Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Computational Insights into the Mechanisms of Au(I)-Catalysed Intramolecular Addition of the Hydroxylamine Group onto Alkynes

Hongli Li, Jiajun Liu, Ogunlana Abosede A., and Xiaoguang Bao*

College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China.

E-mail: xgbao@suda.edu.cn

List of Contents

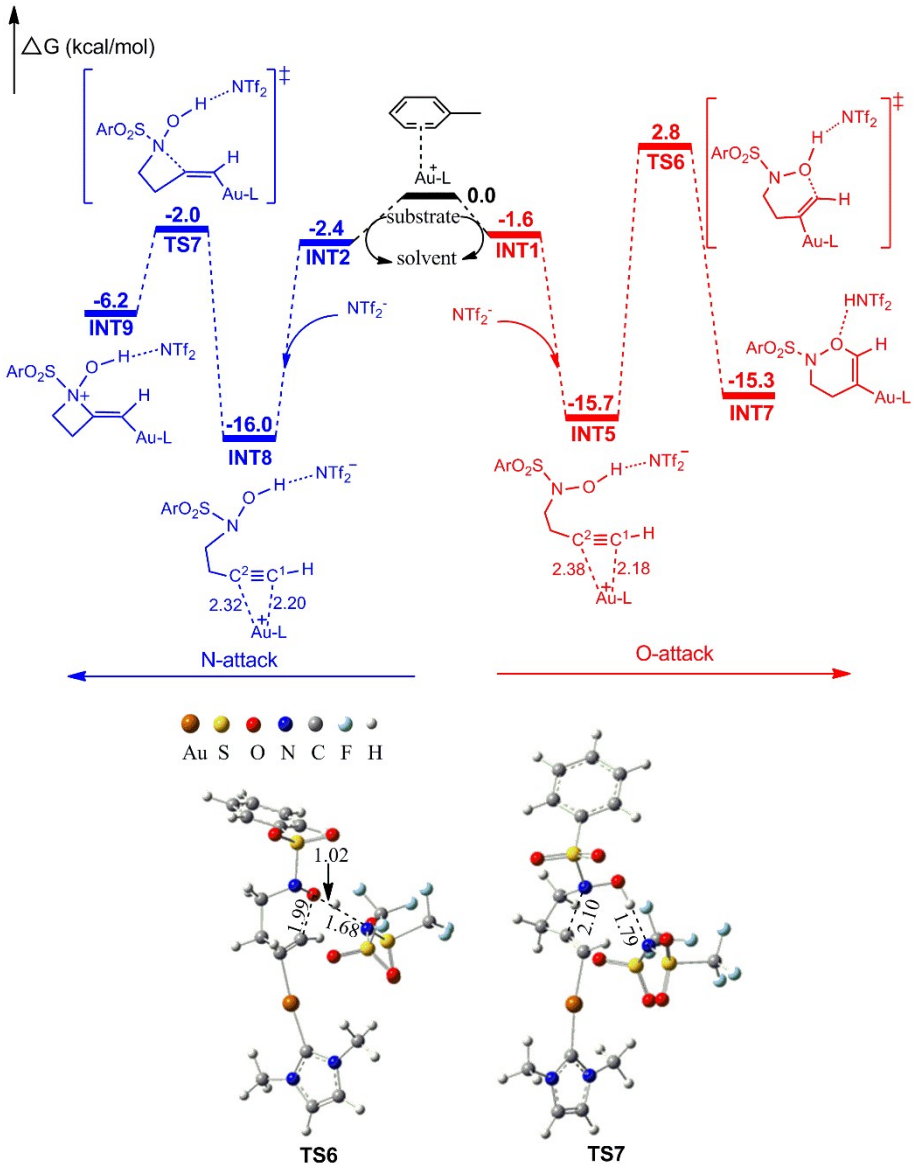

Figure S1. Energy profiles (in kcal mol^{-1}) for the *4-exo* N-attack and *6-endo* O-attack cyclization pathways of **1** catalysed by the cationic NHC-Au(I) and explicit inclusion of the counterion, NTf_2^-. Bond lengths are shown in Å.

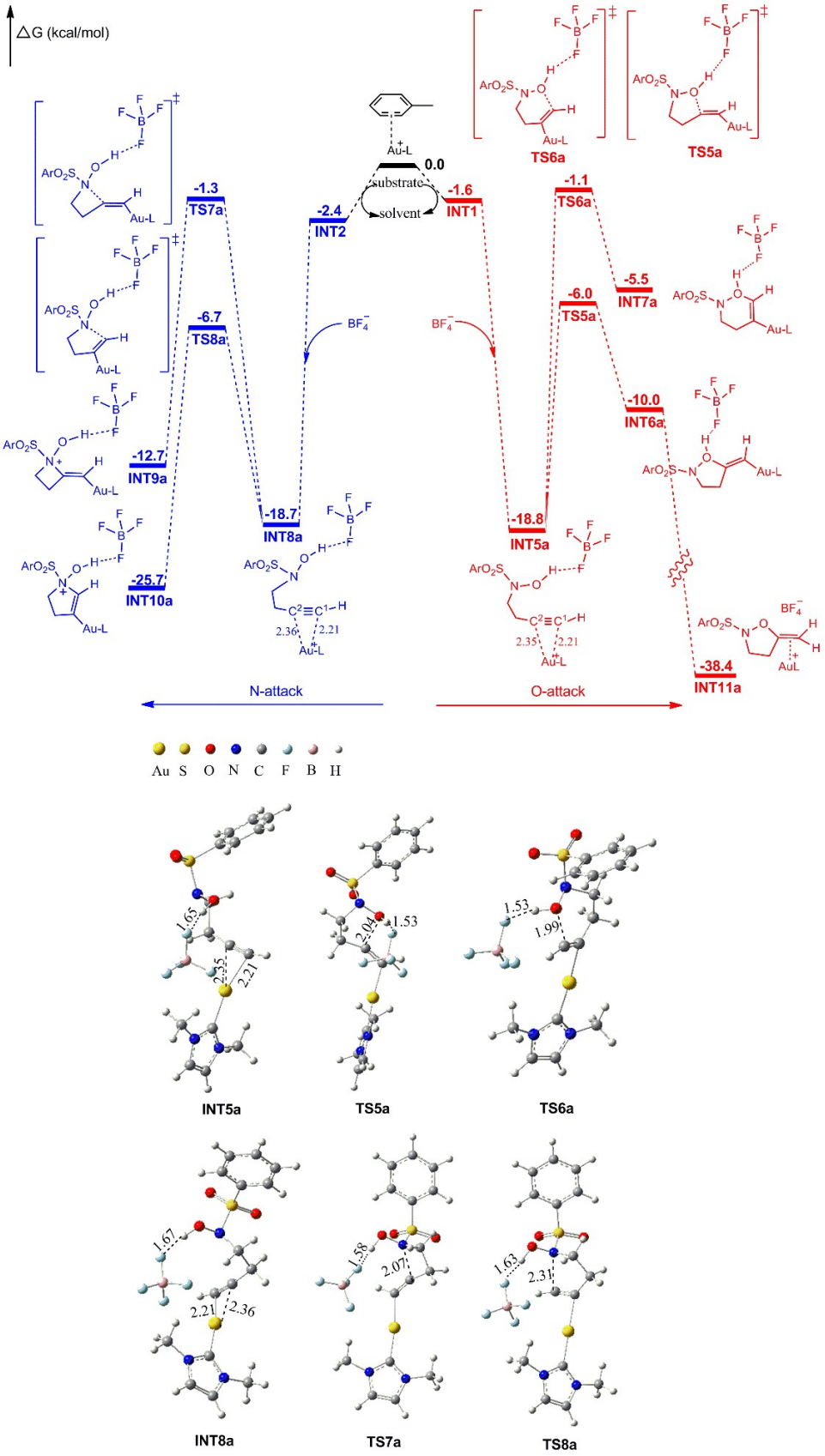

Figure S2. Energy profiles (in kcal mol^{-1}) for the four possible cyclization pathways of **1** catalysed by the cationic NHC-Au(I) and explicit inclusion of the counterion, BF_4^-. Bond lengths are shown in Å.

