Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Computational Insight into the Mechanism of the Pd(0)-Brønsted Acid Cooperatively Catalysed Head-to-Tail Dimerization of Terminal Alkynes

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1. Energy profiles for the OA of the $Ph_2P(O)OH$ acid into the Pd(0) complex.

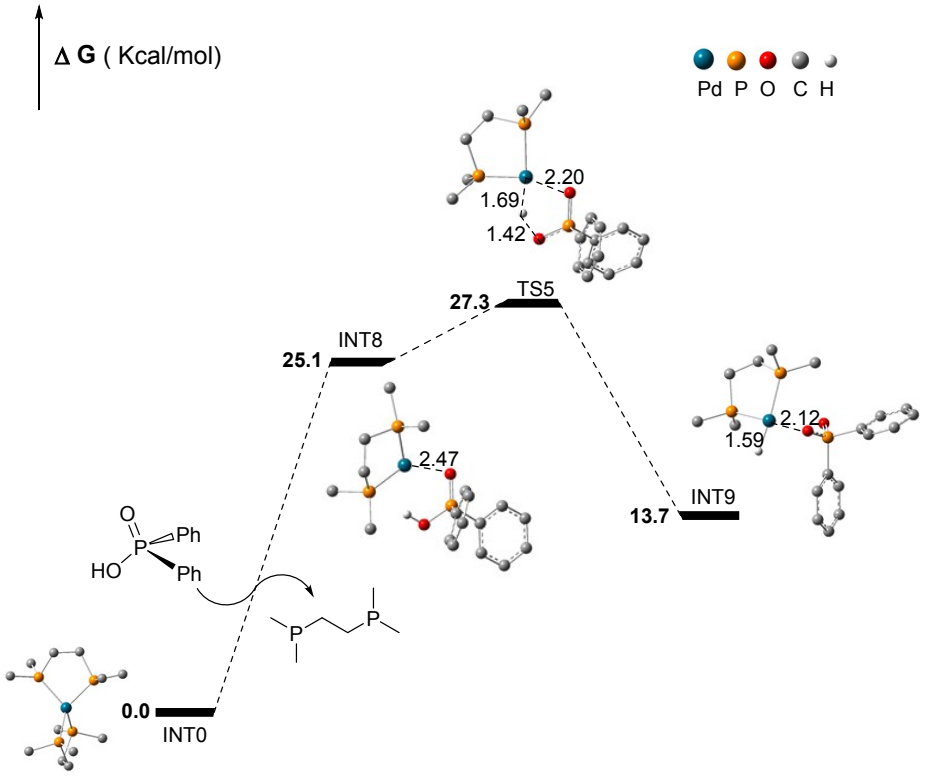

Figure S1. Energy profile (in kcal/mol) for the OA of the $Ph_2P(O)OH$ acid into the Pd(0) complex in the absence of the alkyne. Bond lengths are shown in Å.

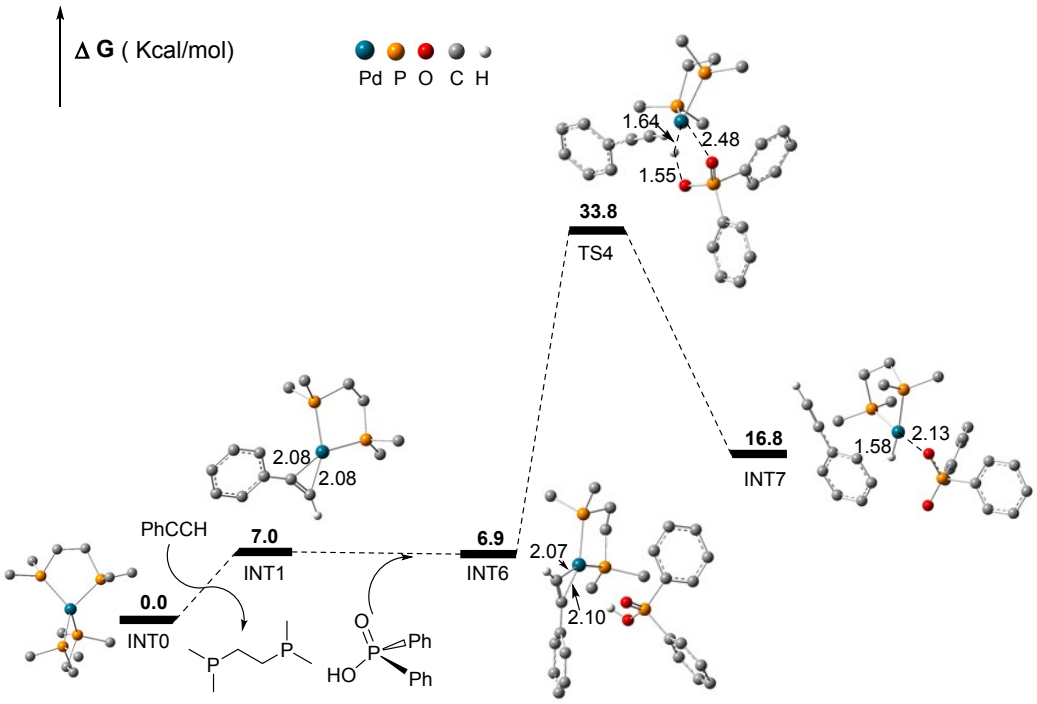

Figure S2. Energy profile (in kcal/mol) for the OA of the $Ph_2P(O)OH$ acid into the Pd(0) complex in the presence of the alkyne. Bond lengths are shown in Å.

2. Computational studies for the head-to-tail dimerization of ethylacetylene.

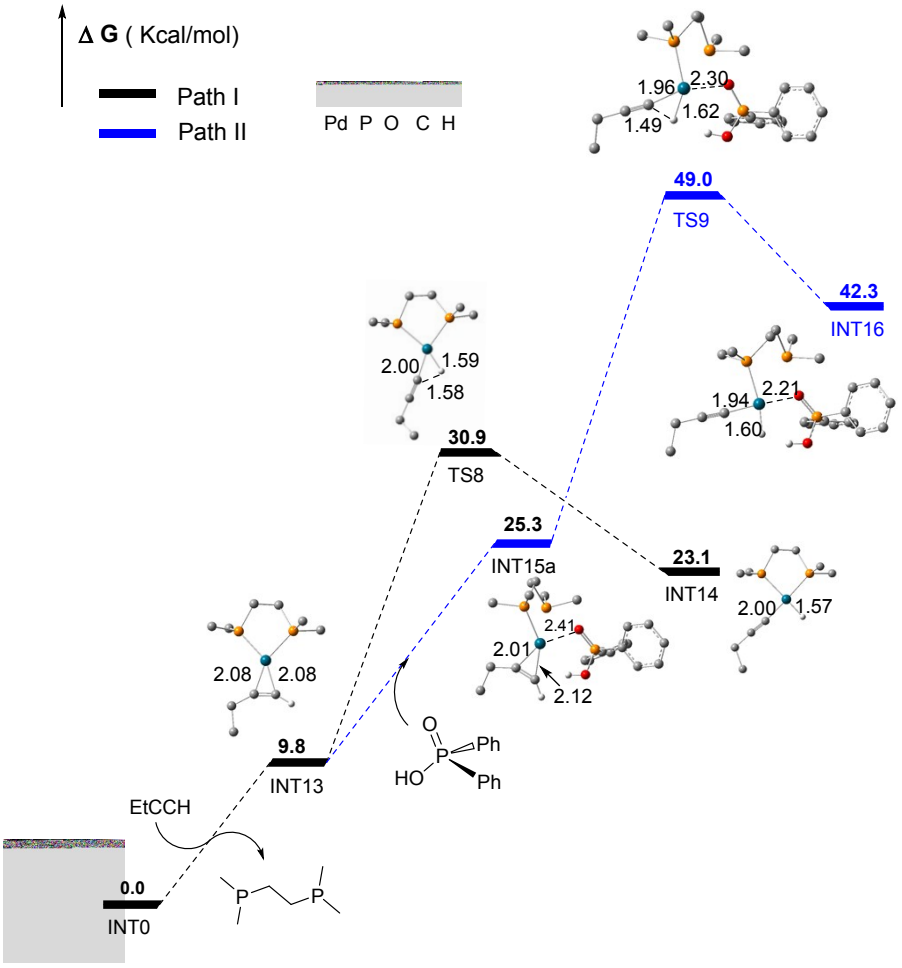

Figure S3. Energy profiles (in kcal/mol) for the OA of the C_{sp}-H bond of ethylacetylene with and without the $Ph_2P(O)OH$ acid. Bond lengths are shown in Å.

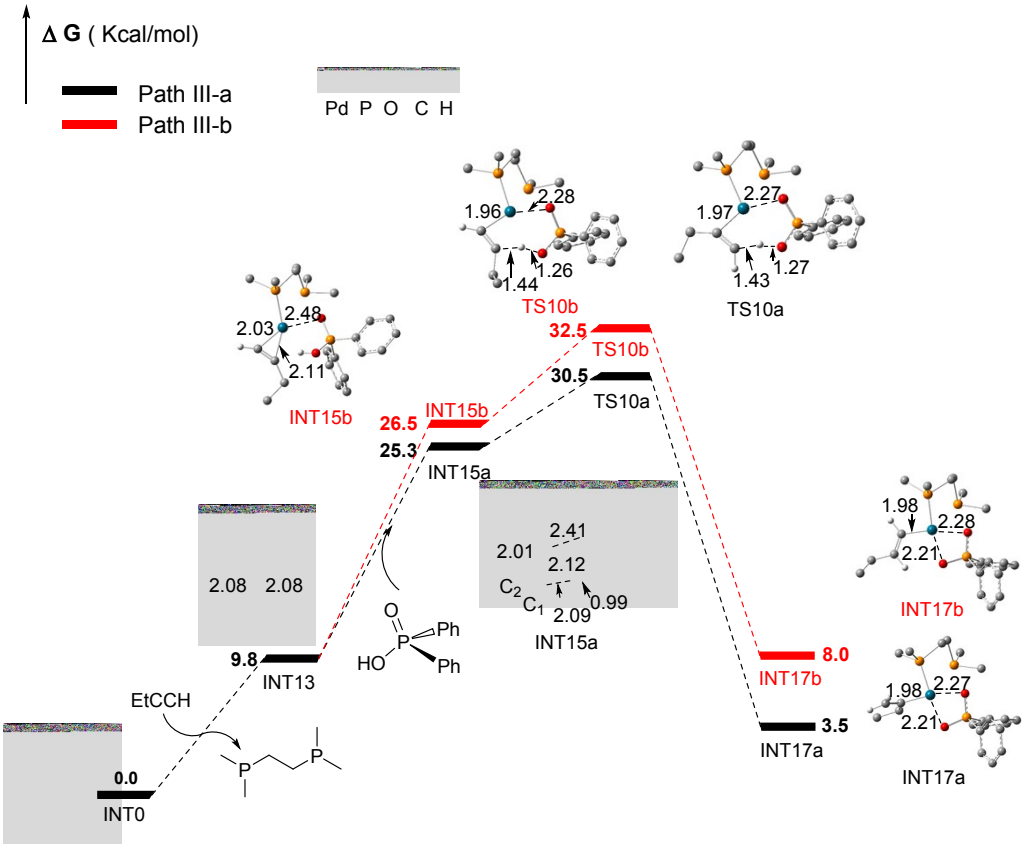

Figure S4. Energy profiles (in kcal/mol) for the two proton transfer steps from the acid to the triple bond of ethylacetylene. Bond lengths are shown in Å.

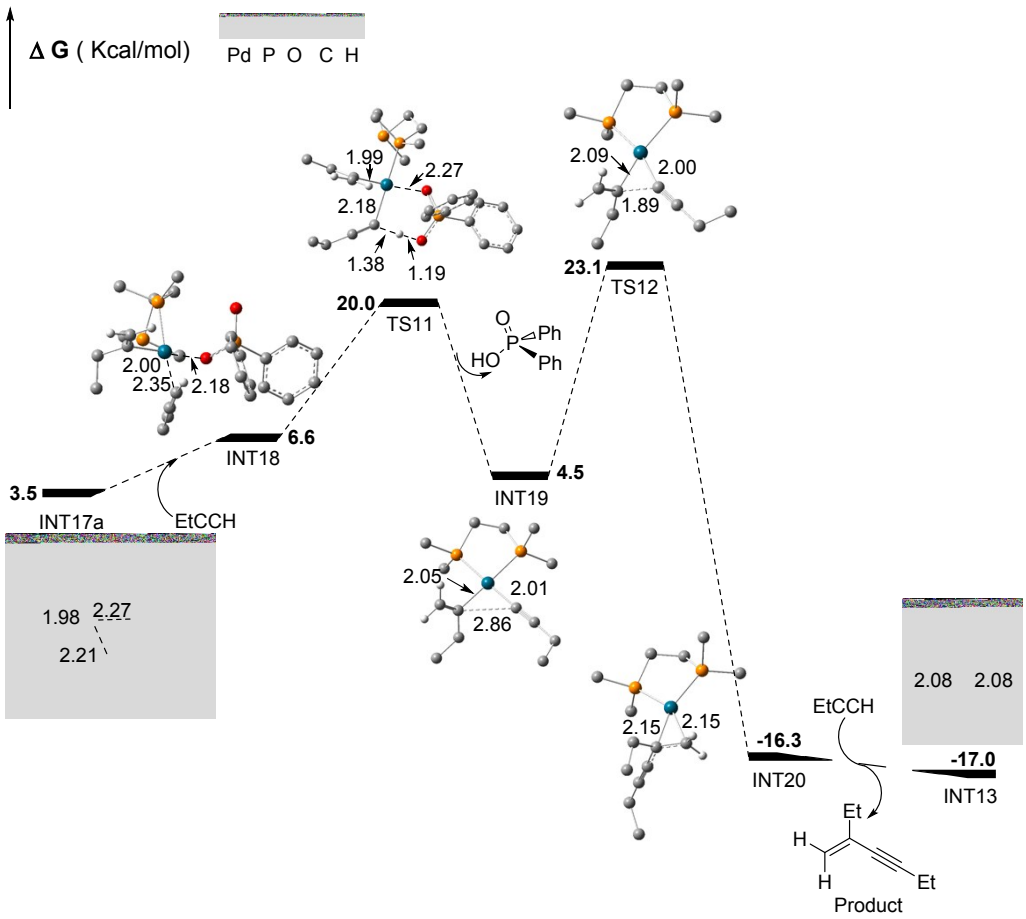

Figure S5. Energy profile (in kcal/mol) for the formation of the alkenyl(alkynyl)palladium intermediate and subsequent RE leading to the final product. Bond lengths are shown in Å.

3. Cartesian Coordinates and Energies

INT0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.276056	-0.287419	-0.710451
2	1	0	3.314393	0.529475	-1.441962
3	1	0	4.160463	-0.914474	-0.879728
4	6	0	3.276127	0.287474	0.710323
5	1	0	3.314658	-0.529397	1.441846
6	1	0	4.160486	0.914628	0.879474
7	15	0	1.709794	-1.241408	-1.069794
8	15	0	1.709833	1.241329	1.069838
9	6	0	1.929634	-1.529328	-2.882760
10	1	0	2.913772	-1.944568	-3.128417
11	1	0	1.157017	-2.219764	-3.232429
12	1	0	1.795927	-0.581378	-3.410829
13	6	0	2.176391	-2.912482	-0.427187
14	1	0	1.370741	-3.618604	-0.645943
15	1	0	3.110747	-3.288563	-0.859571
16	1	0	2.277996	-2.853774	0.659850
17	6	0	2.176251	2.912488	0.427330
18	1	0	1.370519	3.618513	0.646107
19	1	0	3.110560	3.288647	0.859749
20	1	0	2.277889	2.853846	-0.659708
21	6	0	1.929744	1.529155	2.882808
22	1	0	2.913895	1.944373	3.128445
23	1	0	1.157139	2.219607	3.232530
24	1	0	1.796040	0.581189	3.410853
25	6	0	-3.276004	0.710579	-0.287022
26	6	0	-3.276082	-0.710559	0.286981
27	1	0	-3.314173	1.441745	0.530181
28	1	0	-4.160373	0.880196	-0.914029
29	1	0	-4.160488	-0.880090	0.913952
30	1	0	-3.314279	-1.441738	-0.530208
31	46	0	0.000059	0.000058	-0.000049
32	15	0	-1.709715	1.069956	-1.240838
33	15	0	-1.709865	-1.069994	1.240848
34	6	0	-1.929113	-2.883084	1.528571
35	1	0	-1.156907	-3.232389	2.219679
36	1	0	-2.913480	-3.129174	1.943015
37	1	0	-1.794402	-3.411117	0.580730

38	6	0	-2.177174	-0.428110	2.912054
39	1	0	-1.372001	-0.647833	3.618457
40	1	0	-2.278238	0.658986	2.854167
41	1	0	-3.111908	-0.860357	3.287351
42	6	0	-1.929057	2.883059	-1.528484
43	1	0	-1.156995	3.232440	-2.219572
44	1	0	-2.913466	3.129098	-1.942837
45	1	0	-1.794314	3.411041	-0.580638
46	6	0	-2.177164	0.428120	-2.912029
47	1	0	-3.111749	0.860653	-3.287370
48	1	0	-1.371910	0.647467	-3.618456
49	1	0	-2.278634	-0.658949	-2.854021

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1968.64773435
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1968.86091875
Zero-point correction= 0.424687 (Hartree/Particle)
Thermal correction to Energy= 0.452466
Thermal correction to Enthalpy= 0.453410
Thermal correction to Gibbs Free Energy= 0.367894

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.387718	-0.632862	-0.037728
2	6	0	0.798555	-2.340024	-0.014147
3	6	0	1.570498	-1.331197	-0.054067
4	6	0	2.897401	-0.743058	-0.069613
5	6	0	3.120461	0.506083	-0.661027
6	6	0	3.982788	-1.414531	0.510660
7	6	0	4.391035	1.068549	-0.677854
8	1	0	2.275819	1.016354	-1.113587
9	6	0	5.251255	-0.845168	0.504101
10	1	0	3.816746	-2.382342	0.973119
11	6	0	5.461120	0.397219	-0.090243
12	1	0	4.547550	2.034920	-1.148238
13	1	0	6.080971	-1.373734	0.964002
14	1	0	6.452332	0.839977	-0.095189
15	1	0	0.668979	-3.407277	-0.003572
16	6	0	-3.383589	0.879002	0.453576
17	1	0	-3.325979	0.910451	1.548491
18	1	0	-4.439469	0.995450	0.182662
19	6	0	-2.533382	2.007212	-0.145085

20	1	0	-2.682738	2.054430	-1.230698
21	1	0	-2.827382	2.980984	0.263647
22	15	0	-2.745309	-0.795379	-0.062116
23	15	0	-0.716972	1.697062	0.133434
24	6	0	-3.796240	-1.903883	0.964523
25	1	0	-4.863446	-1.692658	0.839431
26	1	0	-3.602048	-2.942118	0.684111
27	1	0	-3.525603	-1.784001	2.016538
28	6	0	-3.523414	-0.992410	-1.720405
29	1	0	-3.307134	-1.993484	-2.101394
30	1	0	-4.608072	-0.844401	-1.687814
31	1	0	-3.080018	-0.272529	-2.413034
32	6	0	-0.471927	2.362207	1.833070
33	1	0	0.590485	2.303699	2.082612
34	1	0	-0.812436	3.398676	1.927766
35	1	0	-1.013691	1.734714	2.545064
36	6	0	0.037605	3.034974	-0.881404
37	1	0	-0.410678	4.011511	-0.670897
38	1	0	1.108696	3.084487	-0.667529
39	1	0	-0.086636	2.803456	-1.942273

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1356.01928444
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1356.20325669
Zero-point correction= 0.325038 (Hartree/Particle)
Thermal correction to Energy= 0.346668
Thermal correction to Enthalpy= 0.347612
Thermal correction to Gibbs Free Energy= 0.273054

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.661176	-0.500546	-0.037312
2	6	0	1.331461	-0.529048	-0.046022
3	6	0	2.551566	-0.444558	-0.036436
4	6	0	3.973564	-0.310773	-0.012913
5	6	0	4.721177	-0.329336	-1.201840
6	6	0	4.656020	-0.155603	1.205058
7	6	0	6.104052	-0.195884	-1.169576
8	1	0	4.202437	-0.450735	-2.147142
9	6	0	6.038763	-0.022544	1.229736
10	1	0	4.085689	-0.142280	2.128189
11	6	0	6.769995	-0.041232	0.044108

12	1	0	6.665209	-0.212771	-2.099316
13	1	0	6.548516	0.096937	2.181224
14	1	0	7.850251	0.064452	0.066151
15	1	0	0.334597	-1.742526	0.053156
16	6	0	-3.923057	0.316556	0.463651
17	1	0	-3.830115	0.459714	1.546955
18	1	0	-4.984635	0.146737	0.250461
19	6	0	-3.401073	1.557830	-0.274998
20	1	0	-3.581335	1.456601	-1.352047
21	1	0	-3.925164	2.461360	0.056512
22	15	0	-2.915982	-1.192368	0.040507
23	15	0	-1.560851	1.733839	-0.052413
24	6	0	-3.585422	-2.440370	1.208337
25	1	0	-4.675279	-2.518311	1.142720
26	1	0	-3.140175	-3.412053	0.981976
27	1	0	-3.301234	-2.171079	2.228431
28	6	0	-3.660088	-1.719088	-1.556245
29	1	0	-3.194942	-2.654790	-1.874885
30	1	0	-4.742386	-1.860977	-1.474116
31	1	0	-3.449069	-0.966804	-2.320193
32	6	0	-1.437740	2.582233	1.573692
33	1	0	-0.384785	2.786708	1.782048
34	1	0	-2.002916	3.519505	1.597479
35	1	0	-1.805529	1.915090	2.357365
36	6	0	-1.138425	3.080563	-1.225932
37	1	0	-1.743524	3.977630	-1.061497
38	1	0	-0.081854	3.330348	-1.102157
39	1	0	-1.281891	2.727830	-2.250092

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1355.97395436
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1356.16458478
Zero-point correction= 0.320661 (Hartree/Particle)
Thermal correction to Energy= 0.342460
Thermal correction to Enthalpy= 0.343404
Thermal correction to Gibbs Free Energy= 0.267377

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.867572	-0.795997	-0.041334
2	6	0	-1.129050	-0.795859	-0.059956
3	6	0	-2.341177	-0.635887	-0.045047

4	6	0	-3.759379	-0.449439	-0.008485
5	6	0	-4.424381	-0.262117	1.214533
6	6	0	-4.520336	-0.438638	-1.188832
7	6	0	-5.800117	-0.070087	1.253052
8	1	0	-3.845210	-0.274815	2.132376
9	6	0	-5.896056	-0.245126	-1.144323
10	1	0	-4.016741	-0.588065	-2.138439
11	6	0	-6.543466	-0.059214	0.074908
12	1	0	-6.295383	0.070581	2.209443
13	1	0	-6.466465	-0.241622	-2.068734
14	1	0	-7.618226	0.090968	0.107446
15	1	0	0.791441	-2.366775	-0.093269
16	6	0	3.694126	1.020525	-0.340287
17	1	0	3.655278	1.125447	-1.431182
18	1	0	4.732896	1.191874	-0.036601
19	6	0	2.746280	2.036071	0.317201
20	1	0	2.872994	2.018252	1.406143
21	1	0	2.968258	3.055042	-0.017409
22	15	0	3.181266	-0.730362	0.037364
23	15	0	0.979255	1.571380	-0.026092
24	6	0	4.246516	-1.725963	-1.068666
25	1	0	5.306253	-1.492722	-0.928383
26	1	0	4.075723	-2.784224	-0.858970
27	1	0	3.964913	-1.539411	-2.107452
28	6	0	3.907958	-1.030727	1.694460
29	1	0	3.720773	-2.068978	1.977385
30	1	0	4.984860	-0.836481	1.706831
31	1	0	3.412019	-0.391359	2.428504
32	6	0	0.609114	2.345097	-1.644164
33	1	0	-0.427393	2.109405	-1.897895
34	1	0	0.746776	3.430379	-1.623857
35	1	0	1.250173	1.908486	-2.413768
36	6	0	-0.023981	2.547273	1.147668
37	1	0	0.115172	3.624458	1.019708
38	1	0	-1.071141	2.283255	0.977131
39	1	0	0.230580	2.261428	2.170891

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1355.98475748
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1356.17978297
Zero-point correction= 0.322610 (Hartree/Particle)
Thermal correction to Energy= 0.344407
Thermal correction to Enthalpy= 0.345351
Thermal correction to Gibbs Free Energy= 0.270032

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.729985	-0.963102	-0.230723
2	6	0	-0.964486	-1.041373	-2.346483
3	6	0	-2.074710	-0.928924	-1.725091
4	1	0	1.071880	-1.369391	-1.907279
5	15	0	2.416903	-0.562319	-0.456838
6	8	0	2.056826	-1.311227	-1.826391
7	8	0	1.479497	-0.877663	0.682123
8	6	0	-1.783427	0.431955	2.957934
9	1	0	-2.380280	0.197356	3.849242
10	1	0	-0.747023	0.542720	3.295306
11	6	0	-2.277529	1.746188	2.340850
12	1	0	-2.299893	2.507876	3.130668
13	1	0	-3.308169	1.631810	1.982969
14	15	0	-1.815468	-1.045047	1.843261
15	15	0	-1.254413	2.402302	0.912583
16	6	0	-1.161264	-2.328595	2.986668
17	1	0	-1.667059	-2.314607	3.957759
18	1	0	-1.289197	-3.311873	2.527432
19	1	0	-0.090798	-2.158996	3.125978
20	6	0	-3.609383	-1.443969	1.802822
21	1	0	-3.751112	-2.383798	1.263399
22	1	0	-4.029346	-1.534246	2.810086
23	1	0	-4.147067	-0.670461	1.248796
24	6	0	0.419391	2.385909	1.697880
25	1	0	1.084427	3.030746	1.116661
26	1	0	0.396975	2.745381	2.733528
27	1	0	0.830758	1.373031	1.663802
28	6	0	-1.654327	4.204565	1.118433
29	1	0	-1.459548	4.569730	2.133502
30	1	0	-1.049978	4.786585	0.416249
31	1	0	-2.707292	4.380972	0.878795
32	6	0	-3.515094	-0.769313	-1.644046
33	6	0	-4.379636	-1.836673	-1.910450
34	6	0	-4.052455	0.460025	-1.236547
35	6	0	-5.754623	-1.677748	-1.767418
36	1	0	-3.962766	-2.790098	-2.218834
37	6	0	-5.427172	0.614988	-1.103866
38	1	0	-3.370191	1.274803	-1.010734

39	6	0	-6.283250	-0.454611	-1.363233
40	1	0	-6.416434	-2.513759	-1.972806
41	1	0	-5.833561	1.572049	-0.790190
42	1	0	-7.356037	-0.334115	-1.250016
43	1	0	-0.588587	-1.066549	-3.359469
44	6	0	2.466237	1.204900	-0.850678
45	6	0	3.480948	2.026962	-0.353098
46	6	0	1.416592	1.769625	-1.583616
47	6	0	3.447705	3.398656	-0.586511
48	1	0	4.299536	1.597795	0.216932
49	6	0	1.384833	3.141002	-1.810964
50	1	0	0.609224	1.143435	-1.952144
51	6	0	2.399379	3.956365	-1.314315
52	1	0	4.239487	4.031762	-0.198959
53	1	0	0.560710	3.571381	-2.370464
54	1	0	2.372769	5.026787	-1.493940
55	6	0	4.103624	-1.092843	-0.118721
56	6	0	4.388465	-1.652752	1.127363
57	6	0	5.115864	-0.952778	-1.073526
58	6	0	5.683481	-2.073743	1.417560
59	1	0	3.590292	-1.757155	1.855365
60	6	0	6.406777	-1.374615	-0.779339
61	1	0	4.893916	-0.514695	-2.041991
62	6	0	6.689326	-1.934582	0.465992
63	1	0	5.904972	-2.512828	2.384940
64	1	0	7.192352	-1.270182	-1.520690
65	1	0	7.698826	-2.263438	0.692843

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.56630885
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.91811661
Zero-point correction= 0.531189 (Hartree/Particle)
Thermal correction to Energy= 0.567190
Thermal correction to Enthalpy= 0.568134
Thermal correction to Gibbs Free Energy= 0.459739

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.725264	-0.856461	-0.032070
2	6	0	-0.922776	-1.179955	-2.220176
3	6	0	-2.007504	-1.052772	-1.514329
4	1	0	0.438413	-1.180422	-1.815408

5	15	0	2.283255	-0.558805	-0.462786
6	8	0	1.703952	-1.171951	-1.760882
7	8	0	1.389075	-0.661485	0.775162
8	6	0	-1.875630	0.854345	2.795474
9	1	0	-2.533409	0.771739	3.670398
10	1	0	-0.854653	0.964806	3.176912
11	6	0	-2.264073	2.084414	1.964632
12	1	0	-2.318842	2.946400	2.641755
13	1	0	-3.266410	1.953910	1.537878
14	15	0	-1.925996	-0.760547	1.903380
15	15	0	-1.093639	2.500990	0.559056
16	6	0	-1.286026	-1.906923	3.183668
17	1	0	-1.790281	-1.768263	4.145375
18	1	0	-1.427031	-2.935950	2.845066
19	1	0	-0.213653	-1.731815	3.297868
20	6	0	-3.717966	-1.142707	1.858326
21	1	0	-3.866096	-2.125410	1.404739
22	1	0	-4.148434	-1.133005	2.864402
23	1	0	-4.237591	-0.414687	1.230903
24	6	0	0.489433	2.614395	1.506300
25	1	0	1.206589	3.191622	0.916348
26	1	0	0.357387	3.104281	2.478413
27	1	0	0.909878	1.613297	1.639353
28	6	0	-1.487165	4.309754	0.421796
29	1	0	-1.403061	4.835726	1.379643
30	1	0	-0.791427	4.764929	-0.289353
31	1	0	-2.500198	4.445044	0.031190
32	6	0	-3.459314	-0.959662	-1.546276
33	6	0	-4.257140	-2.105089	-1.637787
34	6	0	-4.072769	0.293265	-1.409933
35	6	0	-5.643819	-1.998799	-1.588860
36	1	0	-3.780289	-3.075009	-1.737871
37	6	0	-5.458455	0.394330	-1.368007
38	1	0	-3.444034	1.175348	-1.325769
39	6	0	-6.248158	-0.752005	-1.450502
40	1	0	-6.254079	-2.894213	-1.657022
41	1	0	-5.925388	1.369233	-1.265229
42	1	0	-7.329854	-0.671847	-1.408559
43	1	0	-0.810309	-1.285187	-3.295618
44	6	0	2.629269	1.190826	-0.812049
45	6	0	3.651358	1.882849	-0.158779
46	6	0	1.781841	1.878442	-1.685229
47	6	0	3.824338	3.246887	-0.373277
48	1	0	4.317197	1.352640	0.516527

49	6	0	1.950458	3.244100	-1.894189
50	1	0	0.987611	1.341206	-2.194500
51	6	0	2.971645	3.929172	-1.238811
52	1	0	4.624790	3.777190	0.133279
53	1	0	1.286756	3.772564	-2.571568
54	1	0	3.107592	4.993229	-1.406865
55	6	0	3.874137	-1.343149	-0.117293
56	6	0	4.217392	-1.643150	1.202556
57	6	0	4.772097	-1.624183	-1.150945
58	6	0	5.453269	-2.217370	1.487773
59	1	0	3.504093	-1.431539	1.992875
60	6	0	6.005035	-2.198709	-0.863128
61	1	0	4.497375	-1.402424	-2.177644
62	6	0	6.346230	-2.492903	0.456169
63	1	0	5.716873	-2.451713	2.514502
64	1	0	6.700503	-2.421430	-1.666236
65	1	0	7.309393	-2.942565	0.677710

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.55319901
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.90688472
Zero-point correction= 0.525835 (Hartree/Particle)
Thermal correction to Energy= 0.561345
Thermal correction to Enthalpy= 0.562289
Thermal correction to Gibbs Free Energy= 0.455014

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.630666	-1.199668	-0.021353
2	6	0	2.435170	-3.011401	1.426667
3	6	0	2.054135	-1.743805	1.250496
4	1	0	2.058131	-3.822036	0.809546
5	15	0	-1.915986	-0.285188	0.223020
6	8	0	-1.033626	-0.770202	1.386177
7	8	0	-1.255261	-0.591585	-1.134801
8	6	0	1.693570	-0.389285	-3.114538
9	1	0	2.160485	-0.843356	-3.997577
10	1	0	0.608002	-0.476208	-3.233535
11	6	0	2.114717	1.082691	-3.008454
12	1	0	1.896938	1.575331	-3.964649
13	1	0	3.199451	1.153905	-2.864680
14	15	0	2.135013	-1.439960	-1.662742

15	15	0	1.301893	2.042177	-1.623976
16	6	0	2.182329	-3.127223	-2.368423
17	1	0	2.901381	-3.192568	-3.190519
18	1	0	2.464726	-3.833162	-1.584385
19	1	0	1.185961	-3.390654	-2.730563
20	6	0	3.890643	-1.062534	-1.333228
21	1	0	4.289909	-1.834876	-0.673474
22	1	0	4.465637	-1.035389	-2.263541
23	1	0	3.964966	-0.102815	-0.816787
24	6	0	-0.355776	2.309654	-2.391883
25	1	0	-0.910267	3.046115	-1.803468
26	1	0	-0.275643	2.664142	-3.426098
27	1	0	-0.914293	1.370431	-2.352233
28	6	0	2.076209	3.689918	-1.972118
29	1	0	1.973067	3.989956	-3.021077
30	1	0	1.593320	4.444710	-1.344970
31	1	0	3.138249	3.668404	-1.711188
32	6	0	2.581927	-0.618260	2.055480
33	6	0	3.961561	-0.402324	2.159280
34	6	0	1.712000	0.254259	2.726545
35	6	0	4.461810	0.662158	2.904242
36	1	0	4.642847	-1.077833	1.650202
37	6	0	2.215129	1.313264	3.472071
38	1	0	0.641973	0.078535	2.658595
39	6	0	3.590016	1.526177	3.559365
40	1	0	5.534776	0.815117	2.973743
41	1	0	1.528980	1.974849	3.992799
42	1	0	3.978952	2.358473	4.137947
43	1	0	3.106739	-3.283463	2.240427
44	6	0	-2.177399	1.504072	0.397024
45	6	0	-3.279193	2.142674	-0.176271
46	6	0	-1.192727	2.267008	1.031257
47	6	0	-3.393371	3.528653	-0.123893
48	1	0	-4.052644	1.555666	-0.664085
49	6	0	-1.306487	3.652888	1.081744
50	1	0	-0.332076	1.773224	1.469729
51	6	0	-2.405081	4.284870	0.502697
52	1	0	-4.253456	4.018024	-0.570163
53	1	0	-0.536068	4.238690	1.573866
54	1	0	-2.495613	5.366131	0.545701
55	6	0	-3.556181	-1.043603	0.295520
56	6	0	-4.197466	-1.444256	-0.878385
57	6	0	-4.190701	-1.215953	1.528955
58	6	0	-5.470539	-2.005440	-0.819317

59	1	0	-3.686885	-1.322267	-1.828754
60	6	0	-5.460189	-1.779963	1.585241
61	1	0	-3.681353	-0.919056	2.440876
62	6	0	-6.100849	-2.171545	0.410905
63	1	0	-5.967968	-2.318316	-1.732150
64	1	0	-5.949514	-1.918852	2.544162
65	1	0	-7.091600	-2.613434	0.457128

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.60331992
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.95628027
Zero-point correction= 0.534299 (Hartree/Particle)
Thermal correction to Energy= 0.569260
Thermal correction to Enthalpy= 0.570204
Thermal correction to Gibbs Free Energy= 0.465525