Cartesian Coordinates and Energies

Toluene-AuL$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.884747	0.296837	-0.016102
2	6	0	-4.110953	0.491161	-0.162256
3	6	0	-3.604129	1.730843	0.047901
4	1	0	-5.129021	0.155309	-0.288727
5	1	0	-4.093493	2.688399	0.141942
6	7	0	-3.041855	-0.374779	-0.198333
7	7	0	-2.237458	1.591785	0.134758
8	79	0	-0.029786	-0.470940	0.032929
9	6	0	-1.329472	2.702219	0.365451
10	1	0	-1.451905	3.449678	-0.422193
11	1	0	-1.535136	3.155313	1.338540
12	1	0	-0.305122	2.328872	0.350913
13	6	0	-3.174693	-1.806598	-0.409062
14	1	0	-3.788500	-2.242455	0.382957
15	1	0	-3.636366	-1.997576	-1.380951
16	1	0	-2.183420	-2.259763	-0.386296
17	6	0	2.545205	-0.512378	1.542924
18	6	0	1.973019	-1.462192	0.662329
19	6	0	2.099421	-1.261366	-0.732643
20	6	0	2.780913	-0.128833	-1.221485
21	6	0	3.357778	0.790712	-0.351744
22	6	0	3.222436	0.581596	1.037516
23	1	0	2.476250	-0.669283	2.615175
24	1	0	1.601476	-2.408596	1.049640
25	1	0	1.781547	-2.037797	-1.424663
26	1	0	2.885518	0.001638	-2.294975
27	1	0	3.677644	1.291388	1.723982
28	6	0	4.126557	1.973200	-0.862470
29	1	0	3.702612	2.912005	-0.487847
30	1	0	5.167515	1.934008	-0.521416
31	1	0	4.130699	2.012871	-1.954604

Zero-point correction= 0.261824 (Hartree/Particle)
Thermal correction to Energy= 0.278608
Thermal correction to Enthalpy= 0.279552
Thermal correction to Gibbs Free Energy= 0.211475
Sum of electronic and zero-point Energies= -710.726754
Sum of electronic and thermal Energies= -710.709970
Sum of electronic and thermal Enthalpies= -710.709025
Sum of electronic and thermal Free Energies（333K）= -710.785289
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy= -711.5371584

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.238426	0.535266	-0.432937
2	8	0	0.741245	1.268987	-1.552091
3	1	0	1.103659	2.160568	-1.401662
4	6	0	1.504270	-0.844362	-0.873279
5	1	0	0.612647	-1.484749	-0.835671
6	1	0	1.810892	-0.764369	-1.917681
7	6	0	2.617676	-1.492645	-0.022158
8	1	0	2.324338	-1.468594	1.031332
9	1	0	2.723648	-2.544760	-0.316007
10	6	0	3.907063	-0.814912	-0.207826
11	16	0	0.079602	0.713189	0.870216
12	8	0	-0.011350	2.157841	1.063303
13	8	0	0.584072	-0.186249	1.918220
14	6	0	-1.487963	0.091702	0.281172
15	6	0	-1.876825	-1.207135	0.627029
16	6	0	-2.290052	0.912452	-0.519186
17	6	0	-3.096567	-1.691730	0.153836
18	1	0	-1.248400	-1.806696	1.276600
19	6	0	-3.504221	0.411117	-0.985615
20	1	0	-1.974703	1.921887	-0.754039
21	6	0	-3.904369	-0.886350	-0.652772
22	1	0	-3.418742	-2.693428	0.421975
23	1	0	-4.141522	1.036395	-1.603371
24	1	0	-4.853878	-1.267724	-1.016876
25	6	0	4.946002	-0.224993	-0.500416
26	1	0	5.717610	0.310084	-1.017667

Zero-point correction= 0.199730 (Hartree/Particle)
Thermal correction to Energy= 0.214334
Thermal correction to Enthalpy= 0.215278
Thermal correction to Gibbs Free Energy= 0.156822
Sum of electronic and zero-point Energies= -1064.990688
Sum of electronic and thermal Energies= -1064.976084
Sum of electronic and thermal Enthalpies= -1064.975140
Sum of electronic and thermal Free Energies（333K）= -1065.040642

B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy= -1065.783642

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.541492	-1.734508	0.001317
2	8	0	3.072885	-1.614083	-1.312126
3	1	0	3.730126	-2.109496	-1.829012
4	6	0	2.463995	-2.017776	0.915836
5	1	0	2.151647	-3.052735	0.743831
6	1	0	2.892217	-1.958769	1.919738
7	6	0	1.222497	-1.088682	0.855635
8	1	0	0.608419	-1.309141	1.737148
9	1	0	1.521063	-0.036372	0.922520
10	6	0	0.418500	-1.298604	-0.342996
11	16	0	4.675845	-0.496538	0.354872
12	8	0	5.640096	-0.618303	-0.722155
13	8	0	4.994125	-0.705128	1.758232
14	6	0	3.862665	1.074394	0.192618
15	6	0	3.496388	1.762152	1.350014
16	6	0	3.624271	1.596695	-1.078713
17	6	0	2.863547	2.995708	1.225957
18	1	0	3.737224	1.343602	2.322640
19	6	0	2.985423	2.828054	-1.186087
20	1	0	3.956060	1.057621	-1.959145
21	6	0	2.605296	3.523399	-0.038520
22	1	0	2.592999	3.554474	2.117178
23	1	0	2.804657	3.255852	-2.167901
24	1	0	2.125431	4.493862	-0.130296
25	6	0	-0.196237	-1.548841	-1.384394
26	1	0	-0.364219	-1.905588	-2.383566
27	6	0	-3.588947	0.297428	0.173425
28	6	0	-5.259367	1.762653	0.450898
29	6	0	-5.667086	0.572882	0.960373
30	1	0	-5.764261	2.714785	0.388302
31	1	0	-6.595067	0.286817	1.431984
32	7	0	-3.983892	1.573920	-0.025602
33	7	0	-4.630708	-0.312009	0.780243
34	79	0	-1.834805	-0.535206	-0.367101
35	6	0	-4.678707	-1.702139	1.203965
36	1	0	-5.523402	-2.203985	0.726162
37	1	0	-3.753306	-2.194965	0.905476
38	1	0	-4.784087	-1.756258	2.290315
39	6	0	-3.206157	2.614807	-0.677651
40	1	0	-2.187638	2.255288	-0.826015
41	1	0	-3.648442	2.861103	-1.646360
42	1	0	-3.184924	3.505316	-0.045417

Zero-point correction= 0.332268 (Hartree/Particle)
Thermal correction to Energy= 0.357260
Thermal correction to Enthalpy= 0.358205
Thermal correction to Gibbs Free Energy= 0.270933
Sum of electronic and zero-point Energies= -1504.609139
Sum of electronic and thermal Energies= -1504.584147
Sum of electronic and thermal Enthalpies= -1504.583203
Sum of electronic and thermal Free Energies（333K）= -1504.681016
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.910922

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.471262	-1.854324	0.376792
2	8	0	2.479231	-2.123158	-0.581591
3	1	0	2.933914	-1.950964	-1.448508
4	6	0	2.725781	-1.524005	1.580350
5	1	0	2.386291	-2.469240	2.013305
6	1	0	3.398319	-1.041267	2.293060
7	6	0	1.518887	-0.632623	1.223131
8	1	0	0.789215	-0.678623	2.038924
9	1	0	1.829382	0.410474	1.102854
10	6	0	0.866160	-1.112806	0.002566
11	16	0	4.649292	-0.721539	-0.260971
12	8	0	4.537801	-1.032708	-1.688598
13	8	0	5.821844	-0.969994	0.546698
14	6	0	4.134058	0.951511	-0.014124
15	6	0	4.522430	1.607243	1.155755
16	6	0	3.361054	1.576916	-0.993681
17	6	0	4.100630	2.917614	1.354393
18	1	0	5.168215	1.108645	1.872214
19	6	0	2.952236	2.888836	-0.779155
20	1	0	3.117440	1.055282	-1.913464
21	6	0	3.314457	3.552251	0.393061
22	1	0	4.401676	3.449434	2.251758
23	1	0	2.366683	3.400189	-1.537168
24	1	0	2.998480	4.579464	0.549991
25	6	0	-0.112110	-1.286714	-0.798590
26	1	0	-0.076271	-1.857294	-1.721422

27	6	0	-3.783407	0.297802	0.103801
28	6	0	-5.568311	1.655323	0.220579
29	6	0	-5.927419	0.460489	0.750017
30	1	0	-6.129379	2.568024	0.088893
31	1	0	-6.862914	0.126395	1.172401
32	7	0	-4.252931	1.535703	-0.168525
33	7	0	-4.822136	-0.356454	0.669260
34	79	0	-1.932696	-0.444464	-0.290458
35	6	0	-4.804420	-1.733322	1.131701
36	1	0	-5.548641	-2.318845	0.586035
37	1	0	-3.814212	-2.151480	0.949010
38	1	0	-5.021286	-1.769856	2.202335
39	6	0	-3.500988	2.602635	-0.803787
40	1	0	-2.474054	2.266260	-0.949539
41	1	0	-3.942225	2.846088	-1.773867
42	1	0	-3.504885	3.490120	-0.165946

Zero-point correction= 0.332491 (Hartree/Particle)
Thermal correction to Energy= 0.355947
Thermal correction to Enthalpy= 0.356892
Thermal correction to Gibbs Free Energy= 0.273700
Sum of electronic and zero-point Energies= -1504.597573
Sum of electronic and thermal Energies= -1504.574117
Sum of electronic and thermal Enthalpies= -1504.573173
Sum of electronic and thermal Free Energies（333K）= -1504.666415
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.884282