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.337515	0.570299	-1.102489
2	6	0	0.513022	3.459607	-0.842057
3	6	0	1.526556	3.660376	-1.789574
4	6	0	0.628462	4.088403	0.407039
5	6	0	2.617926	4.470774	-1.497224
6	1	0	1.447994	3.176329	-2.758708
7	6	0	1.724099	4.893408	0.695922
8	1	0	-0.153707	3.935684	1.144975
9	6	0	2.724564	5.087828	-0.253697
10	1	0	3.390926	4.617254	-2.245601
11	1	0	1.797466	5.371866	1.668018
12	1	0	3.581183	5.713971	-0.024973
13	6	0	-0.616246	2.585274	-1.118397
14	6	0	-1.858047	2.479698	-1.385050
15	1	0	-2.780408	2.978851	-1.631630
16	1	0	1.189897	1.063124	-1.348476
17	15	0	1.472806	-0.826464	-0.371064
18	8	0	1.932709	0.432457	-1.251273
19	8	0	0.076801	-1.314238	-0.664290
20	6	0	-3.412850	-2.109631	0.037716
21	1	0	-4.188397	-2.823353	-0.269896
22	1	0	-2.488850	-2.682166	0.175707
23	6	0	-3.826871	-1.442274	1.355589
24	1	0	-4.132828	-2.227068	2.059963

25	1	0	-4.706795	-0.806258	1.198962
26	15	0	-3.089641	-0.964787	-1.380170
27	15	0	-2.509745	-0.396878	2.179033
28	6	0	-2.820315	-2.190097	-2.724715
29	1	0	-3.610116	-2.947553	-2.766259
30	1	0	-2.769159	-1.666833	-3.682628
31	1	0	-1.854710	-2.672422	-2.553402
32	6	0	-4.776498	-0.337236	-1.758059
33	1	0	-4.744461	0.208343	-2.704748
34	1	0	-5.513318	-1.144119	-1.831529
35	1	0	-5.084640	0.365039	-0.979491
36	6	0	-1.269744	-1.727960	2.515408
37	1	0	-0.523033	-1.356075	3.223002
38	1	0	-1.731879	-2.632901	2.927428
39	1	0	-0.751040	-1.968645	1.584151
40	6	0	-3.294165	-0.293296	3.859332
41	1	0	-3.574243	-1.274681	4.259571
42	1	0	-2.591317	0.178052	4.552682
43	1	0	-4.188064	0.335938	3.813740
44	6	0	1.681935	-0.348960	1.360082
45	6	0	2.369914	-1.167268	2.259117
46	6	0	1.060196	0.817087	1.819154
47	6	0	2.434709	-0.823321	3.606164
48	1	0	2.853351	-2.074829	1.910628
49	6	0	1.128032	1.157049	3.164883
50	1	0	0.507591	1.448791	1.131458
51	6	0	1.813951	0.337790	4.059167
52	1	0	2.971576	-1.461861	4.300304
53	1	0	0.642321	2.062818	3.512923
54	1	0	1.867046	0.604773	5.110199
55	6	0	2.727228	-2.056559	-0.756975
56	6	0	4.086558	-1.727921	-0.773569
57	6	0	2.319486	-3.366195	-1.015174
58	6	0	5.030744	-2.709763	-1.048527
59	1	0	4.400179	-0.707192	-0.577537
60	6	0	3.269405	-4.346297	-1.288519
61	1	0	1.260059	-3.602344	-1.007031
62	6	0	4.621900	-4.018160	-1.303828
63	1	0	6.085869	-2.456635	-1.066499
64	1	0	2.953963	-5.364717	-1.491027
65	1	0	5.362176	-4.782886	-1.517513

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.56135316

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.91441471

Zero-point correction= 0.530950 (Hartree/Particle)
Thermal correction to Energy= 0.567451
Thermal correction to Enthalpy= 0.568395
Thermal correction to Gibbs Free Energy= 0.456063

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.197813	0.226973	-1.045191
2	6	0	-0.200441	3.700845	-0.246652
3	6	0	1.130984	4.064006	-0.482388
4	6	0	-1.034045	4.607650	0.425158
5	6	0	1.605964	5.306578	-0.074450
6	1	0	1.792878	3.365625	-0.981449
7	6	0	-0.554891	5.845127	0.836054
8	1	0	-2.061782	4.325269	0.632765
9	6	0	0.768757	6.201120	0.585222
10	1	0	2.640555	5.572483	-0.269311
11	1	0	-1.214764	6.531432	1.358413
12	1	0	1.146139	7.166233	0.909280
13	6	0	-0.736219	2.394965	-0.680890
14	6	0	-1.947338	2.026877	-0.997178
15	1	0	-2.926161	2.457021	-1.155308
16	1	0	0.440038	1.527632	-0.684724
17	15	0	1.677822	-0.451064	-0.315804
18	8	0	1.604454	1.067038	-0.626942
19	8	0	0.496520	-1.272733	-0.835645
20	6	0	-3.193564	-2.591938	-0.542796
21	1	0	-3.969855	-3.212663	-1.008864
22	1	0	-2.261981	-3.168281	-0.571361
23	6	0	-3.581798	-2.281318	0.908591
24	1	0	-3.801742	-3.231827	1.411791
25	1	0	-4.507721	-1.693901	0.935630
26	15	0	-2.922965	-1.128978	-1.635415
27	15	0	-2.286730	-1.363262	1.902719
28	6	0	-2.741173	-1.927296	-3.276454
29	1	0	-3.567701	-2.611771	-3.492472
30	1	0	-2.696562	-1.155291	-4.047899
31	1	0	-1.796709	-2.476403	-3.293034
32	6	0	-4.586074	-0.363319	-1.724354
33	1	0	-4.578802	0.412849	-2.493490
34	1	0	-5.360370	-1.099779	-1.960328

35	1	0	-4.812981	0.112177	-0.767223
36	6	0	-0.956105	-2.643579	1.882124
37	1	0	-0.237621	-2.418148	2.674821
38	1	0	-1.352005	-3.654221	2.037786
39	1	0	-0.420259	-2.587182	0.930407
40	6	0	-2.990363	-1.684413	3.589113
41	1	0	-3.181842	-2.748015	3.771969
42	1	0	-2.279591	-1.324238	4.338586
43	1	0	-3.924257	-1.129817	3.719022
44	6	0	1.791654	-0.612225	1.487736
45	6	0	2.492664	-1.656610	2.094245
46	6	0	1.057125	0.276813	2.278237
47	6	0	2.452934	-1.817499	3.476053
48	1	0	3.071253	-2.345539	1.485060
49	6	0	1.009274	0.108432	3.658447
50	1	0	0.523129	1.099326	1.811559
51	6	0	1.704726	-0.939740	4.257946
52	1	0	3.000963	-2.630160	3.942570
53	1	0	0.431060	0.797927	4.265419
54	1	0	1.669094	-1.069198	5.335447
55	6	0	3.216229	-1.099349	-1.002515
56	6	0	4.421344	-0.412826	-0.826073
57	6	0	3.201111	-2.311728	-1.694170
58	6	0	5.601758	-0.939396	-1.337451
59	1	0	4.429407	0.534760	-0.295851
60	6	0	4.385076	-2.836205	-2.205635
61	1	0	2.255769	-2.827093	-1.831029
62	6	0	5.583554	-2.151554	-2.026042
63	1	0	6.537201	-0.405735	-1.202187
64	1	0	4.371722	-3.778237	-2.744920
65	1	0	6.506358	-2.561357	-2.425345

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.54600763
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.90010217
Zero-point correction= 0.527449 (Hartree/Particle)
Thermal correction to Energy= 0.562619
Thermal correction to Enthalpy= 0.563563
Thermal correction to Gibbs Free Energy= 0.455955

INT5b

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

1	46	0	0.649787	0.183789	-0.901336
2	6	0	4.045786	-1.883987	0.679970
3	6	0	4.091111	-3.144742	1.288687
4	6	0	5.255641	-1.203538	0.485405
5	6	0	5.299607	-3.716774	1.670591
6	1	0	3.160640	-3.680959	1.455071
7	6	0	6.464511	-1.773862	0.864320
8	1	0	5.248141	-0.210210	0.046191
9	6	0	6.493938	-3.034849	1.457050
10	1	0	5.308075	-4.697123	2.137442
11	1	0	7.390469	-1.229103	0.704723
12	1	0	7.438914	-3.477692	1.755870
13	6	0	2.734378	-1.333457	0.282158
14	6	0	2.527421	-0.322722	-0.568732
15	1	0	3.371055	0.170583	-1.049503
16	1	0	1.867995	-1.833058	0.714426
17	15	0	-1.736095	-0.869048	-0.145819
18	8	0	-0.359442	-1.515913	0.084464
19	8	0	-1.604150	0.364985	-1.061344
20	6	0	0.084310	3.423242	-1.624722
21	1	0	0.227891	4.174532	-2.411807
22	1	0	-0.916275	2.996357	-1.756257
23	6	0	0.217746	4.085369	-0.246622
24	1	0	-0.423636	4.976033	-0.231897
25	1	0	1.243592	4.442445	-0.094806
26	15	0	1.262689	2.049605	-1.968990
27	15	0	-0.230325	2.995617	1.207297
28	6	0	1.160423	1.878805	-3.788426
29	1	0	1.376911	2.825554	-4.292575
30	1	0	1.869787	1.116883	-4.118748
31	1	0	0.153694	1.545466	-4.051040
32	6	0	2.914003	2.783322	-1.690527
33	1	0	3.682355	2.134442	-2.116844
34	1	0	2.981963	3.768273	-2.161345
35	1	0	3.097269	2.872697	-0.617644
36	6	0	-2.063016	2.963274	0.983438
37	1	0	-2.525180	2.554164	1.886326
38	1	0	-2.474538	3.961232	0.792435
39	1	0	-2.305777	2.287853	0.158487
40	6	0	-0.101290	4.285461	2.532972
41	1	0	-0.647301	5.203241	2.286600
42	1	0	-0.510327	3.875326	3.460851
43	1	0	0.948667	4.533701	2.712825
44	6	0	-2.416551	-0.399363	1.469244

45	6	0	-3.781042	-0.168269	1.656443
46	6	0	-1.525239	-0.168837	2.520497
47	6	0	-4.250487	0.299695	2.879874
48	1	0	-4.479288	-0.355478	0.844971
49	6	0	-1.995263	0.301918	3.742975
50	1	0	-0.467071	-0.353666	2.365415
51	6	0	-3.356445	0.539000	3.922083
52	1	0	-5.311953	0.476832	3.022042
53	1	0	-1.298083	0.481774	4.555548
54	1	0	-3.723536	0.905819	4.876025
55	6	0	-2.918531	-2.034409	-0.863803
56	6	0	-3.155579	-3.265745	-0.245098
57	6	0	-3.597572	-1.705538	-2.037951
58	6	0	-4.064994	-4.159296	-0.798082
59	1	0	-2.626043	-3.522626	0.667968
60	6	0	-4.510403	-2.601663	-2.589022
61	1	0	-3.399752	-0.747802	-2.508852
62	6	0	-4.743570	-3.826168	-1.969720
63	1	0	-4.245005	-5.116180	-0.318370
64	1	0	-5.037352	-2.345161	-3.502933
65	1	0	-5.455136	-4.524826	-2.399432

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.59396337
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.94860142
Zero-point correction= 0.534753 (Hartree/Particle)
Thermal correction to Energy= 0.569895
Thermal correction to Enthalpy= 0.570839
Thermal correction to Gibbs Free Energy= 0.463136

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.704106	-0.532930	0.538506
2	6	0	-2.445086	-1.034278	-0.178265
3	6	0	-3.612336	-1.217516	-0.492123
4	1	0	0.668432	-2.328050	-0.805920
5	15	0	2.334318	-1.094875	-0.274602
6	8	0	1.640536	-2.408148	-0.886556
7	8	0	1.572025	-0.475677	0.872614
8	6	0	-0.545900	2.552807	2.592526
9	1	0	-0.945603	3.008036	3.507908
10	1	0	0.524980	2.388646	2.759381

11	6	0	-0.755502	3.508706	1.411054
12	1	0	-0.288907	4.472998	1.651497
13	1	0	-1.825465	3.703251	1.271751
14	15	0	-1.310205	0.877729	2.390861
15	15	0	-0.080723	2.894954	-0.220755
16	6	0	-1.080408	0.191823	4.081305
17	1	0	-1.466498	0.864639	4.854042
18	1	0	-1.597462	-0.768401	4.148231
19	1	0	-0.015740	0.014827	4.254116
20	6	0	-3.103295	1.260650	2.355938
21	1	0	-3.657992	0.319384	2.365382
22	1	0	-3.412688	1.888713	3.197425
23	1	0	-3.340972	1.757320	1.412282
24	6	0	1.720462	2.867135	0.200223
25	1	0	2.299261	2.831069	-0.727332
26	1	0	2.027535	3.749001	0.774754
27	1	0	1.941889	1.956743	0.763613
28	6	0	-0.141368	4.495175	-1.156355
29	1	0	0.347322	5.318801	-0.623435
30	1	0	0.358025	4.357018	-2.120099
31	1	0	-1.181345	4.769814	-1.354902
32	6	0	-4.990545	-1.385790	-0.828301
33	6	0	-5.665131	-2.581719	-0.533313
34	6	0	-5.703276	-0.351988	-1.458355
35	6	0	-7.007768	-2.734619	-0.856917
36	1	0	-5.121582	-3.385929	-0.048120
37	6	0	-7.045268	-0.512278	-1.780390
38	1	0	-5.188227	0.575158	-1.688295
39	6	0	-7.704517	-1.702602	-1.481689
40	1	0	-7.513036	-3.666694	-0.621806
41	1	0	-7.579949	0.298224	-2.266994
42	1	0	-8.753573	-1.825637	-1.732254
43	1	0	-1.113269	-1.496984	-0.704332
44	6	0	2.550399	0.062670	-1.645087
45	6	0	3.791262	0.646232	-1.912941
46	6	0	1.423529	0.460878	-2.373062
47	6	0	3.904041	1.623265	-2.897899
48	1	0	4.669311	0.345540	-1.349653
49	6	0	1.540789	1.437950	-3.354893
50	1	0	0.450162	0.030427	-2.155222
51	6	0	2.779193	2.020963	-3.615944
52	1	0	4.869090	2.076332	-3.100188
53	1	0	0.660720	1.747952	-3.908663
54	1	0	2.867393	2.785340	-4.381765

55	6	0	3.957172	-1.676239	0.231892
56	6	0	4.463840	-1.236956	1.456448
57	6	0	4.718094	-2.521046	-0.582609
58	6	0	5.731285	-1.641390	1.865239
59	1	0	3.855283	-0.591582	2.081825
60	6	0	5.982352	-2.922893	-0.168118
61	1	0	4.318290	-2.867944	-1.530504
62	6	0	6.488775	-2.480625	1.053301
63	1	0	6.126616	-1.302621	2.817349
64	1	0	6.573573	-3.581591	-0.795785
65	1	0	7.477191	-2.795420	1.373445

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.51928128
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.87694269
Zero-point correction= 0.526466 (Hartree/Particle)
Thermal correction to Energy= 0.562796
Thermal correction to Enthalpy= 0.563740
Thermal correction to Gibbs Free Energy= 0.453195

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.836489	-0.715083	-0.132433
2	6	0	2.715244	-0.901868	0.283174
3	6	0	3.922370	-0.963028	0.450084
4	1	0	-0.771842	-2.596588	1.082283
5	15	0	-2.266886	-1.273574	0.357454
6	8	0	-1.749088	-2.654257	0.976791
7	8	0	-1.305173	-0.643370	-0.630705
8	6	0	0.140956	1.916408	-2.592680
9	1	0	0.422062	2.122031	-3.632593
10	1	0	-0.774386	1.314592	-2.617943
11	6	0	-0.106340	3.244914	-1.865901
12	1	0	-0.866810	3.815564	-2.414957
13	1	0	0.807989	3.849735	-1.881461
14	15	0	1.445631	0.830710	-1.845918
15	15	0	-0.625846	3.087672	-0.079329
16	6	0	2.098774	-0.071143	-3.302776
17	1	0	2.458264	0.611082	-4.079316
18	1	0	2.918956	-0.707546	-2.961481
19	1	0	1.316556	-0.713851	-3.714315
20	6	0	2.817318	1.969863	-1.434794

21	1	0	3.663867	1.356054	-1.118430
22	1	0	3.100507	2.595278	-2.286953
23	1	0	2.525328	2.598184	-0.590187
24	6	0	-2.392231	2.602927	-0.329996
25	1	0	-2.909237	2.588142	0.633736
26	1	0	-2.915428	3.284314	-1.010445
27	1	0	-2.416603	1.588675	-0.735008
28	6	0	-0.858342	4.890887	0.283147
29	1	0	-1.473757	5.395215	-0.470451
30	1	0	-1.341174	5.001267	1.258356
31	1	0	0.114403	5.388103	0.335501
32	6	0	5.340805	-1.021623	0.632732
33	6	0	6.041109	-2.223464	0.442958
34	6	0	6.066320	0.125187	0.993928
35	6	0	7.420047	-2.273421	0.607858
36	1	0	5.486973	-3.114650	0.166916
37	6	0	7.445330	0.069006	1.159107
38	1	0	5.532268	1.057741	1.147602
39	6	0	8.129066	-1.129053	0.966261
40	1	0	7.943785	-3.212838	0.457566
41	1	0	7.988946	0.966261	1.440358
42	1	0	9.205972	-1.171803	1.096933
43	1	0	0.702755	-1.792443	1.043738
44	6	0	-2.624032	-0.137733	1.716591
45	6	0	-3.935438	0.176578	2.082723
46	6	0	-1.552085	0.497398	2.355153
47	6	0	-4.173195	1.122703	3.075479
48	1	0	-4.773193	-0.301860	1.585396
49	6	0	-1.796177	1.441248	3.345738
50	1	0	-0.528528	0.274491	2.064749
51	6	0	-3.105091	1.757003	3.703982
52	1	0	-5.193732	1.366885	3.352147
53	1	0	-0.959975	1.935927	3.828409
54	1	0	-3.292737	2.499310	4.473617
55	6	0	-3.812292	-1.719480	-0.440248
56	6	0	-4.166015	-1.046357	-1.611843
57	6	0	-4.664755	-2.688468	0.098307
58	6	0	-5.372728	-1.336161	-2.239608
59	1	0	-3.487313	-0.311240	-2.032359
60	6	0	-5.870303	-2.973069	-0.533726
61	1	0	-4.380311	-3.220906	1.000432
62	6	0	-6.224489	-2.295521	-1.698891
63	1	0	-5.645678	-0.817497	-3.152748
64	1	0	-6.532292	-3.726986	-0.120463

65	1	0	-7.166479	-2.520370	-2.189084

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2311.52882810
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.88965807
Zero-point correction= 0.528882 (Hartree/Particle)
Thermal correction to Energy= 0.565003
Thermal correction to Enthalpy= 0.565947
Thermal correction to Gibbs Free Energy= 0.456047

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.800532	0.853327	-0.483676
2	6	0	-1.104644	1.882368	-2.135959
3	6	0	-0.478315	2.344526	-1.132392
4	1	0	0.636016	0.724430	0.126424
5	15	0	1.999293	-0.719512	-0.747745
6	8	0	1.517830	0.360458	0.349641
7	8	0	1.806360	-0.378498	-2.180314
8	6	0	-3.802751	-1.586100	0.749377
9	1	0	-4.787298	-2.063837	0.814595
10	1	0	-3.050313	-2.382283	0.697211
11	6	0	-3.539069	-0.696641	1.973332
12	1	0	-3.541728	-1.287026	2.896666
13	1	0	-4.330191	0.056828	2.069002
14	15	0	-3.642461	-0.597249	-0.818335
15	15	0	-1.927496	0.220068	1.790374
16	6	0	-3.851982	-1.871120	-2.129165
17	1	0	-4.682733	-2.552266	-1.918211
18	1	0	-4.040472	-1.363540	-3.078875
19	1	0	-2.929650	-2.443811	-2.241058
20	6	0	-5.278010	0.247190	-0.893784
21	1	0	-5.351377	0.795413	-1.836280
22	1	0	-6.110246	-0.460881	-0.822112
23	1	0	-5.348861	0.975282	-0.082068
24	6	0	-0.735162	-1.006795	2.461568
25	1	0	0.279170	-0.612953	2.368741
26	1	0	-0.950099	-1.242967	3.508815
27	1	0	-0.787237	-1.922049	1.866406
28	6	0	-2.017040	1.445826	3.157600
29	1	0	-2.253735	0.977545	4.118464
30	1	0	-1.051388	1.952728	3.235348

31	1	0	-2.775228	2.196740	2.921809
32	6	0	0.524659	3.220023	-0.551330
33	6	0	0.295669	3.854297	0.674841
34	6	0	1.754496	3.406785	-1.196208
35	6	0	1.264076	4.680378	1.233054
36	1	0	-0.653668	3.688540	1.176136
37	6	0	2.725305	4.222972	-0.627587
38	1	0	1.943719	2.880826	-2.126175
39	6	0	2.483020	4.866018	0.584474
40	1	0	1.071520	5.175194	2.180470
41	1	0	3.678764	4.353280	-1.130356
42	1	0	3.243287	5.504138	1.024462
43	1	0	-1.294833	1.902811	-3.193461
44	6	0	1.112655	-2.240405	-0.285141
45	6	0	-0.098252	-2.516555	-0.927275
46	6	0	1.570791	-3.095904	0.719753
47	6	0	-0.842852	-3.632706	-0.554688
48	1	0	-0.443620	-1.850652	-1.713438
49	6	0	0.823648	-4.210189	1.090201
50	1	0	2.516724	-2.894684	1.213471
51	6	0	-0.386815	-4.476878	0.455862
52	1	0	-1.778553	-3.857083	-1.057515
53	1	0	1.187472	-4.871877	1.869903
54	1	0	-0.969151	-5.348233	0.739818
55	6	0	3.722086	-0.942368	-0.252267
56	6	0	4.619541	-1.406192	-1.217101
57	6	0	4.170473	-0.683897	1.046517
58	6	0	5.952400	-1.623259	-0.882794
59	1	0	4.267982	-1.577391	-2.230018
60	6	0	5.503813	-0.903548	1.377535
61	1	0	3.477617	-0.298304	1.787356
62	6	0	6.393061	-1.375972	0.414914
63	1	0	6.648896	-1.979054	-1.635306
64	1	0	5.851554	-0.699732	2.385458
65	1	0	7.433760	-1.544557	0.674369

ωB97XD/6-31G(d)- LANL2DZ energy= -2311.58645670

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.94506718

Zero-point correction= 0.531688 (Hartree/Particle)

Thermal correction to Energy= 0.567790

Thermal correction to Enthalpy= 0.568734

Thermal correction to Gibbs Free Energy= 0.460915

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.000518	-0.227514	-0.652328
2	6	0	-1.225880	1.388080	-2.567194
3	6	0	-1.667913	2.034703	-1.636511
4	1	0	-0.223270	0.775060	0.340693
5	15	0	1.968891	0.329233	-0.216776
6	8	0	1.204375	1.291511	0.714322
7	8	0	1.303465	-0.089499	-1.518309
8	6	0	-2.344252	-3.119513	0.242636
9	1	0	-3.023110	-3.972128	0.122695
10	1	0	-1.385122	-3.511682	0.603948
11	6	0	-2.908451	-2.114316	1.256016
12	1	0	-3.055205	-2.585260	2.234635
13	1	0	-3.886317	-1.746671	0.922523
14	15	0	-1.993729	-2.324353	-1.407465
15	15	0	-1.801069	-0.629422	1.413474
16	6	0	-1.143073	-3.703540	-2.280722
17	1	0	-1.719745	-4.633503	-2.244055
18	1	0	-0.977527	-3.426160	-3.324648
19	1	0	-0.165956	-3.869473	-1.819947
20	6	0	-3.659311	-2.355804	-2.196971
21	1	0	-3.579142	-1.982373	-3.221196
22	1	0	-4.096319	-3.359568	-2.213249
23	1	0	-4.325044	-1.681923	-1.651142
24	6	0	-0.614573	-1.101737	2.723863
25	1	0	0.119729	-0.298398	2.819082
26	1	0	-1.113883	-1.275575	3.682045
27	1	0	-0.073733	-2.001945	2.419196
28	6	0	-2.861530	0.614310	2.240316
29	1	0	-3.318596	0.218883	3.152733
30	1	0	-2.250045	1.486125	2.486329
31	1	0	-3.638457	0.947357	1.548013
32	6	0	-2.183479	2.880489	-0.592019
33	6	0	-3.551808	3.166337	-0.522472
34	6	0	-1.309979	3.410271	0.368753
35	6	0	-4.044410	3.968086	0.502342
36	1	0	-4.221287	2.754356	-1.270795
37	6	0	-1.812433	4.215673	1.382915
38	1	0	-0.256719	3.147720	0.330235
39	6	0	-3.176985	4.494022	1.455993
40	1	0	-5.107253	4.182618	0.554823

41	1	0	-1.133284	4.621407	2.126226
42	1	0	-3.562355	5.121058	2.254027
43	1	0	-0.794600	0.924485	-3.425168
44	6	0	2.281434	-1.199896	0.739743
45	6	0	1.826651	-2.417408	0.229315
46	6	0	2.867196	-1.169288	2.006831
47	6	0	1.932640	-3.584781	0.981628
48	1	0	1.380267	-2.419346	-0.760737
49	6	0	2.983991	-2.335152	2.757911
50	1	0	3.222450	-0.225897	2.412670
51	6	0	2.509161	-3.543283	2.249730
52	1	0	1.572781	-4.527383	0.577679
53	1	0	3.440534	-2.302517	3.742533
54	1	0	2.595855	-4.451991	2.838040
55	6	0	3.597110	1.064012	-0.532089
56	6	0	4.353985	0.649861	-1.631140
57	6	0	4.110811	2.034408	0.331689
58	6	0	5.613508	1.195589	-1.858274
59	1	0	3.942049	-0.088921	-2.311992
60	6	0	5.371850	2.577949	0.105141
61	1	0	3.504014	2.369947	1.167115
62	6	0	6.124237	2.157014	-0.988444
63	1	0	6.196265	0.875060	-2.716645
64	1	0	5.764880	3.334299	0.777939
65	1	0	7.106882	2.583497	-1.167035

ωB97XD/6-31G(d)- LANL2DZ energy= -2311.53939306
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.89702051
Zero-point correction= 0.525839 (Hartree/Particle)
Thermal correction to Energy= 0.561584
Thermal correction to Enthalpy= 0.562528
Thermal correction to Gibbs Free Energy= 0.455866

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.758528	0.223431	0.079527
2	6	0	-5.215322	-1.878559	0.646185
3	6	0	-4.240853	-2.136092	-0.023094
4	1	0	-0.529196	0.312171	-1.467877
5	15	0	2.210365	-0.679427	-0.584349
6	8	0	2.175165	-1.591816	-1.773496

7	8	0	1.096583	-0.722180	0.495613
8	6	0	-2.647020	1.712523	2.434261
9	1	0	-3.253670	1.660813	3.344668
10	1	0	-2.095354	2.659590	2.465016
11	6	0	-3.531399	1.655924	1.180231
12	1	0	-4.204247	2.519084	1.126999
13	1	0	-4.152301	0.751480	1.193196
14	15	0	-1.382133	0.352504	2.386446
15	15	0	-2.507215	1.534483	-0.363269
16	6	0	-0.143245	0.823941	3.647600
17	1	0	-0.585317	0.952184	4.639880
18	1	0	0.617540	0.040276	3.682804
19	1	0	0.345794	1.752198	3.342115
20	6	0	-2.247966	-1.072732	3.146959
21	1	0	-1.550772	-1.912251	3.211303
22	1	0	-2.618640	-0.836607	4.149108
23	1	0	-3.082912	-1.371795	2.506641
24	6	0	-1.974215	3.249938	-0.712542
25	1	0	-1.399187	3.251056	-1.641359
26	1	0	-2.825877	3.931820	-0.797668
27	1	0	-1.304828	3.588058	0.081703
28	6	0	-3.738525	1.174282	-1.659616
29	1	0	-4.469214	1.985107	-1.734957
30	1	0	-3.226297	1.044009	-2.614542
31	1	0	-4.251269	0.243133	-1.410533
32	6	0	-3.079334	-2.390485	-0.824841
33	6	0	-3.136336	-2.232970	-2.216203
34	6	0	-1.863260	-2.740502	-0.220471
35	6	0	-1.984627	-2.383634	-2.980235
36	1	0	-4.081823	-1.980814	-2.686512
37	6	0	-0.717923	-2.884809	-0.991790
38	1	0	-1.817393	-2.871939	0.855340
39	6	0	-0.771506	-2.688646	-2.369297
40	1	0	-2.033243	-2.241559	-4.055408
41	1	0	0.236989	-3.080890	-0.521195
42	1	0	0.152188	-2.734975	-2.934593
43	1	0	-6.095593	-1.706430	1.221946
44	6	0	2.278535	1.064979	-1.137806
45	6	0	2.077613	2.115589	-0.236796
46	6	0	2.468013	1.354497	-2.488179
47	6	0	2.056969	3.433640	-0.679812
48	1	0	1.918411	1.890759	0.814642
49	6	0	2.444400	2.673893	-2.936507
50	1	0	2.609648	0.530101	-3.180543

51	6	0	2.237097	3.713896	-2.034153
52	1	0	1.904375	4.244037	0.028058
53	1	0	2.588186	2.890278	-3.991113
54	1	0	2.221432	4.742432	-2.383467
55	6	0	3.751740	-0.926170	0.359538
56	6	0	3.873399	-0.495498	1.683670
57	6	0	4.841560	-1.539871	-0.260930
58	6	0	5.069757	-0.664777	2.373097
59	1	0	3.016322	-0.040467	2.171521
60	6	0	6.038861	-1.712626	0.428074
61	1	0	4.729668	-1.890858	-1.282358
62	6	0	6.155188	-1.271320	1.743763
63	1	0	5.158065	-0.328312	3.402253
64	1	0	6.881818	-2.193276	-0.059606
65	1	0	7.090153	-1.404105	2.280331

ωB97XD/6-31G(d)- LANL2DZ energy= -2311.55942582
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2311.92658597
Zero-point correction= 0.527952 (Hartree/Particle)
Thermal correction to Energy= 0.563460
Thermal correction to Enthalpy= 0.564404
Thermal correction to Gibbs Free Energy= 0.458229

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.147377	-0.839137	-0.604839
2	1	0	-0.630604	0.393063	-1.914617
3	15	0	-1.835077	-0.367179	-0.362862
4	8	0	-1.606248	0.361787	-1.782541
5	8	0	-1.127249	-1.670254	-0.134344
6	6	0	4.196625	-0.029789	0.191988
7	1	0	4.973186	0.129895	0.950627
8	1	0	4.697410	-0.419641	-0.702848
9	6	0	3.490883	1.290752	-0.139164
10	1	0	4.210914	2.031568	-0.509397
11	1	0	3.034967	1.709757	0.766292
12	15	0	3.002940	-1.354783	0.754940
13	15	0	2.103096	1.076251	-1.374768
14	6	0	4.184689	-2.766649	0.937665
15	1	0	5.068417	-2.496394	1.526850
16	1	0	3.674500	-3.602059	1.424552

17	1	0	4.504786	-3.101560	-0.052674
18	6	0	2.798466	-0.875259	2.529383
19	1	0	2.202126	-1.634405	3.042920
20	1	0	3.759851	-0.765252	3.043569
21	1	0	2.251059	0.069729	2.579676
22	6	0	3.050129	1.065752	-2.960402
23	1	0	3.753005	1.903596	-3.026073
24	1	0	3.599892	0.124899	-3.042904
25	1	0	2.352079	1.116298	-3.800113
26	6	0	1.451075	2.806353	-1.381837
27	1	0	2.242855	3.549833	-1.527536
28	1	0	0.710084	2.915048	-2.179126
29	1	0	0.948104	2.995787	-0.429337
30	6	0	-3.628732	-0.547482	-0.339178
31	6	0	-4.486972	0.438695	-0.834891
32	6	0	-4.156842	-1.709120	0.227856
33	6	0	-5.863555	0.262102	-0.758492
34	1	0	-4.079506	1.333133	-1.295287
35	6	0	-5.535725	-1.881676	0.302614
36	1	0	-3.478974	-2.474903	0.591572
37	6	0	-6.387734	-0.896279	-0.187438
38	1	0	-6.529768	1.025311	-1.148047
39	1	0	-5.944646	-2.786996	0.739635
40	1	0	-7.463260	-1.031711	-0.128074
41	6	0	-1.360107	0.862198	0.881445
42	6	0	-1.586614	2.226734	0.685842
43	6	0	-0.731365	0.423641	2.049836
44	6	0	-1.184286	3.146046	1.649508
45	1	0	-2.053921	2.572575	-0.231183
46	6	0	-0.329918	1.345414	3.011786
47	1	0	-0.538695	-0.636818	2.179182
48	6	0	-0.554366	2.705527	2.811878
49	1	0	-1.356326	4.206060	1.491358
50	1	0	0.161414	1.001123	3.916655
51	1	0	-0.238596	3.424002	3.561932

ωB97XD/6-31G(d)- LANL2DZ energy= -2003.25429671

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2003.53559958

Zero-point correction= 0.418526 (Hartree/Particle)

Thermal correction to Energy= 0.447169

Thermal correction to Enthalpy= 0.448113

Thermal correction to Gibbs Free Energy= 0.356736

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.297049	-0.146830	-0.039642
2	1	0	0.241927	-0.393998	-1.289398
3	15	0	-1.731054	-0.092980	-0.218121
4	8	0	-1.162868	-0.444163	-1.605798
5	8	0	-0.682925	0.052082	0.893457
6	6	0	4.588766	-0.162569	0.709146
7	1	0	5.479452	0.292711	1.157513
8	1	0	4.688369	-1.248143	0.830733
9	6	0	4.495950	0.189921	-0.782284
10	1	0	5.367649	-0.188501	-1.328782
11	1	0	4.482930	1.278861	-0.911157
12	15	0	3.056048	0.338500	1.647627
13	15	0	2.923915	-0.452630	-1.543746
14	6	0	3.412547	-0.376335	3.307250
15	1	0	4.400598	-0.089435	3.682084
16	1	0	2.651081	-0.034654	4.012907
17	1	0	3.350823	-1.466163	3.251577
18	6	0	3.376274	2.129442	1.942624
19	1	0	2.591129	2.529931	2.588902
20	1	0	4.351297	2.306523	2.408379
21	1	0	3.325561	2.665265	0.991287
22	6	0	3.356178	-2.190111	-1.953251
23	1	0	4.243996	-2.247961	-2.591270
24	1	0	3.535185	-2.743565	-1.028299
25	1	0	2.508902	-2.655470	-2.461763
26	6	0	2.924229	0.354226	-3.189605
27	1	0	3.866099	0.190976	-3.723159
28	1	0	2.095875	-0.047122	-3.777910
29	1	0	2.756223	1.426110	-3.062847
30	6	0	-2.941523	-1.360667	0.248608
31	6	0	-3.366151	-2.308266	-0.684337
32	6	0	-3.464831	-1.384755	1.544915
33	6	0	-4.308078	-3.269389	-0.325649
34	1	0	-2.943125	-2.286726	-1.683787
35	6	0	-4.405542	-2.343966	1.901268
36	1	0	-3.126810	-0.653734	2.273510
37	6	0	-4.829354	-3.285778	0.964828
38	1	0	-4.634403	-4.005888	-1.053640
39	1	0	-4.809860	-2.360222	2.908816
40	1	0	-5.565074	-4.033976	1.244168

41	6	0	-2.669953	1.458933	-0.312623
42	6	0	-3.596846	1.669950	-1.337464
43	6	0	-2.471700	2.448453	0.651677
44	6	0	-4.321363	2.855223	-1.392626
45	1	0	-3.743495	0.905002	-2.094698
46	6	0	-3.196015	3.636549	0.594232
47	1	0	-1.740678	2.274989	1.435307
48	6	0	-4.122275	3.838902	-0.425007
49	1	0	-5.041186	3.014571	-2.189733
50	1	0	-3.038186	4.404460	1.345720
51	1	0	-4.687719	4.765057	-0.468829

ωB97XD/6-31G(d)- LANL2DZ energy= -2003.23433333
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2003.52431654
Zero-point correction= 0.412490 (Hartree/Particle)
Thermal correction to Energy= 0.440732
Thermal correction to Enthalpy= 0.441676
Thermal correction to Gibbs Free Energy= 0.348948