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.578403	-1.055650	0.059106
2	8	0	2.204436	-0.454133	-1.196239
3	1	0	2.397601	-1.184448	-1.824221
4	6	0	2.155672	-0.147772	1.121069
5	1	0	2.709300	-0.451368	2.014356
6	1	0	2.418098	0.889839	0.873384
7	6	0	0.656740	-0.301091	1.360303
8	1	0	0.444771	-1.281561	1.802421
9	1	0	0.319683	0.450214	2.082040
10	6	0	-0.121361	-0.179251	0.088532
11	16	0	4.284236	-1.406547	-0.050596
12	8	0	4.356453	-1.979119	-1.389607
13	8	0	4.547460	-2.146517	1.166680
14	6	0	5.161821	0.124484	-0.016076
15	6	0	5.668139	0.580184	1.202234
16	6	0	5.322020	0.845054	-1.200608
17	6	0	6.344223	1.795222	1.229020
18	1	0	5.560066	-0.024608	2.097174
19	6	0	5.998455	2.058602	-1.153874
20	1	0	4.949966	0.446076	-2.138072
21	6	0	6.503665	2.531936	0.056505
22	1	0	6.757881	2.160194	2.164116
23	1	0	6.143727	2.629298	-2.065980
24	1	0	7.037958	3.477162	0.083372
25	6	0	0.282775	-0.214800	-1.118782
26	6	0	-4.218274	0.205864	0.006117
27	6	0	-6.407127	-0.281763	0.087690
28	6	0	-6.289207	1.068580	0.059356
29	1	0	-7.280565	-0.914862	0.126157
30	1	0	-7.039543	1.844514	0.068190
31	7	0	-5.129130	-0.791361	0.054631
32	7	0	-4.942337	1.347035	0.009593
33	79	0	-2.195818	0.024741	-0.031787
34	1	0	0.138266	-0.135971	-2.180491
35	6	0	-4.400064	2.693945	-0.028013
36	1	0	-3.315272	2.632522	-0.118614
37	1	0	-4.803975	3.232273	-0.888995
38	1	0	-4.656730	3.226386	0.891448
39	6	0	-4.829110	-2.212721	0.072564
40	1	0	-5.310019	-2.704216	-0.776799
41	1	0	-3.749246	-2.344206	0.000075
42	1	0	-5.185680	-2.657893	1.004909

Zero-point correction= 0.332931 (Hartree/Particle)
Thermal correction to Energy= 0.356564
Thermal correction to Enthalpy= 0.357508
Thermal correction to Gibbs Free Energy= 0.274604
Sum of electronic and zero-point Energies= -1504.593740
Sum of electronic and thermal Energies= -1504.570107
Sum of electronic and thermal Enthalpies= -1504.569163
Sum of electronic and thermal Free Energies（333K）= -1504.662086
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.883223

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.561854	0.199421	0.354414

2	8	0	-1.499783	1.613784	0.295062
3	1	0	-1.472752	1.852831	1.239633
4	6	0	-1.359454	-0.290676	-1.004884
5	1	0	-2.229835	-0.122208	-1.655384
6	1	0	-0.530994	0.303032	-1.402308
7	6	0	-0.987879	-1.776139	-1.018634
8	1	0	-1.848546	-2.388941	-0.725251
9	1	0	-0.702752	-2.060661	-2.038275
10	6	0	0.079606	-2.130533	-0.086010
11	16	0	-3.057041	-0.237007	1.121299
12	8	0	-3.042131	0.601363	2.311000
13	8	0	-3.018047	-1.691647	1.175027
14	6	0	-4.375933	0.268354	0.058212
15	6	0	-4.981346	-0.683355	-0.763882
16	6	0	-4.773039	1.606483	0.051534
17	6	0	-6.004691	-0.278789	-1.614811
18	1	0	-4.677275	-1.723624	-0.704154
19	6	0	-5.794581	1.994148	-0.807916
20	1	0	-4.306852	2.318824	0.722819
21	6	0	-6.405165	1.055795	-1.639033
22	1	0	-6.497737	-1.008658	-2.249729
23	1	0	-6.123038	3.028923	-0.820645
24	1	0	-7.207806	1.365238	-2.302130
25	6	0	0.881604	-2.560829	0.745021
26	6	0	3.264883	0.757011	-0.165368
27	6	0	5.067660	1.960174	-0.723732
28	6	0	4.212779	2.781378	-0.061765
29	1	0	6.036783	2.151187	-1.158972
30	1	0	4.293679	3.827137	0.192819
31	7	0	4.467573	0.724746	-0.778007
32	7	0	3.114100	2.026205	0.270110
33	79	0	1.965119	-0.758201	0.098623
34	1	0	1.334842	-3.157891	1.514019
35	6	0	5.074071	-0.438616	-1.404640
36	1	0	4.359185	-1.261434	-1.387649
37	1	0	5.331762	-0.206048	-2.440500
38	1	0	5.974212	-0.729362	-0.857321
39	6	0	1.971306	2.519886	1.024868
40	1	0	1.044530	2.149544	0.581406
41	1	0	2.039878	2.195578	2.066480
42	1	0	1.972978	3.610170	0.985025

Zero-point correction= 0.332525 (Hartree/Particle)
Thermal correction to Energy= 0.357266
Thermal correction to Enthalpy= 0.358210
Thermal correction to Gibbs Free Energy= 0.272781
Sum of electronic and zero-point Energies= -1504.615070
Sum of electronic and thermal Energies= -1504.590328
Sum of electronic and thermal Enthalpies= -1504.589384
Sum of electronic and thermal Free Energies（333K）= -1504.685139
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.914201

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.568969	-0.869673	0.013183
2	8	0	-3.148989	-2.095233	-0.296789
3	1	0	-2.925060	-2.225599	-1.236525
4	6	0	-2.394882	-0.733090	1.473684
5	1	0	-3.215162	-0.201926	1.966281
6	1	0	-2.339255	-1.751004	1.863163
7	6	0	-1.036116	-0.034766	1.505501
8	1	0	-1.139118	1.054451	1.545211
9	1	0	-0.380007	-0.366822	2.316944
10	6	0	-0.528769	-0.444397	0.179648
11	16	0	-3.463034	0.422068	-0.804015
12	8	0	-3.484339	-0.063835	-2.173042
13	8	0	-2.767230	1.628487	-0.389210
14	6	0	-5.082726	0.397135	-0.113879
15	6	0	-5.395140	1.313165	0.893076
16	6	0	-6.008997	-0.534943	-0.585090
17	6	0	-6.671002	1.282656	1.445044
18	1	0	-4.661355	2.049308	1.205877
19	6	0	-7.277787	-0.551006	-0.018422
20	1	0	-5.745655	-1.213581	-1.388608
21	6	0	-7.604617	0.351044	0.993587
22	1	0	-6.939562	1.993967	2.219958
23	1	0	-8.016205	-1.262891	-0.373952
24	1	0	-8.600401	0.334706	1.426824
25	6	0	0.286418	-0.689745	-0.759835
26	6	0	4.190562	0.212371	0.142929
27	6	0	6.142112	1.309131	0.302111
28	6	0	6.365992	0.021262	0.660892
29	1	0	6.811421	2.154052	0.244862
30	1	0	7.268908	-0.478115	0.977893
31	7	0	4.805156	1.406100	-0.011257
32	7	0	5.159561	-0.633706	0.557019
33	79	0	2.240439	-0.220529	-0.219497
34	1	0	0.102790	-1.050630	-1.764389
35	6	0	4.169276	2.635102	-0.453474

36	1	0	3.105602	2.446707	-0.601452
37	1	0	4.296623	3.412353	0.304193
38	1	0	4.611316	2.965537	-1.396885
39	6	0	4.982014	-2.045213	0.849115
40	1	0	3.927838	-2.297355	0.730812
41	1	0	5.576938	-2.647808	0.157959
42	1	0	5.290389	-2.253244	1.876726

Zero-point correction= 0.331696 (Hartree/Particle)
Thermal correction to Energy= 0.355944
Thermal correction to Enthalpy= 0.356888
Thermal correction to Gibbs Free Energy= 0.270728
Sum of electronic and zero-point Energies= -1504.602448
Sum of electronic and thermal Energies= -1504.578200
Sum of electronic and thermal Enthalpies= -1504.577256
Sum of electronic and thermal Free Energies（333K）= -1504.673821
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.889376

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.312454	-0.778375	0.206636
2	8	0	-2.706499	-1.836910	-0.601580
3	1	0	-2.186345	-1.720005	-1.420579
4	6	0	-2.470998	-1.072728	1.672639
5	1	0	-3.250201	-0.460734	2.128735
6	1	0	-2.701400	-2.133337	1.775435
7	6	0	-1.003351	-0.681575	1.917151
8	1	0	-0.885866	0.266359	2.449754
9	1	0	-0.393789	-1.451059	2.396871
10	6	0	-0.831828	-0.565194	0.425746
11	16	0	-3.186683	0.768010	-0.438094
12	8	0	-2.852165	0.685226	-1.846107
13	8	0	-2.715701	1.801251	0.458525
14	6	0	-4.879454	0.414015	-0.153542
15	6	0	-5.488569	0.962035	0.979255
16	6	0	-5.574551	-0.373407	-1.074725
17	6	0	-6.835122	0.695652	1.195042
18	1	0	-4.925349	1.604350	1.649057
19	6	0	-6.919143	-0.627830	-0.836552
20	1	0	-5.077376	-0.758671	-1.957782
21	6	0	-7.542887	-0.099085	0.293716
22	1	0	-7.334919	1.118479	2.060827
23	1	0	-7.483869	-1.232523	-1.539042
24	1	0	-8.595884	-0.299759	0.467947
25	6	0	0.087217	-0.393623	-0.512960
26	6	0	4.086309	0.147956	0.044955
27	6	0	6.290634	-0.209975	0.315754
28	6	0	6.096983	1.130433	0.272124
29	1	0	7.192669	-0.791297	0.431833
30	1	0	6.796835	1.949130	0.342957
31	7	0	5.050060	-0.791967	0.175648
32	7	0	4.744095	1.328164	0.106187
33	79	0	2.074803	-0.140372	-0.207947
34	1	0	-0.281086	-0.364656	-1.542981
35	6	0	4.127154	2.638519	0.008296
36	1	0	3.054039	2.508382	-0.135301
37	1	0	4.303458	3.205117	0.926453
38	1	0	4.541487	3.183502	-0.843881
39	6	0	4.828868	-2.226040	0.163549
40	1	0	3.761132	-2.411232	0.042191
41	1	0	5.371076	-2.681740	-0.669204
42	1	0	5.168310	-2.665320	1.105358

Zero-point correction= 0.333765 (Hartree/Particle)
Thermal correction to Energy= 0.357947
Thermal correction to Enthalpy= 0.358891
Thermal correction to Gibbs Free Energy= 0.274580
Sum of electronic and zero-point Energies= -1504.617895
Sum of electronic and thermal Energies= -1504.593713
Sum of electronic and thermal Enthalpies= -1504.592769
Sum of electronic and thermal Free Energies（333K）= -1504.687266
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1505.897586

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.494492	-0.983902	0.380577
2	8	0	3.261272	-2.079574	0.800213
3	1	0	3.069646	-2.142618	1.751356
4	6	0	2.189275	-1.140551	-1.038573
5	1	0	3.013488	-0.796997	-1.676152
6	1	0	2.076645	-2.217826	-1.178706
7	6	0	0.884438	-0.414516	-1.421961
8	1	0	1.067567	0.646730	-1.619075
9	1	0	0.466148	-0.857885	-2.329851
10	6	0	-0.035313	-0.502905	-0.262660

11	16	0	3.318737	0.484162	0.854256
12	8	0	3.459384	0.305145	2.290333
13	8	0	2.512162	1.542065	0.263475
14	6	0	4.904180	0.447804	0.081665
15	6	0	5.083782	1.148377	-1.112399
16	6	0	5.935780	-0.280343	0.675481
17	6	0	6.330141	1.106388	-1.727955
18	1	0	4.270477	1.737409	-1.524289
19	6	0	7.173806	-0.312387	0.044576
20	1	0	5.773729	-0.789714	1.618708
21	6	0	7.367845	0.374574	-1.153194
22	1	0	6.494013	1.654586	-2.650673
23	1	0	7.991608	-0.867837	0.493232
24	1	0	8.339883	0.348107	-1.637009
25	6	0	0.185369	-0.711477	0.954217
26	6	0	-4.090897	0.208363	-0.048752
27	6	0	-6.057641	1.280169	0.049942
28	6	0	-6.314909	-0.025847	-0.210303
29	1	0	-6.723463	2.120414	0.176119
30	1	0	-7.248834	-0.547149	-0.356118
31	7	0	-4.691018	1.403685	0.144365
32	7	0	-5.098285	-0.665211	-0.267763
33	79	0	-2.101011	-0.174070	-0.042705
34	1	0	0.166711	-0.810870	2.022390
35	6	0	-4.948129	-2.086405	-0.529858
36	1	0	-3.888608	-2.340787	-0.493301
37	1	0	-5.483505	-2.661877	0.229332
38	1	0	-5.343551	-2.326170	-1.520094
39	6	0	-4.014449	2.660757	0.417735
40	1	0	-4.349734	3.060830	1.377749
41	1	0	-2.939744	2.481987	0.458308
42	1	0	-4.230930	3.379480	-0.376507

Zero-point correction= 0.331854 (Hartree/Particle)
Thermal correction to Energy= 0.356112
Thermal correction to Enthalpy= 0.357056
Thermal correction to Gibbs Free Energy= 0.272610
Sum of electronic and zero-point Energies= -1504.603506
Sum of electronic and thermal Energies= -1504.579249
Sum of electronic and thermal Enthalpies= -1504.578305
Sum of electronic and thermal Free Energies（333K）= -1504.672954
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.896595

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.203512	-0.524640	0.811758
2	8	0	2.867084	-1.046526	1.929470
3	1	0	2.851152	-0.315699	2.580630
4	6	0	2.145896	-1.578210	-0.248254
5	1	0	3.012895	-1.485958	-0.904701
6	1	0	2.210251	-2.522934	0.295632
7	6	0	0.778819	-1.374757	-0.900760
8	1	0	0.854175	-0.807445	-1.835735
9	1	0	0.309139	-2.332551	-1.142774
10	6	0	-0.019107	-0.579833	0.107905
11	16	0	3.215285	1.037968	0.329422
12	8	0	3.293442	1.659989	1.642292
13	8	0	2.475734	1.583138	-0.787649
14	6	0	4.777543	0.427860	-0.181144
15	6	0	5.014307	0.277601	-1.551132
16	6	0	5.745476	0.142758	0.784916
17	6	0	6.259891	-0.186007	-1.955536
18	1	0	4.249215	0.545729	-2.273110
19	6	0	6.982963	-0.320552	0.356307
20	1	0	5.540791	0.300695	1.837889
21	6	0	7.235488	-0.487660	-1.005241
22	1	0	6.472959	-0.301030	-3.013611
23	1	0	7.754802	-0.543157	1.086204
24	1	0	8.207571	-0.846717	-1.330038
25	6	0	0.818359	-0.130872	1.052167
26	6	0	-4.019471	0.156659	-0.120185
27	6	0	-5.993627	1.220881	-0.293077
28	6	0	-6.252848	-0.104527	-0.181951
29	1	0	-6.657763	2.065601	-0.395370
30	1	0	-7.187622	-0.644089	-0.169436
31	7	0	-4.623998	1.359288	-0.253491
32	7	0	-5.033893	-0.736958	-0.077479
33	79	0	-2.009402	-0.219227	-0.002832
34	1	0	0.658979	0.519039	1.903487
35	6	0	-4.881022	-2.174077	0.054284
36	1	0	-3.819338	-2.403171	0.150513
37	1	0	-5.408032	-2.525444	0.945163
38	1	0	-5.281400	-2.676632	-0.830250
39	6	0	-3.940807	2.637349	-0.337047
40	1	0	-4.197337	3.257880	0.525793
41	1	0	-2.865252	2.458046	-0.346152
42	1	0	-4.227615	3.152975	-1.257130

Zero-point correction= 0.335557 (Hartree/Particle)

Thermal correction to Energy= 0.359240
Thermal correction to Enthalpy= 0.360184
Thermal correction to Gibbs Free Energy= 0.275948
Sum of electronic and zero-point Energies= -1504.645718
Sum of electronic and thermal Energies= -1504.622034
Sum of electronic and thermal Enthalpies= -1504.621090
Sum of electronic and thermal Free Energies（333K）= -1504.715502
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1505.927426

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.976622	-1.816835	0.386571
2	8	0	-1.845131	-1.139754	-0.834679
3	1	0	-1.684089	-0.199038	-0.575546
4	6	0	-0.721689	-2.474953	0.747712
5	1	0	-0.101689	-1.714053	1.230768
6	1	0	-0.962247	-3.242615	1.488998
7	6	0	0.025037	-3.110785	-0.440305
8	1	0	0.778601	-3.809198	-0.057746
9	1	0	-0.673936	-3.689687	-1.059246
10	6	0	0.668225	-2.136813	-1.315909
11	16	0	-3.283716	-2.908760	0.194839
12	8	0	-3.378765	-3.597379	1.478463
13	8	0	-3.154679	-3.682703	-1.039766
14	6	0	-4.629173	-1.771453	0.013809
15	6	0	-5.234646	-1.264341	1.160622
16	6	0	-5.056874	-1.422627	-1.263729
17	6	0	-6.298507	-0.380298	1.017630
18	1	0	-4.876879	-1.567891	2.139137
19	6	0	-6.121295	-0.536068	-1.391167
20	1	0	-4.558523	-1.843818	-2.130066
21	6	0	-6.738064	-0.017262	-0.254445
22	1	0	-6.785711	0.024750	1.899822
23	1	0	-6.467931	-0.248903	-2.379581
24	1	0	-7.568929	0.675030	-0.360273
25	6	0	1.139757	-1.336551	-2.128766
26	1	0	1.155602	-0.645136	-2.951491
27	6	0	4.220520	-0.480208	0.550967
28	6	0	5.546804	0.660823	1.942390
29	6	0	6.249626	-0.414729	1.503227
30	1	0	5.819502	1.454391	2.620759
31	1	0	7.255279	-0.741467	1.718592
32	7	0	4.311582	0.603739	1.347291
33	7	0	5.419108	-1.102109	0.649864
34	79	0	2.638072	-1.030268	-0.571372
35	6	0	5.798371	-2.317984	-0.043035
36	1	0	4.953212	-2.651500	-0.645970
37	1	0	6.653994	-2.125558	-0.695952
38	1	0	6.056533	-3.095760	0.680757
39	6	0	3.233488	1.562050	1.576735
40	1	0	3.644973	2.425894	2.100218
41	1	0	2.807859	1.883057	0.624798
42	1	0	2.448253	1.104197	2.180174
43	7	0	-0.864921	1.439648	-0.165139
44	16	0	-0.394814	1.674634	1.368009
45	8	0	0.077995	0.427517	1.976653
46	8	0	0.382213	2.885831	1.610860
47	6	0	-2.059172	1.975062	2.109018
48	9	0	-2.588911	3.081097	1.604022
49	9	0	-1.907356	2.124119	3.421557
50	9	0	-2.868987	0.950694	1.876915
51	16	0	-0.007718	1.972135	-1.419014
52	8	0	1.429234	2.096119	-1.160408
53	8	0	-0.446734	1.237805	-2.599699
54	6	0	-0.606663	3.698801	-1.712370
55	9	0	-0.000589	4.176909	-2.795594
56	9	0	-1.917882	3.686356	-1.917392
57	9	0	-0.333290	4.481243	-0.679171