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.396778	0.354060	-0.658869
2	1	0	-1.200371	1.876414	-0.995527
3	15	0	1.445568	0.013568	0.226018
4	8	0	0.772947	-0.205770	1.558181
5	8	0	0.622554	-0.138896	-1.080407
6	6	0	-3.372878	-1.626384	1.189799
7	1	0	-3.905343	-2.562430	1.389007
8	1	0	-2.941535	-1.284242	2.137240
9	6	0	-4.325794	-0.562926	0.622167
10	1	0	-5.112107	-0.304565	1.339872
11	1	0	-4.821087	-0.940653	-0.280116
12	15	0	-1.948603	-1.887431	0.029052
13	15	0	-3.390738	0.964606	0.128125
14	6	0	-0.743902	-2.893572	0.955163
15	1	0	-1.211963	-3.760908	1.429559
16	1	0	0.027552	-3.229116	0.256613
17	1	0	-0.253822	-2.238306	1.680729
18	6	0	-2.631951	-3.044091	-1.222978
19	1	0	-1.852729	-3.268177	-1.955366
20	1	0	-2.976565	-3.977627	-0.767728

21	1	0	-3.463048	-2.571049	-1.752407
22	6	0	-3.207146	1.890633	1.693331
23	1	0	-4.173330	2.056294	2.179510
24	1	0	-2.544021	1.330949	2.357123
25	1	0	-2.727645	2.848385	1.481406
26	6	0	-4.591808	1.938766	-0.843347
27	1	0	-5.530224	2.074229	-0.297746
28	1	0	-4.152082	2.914112	-1.062182
29	1	0	-4.788698	1.433439	-1.791282
30	6	0	2.824362	-1.164294	0.038560
31	6	0	3.252950	-1.894914	1.148113
32	6	0	3.452266	-1.357980	-1.195183
33	6	0	4.297123	-2.808951	1.028287
34	1	0	2.750276	-1.741325	2.098413
35	6	0	4.496616	-2.268706	-1.315142
36	1	0	3.110034	-0.799693	-2.061379
37	6	0	4.920164	-2.994566	-0.202701
38	1	0	4.624886	-3.375721	1.894889
39	1	0	4.980162	-2.416358	-2.276276
40	1	0	5.734244	-3.707334	-0.297428
41	6	0	2.200579	1.669078	0.163538
42	6	0	2.733449	2.240225	1.321393
43	6	0	2.261208	2.372753	-1.041182
44	6	0	3.332454	3.495179	1.272503
45	1	0	2.661504	1.699199	2.260291
46	6	0	2.858339	3.629192	-1.090122
47	1	0	1.820517	1.929119	-1.928860
48	6	0	3.398121	4.188692	0.065645
49	1	0	3.746391	3.935372	2.174935
50	1	0	2.901441	4.172951	-2.029313
51	1	0	3.867018	5.167646	0.026806

ωB97XD/6-31G(d)- LANL2DZ energy= -2003.25554419
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2003.55174509
Zero-point correction= 0.416142 (Hartree/Particle)
Thermal correction to Energy= 0.444274
Thermal correction to Enthalpy= 0.445219
Thermal correction to Gibbs Free Energy= 0.354653

INT10

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

1	46	0	0.458325	0.390007	-0.539990
2	6	0	2.042300	2.446644	-1.725129
3	6	0	2.128817	1.486907	-0.795969
4	1	0	1.107166	2.662229	-2.234589
5	15	0	-2.685013	-0.312018	-1.200779
6	8	0	-2.471796	-0.358665	-2.690559
7	8	0	-1.479441	-0.571188	-0.264287
8	6	0	-1.056211	0.827170	2.479005
9	1	0	-1.600884	1.620032	3.005812
10	1	0	-1.761950	0.310285	1.823759
11	6	0	-0.444413	-0.145759	3.494552
12	1	0	-1.259053	-0.585784	4.084456
13	1	0	0.190385	0.402569	4.201221
14	15	0	0.135011	1.642799	1.332212
15	15	0	0.615229	-1.519891	2.799745
16	6	0	-0.639630	3.242198	0.917124
17	1	0	-0.817560	3.834578	1.819518
18	1	0	0.034225	3.782449	0.247859
19	1	0	-1.585198	3.072742	0.401274
20	6	0	1.540167	2.134834	2.392181
21	1	0	2.191002	2.812738	1.837441
22	1	0	1.163739	2.638335	3.287889
23	1	0	2.126517	1.258035	2.672691
24	6	0	-0.670992	-2.625966	2.078171
25	1	0	-0.210453	-3.582440	1.813698
26	1	0	-1.492474	-2.817265	2.778973
27	1	0	-1.060601	-2.169153	1.163061
28	6	0	0.941063	-2.397527	4.399835
29	1	0	0.017431	-2.608888	4.950456
30	1	0	1.449129	-3.344371	4.197201
31	1	0	1.598823	-1.793084	5.031016
32	6	0	2.896498	-1.514716	-2.165940
33	6	0	3.965204	-0.734173	-2.621506
34	6	0	5.270816	-1.135912	-2.372594
35	6	0	5.518738	-2.319094	-1.681738
36	6	0	4.457367	-3.106540	-1.240263
37	6	0	3.148582	-2.707560	-1.477110
38	1	0	3.757239	0.198238	-3.134232
39	1	0	6.096638	-0.517427	-2.707856
40	1	0	6.540858	-2.625899	-1.483784
41	1	0	4.650229	-4.030514	-0.704680
42	1	0	2.312655	-3.301223	-1.122060
43	6	0	1.544394	-1.082764	-2.373847
44	6	0	0.398490	-0.747044	-2.625423

45	1	0	-0.639023	-0.599239	-2.928477
46	6	0	3.377210	1.171654	-0.054726
47	6	0	3.502602	-0.033194	0.646306
48	6	0	4.458400	2.064999	-0.017022
49	6	0	4.671581	-0.355219	1.325042
50	1	0	2.667607	-0.725504	0.666422
51	6	0	5.628546	1.746560	0.662197
52	1	0	4.380398	3.028451	-0.511176
53	6	0	5.744692	0.530532	1.331637
54	1	0	4.738828	-1.304310	1.847724
55	1	0	6.450030	2.456810	0.675954
56	1	0	6.659553	0.283407	1.861499
57	1	0	2.904919	3.029784	-2.046243
58	6	0	-3.962304	-1.496885	-0.684297
59	6	0	-4.060464	-1.940887	0.637467
60	6	0	-4.876056	-1.962828	-1.632289
61	6	0	-5.065300	-2.828092	1.009427
62	1	0	-3.334897	-1.603410	1.371556
63	6	0	-5.879548	-2.853095	-1.261314
64	1	0	-4.778964	-1.630523	-2.661293
65	6	0	-5.977096	-3.283299	0.059627
66	1	0	-5.134190	-3.171434	2.037402
67	1	0	-6.584311	-3.214730	-2.003817
68	1	0	-6.759033	-3.979154	0.348523
69	6	0	-3.350044	1.336792	-0.766665
70	6	0	-3.960106	1.607169	0.462210
71	6	0	-3.191734	2.374004	-1.689122
72	6	0	-4.388852	2.894867	0.770411
73	1	0	-4.116006	0.804500	1.177845
74	6	0	-3.617186	3.664439	-1.381598
75	1	0	-2.740254	2.148304	-2.650353
76	6	0	-4.213531	3.926575	-0.150582
77	1	0	-4.866245	3.092869	1.725394
78	1	0	-3.490182	4.463269	-2.105948
79	1	0	-4.549542	4.931142	0.088128

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2619.91209672

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2620.33607024

Zero-point correction= 0.647000 (Hartree/Particle)

Thermal correction to Energy= 0.689598

Thermal correction to Enthalpy= 0.690542

Thermal correction to Gibbs Free Energy= 0.568733

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.272110	-0.104425	0.311017
2	6	0	-1.804557	-1.303025	2.441937
3	6	0	-1.906108	-0.461475	1.405849
4	1	0	-0.856989	-1.757122	2.717610
5	15	0	2.605233	-0.985046	-0.593543
6	8	0	1.957170	-2.261765	-1.211140
7	8	0	1.740323	0.268645	-0.665130
8	6	0	1.140808	2.987453	0.895538
9	1	0	1.654747	3.533061	1.696648
10	1	0	1.895036	2.432366	0.328513
11	6	0	0.398931	3.981293	-0.007202
12	1	0	1.133940	4.662631	-0.455424
13	1	0	-0.270845	4.602659	0.599871
14	15	0	0.083042	1.695090	1.681004
15	15	0	-0.655127	3.235817	-1.358772
16	6	0	1.041604	1.204797	3.159262
17	1	0	1.206307	2.051267	3.832879
18	1	0	0.491414	0.418962	3.682335
19	1	0	2.002879	0.792937	2.842480
20	6	0	-1.338972	2.610097	2.373051
21	1	0	-1.882294	1.951139	3.053009
22	1	0	-1.004305	3.500844	2.913215
23	1	0	-2.019389	2.892119	1.566397
24	6	0	0.659933	2.673606	-2.527893
25	1	0	0.197135	2.405174	-3.481971
26	1	0	1.411999	3.451418	-2.707952
27	1	0	1.138244	1.778011	-2.121671
28	6	0	-1.146783	4.823670	-2.180517
29	1	0	-0.284247	5.458504	-2.413849
30	1	0	-1.674816	4.599017	-3.111413
31	1	0	-1.831807	5.381361	-1.535460
32	6	0	-3.126686	-2.474225	-1.485874
33	6	0	-3.985449	-2.839087	-0.437947
34	6	0	-5.339592	-3.026644	-0.678350
35	6	0	-5.850534	-2.869575	-1.965123
36	6	0	-5.002581	-2.518773	-3.013550
37	6	0	-3.648760	-2.315065	-2.777225
38	1	0	-3.574016	-2.938465	0.561063
39	1	0	-6.000999	-3.292730	0.140086
40	1	0	-6.909892	-3.018332	-2.150300

41	1	0	-5.401001	-2.393660	-4.015665
42	1	0	-2.982339	-2.023663	-3.582442
43	6	0	-1.753516	-2.192092	-1.204466
44	6	0	-0.599864	-1.902102	-0.882885
45	1	0	0.854777	-2.183456	-1.098020
46	6	0	-3.180527	0.194866	1.022903
47	6	0	-3.416003	0.607160	-0.294414
48	6	0	-4.185816	0.427584	1.973955
49	6	0	-4.626078	1.186670	-0.658154
50	1	0	-2.640629	0.462073	-1.038391
51	6	0	-5.393765	1.012473	1.613392
52	1	0	-4.010665	0.160630	3.012163
53	6	0	-5.622598	1.388166	0.291812
54	1	0	-4.787672	1.480114	-1.690644
55	1	0	-6.156170	1.181901	2.368210
56	1	0	-6.566077	1.845050	0.008966
57	1	0	-2.674699	-1.608038	3.023022
58	6	0	4.175849	-0.688885	-1.426058
59	6	0	4.413446	0.557494	-2.007555
60	6	0	5.153231	-1.686811	-1.487569
61	6	0	5.624479	0.804602	-2.648198
62	1	0	3.644457	1.322069	-1.957854
63	6	0	6.361221	-1.435908	-2.127241
64	1	0	4.967626	-2.656960	-1.036034
65	6	0	6.596281	-0.189901	-2.706819
66	1	0	5.807556	1.772474	-3.103929
67	1	0	7.119459	-2.210689	-2.175821
68	1	0	7.540872	0.003695	-3.205717
69	6	0	2.989266	-1.354588	1.140412
70	6	0	4.065648	-0.742676	1.787775
71	6	0	2.114438	-2.166424	1.870064
72	6	0	4.264516	-0.936842	3.152136
73	1	0	4.751934	-0.117810	1.222886
74	6	0	2.310658	-2.351724	3.234809
75	1	0	1.280063	-2.647162	1.366644
76	6	0	3.383973	-1.736913	3.876377
77	1	0	5.106498	-0.464770	3.648561
78	1	0	1.628988	-2.982026	3.797296
79	1	0	3.538276	-1.887154	4.940347

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2619.89050895

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2620.31118640

Zero-point correction= 0.643550 (Hartree/Particle)

Thermal correction to Energy= 0.685899

Thermal correction to Enthalpy= 0.686843
Thermal correction to Gibbs Free Energy= 0.565058

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.834286	-0.260772	0.300879
2	6	0	1.117538	1.826449	2.433117
3	6	0	0.797392	1.606733	1.152676
4	1	0	1.400590	1.019424	3.104532
5	6	0	3.604259	-2.138384	-0.112612
6	1	0	4.646920	-2.217667	-0.439103
7	1	0	3.520462	-2.679356	0.837512
8	6	0	2.647554	-2.748127	-1.149746
9	1	0	2.824036	-3.822607	-1.266680
10	1	0	2.812306	-2.285463	-2.130163
11	15	0	3.153689	-0.369890	0.256006
12	15	0	0.883158	-2.388303	-0.685234
13	6	0	4.117066	0.037811	1.753080
14	1	0	5.190953	-0.095150	1.595425
15	1	0	3.901342	1.075345	2.019203
16	1	0	3.785701	-0.595453	2.579493
17	6	0	3.995643	0.586491	-1.061127
18	1	0	3.839296	1.651237	-0.870684
19	1	0	5.068726	0.376019	-1.094489
20	1	0	3.546564	0.349913	-2.028938
21	6	0	0.386603	-3.760157	0.418305
22	1	0	-0.647858	-3.577841	0.720216
23	1	0	0.465068	-4.734732	-0.072177
24	1	0	1.005847	-3.750488	1.318596
25	6	0	-0.092558	-2.675921	-2.200602
26	1	0	0.009269	-3.697917	-2.576237
27	1	0	-1.137539	-2.466271	-1.957202
28	1	0	0.219758	-1.966305	-2.970176
29	6	0	-3.804650	-0.598949	0.222985
30	6	0	-4.588018	0.290738	-0.529906
31	6	0	-5.966800	0.132696	-0.602359
32	6	0	-6.594317	-0.910665	0.075022
33	6	0	-5.828703	-1.795531	0.830762
34	6	0	-4.449268	-1.643951	0.904195
35	1	0	-4.097223	1.106058	-1.051415
36	1	0	-6.556565	0.829035	-1.191309

37	1	0	-7.671449	-1.032484	0.015149
38	1	0	-6.309005	-2.610076	1.365227
39	1	0	-3.851362	-2.330259	1.495740
40	6	0	-2.382389	-0.450660	0.283832
41	6	0	-1.169517	-0.304014	0.325794
42	6	0	0.361929	2.720793	0.278321
43	6	0	0.828897	2.836142	-1.038029
44	6	0	-0.539702	3.689240	0.740409
45	6	0	0.443466	3.896548	-1.850243
46	1	0	1.497269	2.071946	-1.426290
47	6	0	-0.936659	4.744968	-0.073828
48	1	0	-0.947990	3.589509	1.741215
49	6	0	-0.441657	4.858842	-1.370271
50	1	0	0.828494	3.968798	-2.863572
51	1	0	-1.643976	5.478152	0.303096
52	1	0	-0.753587	5.681690	-2.006342
53	1	0	1.087448	2.826802	2.868705

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1664.33877204
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1664.59890034
Zero-point correction= 0.439835 (Hartree/Particle)
Thermal correction to Energy= 0.468861
Thermal correction to Enthalpy= 0.469806
Thermal correction to Gibbs Free Energy= 0.376685

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.941550	-0.286737	0.338575
2	6	0	-0.361218	1.215480	2.509135
3	6	0	-0.425358	1.079178	1.169579
4	1	0	-0.052099	0.395638	3.148440
5	6	0	4.317435	-0.541913	-0.161846
6	1	0	5.248155	-0.116352	-0.553628
7	1	0	4.559360	-1.023728	0.793204
8	6	0	3.730780	-1.575854	-1.136090
9	1	0	4.426576	-2.408581	-1.289576
10	1	0	3.561465	-1.113015	-2.116085
11	15	0	3.075320	0.791963	0.212924
12	15	0	2.075214	-2.191807	-0.543057
13	6	0	3.824604	1.663982	1.642598
14	1	0	4.843163	2.006939	1.436671

15	1	0	3.196180	2.522461	1.893331
16	1	0	3.833460	0.994534	2.506331
17	6	0	3.347376	1.988773	-1.157770
18	1	0	2.689717	2.849533	-1.011110
19	1	0	4.386669	2.328262	-1.210409
20	1	0	3.073295	1.519598	-2.106725
21	6	0	2.553475	-3.521089	0.634778
22	1	0	1.648263	-4.015462	0.995589
23	1	0	3.213175	-4.263167	0.173734
24	1	0	3.055046	-3.077416	1.498539
25	6	0	1.468679	-3.150868	-1.984991
26	1	0	2.193579	-3.899152	-2.320168
27	1	0	0.535716	-3.647740	-1.707785
28	1	0	1.247799	-2.463808	-2.805467
29	6	0	-3.554524	-1.247459	0.131641
30	6	0	-4.337309	-0.440143	-0.713291
31	6	0	-5.682056	-0.723040	-0.911845
32	6	0	-6.276349	-1.810444	-0.273528
33	6	0	-5.510899	-2.614259	0.568469
34	6	0	-4.163855	-2.340164	0.770652
35	1	0	-3.872710	0.413148	-1.197277
36	1	0	-6.273235	-0.087916	-1.564972
37	1	0	-7.328543	-2.027288	-0.429556
38	1	0	-5.966633	-3.462840	1.070307
39	1	0	-3.566047	-2.966805	1.424610
40	6	0	-2.179575	-0.936153	0.332042
41	6	0	-1.025809	-0.554405	0.507354
42	6	0	-0.932312	2.184589	0.309382
43	6	0	-0.381557	2.439421	-0.951364
44	6	0	-1.995605	2.988838	0.737752
45	6	0	-0.840621	3.489943	-1.738060
46	1	0	0.408128	1.789015	-1.317306
47	6	0	-2.460507	4.038115	-0.048583
48	1	0	-2.470135	2.773372	1.690133
49	6	0	-1.880684	4.298695	-1.287522
50	1	0	-0.391504	3.670408	-2.710472
51	1	0	-3.286962	4.648136	0.303982
52	1	0	-2.247154	5.114393	-1.903265
53	1	0	-0.638700	2.148101	2.995538

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1664.31506377

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1664.56788204

Zero-point correction= 0.438686 (Hartree/Particle)

Thermal correction to Energy= 0.467343

Thermal correction to Enthalpy= 0.468287
Thermal correction to Gibbs Free Energy= 0.376500