Zero-point correction= 0.388987 (Hartree/Particle)
Thermal correction to Energy= 0.437864
Thermal correction to Enthalpy= 0.438919
Thermal correction to Gibbs Free Energy= 0.292400
Sum of electronic and zero-point Energies= -3330.598490
Sum of electronic and thermal Energies= -3330.549613
Sum of electronic and thermal Enthalpies= -3330.548558
Sum of electronic and thermal Free Energies(333K)= -3330.695077
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.991125

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.491839	-1.536779	0.958951
2	8	0	-1.860531	-1.168118	-0.236738
3	1	0	-1.591587	-0.201193	-0.119430
4	6	0	-1.454927	-2.025754	1.878607

5	1	0	-1.016454	-1.145445	2.353946
6	1	0	-1.930483	-2.652142	2.636860
7	6	0	-0.377990	-2.785252	1.094401
8	1	0	0.500708	-2.924870	1.735319
9	1	0	-0.734453	-3.773097	0.779197
10	6	0	0.054467	-2.027415	-0.072285
11	16	0	-3.657433	-2.741103	0.528836
12	8	0	-4.199104	-3.170489	1.811900
13	8	0	-3.076708	-3.705620	-0.399225
14	6	0	-4.844094	-1.752133	-0.332684
15	6	0	-5.902553	-1.203254	0.387023
16	6	0	-4.698186	-1.555636	-1.703728
17	6	0	-6.839277	-0.431438	-0.291692
18	1	0	-5.985767	-1.391041	1.452617
19	6	0	-5.640357	-0.776083	-2.366352
20	1	0	-3.863506	-2.005459	-2.230112
21	6	0	-6.705277	-0.217053	-1.662438
22	1	0	-7.674609	0.002372	0.250088
23	1	0	-5.541302	-0.605081	-3.434094
24	1	0	-7.438206	0.389752	-2.186990
25	6	0	0.784196	-1.554117	-0.994574
26	1	0	0.437590	-0.994242	-1.860906
27	6	0	4.594021	-0.533001	0.016649
28	6	0	6.152344	0.889209	0.770373
29	6	0	6.795297	-0.220572	0.327001
30	1	0	6.533710	1.800708	1.204139
31	1	0	7.845281	-0.467689	0.296730
32	7	0	4.808577	0.679201	0.571568
33	7	0	5.821030	-1.080154	-0.131183
34	79	0	2.762178	-1.232354	-0.479300
35	6	0	6.083697	-2.386866	-0.699563
36	1	0	5.129775	-2.837682	-0.975962
37	1	0	6.709820	-2.290536	-1.590881
38	1	0	6.586610	-3.022680	0.034431
39	6	0	3.749363	1.623871	0.916201
40	1	0	4.209170	2.535944	1.299225
41	1	0	3.148101	1.862977	0.036581
42	1	0	3.100156	1.196997	1.682975
43	7	0	-0.765272	1.339850	0.050410
44	16	0	-0.093775	1.794047	1.458544
45	8	0	0.351114	0.615569	2.205192
46	8	0	0.787897	2.951429	1.393213
47	6	0	-1.617274	2.351582	2.341140
48	9	0	-2.180468	3.365673	1.698571
49	9	0	-1.280224	2.741765	3.565637
50	9	0	-2.485360	1.347994	2.427441
51	16	0	-0.208863	1.835182	-1.387435
52	8	0	1.212894	2.157721	-1.411979
53	8	0	-0.755826	0.912479	-2.376906
54	6	0	-1.093105	3.431553	-1.691263
55	9	0	-0.700298	3.925599	-2.860171
56	9	0	-2.403002	3.219160	-1.725336
57	9	0	-0.817638	4.304691	-0.731800

Zero-point correction= 0.388729 (Hartree/Particle)
Thermal correction to Energy= 0.436376
Thermal correction to Enthalpy= 0.437431
Thermal correction to Gibbs Free Energy= 0.293299
Sum of electronic and zero-point Energies= -3330.592566
Sum of electronic and thermal Energies= -3330.544919
Sum of electronic and thermal Enthalpies= -3330.543864
Sum of electronic and thermal Free Energies(333K)= -3330.687996
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.974302

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.877914	-1.703286	-1.688880
2	8	0	1.272572	-1.032504	-0.600375
3	1	0	1.870391	0.571088	-0.583131
4	6	0	0.844840	-1.729928	-2.743959
5	1	0	0.943585	-0.789914	-3.293320
6	1	0	1.045929	-2.566348	-3.416648
7	6	0	-0.478332	-1.800617	-1.986535
8	1	0	-1.288870	-1.291633	-2.512990
9	1	0	-0.773069	-2.838863	-1.801445
10	6	0	-0.156763	-1.111066	-0.693194
11	16	0	2.315390	-3.297807	-1.138726
12	8	0	2.923027	-3.909503	-2.314524
13	8	0	1.208545	-3.947759	-0.442378
14	6	0	3.560429	-2.879504	0.048177
15	6	0	4.860695	-2.645751	-0.392015
16	6	0	3.209012	-2.800459	1.392921
17	6	0	5.832734	-2.319285	0.546595
18	1	0	5.097521	-2.726476	-1.447988
19	6	0	4.192235	-2.469505	2.319419
20	1	0	2.186062	-3.001393	1.693666
21	6	0	5.497581	-2.228697	1.896240
22	1	0	6.852133	-2.130587	0.223620
23	1	0	3.938389	-2.400936	3.373326

24	1	0	6.261010	-1.967572	2.623864
25	6	0	-0.896708	-0.573616	0.270308
26	1	0	-0.328868	-0.154172	1.103168
27	6	0	-4.964284	-0.384775	0.377210
28	6	0	-7.089968	0.350347	0.202246
29	6	0	-7.136183	-0.921949	0.665772
30	1	0	-7.879534	1.052475	-0.018276
31	1	0	-7.974078	-1.549408	0.928989
32	7	0	-5.757330	0.658366	0.032845
33	7	0	-5.830453	-1.351472	0.765566
34	79	0	-2.912106	-0.484411	0.313758
35	6	0	-5.441790	-2.670974	1.224080
36	1	0	-4.352540	-2.728724	1.214961
37	1	0	-5.805659	-2.837486	2.241901
38	1	0	-5.850790	-3.436918	0.559069
39	6	0	-5.273512	1.936261	-0.451575
40	1	0	-5.677692	2.138296	-1.447516
41	1	0	-5.570056	2.736156	0.232940
42	1	0	-4.184908	1.890283	-0.505301
43	7	0	2.156974	1.575317	-0.505446
44	16	0	3.376285	1.922110	0.592212
45	8	0	4.358803	0.863456	0.545580
46	8	0	3.704930	3.325545	0.511344
47	6	0	2.434785	1.665714	2.168539
48	9	0	1.392792	2.482045	2.217508
49	9	0	3.249076	1.920107	3.181333
50	9	0	2.016883	0.408287	2.236549
51	16	0	1.535637	2.570083	-1.699413
52	8	0	2.520862	3.515201	-2.163214
53	8	0	0.810012	1.679781	-2.582387
54	6	0	0.262882	3.541818	-0.766489
55	9	0	-0.393118	4.292947	-1.640750
56	9	0	-0.581086	2.720513	-0.164259
57	9	0	0.853758	4.313446	0.130918

Zero-point correction= 0.391170 (Hartree/Particle)
Thermal correction to Energy= 0.430872
Thermal correction to Enthalpy= 0.431816
Thermal correction to Gibbs Free Energy= 0.308133
Sum of electronic and zero-point Energies= -3330.624445
Sum of electronic and thermal Energies= -3330.584743
Sum of electronic and thermal Enthalpies= -3330.583799
Sum of electronic and thermal Free Energies(333K)= -3330.722435
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.998253

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.412582	-0.902206	-1.005363
2	8	0	1.965140	-0.591658	0.302860
3	1	0	1.553663	0.336206	0.204306
4	6	0	1.936406	-2.221936	-1.422139
5	1	0	2.453893	-2.429488	-2.361492
6	1	0	2.206182	-2.991443	-0.682862
7	6	0	0.428023	-2.214603	-1.643334
8	1	0	0.157286	-1.449330	-2.380074
9	1	0	0.115222	-3.187418	-2.037115
10	6	0	-0.289099	-1.907303	-0.370201
11	16	0	4.129828	-0.719139	-0.993555
12	8	0	4.364298	0.634818	-0.531399
13	8	0	4.547777	-1.191986	-2.305864
14	6	0	4.727194	-1.848121	0.239762
15	6	0	5.205277	-3.095330	-0.159144
16	6	0	4.688124	-1.471513	1.582166
17	6	0	5.652540	-3.985218	0.812745
18	1	0	5.243766	-3.343007	-1.215332
19	6	0	5.133786	-2.374037	2.541899
20	1	0	4.323795	-0.487945	1.857870
21	6	0	5.612707	-3.625841	2.158408
22	1	0	6.038511	-4.956802	0.517859
23	1	0	5.112139	-2.096171	3.591619
24	1	0	5.963655	-4.323710	2.913747
25	6	0	0.169684	-1.361568	0.680991
26	6	0	-4.293543	-1.138702	0.037330
27	6	0	-6.122355	0.152857	-0.018042
28	6	0	-6.519756	-1.099868	0.321129
29	1	0	-6.688016	1.062473	-0.148702
30	1	0	-7.498481	-1.499269	0.538060
31	7	0	-4.760110	0.107719	-0.190346
32	7	0	-5.382991	-1.876345	0.348779
33	79	0	-2.338069	-1.655882	-0.069317
34	1	0	0.155653	-0.913505	1.661504
35	6	0	-5.366876	-3.289584	0.668032
36	1	0	-4.333153	-3.636006	0.638697
37	1	0	-5.774249	-3.452456	1.669612
38	1	0	-5.957869	-3.848400	-0.063058
39	6	0	-3.921813	1.256276	-0.525185
40	1	0	-3.357593	1.591722	0.348073
41	1	0	-3.221283	0.983990	-1.315746
42	1	0	-4.564083	2.063018	-0.881405