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.143064	-0.240069	0.624420
2	6	0	0.533585	0.655530	2.485439
3	6	0	-0.206669	1.225649	1.411201
4	1	0	0.038362	-0.070115	3.122774
5	6	0	2.091917	-1.656223	-2.314094
6	1	0	1.781078	-2.124730	-3.254606
7	1	0	3.003215	-1.083862	-2.525667
8	6	0	2.379843	-2.719103	-1.241675
9	1	0	3.209872	-3.367603	-1.546778
10	1	0	1.501207	-3.362304	-1.109229
11	15	0	0.821045	-0.436808	-1.707649
12	15	0	2.727912	-1.955175	0.427939
13	6	0	0.979840	0.969750	-2.875916
14	1	0	0.827155	0.675152	-3.918913
15	1	0	0.244673	1.730006	-2.597070
16	1	0	1.969953	1.418614	-2.763405
17	6	0	-0.775570	-1.196593	-2.204719
18	1	0	-1.588516	-0.552165	-1.858852
19	1	0	-0.853104	-1.344069	-3.286605
20	1	0	-0.889174	-2.157691	-1.696771
21	6	0	4.491463	-1.456690	0.242379
22	1	0	4.860955	-1.079220	1.199047
23	1	0	5.122836	-2.289439	-0.085049
24	1	0	4.560638	-0.643385	-0.484462
25	6	0	2.877660	-3.460662	1.475003
26	1	0	3.577169	-4.190059	1.052919
27	1	0	3.221433	-3.169671	2.470749
28	1	0	1.893656	-3.924013	1.581639
29	6	0	-3.819351	-0.428026	0.492908
30	6	0	-4.644992	0.113887	-0.504903
31	6	0	-5.837203	-0.511978	-0.848284
32	6	0	-6.227559	-1.684680	-0.205963
33	6	0	-5.414914	-2.229293	0.786046
34	6	0	-4.221773	-1.609945	1.135114
35	1	0	-4.341864	1.029789	-1.002394
36	1	0	-6.466337	-0.080540	-1.620910

37	1	0	-7.160076	-2.170270	-0.475497
38	1	0	-5.712825	-3.142803	1.291552
39	1	0	-3.586478	-2.030859	1.907443
40	6	0	-2.583176	0.195928	0.840883
41	6	0	-1.502098	0.671690	1.121505
42	6	0	0.127128	2.540471	0.777163
43	6	0	-0.763682	3.141071	-0.121796
44	6	0	1.344541	3.191425	1.024145
45	6	0	-0.447631	4.337027	-0.758254
46	1	0	-1.715446	2.658482	-0.319496
47	6	0	1.658219	4.387013	0.389323
48	1	0	2.065418	2.749885	1.704126
49	6	0	0.766950	4.968361	-0.509953
50	1	0	-1.160196	4.778448	-1.449275
51	1	0	2.610029	4.867034	0.597626
52	1	0	1.014606	5.902134	-1.004797
53	1	0	1.317304	1.228507	2.970931

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1664.38324164
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1664.63147364
Zero-point correction= 0.440738 (Hartree/Particle)
Thermal correction to Energy= 0.469399
Thermal correction to Enthalpy= 0.470343
Thermal correction to Gibbs Free Energy= 0.376373

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.439229	-0.443353	-0.003127
2	6	0	-1.964579	-1.859556	-0.080808
3	6	0	-2.505207	-0.716537	0.007452
4	1	0	-2.049989	-2.927735	-0.160610
5	6	0	2.825419	0.399694	-0.375262
6	1	0	2.791624	0.539400	-1.462714
7	1	0	3.877047	0.256408	-0.100461
8	6	0	2.231920	1.627414	0.327374
9	1	0	2.357608	1.533027	1.412961
10	1	0	2.746517	2.545930	0.021608
11	15	0	1.824449	-1.130562	-0.005727
12	15	0	0.398954	1.756766	0.010532
13	6	0	2.612910	-2.353411	-1.133531
14	1	0	3.700222	-2.392528	-1.008721

15	1	0	2.193972	-3.342583	-0.932098
16	1	0	2.376871	-2.094978	-2.168897
17	6	0	2.523559	-1.642663	1.620801
18	1	0	2.072588	-2.592604	1.918141
19	1	0	3.612741	-1.753084	1.589284
20	1	0	2.255158	-0.899807	2.376087
21	6	0	0.365893	2.637307	-1.608371
22	1	0	-0.671991	2.855800	-1.872060
23	1	0	0.938261	3.570770	-1.587061
24	1	0	0.771161	1.979623	-2.381555
25	6	0	-0.071210	3.113105	1.163531
26	1	0	0.554922	4.002510	1.036860
27	1	0	-1.115655	3.382395	0.986574
28	1	0	0.013427	2.754994	2.192665
29	6	0	-3.702590	0.155264	0.085509
30	6	0	-5.018253	-0.622464	-0.007392
31	1	0	-3.648536	0.903402	-0.713854
32	1	0	-3.663366	0.719456	1.024821
33	1	0	-5.879080	0.050190	0.063849
34	1	0	-5.079936	-1.160215	-0.957830
35	1	0	-5.087257	-1.358103	0.798959

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1203.64696736
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1203.79718880
Zero-point correction= 0.299504 (Hartree/Particle)
Thermal correction to Energy= 0.319690
Thermal correction to Enthalpy= 0.320634
Thermal correction to Gibbs Free Energy= 0.250065

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.315745	-0.408668	0.065642
2	6	0	2.308400	-0.251078	0.145250
3	6	0	3.511794	-0.052743	0.191276
4	1	0	1.409003	-1.550654	0.213849
5	6	0	-3.047096	0.085506	0.295380
6	1	0	-3.070212	0.255711	1.378627
7	1	0	-4.062136	-0.196772	-0.007491
8	6	0	-2.589617	1.360888	-0.427000
9	1	0	-2.666854	1.223400	-1.512327
10	1	0	-3.228471	2.211602	-0.163311

11	15	0	-1.858404	-1.318426	0.001064
12	15	0	-0.801394	1.729986	-0.058040
13	6	0	-2.503285	-2.603738	1.143325
14	1	0	-3.575965	-2.772031	1.004196
15	1	0	-1.966930	-3.538890	0.965238
16	1	0	-2.314186	-2.299536	2.175491
17	6	0	-2.414329	-1.950126	-1.634973
18	1	0	-1.854151	-2.856461	-1.876806
19	1	0	-3.486462	-2.171965	-1.645271
20	1	0	-2.189964	-1.206926	-2.403993
21	6	0	-0.915806	2.621699	1.546682
22	1	0	0.080648	2.970937	1.827849
23	1	0	-1.601033	3.474293	1.499265
24	1	0	-1.252492	1.927656	2.320833
25	6	0	-0.440411	3.096994	-1.230614
26	1	0	-1.171608	3.908305	-1.156713
27	1	0	0.556851	3.489932	-1.018344
28	1	0	-0.435582	2.705104	-2.250649
29	6	0	4.955685	0.188185	0.234090
30	6	0	5.771347	-0.945947	-0.402181
31	1	0	5.268408	0.318921	1.277857
32	1	0	5.190996	1.133171	-0.272581
33	1	0	6.843765	-0.734478	-0.341789
34	1	0	5.576603	-1.892933	0.108241
35	1	0	5.502387	-1.070887	-1.454468

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1203.60169378
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1203.75839502
Zero-point correction= 0.295225 (Hartree/Particle)
Thermal correction to Energy= 0.315498
Thermal correction to Enthalpy= 0.316442
Thermal correction to Gibbs Free Energy= 0.244891

INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.098973	-0.720471	-0.028709
2	6	0	-2.086632	-0.515275	-0.013906
3	6	0	-3.278131	-0.251063	0.019095
4	1	0	-0.349970	-2.272264	-0.102606
5	6	0	2.876284	0.822683	-0.388966
6	1	0	2.813071	0.934045	-1.478139

7	1	0	3.935727	0.894907	-0.118034
8	6	0	2.049582	1.922431	0.297414
9	1	0	2.207583	1.889413	1.381820
10	1	0	2.356332	2.916504	-0.044961
11	15	0	2.213031	-0.874676	0.002978
12	15	0	0.236923	1.621395	0.009447
13	6	0	3.172158	-1.955446	-1.121421
14	1	0	4.249288	-1.795357	-1.014291
15	1	0	2.935247	-2.997548	-0.895297
16	1	0	2.873595	-1.759000	-2.153615
17	6	0	2.950712	-1.234002	1.644222
18	1	0	2.685190	-2.252724	1.935593
19	1	0	4.040053	-1.129379	1.630659
20	1	0	2.527772	-0.554086	2.387620
21	6	0	-0.120201	2.446697	-1.585771
22	1	0	-1.177914	2.287053	-1.809451
23	1	0	0.096293	3.518876	-1.556932
24	1	0	0.463255	1.974820	-2.380031
25	6	0	-0.640415	2.661312	1.228328
26	1	0	-0.437894	3.727930	1.096043
27	1	0	-1.708245	2.462675	1.102422
28	1	0	-0.360320	2.354132	2.238654
29	6	0	-4.724172	-0.013805	0.068416
30	6	0	-5.548410	-1.305715	-0.017099
31	1	0	-5.019914	0.658716	-0.747760
32	1	0	-4.977554	0.514001	0.997589
33	1	0	-6.620664	-1.091845	0.044510
34	1	0	-5.350921	-1.823596	-0.959413
35	1	0	-5.281198	-1.983287	0.797994

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1203.61182991
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1203.77299922
Zero-point correction= 0.297232 (Hartree/Particle)
Thermal correction to Energy= 0.317540
Thermal correction to Enthalpy= 0.318484
Thermal correction to Gibbs Free Energy= 0.247156

INT15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.244460	-1.024286	0.417188
2	6	0	1.249678	-1.202570	2.531870

3	6	0	2.424255	-1.227958	2.031020
4	1	0	-0.711538	-1.488576	1.855470
5	15	0	-1.903944	-0.547112	0.350953
6	8	0	-1.683548	-1.418689	1.674862
7	8	0	-0.860774	-0.760547	-0.717498
8	6	0	2.207062	0.344172	-2.785738
9	1	0	2.732836	0.088597	-3.715175
10	1	0	1.138166	0.381322	-3.024184
11	6	0	2.686130	1.714252	-2.289586
12	1	0	2.586083	2.433997	-3.112898
13	1	0	3.753756	1.673468	-2.041016
14	15	0	2.418751	-1.062683	-1.600785
15	15	0	1.777853	2.391057	-0.799107
16	6	0	1.961487	-2.470061	-2.693556
17	1	0	2.495077	-2.448418	-3.649686
18	1	0	2.177416	-3.409206	-2.178525
19	1	0	0.884300	-2.426799	-2.873490
20	6	0	4.251447	-1.215404	-1.528061
21	1	0	4.507812	-2.138501	-1.001834
22	1	0	4.705347	-1.230879	-2.524582
23	1	0	4.663244	-0.380243	-0.955795
24	6	0	0.084102	2.502682	-1.534121
25	1	0	-0.543841	3.128764	-0.893821
26	1	0	0.099865	2.931588	-2.543352
27	1	0	-0.363859	1.505716	-1.562024
28	6	0	2.288887	4.167012	-0.983024
29	1	0	2.099592	4.560726	-1.988538
30	1	0	1.733070	4.773350	-0.261696
31	1	0	3.354136	4.275178	-0.758349
32	1	0	0.743362	-1.213791	3.486067
33	6	0	-1.992978	1.180918	0.886246
34	6	0	-2.999439	2.029956	0.419364
35	6	0	-0.977302	1.693902	1.701159
36	6	0	-2.991073	3.379070	0.762158
37	1	0	-3.789462	1.641206	-0.216233
38	6	0	-0.971393	3.042573	2.038569
39	1	0	-0.177372	1.045729	2.048347
40	6	0	-1.977127	3.885900	1.570701
41	1	0	-3.775142	4.034310	0.396266
42	1	0	-0.175603	3.434017	2.663920
43	1	0	-1.970072	4.938967	1.835000
44	6	0	-3.551389	-1.032685	-0.188873
45	6	0	-3.764718	-1.287353	-1.544278
46	6	0	-4.610026	-1.134406	0.719188

47	6	0	-5.034477	-1.642651	-1.991487
48	1	0	-2.931023	-1.213927	-2.235487
49	6	0	-5.875072	-1.491607	0.268388
50	1	0	-4.440479	-0.941772	1.774006
51	6	0	-6.086915	-1.743444	-1.086352
52	1	0	-5.200988	-1.842458	-3.045080
53	1	0	-6.695787	-1.575740	0.973441
54	1	0	-7.076647	-2.020871	-1.435966
55	6	0	3.893852	-1.301655	2.215578
56	6	0	4.298607	-1.352240	3.691195
57	1	0	4.352687	-0.435170	1.725036
58	1	0	4.273129	-2.184797	1.687800
59	1	0	5.386104	-1.407839	3.799339
60	1	0	3.944875	-0.460113	4.215516
61	1	0	3.858847	-2.226175	4.179887

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.19369995
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.51244718
Zero-point correction= 0.505930 (Hartree/Particle)
Thermal correction to Energy= 0.540487
Thermal correction to Enthalpy= 0.541431
Thermal correction to Gibbs Free Energy= 0.436415

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.272791	-0.960145	0.312770
2	6	0	-2.776956	-1.844993	-0.578408
3	6	0	-3.823906	-2.289142	-1.021172
4	1	0	0.582192	-2.481012	-0.772988
5	15	0	1.890395	-0.925851	-0.116356
6	8	0	1.554729	-2.369438	-0.736193
7	8	0	0.890975	-0.451562	0.910920
8	6	0	-1.768495	2.157725	2.390248
9	1	0	-2.309337	2.473150	3.291646
10	1	0	-0.717665	2.032096	2.675115
11	6	0	-1.900097	3.245420	1.316902
12	1	0	-1.494862	4.184956	1.715786
13	1	0	-2.959676	3.427062	1.101477
14	15	0	-2.378609	0.475270	1.899800
15	15	0	-1.062000	2.858050	-0.306271
16	6	0	-2.597701	-0.297749	3.555566

17	1	0	-3.228400	0.308939	4.213918
18	1	0	-3.053375	-1.282255	3.424287
19	1	0	-1.618775	-0.437770	4.021406
20	6	0	-4.111976	0.799570	1.394933
21	1	0	-4.588333	-0.165156	1.202418
22	1	0	-4.674916	1.356428	2.150907
23	1	0	-4.109518	1.350323	0.451112
24	6	0	0.698754	2.896227	0.259109
25	1	0	1.355343	2.955181	-0.613959
26	1	0	0.902956	3.750043	0.915838
27	1	0	0.924724	1.962216	0.780771
28	6	0	-1.170291	4.546710	-1.066325
29	1	0	-0.781445	5.331160	-0.407180
30	1	0	-0.596658	4.555618	-1.997892
31	1	0	-2.211163	4.776276	-1.312324
32	1	0	-1.331947	-2.096610	-0.841845
33	6	0	2.018971	0.227505	-1.502946
34	6	0	3.204527	0.911885	-1.781707
35	6	0	0.866219	0.506362	-2.246776
36	6	0	3.236655	1.868631	-2.792477
37	1	0	4.102168	0.708002	-1.206506
38	6	0	0.903107	1.463606	-3.253552
39	1	0	-0.070495	0.002891	-2.019464
40	6	0	2.086603	2.146742	-3.526042
41	1	0	4.160168	2.398470	-3.002586
42	1	0	0.000264	1.682597	-3.813981
43	1	0	2.111890	2.897269	-4.309945
44	6	0	3.525082	-1.153711	0.594325
45	6	0	3.792364	-0.554505	1.826819
46	6	0	4.518555	-1.888463	-0.060764
47	6	0	5.051695	-0.689619	2.403097
48	1	0	3.006056	-0.000277	2.329326
49	6	0	5.774889	-2.019491	0.519726
50	1	0	4.306157	-2.361974	-1.014271
51	6	0	6.040751	-1.419008	1.749487
52	1	0	5.258541	-0.228634	3.363373
53	1	0	6.546067	-2.592967	0.015778
54	1	0	7.021969	-1.525735	2.201411
55	6	0	-5.074562	-2.821286	-1.567364
56	6	0	-4.899709	-3.449538	-2.957115
57	1	0	-5.825868	-2.022994	-1.621042
58	1	0	-5.479294	-3.572190	-0.877125
59	1	0	-5.850164	-3.846332	-3.327850
60	1	0	-4.533426	-2.706973	-3.671166

61	1	0	-4.174092	-4.266415	-2.920646

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.14672617
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.47025456
Zero-point correction= 0.501509 (Hartree/Particle)
Thermal correction to Energy= 0.536104
Thermal correction to Enthalpy= 0.537048
Thermal correction to Gibbs Free Energy= 0.431949

INT16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.424262	-0.936895	-0.035811
2	6	0	3.231345	-1.381016	0.506754
3	6	0	4.394920	-1.627171	0.771082
4	1	0	-0.434697	-2.619495	1.016068
5	15	0	-1.749884	-1.148683	0.232552
6	8	0	-1.411160	-2.570941	0.877961
7	8	0	-0.667188	-0.612218	-0.682435
8	6	0	1.278437	1.890440	-2.407050
9	1	0	1.711526	2.096789	-3.393202
10	1	0	0.316120	1.393777	-2.573578
11	6	0	1.078804	3.215572	-1.659633
12	1	0	0.445239	3.875508	-2.266793
13	1	0	2.043148	3.724664	-1.547346
14	15	0	2.359845	0.645569	-1.555290
15	15	0	0.346980	3.056186	0.050049
16	6	0	3.126606	-0.242889	-2.965391
17	1	0	3.661321	0.436107	-3.636978
18	1	0	3.820756	-0.979206	-2.552774
19	1	0	2.354064	-0.776734	-3.524460
20	6	0	3.761217	1.623147	-0.900191
21	1	0	4.483760	0.909094	-0.498446
22	1	0	4.225460	2.243193	-1.673115
23	1	0	3.414812	2.249779	-0.075330
24	6	0	-1.410818	2.718175	-0.410502
25	1	0	-2.035400	2.745884	0.487097
26	1	0	-1.792934	3.443082	-1.138391
27	1	0	-1.470947	1.709783	-0.826870
28	6	0	0.211905	4.862146	0.446528
29	1	0	-0.296102	5.428131	-0.342507
30	1	0	-0.346182	4.983699	1.379331

31	1	0	1.208965	5.285766	0.598077
32	1	0	1.093875	-2.078056	1.035875
33	6	0	-2.083817	0.015515	1.573689
34	6	0	-3.375094	0.476862	1.842367
35	6	0	-0.998762	0.521721	2.298816
36	6	0	-3.579293	1.441816	2.824443
37	1	0	-4.220693	0.097612	1.277361
38	6	0	-1.209081	1.484672	3.278705
39	1	0	0.011741	0.183238	2.083132
40	6	0	-2.497001	1.948014	3.539263
41	1	0	-4.582981	1.802405	3.025215
42	1	0	-0.361607	1.881068	3.827750
43	1	0	-2.657075	2.705048	4.300821
44	6	0	-3.282219	-1.450731	-0.654511
45	6	0	-3.530854	-0.739069	-1.830276
46	6	0	-4.227729	-2.359477	-0.169370
47	6	0	-4.725843	-0.932787	-2.515841
48	1	0	-2.782352	-0.049535	-2.207708
49	6	0	-5.420608	-2.547419	-0.858128
50	1	0	-4.023564	-2.921509	0.736380
51	6	0	-5.669530	-1.833266	-2.028527
52	1	0	-4.917824	-0.386218	-3.433376
53	1	0	-6.153672	-3.255798	-0.486377
54	1	0	-6.601859	-1.982916	-2.563946
55	6	0	5.776902	-1.962536	1.128734
56	6	0	5.874872	-3.159698	2.083984
57	1	0	6.259470	-1.090725	1.589491
58	1	0	6.350371	-2.178879	0.217982
59	1	0	6.920186	-3.382317	2.321776
60	1	0	5.343092	-2.951436	3.016060
61	1	0	5.424453	-4.047570	1.632547

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.15648926
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.48323636
Zero-point correction= 0.504042 (Hartree/Particle)
Thermal correction to Energy= 0.538415
Thermal correction to Enthalpy= 0.539359
Thermal correction to Gibbs Free Energy= 0.434261

TS10a

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

1	46	0	1.217345	-1.050996	0.116658
2	6	0	1.077070	-2.023763	2.092356
3	6	0	2.260407	-1.865316	1.574328
4	1	0	-0.208873	-1.748185	1.573188
5	15	0	-1.822063	-0.611068	0.278107
6	8	0	-1.457386	-1.613357	1.398327
7	8	0	-0.760950	-0.426346	-0.809440
8	6	0	2.219891	1.019925	-2.529409
9	1	0	2.753958	0.957081	-3.486035
10	1	0	1.150523	0.920698	-2.745310
11	6	0	2.513137	2.373739	-1.871017
12	1	0	2.251121	3.167032	-2.583267
13	1	0	3.588239	2.472894	-1.678341
14	15	0	2.674091	-0.471065	-1.534815
15	15	0	1.613686	2.690747	-0.262169
16	6	0	2.829806	-1.749541	-2.843839
17	1	0	3.537186	-1.448026	-3.623025
18	1	0	3.162866	-2.686817	-2.392118
19	1	0	1.847069	-1.919783	-3.290150
20	6	0	4.423512	-0.152050	-1.084584
21	1	0	4.862065	-1.069506	-0.685021
22	1	0	5.008303	0.180245	-1.948394
23	1	0	4.459003	0.610526	-0.303000
24	6	0	-0.096130	2.866566	-0.935173
25	1	0	-0.741845	3.310249	-0.172532
26	1	0	-0.118064	3.497374	-1.831899
27	1	0	-0.491501	1.872786	-1.162869
28	6	0	2.057395	4.483047	-0.081082
29	1	0	1.828095	5.064132	-0.981728
30	1	0	1.497097	4.905143	0.758022
31	1	0	3.123121	4.586157	0.143485
32	1	0	0.788656	-2.438573	3.054266
33	6	0	-2.135561	0.991229	1.075265
34	6	0	-3.166185	1.841951	0.673336
35	6	0	-1.237817	1.414966	2.060708
36	6	0	-3.297409	3.104464	1.246100
37	1	0	-3.869955	1.518932	-0.088465
38	6	0	-1.363948	2.679248	2.625758
39	1	0	-0.436837	0.753569	2.379194
40	6	0	-2.394223	3.525637	2.218770
41	1	0	-4.103120	3.760468	0.931405
42	1	0	-0.658762	3.003247	3.384702
43	1	0	-2.496674	4.510230	2.664979
44	6	0	-3.376280	-1.137958	-0.476960

45	6	0	-3.591895	-0.912464	-1.838347
46	6	0	-4.374242	-1.738441	0.295439
47	6	0	-4.800898	-1.279272	-2.422530
48	1	0	-2.802380	-0.460201	-2.430427
49	6	0	-5.580306	-2.105645	-0.291502
50	1	0	-4.195411	-1.925131	1.349714
51	6	0	-5.794492	-1.873481	-1.648840
52	1	0	-4.966337	-1.105827	-3.481304
53	1	0	-6.353267	-2.576358	0.307912
54	1	0	-6.737121	-2.160178	-2.105191
55	6	0	3.698394	-2.108989	1.858810
56	6	0	3.928058	-2.750090	3.229325
57	1	0	4.237620	-1.156838	1.790025
58	1	0	4.109048	-2.750142	1.068519
59	1	0	4.994013	-2.918135	3.407870
60	1	0	3.543893	-2.103731	4.023424
61	1	0	3.411675	-3.711674	3.296680

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.18134493
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.50247324
Zero-point correction= 0.501961 (Hartree/Particle)
Thermal correction to Energy= 0.535403
Thermal correction to Enthalpy= 0.536347
Thermal correction to Gibbs Free Energy= 0.434696

INT17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.895328	-1.074939	0.112005
2	6	0	2.502232	-3.137056	1.414574
3	6	0	2.090872	-1.869593	1.474520
4	1	0	2.281374	-3.774301	0.562889
5	15	0	-1.710620	-0.331389	0.128033
6	8	0	-0.984514	-1.047202	1.278664
7	8	0	-0.822822	-0.260623	-1.129746
8	6	0	2.467316	0.482803	-2.430805
9	1	0	3.084811	0.244715	-3.305724
10	1	0	1.418279	0.425444	-2.741399
11	6	0	2.808895	1.892564	-1.929630
12	1	0	2.668898	2.599559	-2.757250
13	1	0	3.869234	1.943791	-1.654936
14	15	0	2.703557	-0.866197	-1.190992

15	15	0	1.819704	2.485311	-0.456259
16	6	0	3.036098	-2.339850	-2.223315
17	1	0	3.887069	-2.174479	-2.890926
18	1	0	3.248006	-3.188448	-1.569039
19	1	0	2.146471	-2.570451	-2.813895
20	6	0	4.322904	-0.514954	-0.420622
21	1	0	4.592183	-1.362076	0.212830
22	1	0	5.093714	-0.355343	-1.180480
23	1	0	4.238180	0.373572	0.209050
24	6	0	0.229338	2.871358	-1.307522
25	1	0	-0.413652	3.442161	-0.631622
26	1	0	0.389424	3.452134	-2.223456
27	1	0	-0.284137	1.933906	-1.539856
28	6	0	2.541268	4.189700	-0.346095
29	1	0	2.544844	4.705588	-1.312900
30	1	0	1.950060	4.779935	0.359698
31	1	0	3.565728	4.141261	0.034298
32	1	0	3.036507	-3.604265	2.240394
33	6	0	-2.143462	1.346845	0.669501
34	6	0	-3.092643	2.106753	-0.017989
35	6	0	-1.427254	1.923264	1.720815
36	6	0	-3.316327	3.433535	0.333930
37	1	0	-3.656345	1.659749	-0.832547
38	6	0	-1.651063	3.251530	2.072748
39	1	0	-0.695016	1.322298	2.250831
40	6	0	-2.592448	4.007619	1.377611
41	1	0	-4.053585	4.020903	-0.204533
42	1	0	-1.092942	3.696039	2.891096
43	1	0	-2.766502	5.043947	1.651223
44	6	0	-3.277328	-1.135388	-0.289908
45	6	0	-3.569084	-1.424710	-1.624118
46	6	0	-4.202336	-1.454142	0.708804
47	6	0	-4.780193	-2.025244	-1.958761
48	1	0	-2.836574	-1.178909	-2.386505
49	6	0	-5.409292	-2.056183	0.372577
50	1	0	-3.972635	-1.236302	1.747824
51	6	0	-5.699075	-2.339153	-0.961644
52	1	0	-5.004961	-2.248401	-2.997207
53	1	0	-6.125433	-2.307254	1.148685
54	1	0	-6.643159	-2.808353	-1.221681
55	6	0	2.322645	-0.920047	2.622879
56	6	0	3.209222	-1.454249	3.748633
57	1	0	1.339499	-0.642424	3.023558
58	1	0	2.746572	0.011542	2.225763

59	1	0	3.341426	-0.693561	4.523240
60	1	0	2.765625	-2.337607	4.217359
61	1	0	4.199325	-1.732855	3.372845

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.23059285
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.55006423
Zero-point correction= 0.508242 (Hartree/Particle)
Thermal correction to Energy= 0.541847
Thermal correction to Enthalpy= 0.542792
Thermal correction to Gibbs Free Energy= 0.439274

INT15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.264801	0.860772	-0.917869
2	6	0	-0.476907	2.817263	-0.921130
3	6	0	-1.671572	2.802543	-1.350233
4	1	0	-2.547049	3.298006	-1.730584
5	1	0	0.998851	1.088569	-1.925667
6	15	0	1.609758	-0.335193	-0.466173
7	8	0	1.799336	0.534540	-1.807779
8	8	0	0.264845	-0.986134	-0.301514
9	6	0	-2.870326	-2.293640	-0.215237
10	1	0	-3.436971	-3.096155	-0.705336
11	1	0	-1.827777	-2.624224	-0.150977
12	6	0	-3.449061	-2.061949	1.185969
13	1	0	-3.532969	-3.031412	1.695161
14	1	0	-4.468625	-1.664346	1.111848
15	15	0	-2.858622	-0.824438	-1.347097
16	15	0	-2.487259	-0.904645	2.291750
17	6	0	-2.605800	-1.681015	-2.957874
18	1	0	-3.352158	-2.462649	-3.137004
19	1	0	-2.650094	-0.945351	-3.764527
20	1	0	-1.607340	-2.125906	-2.961873
21	6	0	-4.646651	-0.396165	-1.440533
22	1	0	-4.789317	0.327615	-2.247255
23	1	0	-5.275490	-1.273340	-1.627802
24	1	0	-4.955948	0.082401	-0.508112
25	6	0	-0.998377	-1.961117	2.603032
26	1	0	-0.408324	-1.525549	3.415282
27	1	0	-1.264660	-2.990052	2.871866
28	1	0	-0.379525	-1.960194	1.701260

29	6	0	-3.424839	-1.235442	3.859473
30	1	0	-3.531129	-2.306254	4.068439
31	1	0	-2.906974	-0.764556	4.699974
32	1	0	-4.421534	-0.789472	3.793000
33	6	0	1.980629	0.762072	0.922295
34	6	0	3.223355	1.391610	1.030896
35	6	0	0.986891	1.008992	1.871625
36	6	0	3.468660	2.269313	2.080460
37	1	0	3.999290	1.198964	0.295299
38	6	0	1.236896	1.886841	2.921860
39	1	0	0.011819	0.544554	1.762521
40	6	0	2.474448	2.516845	3.025725
41	1	0	4.432658	2.760944	2.162064
42	1	0	0.458567	2.085780	3.651454
43	1	0	2.665664	3.206573	3.842103
44	6	0	2.956058	-1.520632	-0.621300
45	6	0	4.108133	-1.241437	-1.362058
46	6	0	2.836526	-2.740504	0.049655
47	6	0	5.136455	-2.176264	-1.421743
48	1	0	4.188155	-0.304158	-1.903242
49	6	0	3.866535	-3.672621	-0.014833
50	1	0	1.930270	-2.959724	0.606281
51	6	0	5.016740	-3.388952	-0.747187
52	1	0	6.029655	-1.960793	-1.999372
53	1	0	3.769476	-4.622381	0.501056
54	1	0	5.819184	-4.118306	-0.797231
55	6	0	0.718447	3.613731	-0.537299
56	6	0	0.575407	5.100258	-0.869797
57	1	0	1.612225	3.204575	-1.023554
58	1	0	0.892976	3.481381	0.536949
59	1	0	1.467082	5.657395	-0.564897
60	1	0	0.429559	5.245010	-1.944185
61	1	0	-0.290190	5.526045	-0.354411

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.19216503
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.51062210
Zero-point correction= 0.506069 (Hartree/Particle)
Thermal correction to Energy= 0.540783
Thermal correction to Enthalpy= 0.541727
Thermal correction to Gibbs Free Energy= 0.436382

TS10b

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	46	0	1.229717	-1.232081	0.134458
2	6	0	0.746016	-2.207316	2.074309
3	6	0	1.967899	-2.249375	1.642418
4	1	0	2.944641	-2.619640	1.916962
5	1	0	-0.383092	-1.590147	1.410876
6	15	0	-1.665754	-0.199415	0.005933
7	8	0	-1.560079	-1.182233	1.200322
8	8	0	-0.493246	-0.235676	-0.974367
9	6	0	3.161344	0.789575	-2.026039
10	1	0	3.944003	0.731767	-2.793612
11	1	0	2.219761	1.005325	-2.543179
12	6	0	3.493818	1.911658	-1.034683
13	1	0	3.686779	2.829025	-1.605981
14	1	0	4.421111	1.679524	-0.497016
15	15	0	2.973776	-0.897131	-1.297177
16	15	0	2.163476	2.265740	0.233733
17	6	0	2.918533	-1.933949	-2.811116
18	1	0	3.764195	-1.731437	-3.476221
19	1	0	2.925115	-2.988101	-2.524310
20	1	0	1.982723	-1.734416	-3.338663
21	6	0	4.649518	-1.240915	-0.634527
22	1	0	4.713118	-2.298938	-0.367752
23	1	0	5.431490	-1.005206	-1.363207
24	1	0	4.806199	-0.654753	0.273884
25	6	0	0.840033	2.855865	-0.913258
26	1	0	0.096796	3.415787	-0.339116
27	1	0	1.239085	3.504038	-1.702770
28	1	0	0.333638	1.990817	-1.350306
29	6	0	2.802973	3.905423	0.821288
30	1	0	2.977817	4.610325	0.000462
31	1	0	2.069454	4.341817	1.505664
32	1	0	3.737013	3.767499	1.373801
33	6	0	-1.824575	1.464094	0.715934
34	6	0	-2.599734	2.459185	0.117626
35	6	0	-1.061675	1.771178	1.846408
36	6	0	-2.607977	3.749896	0.639040
37	1	0	-3.199270	2.225803	-0.757884
38	6	0	-1.064617	3.062869	2.362768
39	1	0	-0.461094	0.996358	2.313216
40	6	0	-1.837020	4.053575	1.758941
41	1	0	-3.215132	4.518675	0.171305
42	1	0	-0.467082	3.295247	3.238921

43	1	0	-1.843554	5.060116	2.166210
44	6	0	-3.208790	-0.540172	-0.869870
45	6	0	-4.344304	-0.948965	-0.164960
46	6	0	-3.276370	-0.359820	-2.253196
47	6	0	-5.539556	-1.169742	-0.839942
48	1	0	-4.280427	-1.103073	0.907720
49	6	0	-4.475467	-0.578660	-2.925829
50	1	0	-2.382525	-0.060055	-2.791483
51	6	0	-5.605907	-0.980684	-2.219205
52	1	0	-6.419925	-1.491730	-0.292624
53	1	0	-4.527771	-0.438927	-4.001121
54	1	0	-6.541153	-1.151338	-2.743745
55	6	0	0.017675	-2.743790	3.280646
56	6	0	-0.907524	-3.907971	2.911756
57	1	0	-0.580781	-1.938295	3.720010
58	1	0	0.748005	-3.061784	4.032334
59	1	0	-1.436894	-4.273689	3.796938
60	1	0	-1.646255	-3.584784	2.174139
61	1	0	-0.334614	-4.736490	2.485464

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.17720896
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.49733385
Zero-point correction= 0.501597 (Hartree/Particle)
Thermal correction to Energy= 0.535284
Thermal correction to Enthalpy= 0.536229
Thermal correction to Gibbs Free Energy= 0.433440

INT17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.061562	-0.859480	-0.143571
2	6	0	1.792937	-2.505807	2.059370
3	6	0	2.315724	-1.808796	1.050833
4	1	0	3.399031	-1.750220	0.940364
5	1	0	0.709486	-2.555484	2.172391
6	15	0	-1.596885	-0.302732	-0.033478
7	8	0	-0.836922	-1.226707	0.933567
8	8	0	-0.700207	0.093955	-1.223331
9	6	0	2.446397	1.415122	-2.209504
10	1	0	3.061189	1.502776	-3.114453
11	1	0	1.396824	1.456984	-2.521650
12	6	0	2.773434	2.564617	-1.246936

13	1	0	2.730132	3.505315	-1.810706
14	1	0	3.802571	2.471002	-0.879288
15	15	0	2.700734	-0.285396	-1.547806
16	15	0	1.644383	2.704642	0.239833
17	6	0	2.686519	-1.304122	-3.069014
18	1	0	3.437261	-0.962550	-3.788268
19	1	0	2.876743	-2.347285	-2.807607
20	1	0	1.693195	-1.240570	-3.519543
21	6	0	4.452675	-0.311779	-1.026273
22	1	0	4.772207	-1.344637	-0.870013
23	1	0	5.087784	0.145438	-1.790479
24	1	0	4.565060	0.228897	-0.083911
25	6	0	0.117355	3.283233	-0.622065
26	1	0	-0.596147	3.651395	0.120723
27	1	0	0.328784	4.081929	-1.342844
28	1	0	-0.346399	2.431193	-1.126815
29	6	0	2.273390	4.330224	0.874711
30	1	0	2.318850	5.099303	0.095245
31	1	0	1.605105	4.678300	1.667564
32	1	0	3.269329	4.205056	1.309386
33	6	0	-2.119103	1.170611	0.888840
34	6	0	-3.123081	2.018992	0.416164
35	6	0	-1.415317	1.509507	2.047151
36	6	0	-3.415105	3.200740	1.089877
37	1	0	-3.676400	1.755524	-0.481409
38	6	0	-1.706455	2.693104	2.719227
39	1	0	-0.640057	0.839992	2.406008
40	6	0	-2.703422	3.539993	2.239584
41	1	0	-4.195393	3.858414	0.719546
42	1	0	-1.156884	2.953109	3.618757
43	1	0	-2.930418	4.463560	2.763764
44	6	0	-3.115524	-1.069247	-0.650960
45	6	0	-4.102506	-1.500947	0.240776
46	6	0	-3.298070	-1.243006	-2.023594
47	6	0	-5.260475	-2.101960	-0.238376
48	1	0	-3.961742	-1.364714	1.309301
49	6	0	-4.459963	-1.843744	-2.501882
50	1	0	-2.523510	-0.903878	-2.704100
51	6	0	-5.439004	-2.273021	-1.610485
52	1	0	-6.023678	-2.438244	0.456378
53	1	0	-4.600838	-1.978624	-3.569815
54	1	0	-6.344268	-2.741683	-1.984500
55	6	0	2.603457	-3.256960	3.084069
56	6	0	2.283425	-4.755459	3.090604