43	7	0	0.512858	1.660572	0.160692
44	16	0	-0.207293	2.119642	-1.227742
45	8	0	-0.433416	0.948498	-2.071092
46	8	0	-1.280565	3.091798	-1.065799
47	16	0	-0.071885	1.987308	1.630956
48	8	0	-1.519649	2.138840	1.704268
49	8	0	0.593757	1.052530	2.538576
50	6	0	1.197321	3.025652	-2.016864
51	6	0	0.627092	3.645580	2.054689
52	9	0	0.274582	3.955798	3.297856
53	9	0	0.155190	4.563383	1.222395
54	9	0	1.949544	3.612713	1.970277
55	9	0	2.233562	2.219250	-2.179189
56	9	0	0.793315	3.471361	-3.202394
57	9	0	1.549882	4.057037	-1.259636

Zero-point correction= 0.389469 (Hartree/Particle)
Thermal correction to Energy= 0.436813
Thermal correction to Enthalpy= 0.437868
Thermal correction to Gibbs Free Energy= 0.296518
Sum of electronic and zero-point Energies= -3330.580670
Sum of electronic and thermal Energies= -3330.533326
Sum of electronic and thermal Enthalpies= -3330.532271
Sum of electronic and thermal Free Energies(333K)= -3330.673621
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.965814

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.058838	1.733317	1.142422
2	8	0	0.862175	1.158144	-0.146384
3	1	0	1.666616	-0.576437	-0.199210
4	6	0	0.213226	2.923125	1.286869
5	1	0	0.529371	3.422247	2.206365
6	1	0	0.360197	3.600602	0.433214
7	6	0	-1.230159	2.437814	1.361341
8	1	0	-1.425155	2.014660	2.355301
9	1	0	-1.896463	3.303838	1.258189
10	6	0	-1.525465	1.416481	0.291829
11	16	0	2.742022	1.990755	1.289615
12	8	0	3.345700	0.710582	0.950492
13	8	0	2.893381	2.598128	2.602840
14	6	0	3.203643	3.181556	0.056942
15	6	0	3.336565	4.516790	0.435971
16	6	0	3.403674	2.766712	-1.259726
17	6	0	3.679507	5.458234	-0.529077
18	1	0	3.193987	4.796937	1.474820
19	6	0	3.741433	3.722652	-2.212656
20	1	0	3.310688	1.719863	-1.529630
21	6	0	3.877946	5.061405	-1.850059
22	1	0	3.797060	6.500707	-0.247395
23	1	0	3.903735	3.416110	-3.241871
24	1	0	4.146314	5.799630	-2.600933
25	6	0	-0.498158	0.894666	-0.380615
26	6	0	-5.173858	-0.277688	-0.382025
27	6	0	-6.710703	-1.900709	-0.674024
28	6	0	-7.353121	-0.711383	-0.768716
29	1	0	-7.079023	-2.912111	-0.754358
30	1	0	-8.392394	-0.479975	-0.945893
31	7	0	-5.383681	-1.615012	-0.437387
32	7	0	-6.397382	0.265508	-0.588320
33	79	0	-3.372629	0.650025	-0.057436
34	1	0	-0.553697	0.181561	-1.195477
35	6	0	-6.669661	1.688079	-0.614764
36	1	0	-5.724191	2.216445	-0.485183
37	1	0	-7.113255	1.968575	-1.574397
38	1	0	-7.351684	1.958896	0.196499
39	6	0	-4.352481	-2.625054	-0.277545
40	1	0	-4.241578	-3.198533	-1.202068
41	1	0	-3.407433	-2.131345	-0.045789
42	1	0	-4.616476	-3.299322	0.541717
43	7	0	1.848409	-1.571751	-0.426461
44	16	0	0.989635	-2.728013	0.436299
45	8	0	-0.396903	-2.320751	0.517744
46	8	0	1.399349	-4.039848	-0.007476
47	16	0	2.851929	-1.810901	-1.747110
48	8	0	2.395092	-2.927276	-2.538199
49	8	0	3.058813	-0.486126	-2.295836
50	6	0	1.709897	-2.443868	2.122932
51	6	0	4.456160	-2.330132	-0.972488
52	9	0	5.327864	-2.496335	-1.958541
53	9	0	4.291637	-3.471700	-0.325153
54	9	0	4.885950	-1.399278	-0.145443
55	9	0	1.444233	-1.210499	2.513007
56	9	0	1.144814	-3.312075	2.950505
57	9	0	3.016492	-2.641574	2.091213

Zero-point correction= 0.391875 (Hartree/Particle)
Thermal correction to Energy= 0.439664
Thermal correction to Enthalpy= 0.440719

Thermal correction to Gibbs Free Energy= 0.295355
Sum of electronic and zero-point Energies= -3330.619409
Sum of electronic and thermal Energies= -3330.571620
Sum of electronic and thermal Enthalpies= -3330.570565
Sum of electronic and thermal Free Energies(333K)= -3330.715929
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.993444

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.441357	-0.969243	-0.519411
2	8	0	2.750864	0.305582	-0.037250
3	1	0	2.038889	0.877740	-0.408077
4	6	0	1.834052	-1.798412	0.522488
5	1	0	2.572367	-2.337614	1.133860
6	1	0	1.301119	-1.095090	1.167148
7	6	0	0.851098	-2.802104	-0.095981
8	1	0	1.401107	-3.541438	-0.689207
9	1	0	0.314061	-3.331146	0.698616
10	6	0	-0.076767	-2.117597	-0.997433
11	16	0	3.820564	-1.597315	-1.286620
12	8	0	4.163325	-0.687094	-2.361003
13	8	0	3.486413	-2.999578	-1.532857
14	6	0	5.115490	-1.549215	-0.070046
15	6	0	5.461277	-2.722038	0.598771
16	6	0	5.749219	-0.337204	0.203248
17	6	0	6.462446	-2.676862	1.564943
18	1	0	4.965148	-3.651700	0.338622
19	6	0	6.743872	-0.306616	1.174314
20	1	0	5.462819	0.555210	-0.341563
21	6	0	7.098189	-1.471604	1.853548
22	1	0	6.749724	-3.584965	2.087466
23	1	0	7.247098	0.629384	1.398923
24	1	0	7.879098	-1.440054	2.608544
25	6	0	-0.648916	-1.466625	-1.873862
26	6	0	-3.943440	-1.428431	0.708816
27	6	0	-5.969942	-1.832558	1.576837
28	6	0	-5.549286	-0.627175	2.040515
29	1	0	-6.881973	-2.381662	1.753316
30	1	0	-6.023420	0.079605	2.703823
31	7	0	-4.970135	-2.308554	0.761729
32	7	0	-4.310127	-0.399320	1.497729
33	79	0	-2.232777	-1.568230	-0.346630
34	1	0	-0.846664	-0.843217	-2.727324
35	6	0	-5.035113	-3.570997	0.051350
36	1	0	-5.203671	-4.387558	0.758385
37	1	0	-5.845045	-3.548098	-0.682917
38	1	0	-4.086901	-3.728593	-0.463554
39	6	0	-3.490235	0.784885	1.741057
40	1	0	-3.222157	1.257734	0.795415
41	1	0	-4.062669	1.484161	2.351324
42	1	0	-2.576040	0.504570	2.266512
43	7	0	0.404691	1.922842	-0.244921
44	16	0	-0.634214	2.001955	-1.469998
45	8	0	-0.000234	1.413309	-2.643283
46	8	0	-1.999649	1.585734	-1.131330
47	6	0	-0.757891	3.804202	-1.871505
48	9	0	-1.245019	4.484788	-0.843591
49	9	0	-1.567526	3.952541	-2.916321
50	9	0	0.442578	4.276849	-2.179755
51	16	0	-0.084119	2.020002	1.297409
52	8	0	-1.284048	2.818151	1.534042
53	8	0	0.011893	0.718212	1.965701
54	6	0	1.304904	3.034623	1.971492
55	9	0	1.095948	3.196705	3.275126
56	9	0	2.472985	2.435736	1.789844
57	9	0	1.321925	4.222978	1.382741

Zero-point correction= 0.389039 (Hartree/Particle)
Thermal correction to Energy= 0.437993
Thermal correction to Enthalpy= 0.439048
Thermal correction to Gibbs Free Energy= 0.292507
Sum of electronic and zero-point Energies= -3330.596284
Sum of electronic and thermal Energies= -3330.547330
Sum of electronic and thermal Enthalpies= -3330.546275
Sum of electronic and thermal Free Energies(333K)= -3330.692816
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.991684