57	1	0	2.393114	-2.842806	4.079259
58	1	0	3.673366	-3.103021	2.899750
59	1	0	2.850023	-5.279540	3.866794
60	1	0	1.218187	-4.924888	3.277691
61	1	0	2.525446	-5.207439	2.123950

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2159.22387919
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2159.54397100
Zero-point correction= 0.509076 (Hartree/Particle)
Thermal correction to Energy= 0.542715
Thermal correction to Enthalpy= 0.543659
Thermal correction to Gibbs Free Energy= 0.440341

INT18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.050140	0.762720	0.188597
2	6	0	-2.517000	3.159699	-0.557092
3	6	0	-2.614315	2.013127	0.121216
4	1	0	-1.632005	3.423639	-1.132355
5	15	0	1.819582	-0.235063	-0.792377
6	8	0	1.521004	-0.455667	-2.250701
7	8	0	0.705982	-0.525576	0.241397
8	6	0	-1.420918	-1.841102	-2.125737
9	1	0	-1.492129	-1.962549	-3.213652
10	1	0	-0.360860	-1.924923	-1.873734
11	6	0	-2.276388	-2.909469	-1.438170
12	1	0	-1.888754	-3.896950	-1.719154
13	1	0	-3.307593	-2.863315	-1.809228
14	15	0	-1.886505	-0.094509	-1.774217
15	15	0	-2.360408	-2.800792	0.421150
16	6	0	-1.212507	0.809093	-3.209342
17	1	0	-1.699009	0.475740	-4.131091
18	1	0	-1.380709	1.880026	-3.075527
19	1	0	-0.140927	0.587561	-3.248218
20	6	0	-3.693398	-0.069057	-2.064213
21	1	0	-4.046967	0.963048	-2.032221
22	1	0	-3.914109	-0.504825	-3.043274
23	1	0	-4.206781	-0.644357	-1.291017
24	6	0	-0.662576	-3.392171	0.838998
25	1	0	-0.595958	-3.580235	1.914724
26	1	0	-0.409184	-4.314216	0.303918

27	1	0	0.053717	-2.603255	0.587459
28	6	0	-3.332729	-4.349632	0.724963
29	1	0	-2.888349	-5.221558	0.232276
30	1	0	-3.380666	-4.542706	1.800260
31	1	0	-4.357429	-4.223476	0.363336
32	6	0	-0.233005	1.491116	2.459702
33	6	0	-0.023272	2.335595	1.607770
34	1	0	0.263876	3.145951	0.970389
35	1	0	-3.320976	3.896665	-0.540520
36	6	0	2.307574	1.510340	-0.532908
37	6	0	3.056146	1.922059	0.572191
38	6	0	1.802186	2.476837	-1.406434
39	6	0	3.282995	3.274611	0.809436
40	1	0	3.461108	1.180718	1.254983
41	6	0	2.013763	3.832008	-1.164283
42	1	0	1.242349	2.155320	-2.278737
43	6	0	2.752872	4.232870	-0.052445
44	1	0	3.867905	3.582925	1.670669
45	1	0	1.615132	4.574584	-1.849302
46	1	0	2.925085	5.288417	0.134994
47	6	0	3.241462	-1.234152	-0.260227
48	6	0	3.407200	-1.605759	1.076839
49	6	0	4.187869	-1.636412	-1.205668
50	6	0	4.513857	-2.354180	1.467031
51	1	0	2.657882	-1.310256	1.805074
52	6	0	5.292236	-2.388625	-0.816789
53	1	0	4.038026	-1.367386	-2.246797
54	6	0	5.458101	-2.743734	0.520015
55	1	0	4.638538	-2.637747	2.507832
56	1	0	6.022587	-2.702034	-1.556474
57	1	0	6.320978	-3.329348	0.823207
58	6	0	-3.850047	1.649024	0.907796
59	6	0	-3.604608	1.356732	2.389635
60	1	0	-4.312094	0.760206	0.462832
61	1	0	-4.579753	2.464968	0.810871
62	1	0	-4.554461	1.200269	2.909560
63	1	0	-3.007374	0.447942	2.505847
64	1	0	-3.077837	2.185592	2.872110
65	6	0	-0.379855	0.581166	3.600822
66	6	0	-0.417800	-0.901326	3.221319
67	1	0	-1.287122	0.855934	4.149968
68	1	0	0.465780	0.776058	4.270517
69	1	0	-0.428467	-1.515029	4.126247
70	1	0	-1.312285	-1.127957	2.633810

71	1	0	0.442314	-1.165083	2.604461

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2315.17362621
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2315.52917032
Zero-point correction= 0.597454 (Hartree/Particle)
Thermal correction to Energy= 0.636517
Thermal correction to Enthalpy= 0.637461
Thermal correction to Gibbs Free Energy= 0.525752

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.020522	-0.275507	0.189975
2	6	0	2.895499	-2.159298	-0.986738
3	6	0	2.797231	-1.078146	-0.210000
4	1	0	2.018625	-2.634458	-1.419278
5	15	0	-2.082456	-0.480421	0.701472
6	8	0	-1.734935	-1.356464	1.930028
7	8	0	-1.064376	0.613962	0.383582
8	6	0	0.301637	2.415433	-1.851041
9	1	0	0.011136	2.633712	-2.886036
10	1	0	-0.612825	2.243554	-1.274566
11	6	0	1.096252	3.597762	-1.281380
12	1	0	0.437766	4.475152	-1.240126
13	1	0	1.915805	3.854617	-1.963894
14	15	0	1.177545	0.792263	-1.832144
15	15	0	1.875951	3.329281	0.395808
16	6	0	0.310850	-0.164886	-3.128017
17	1	0	0.371085	0.333472	-4.100447
18	1	0	0.765616	-1.155811	-3.196529
19	1	0	-0.736321	-0.291096	-2.842721
20	6	0	2.810295	1.131018	-2.583748
21	1	0	3.318744	0.177782	-2.740671
22	1	0	2.700463	1.655717	-3.537424
23	1	0	3.411153	1.734369	-1.899471
24	6	0	0.373578	3.347169	1.469348
25	1	0	0.683571	3.369507	2.517994
26	1	0	-0.258821	4.220515	1.269824
27	1	0	-0.204221	2.431833	1.309076
28	6	0	2.483442	5.060470	0.662924
29	1	0	1.689832	5.805827	0.537438
30	1	0	2.889388	5.150355	1.674319

31	1	0	3.290919	5.283773	-0.040595
32	6	0	1.751664	-1.921475	2.690083
33	6	0	0.835378	-1.453800	2.018209
34	1	0	-0.548329	-1.415488	2.017710
35	1	0	3.854563	-2.631573	-1.196632
36	6	0	-3.705236	0.267238	0.952754
37	6	0	-3.859344	1.644137	0.784587
38	6	0	-4.804831	-0.519444	1.308665
39	6	0	-5.107970	2.231849	0.968381
40	1	0	-2.994074	2.243643	0.518386
41	6	0	-6.050097	0.070307	1.491317
42	1	0	-4.681292	-1.589322	1.447961
43	6	0	-6.201582	1.445530	1.319730
44	1	0	-5.227594	3.302859	0.838921
45	1	0	-6.902830	-0.540309	1.770862
46	1	0	-7.174901	1.904685	1.463243
47	6	0	-2.219868	-1.573815	-0.742822
48	6	0	-3.104698	-1.302604	-1.789137
49	6	0	-1.310594	-2.630373	-0.865478
50	6	0	-3.075699	-2.072272	-2.949787
51	1	0	-3.821038	-0.490799	-1.696251
52	6	0	-1.276302	-3.390864	-2.029683
53	1	0	-0.626496	-2.850249	-0.050504
54	6	0	-2.156389	-3.111069	-3.073206
55	1	0	-3.770310	-1.859732	-3.756495
56	1	0	-0.564004	-4.205245	-2.119376
57	1	0	-2.130629	-3.706838	-3.980568
58	6	0	2.869999	-2.515685	3.417201
59	6	0	3.619438	-3.568736	2.589526
60	1	0	2.482258	-2.965129	4.339865
61	1	0	3.559509	-1.723193	3.734176
62	1	0	4.472546	-3.962900	3.149166
63	1	0	2.954891	-4.397435	2.332647
64	1	0	3.979932	-3.132315	1.654726
65	6	0	3.959580	-0.371673	0.441671
66	6	0	5.350078	-0.822544	-0.007453
67	1	0	3.859569	-0.499922	1.527015
68	1	0	3.847492	0.707915	0.282100
69	1	0	6.122323	-0.239820	0.503035
70	1	0	5.526677	-1.878971	0.219080
71	1	0	5.480841	-0.687557	-1.086175

ωB97XD/6-31G(d,p)-LANL2DZ energy= -2315.14799839

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -2315.50076649

Zero-point correction= 0.591532 (Hartree/Particle)
Thermal correction to Energy= 0.630616
Thermal correction to Enthalpy= 0.631560
Thermal correction to Gibbs Free Energy= 0.518753

INT19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.022475	0.077096	-0.112524
2	6	0	0.717074	2.669222	-1.415355
3	6	0	0.820701	1.959428	-0.287439
4	1	0	0.217091	2.274756	-2.297186
5	6	0	-3.307769	-0.548743	-0.175701
6	1	0	-4.305172	-0.281048	0.189986
7	1	0	-3.406864	-0.775753	-1.243987
8	6	0	-2.752281	-1.772387	0.571237
9	1	0	-3.359507	-2.662627	0.374833
10	1	0	-2.779043	-1.594618	1.652842
11	15	0	-2.142304	0.899544	-0.060262
12	15	0	-0.966872	-2.047075	0.126529
13	6	0	-2.763859	2.067780	-1.320215
14	1	0	-3.804808	2.348882	-1.137654
15	1	0	-2.123966	2.953266	-1.299823
16	1	0	-2.674222	1.612756	-2.309587
17	6	0	-2.584589	1.711756	1.521128
18	1	0	-1.971304	2.610457	1.624382
19	1	0	-3.643529	1.983716	1.564262
20	1	0	-2.342891	1.044400	2.351823
21	6	0	-1.022927	-3.069770	-1.392221
22	1	0	0.006617	-3.255640	-1.707732
23	1	0	-1.537834	-4.021910	-1.232641
24	1	0	-1.521665	-2.513480	-2.189852
25	6	0	-0.325891	-3.196807	1.393003
26	1	0	-0.841802	-4.161052	1.387233
27	1	0	0.739559	-3.335067	1.191244
28	1	0	-0.419823	-2.733757	2.378128
29	6	0	2.979702	-1.212617	0.027246
30	6	0	1.880850	-0.685744	-0.052579
31	1	0	1.166765	3.656195	-1.528908
32	6	0	1.540643	2.458745	0.944204
33	6	0	2.123854	3.870356	0.868878
34	1	0	2.335454	1.736656	1.164868

35	1	0	0.853046	2.394536	1.800238
36	1	0	2.610572	4.135350	1.812653
37	1	0	2.871936	3.944103	0.073505
38	1	0	1.347511	4.616457	0.667657
39	6	0	4.336952	-1.761796	0.106622
40	6	0	5.397682	-0.807283	-0.459089
41	1	0	4.388157	-2.718654	-0.429480
42	1	0	4.577957	-1.990471	1.153245
43	1	0	6.399561	-1.240729	-0.371951
44	1	0	5.199895	-0.597099	-1.513520
45	1	0	5.381222	0.144091	0.079204

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1359.59496284
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1359.7864731
Zero-point correction= 0.389790 (Hartree/Particle)
Thermal correction to Energy= 0.415402
Thermal correction to Enthalpy= 0.416347
Thermal correction to Gibbs Free Energy= 0.333386

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.023198	-0.130919	0.161545
2	6	0	1.519453	-2.137578	1.714880
3	6	0	1.404704	-1.671505	0.459076
4	1	0	1.328947	-1.504255	2.574686
5	6	0	-3.371075	0.318461	0.038963
6	1	0	-4.342216	0.049126	-0.391682
7	1	0	-3.526229	0.469499	1.114225
8	6	0	-2.824878	1.606493	-0.596796
9	1	0	-3.499682	2.450838	-0.414916
10	1	0	-2.747623	1.482254	-1.683837
11	15	0	-2.154843	-1.082571	-0.133389
12	15	0	-1.106999	1.973640	0.018788
13	6	0	-2.886196	-2.365601	0.959213
14	1	0	-3.942141	-2.550734	0.738021
15	1	0	-2.324091	-3.294908	0.836151
16	1	0	-2.782555	-2.050900	2.000548
17	6	0	-2.560007	-1.733039	-1.807580
18	1	0	-1.971100	-2.635289	-1.991337
19	1	0	-3.623797	-1.968626	-1.915560
20	1	0	-2.275124	-0.993165	-2.559803

21	6	0	-1.443641	2.843280	1.605410
22	1	0	-0.497228	3.196857	2.022122
23	1	0	-2.122905	3.692551	1.477788
24	1	0	-1.876035	2.137903	2.319685
25	6	0	-0.583696	3.358107	-1.068430
26	1	0	-1.304777	4.181559	-1.071257
27	1	0	0.385361	3.725964	-0.721292
28	1	0	-0.453093	2.984872	-2.087172
29	6	0	3.119923	0.580313	0.015065
30	6	0	2.009727	0.100164	0.205498
31	1	0	1.850132	-3.153873	1.917586
32	6	0	4.444978	1.163849	-0.191856
33	6	0	4.415994	2.692616	-0.337631
34	1	0	4.900255	0.723797	-1.088583
35	1	0	5.101183	0.891168	0.645002
36	1	0	5.424166	3.091225	-0.490254
37	1	0	3.795734	2.983810	-1.190167
38	1	0	3.993847	3.154194	0.559326
39	6	0	1.704602	-2.513766	-0.767368
40	6	0	2.784677	-3.579376	-0.572113
41	1	0	2.005697	-1.844824	-1.577673
42	1	0	0.768520	-2.987293	-1.096366
43	1	0	2.997669	-4.088396	-1.517347
44	1	0	3.709630	-3.120764	-0.210015
45	1	0	2.480578	-4.340829	0.152086

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1359.56908671
ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1359.75379981
Zero-point correction= 0.388142 (Hartree/Particle)
Thermal correction to Energy= 0.413692
Thermal correction to Enthalpy= 0.414636
Thermal correction to Gibbs Free Energy= 0.330447

INT20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.363111	-0.647694	0.038512
2	6	0	-1.006422	-2.219211	-0.502960
3	6	0	-1.671373	-1.283170	0.324819
4	1	0	-1.166108	-2.210548	-1.577167
5	6	0	2.543708	1.911684	0.591337
6	1	0	2.712268	2.994455	0.558705

7	1	0	3.094259	1.526142	1.458169
8	6	0	3.051495	1.239212	-0.692113
9	1	0	4.136827	1.359366	-0.793129
10	1	0	2.592609	1.714204	-1.567900
11	15	0	0.745880	1.522759	0.889211
12	15	0	2.578342	-0.566402	-0.767956
13	6	0	0.490551	2.209811	2.578209
14	1	0	0.820621	3.250904	2.657770
15	1	0	-0.573485	2.152937	2.822390
16	1	0	1.036338	1.602499	3.304780
17	6	0	-0.116693	2.770235	-0.151266
18	1	0	-1.193644	2.608417	-0.049612
19	1	0	0.137144	3.799853	0.121588
20	1	0	0.137639	2.596609	-1.200090
21	6	0	3.861954	-1.325588	0.315328
22	1	0	3.782893	-2.413713	0.250934
23	1	0	4.875485	-1.020978	0.033410
24	1	0	3.673641	-1.040987	1.353560
25	6	0	3.208256	-1.014960	-2.439209
26	1	0	4.258872	-0.738482	-2.577809
27	1	0	3.099818	-2.092966	-2.582411
28	1	0	2.600939	-0.514432	-3.197725
29	6	0	-3.216367	0.610279	-0.711936
30	6	0	-2.499817	-0.261448	-0.269184
31	1	0	-0.713658	-3.176822	-0.077973
32	6	0	-4.097099	1.625960	-1.293200
33	6	0	-5.285571	1.021922	-2.053568
34	1	0	-3.516727	2.266545	-1.969386
35	1	0	-4.467820	2.283314	-0.496963
36	1	0	-5.918863	1.810240	-2.471810
37	1	0	-4.935563	0.387494	-2.871979
38	1	0	-5.894945	0.405071	-1.387934
39	6	0	-2.006425	-1.624070	1.773088
40	6	0	-3.381084	-2.284919	1.913246
41	1	0	-1.975076	-0.710171	2.376539
42	1	0	-1.230098	-2.290497	2.164561
43	1	0	-3.610808	-2.501391	2.961526
44	1	0	-4.163221	-1.628483	1.519277
45	1	0	-3.416484	-3.224431	1.352754

ωB97XD/6-31G(d,p)-LANL2DZ energy= -1359.64052425

ωB97XD/6-311++G(d,p)-LANL2TZ(f)/SMD energy= -1359.82082938

Zero-point correction= 0.390994 (Hartree/Particle)

Thermal correction to Energy= 0.416278

Thermal correction to Enthalpy= 0.417222
Thermal correction to Gibbs Free Energy= 0.334583