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.390921	-1.179754	-0.140976
2	8	0	-2.783140	0.120956	0.110935
3	1	0	-1.934276	0.622219	0.280989
4	6	0	-2.198567	-1.486935	-1.578887
5	1	0	-3.026024	-2.051051	-2.018651
6	1	0	-2.090790	-0.521623	-2.072456

7	6	0	-0.864590	-2.232753	-1.526796
8	1	0	-0.997944	-3.319057	-1.551066
9	1	0	-0.164765	-1.922411	-2.309826
10	6	0	-0.384263	-1.807359	-0.198703
11	16	0	-3.404310	-2.258640	0.760256
12	8	0	-3.188755	-1.935657	2.155331
13	8	0	-3.092663	-3.567251	0.197846
14	6	0	-5.054123	-1.810226	0.298463
15	6	0	-5.723126	-2.586793	-0.646292
16	6	0	-5.641962	-0.689236	0.884006
17	6	0	-7.014682	-2.224506	-1.015801
18	1	0	-5.240910	-3.468038	-1.057409
19	6	0	-6.931286	-0.339018	0.499894
20	1	0	-5.094039	-0.113883	1.621780
21	6	0	-7.613209	-1.102280	-0.446941
22	1	0	-7.555266	-2.822558	-1.743634
23	1	0	-7.406121	0.531184	0.943287
24	1	0	-8.621667	-0.822843	-0.739311
25	6	0	0.366210	-1.543880	0.784978
26	6	0	4.312864	-1.211647	-0.256326
27	6	0	6.526368	-1.456361	-0.546763
28	6	0	6.192981	-0.200337	-0.936907
29	1	0	7.479033	-1.962639	-0.522500
30	1	0	6.799206	0.603336	-1.325481
31	7	0	5.359229	-2.059884	-0.133872
32	7	0	4.837510	-0.069702	-0.749450
33	79	0	2.362174	-1.495987	0.208327
34	1	0	0.112301	-1.149495	1.764083
35	6	0	5.278353	-3.411175	0.383500
36	1	0	5.669985	-4.118347	-0.352842
37	1	0	5.850180	-3.494670	1.312013
38	1	0	4.230940	-3.639979	0.583934
39	6	0	4.061653	1.126266	-1.061574
40	1	0	3.401144	1.376837	-0.229933
41	1	0	4.754253	1.951422	-1.235516
42	1	0	3.457917	0.964944	-1.956790
43	7	0	-0.490132	1.671643	0.124826
44	16	0	0.368098	1.902961	1.474049
45	8	0	-0.293861	1.140535	2.523753
46	8	0	1.814217	1.792969	1.305679
47	6	0	0.070524	3.676519	1.904474
48	9	0	0.558075	4.467538	0.955993
49	9	0	0.675718	3.951012	3.054958
50	9	0	-1.231509	3.901239	2.032700
51	16	0	0.044253	1.984270	-1.369770
52	8	0	1.297155	2.723419	-1.458683
53	8	0	-0.140528	0.802089	-2.212729
54	6	0	-1.276680	3.142897	-1.939340
55	9	0	-1.016200	3.508482	-3.190455
56	9	0	-2.458818	2.534542	-1.902411
57	9	0	-1.317441	4.222795	-1.169419

Zero-point correction= 0.388288 (Hartree/Particle)
Thermal correction to Energy= 0.436293
Thermal correction to Enthalpy= 0.437348
Thermal correction to Gibbs Free Energy= 0.293254
Sum of electronic and zero-point Energies= -3330.584208
Sum of electronic and thermal Energies= -3330.536203
Sum of electronic and thermal Enthalpies= -3330.535148
Sum of electronic and thermal Free Energies(333K)= -3330.679242
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.970054

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.061859	-1.394548	0.488510
2	8	0	2.499096	-0.227180	-0.084342
3	1	0	1.723857	0.443292	-0.075843
4	6	0	2.115487	-1.499349	1.996208
5	1	0	2.921080	-2.148940	2.340161
6	1	0	2.210907	-0.483366	2.377586
7	6	0	0.677007	-2.035004	2.012309
8	1	0	0.607862	-3.104229	2.232063
9	1	0	-0.006847	-1.461928	2.641140
10	6	0	0.586606	-1.705664	0.545555
11	16	0	3.009433	-2.730167	-0.413793
12	8	0	2.499679	-2.680275	-1.765536
13	8	0	2.865574	-3.888140	0.451869
14	6	0	4.664959	-2.127228	-0.353322
15	6	0	5.524758	-2.642249	0.616146
16	6	0	5.075179	-1.179361	-1.291157
17	6	0	6.837124	-2.183382	0.647377
18	1	0	5.173057	-3.400504	1.308412
19	6	0	6.389613	-0.732190	-1.240861
20	1	0	4.374783	-0.806222	-2.030109
21	6	0	7.264058	-1.230270	-0.275255
22	1	0	7.527182	-2.575316	1.388460
23	1	0	6.731739	0.007620	-1.958008
24	1	0	8.290250	-0.874994	-0.245152
25	6	0	-0.286248	-1.509369	-0.431159

26	6	0	-4.300474	-1.147614	0.052275
27	6	0	-6.527269	-1.412003	0.253842
28	6	0	-6.245644	-0.102694	0.467749
29	1	0	-7.465889	-1.944596	0.250713
30	1	0	-6.891589	0.731388	0.695190
31	7	0	-5.323072	-2.033080	0.002282
32	7	0	-4.883343	0.038585	0.336772
33	79	0	-2.292176	-1.443148	-0.199233
34	1	0	0.142489	-1.191410	-1.383920
35	6	0	-5.176613	-3.443633	-0.291895
36	1	0	-5.558122	-4.043894	0.539149
37	1	0	-5.720423	-3.698161	-1.206266
38	1	0	-4.115520	-3.653609	-0.433118
39	6	0	-4.156748	1.288215	0.524756
40	1	0	-3.352167	1.369485	-0.207385
41	1	0	-4.852879	2.118337	0.388866
42	1	0	-3.724068	1.334626	1.526786
43	7	0	0.667751	1.717771	-0.041393
44	16	0	-0.067110	1.975650	-1.469249
45	8	0	0.676752	1.187710	-2.440237
46	8	0	-1.521646	1.916260	-1.429255
47	6	0	0.315530	3.737752	-1.885507
48	9	0	-0.360409	4.557620	-1.089877
49	9	0	-0.041036	3.962154	-3.145684
50	9	0	1.616070	3.973447	-1.754052
51	16	0	0.077923	2.127117	1.410775
52	8	0	-1.226731	2.771708	1.407435
53	8	0	0.346131	1.028315	2.336929
54	6	0	1.288180	3.422011	1.936317
55	9	0	0.959064	3.847977	3.151543
56	9	0	2.512987	2.904418	1.975909
57	9	0	1.279554	4.451429	1.098669

Zero-point correction= 0.390185 (Hartree/Particle)
Thermal correction to Energy= 0.437851
Thermal correction to Enthalpy= 0.438906
Thermal correction to Gibbs Free Energy= 0.295602
Sum of electronic and zero-point Energies= -3330.600894
Sum of electronic and thermal Energies= -3330.553229
Sum of electronic and thermal Enthalpies= -3330.552174
Sum of electronic and thermal Free Energies(333K)= -3330.695478
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.979183

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.296156	-1.114969	0.063324
2	8	0	-2.742981	0.202088	-0.000696
3	1	0	-1.946013	0.743791	0.239577
4	6	0	-1.975674	-1.662138	-1.255107
5	1	0	-2.829418	-2.183451	-1.704458
6	1	0	-1.729796	-0.787384	-1.859179
7	6	0	-0.750396	-2.600105	-1.197550
8	1	0	-1.045715	-3.613936	-0.908320
9	1	0	-0.277513	-2.645921	-2.182194
10	6	0	0.155129	-2.064652	-0.152038
11	16	0	-3.376447	-2.019199	1.041178
12	8	0	-3.317640	-1.428338	2.363956
13	8	0	-2.998592	-3.405745	0.788145
14	6	0	-4.986109	-1.736050	0.351998
15	6	0	-5.538125	-2.706035	-0.482815
16	6	0	-5.658929	-0.551620	0.649559
17	6	0	-6.794631	-2.478922	-1.036011
18	1	0	-4.994230	-3.626916	-0.668184
19	6	0	-6.911683	-0.338004	0.085575
20	1	0	-5.203423	0.176983	1.310614
21	6	0	-7.475913	-1.296689	-0.754968
22	1	0	-7.243455	-3.228200	-1.681739
23	1	0	-7.450613	0.578949	0.305382
24	1	0	-8.456578	-1.122650	-1.189361
25	6	0	-0.086484	-1.390029	0.877639
26	6	0	4.191470	-1.246482	-0.218177
27	6	0	6.431487	-1.333355	-0.130222
28	6	0	6.082301	-0.140188	-0.675724
29	1	0	7.399457	-1.759241	0.084461
30	1	0	6.688634	0.680604	-1.026456
31	7	0	5.257284	-1.997290	0.141596
32	7	0	4.710401	-0.108186	-0.723659
33	79	0	2.218728	-1.665100	-0.060070
34	1	0	-0.109583	-0.784795	1.772614
35	6	0	3.915623	1.016483	-1.209332
36	1	0	4.592547	1.762039	-1.628856
37	1	0	3.228923	0.678827	-1.987141
38	1	0	3.341127	1.456604	-0.392142
39	6	0	5.187554	-3.315267	0.741311
40	1	0	5.667937	-3.305192	1.723398
41	1	0	4.137786	-3.586882	0.857384
42	1	0	5.682660	-4.047857	0.097919
43	7	0	-0.409461	1.751623	0.131007
44	16	0	0.477941	1.992912	1.453697

45	8	0	-0.130148	1.194853	2.515773
46	8	0	1.922124	1.915219	1.252051
47	6	0	0.143142	3.747902	1.928374
48	9	0	0.570198	4.565268	0.973833
49	9	0	0.783437	4.022404	3.059180
50	9	0	-1.158793	3.928011	2.108431
51	16	0	0.099298	2.059141	-1.378111
52	8	0	1.329317	2.834578	-1.485317
53	8	0	-0.052740	0.858720	-2.199137
54	6	0	-1.254778	3.184386	-1.937808
55	9	0	-1.034433	3.515120	-3.205996
56	9	0	-2.429824	2.573009	-1.844787
57	9	0	-1.274805	4.285881	-1.197140

Zero-point correction= 0.388921 (Hartree/Particle)
Thermal correction to Energy= 0.436870
Thermal correction to Enthalpy= 0.437925
Thermal correction to Gibbs Free Energy= 0.294340
Sum of electronic and zero-point Energies= -3330.586579
Sum of electronic and thermal Energies= -3330.538630
Sum of electronic and thermal Enthalpies= -3330.537575
Sum of electronic and thermal Free Energies(333K)= -3330.681160
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.977321

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.950193	-1.326954	-0.078818
2	8	0	-2.622145	-0.133024	0.156513
3	1	0	-1.907992	0.598104	0.160272
4	6	0	-1.834298	-1.652877	-1.543338
5	1	0	-2.633224	-2.339378	-1.826704
6	1	0	-1.960872	-0.693434	-2.044427
7	6	0	-0.412412	-2.184546	-1.713347
8	1	0	-0.390866	-3.275237	-1.819725
9	1	0	0.057343	-1.749285	-2.600113
10	6	0	0.307114	-1.778679	-0.449482
11	16	0	-2.991930	-2.591248	0.863794
12	8	0	-2.752514	-2.273063	2.254662
13	8	0	-2.607754	-3.854903	0.258723
14	6	0	-4.645054	-2.177429	0.409963
15	6	0	-5.270428	-2.930079	-0.583488
16	6	0	-5.292870	-1.141427	1.082969
17	6	0	-6.585053	-2.623360	-0.917496
18	1	0	-4.741430	-3.749782	-1.059102
19	6	0	-6.605401	-0.850010	0.733316
20	1	0	-4.772326	-0.583736	1.853428
21	6	0	-7.246043	-1.585337	-0.263647
22	1	0	-7.094441	-3.200191	-1.683497
23	1	0	-7.129609	-0.046109	1.240936
24	1	0	-8.272783	-1.350060	-0.529413
25	6	0	-0.587194	-1.356428	0.451759
26	6	0	4.292632	-1.149656	-0.014933
27	6	0	6.509914	-1.221380	0.362338
28	6	0	6.186092	0.055970	0.039856
29	1	0	7.457836	-1.671082	0.614756
30	1	0	6.798711	0.940373	-0.044215
31	7	0	5.336241	-1.942146	0.321899
32	7	0	4.829873	0.078465	-0.186352
33	79	0	2.306029	-1.586055	-0.217120
34	1	0	-0.490391	-0.990302	1.465222
35	6	0	4.061324	1.263656	-0.551389
36	1	0	4.743153	2.114531	-0.600282
37	1	0	3.590964	1.121949	-1.526059
38	1	0	3.283173	1.459714	0.188552
39	6	0	5.235165	-3.356795	0.615878
40	1	0	5.554626	-3.552598	1.643477
41	1	0	4.192567	-3.655682	0.499865
42	1	0	5.857213	-3.931927	-0.076054
43	7	0	-0.780837	1.829817	0.083006
44	16	0	0.000125	2.055873	1.489441
45	8	0	-0.768722	1.326780	2.487982
46	8	0	1.446387	1.895793	1.422877
47	6	0	-0.259513	3.843879	1.888815
48	9	0	0.451121	4.606156	1.066629
49	9	0	0.137205	4.062965	3.137866
50	9	0	-1.544285	4.160850	1.778859
51	16	0	-0.177244	2.166263	-1.384661
52	8	0	1.158202	2.744951	-1.400639
53	8	0	-0.501175	1.057314	-2.278946
54	6	0	-1.318865	3.513542	-1.929871
55	9	0	-0.987898	3.881723	-3.163270
56	9	0	-2.573529	3.075172	-1.929778
57	9	0	-1.225683	4.564127	-1.123256

Zero-point correction= 0.392004 (Hartree/Particle)
Thermal correction to Energy= 0.431228
Thermal correction to Enthalpy= 0.432172
Thermal correction to Gibbs Free Energy= 0.312696
Sum of electronic and zero-point Energies= -3330.629075

Sum of electronic and thermal Energies= -3330.589851
Sum of electronic and thermal Enthalpies= -3330.588907
Sum of electronic and thermal Free Energies(333K)= -3330.722820
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3333.009786

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.613825	0.139014	-1.442464
2	8	0	2.802872	0.225895	-0.287986
3	1	0	-0.287318	1.080759	-0.183055
4	6	0	2.681563	-0.120626	-2.555333
5	1	0	2.339643	0.856630	-2.910772
6	1	0	3.214889	-0.625057	-3.363416
7	6	0	1.549650	-0.916678	-1.915264
8	1	0	0.577421	-0.730103	-2.375686
9	1	0	1.755607	-1.992297	-1.936200
10	6	0	1.587534	-0.420057	-0.498083
11	16	0	4.731744	-1.173343	-1.200842
12	8	0	5.472724	-1.235050	-2.456316
13	8	0	4.067634	-2.357009	-0.660533
14	6	0	5.757029	-0.478231	0.065942
15	6	0	6.796050	0.372548	-0.302679
16	6	0	5.509200	-0.809082	1.394660
17	6	0	7.604668	0.908299	0.693401
18	1	0	6.964508	0.596353	-1.351120
19	6	0	6.325822	-0.264226	2.380609
20	1	0	4.695473	-1.484182	1.637588
21	6	0	7.367772	0.591734	2.030322
22	1	0	8.421665	1.572147	0.426077
23	1	0	6.148215	-0.509433	3.423687
24	1	0	8.002468	1.013887	2.804716
25	6	0	0.670953	-0.464889	0.482519
26	1	0	1.010295	-0.027491	1.425372
27	6	0	-2.794802	-2.621451	0.375694
28	6	0	-4.738702	-3.540526	-0.301605
29	6	0	-4.486790	-3.998566	0.948256
30	1	0	-5.558364	-3.737121	-0.975791
31	1	0	-5.042425	-4.674247	1.580466
32	7	0	-3.695381	-2.703399	-0.633068
33	7	0	-3.296536	-3.426843	1.342971
34	79	0	-1.059812	-1.528991	0.422325
35	6	0	-2.667926	-3.663720	2.627182
36	1	0	-2.464458	-4.730661	2.755117
37	1	0	-1.727532	-3.111666	2.654200
38	1	0	-3.316819	-3.315112	3.435823
39	6	0	-3.593305	-1.997749	-1.896667
40	1	0	-3.619656	-2.712344	-2.723863
41	1	0	-4.417714	-1.287023	-2.000219
42	1	0	-2.650501	-1.450789	-1.918961
43	7	0	-0.831045	1.979377	-0.363266
44	16	0	-0.507155	3.266522	0.664944
45	8	0	0.894120	3.223084	1.010759
46	8	0	-1.185536	4.446232	0.181939
47	6	0	-1.419729	2.702980	2.177718
48	9	0	-2.705440	2.538239	1.897737
49	9	0	-1.283770	3.636441	3.106797
50	9	0	-0.912442	1.559915	2.613882
51	16	0	-1.717490	2.001169	-1.772625
52	8	0	-1.607669	3.261850	-2.463714
53	8	0	-1.436424	0.727881	-2.411558
54	6	0	-3.468629	1.879785	-1.172084
55	9	0	-4.236604	1.629158	-2.227073
56	9	0	-3.587586	0.883173	-0.303688
57	9	0	-3.842354	3.012082	-0.606406

Zero-point correction= 0.390550 (Hartree/Particle)
Thermal correction to Energy= 0.438170
Thermal correction to Enthalpy= 0.439225
Thermal correction to Gibbs Free Energy= 0.294358
Sum of electronic and zero-point Energies= -3330.626821
Sum of electronic and thermal Energies= -3330.579201
Sum of electronic and thermal Enthalpies= -3330.578146
Sum of electronic and thermal Free Energies(333K)= -3330.723012
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.997862

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.633927	-0.479907	-1.431548
2	8	0	-2.805655	-0.481367	-0.274447
3	1	0	0.312620	-0.945217	-0.068129
4	6	0	-2.704468	-0.340066	-2.569989
5	1	0	-2.413001	-1.353325	-2.862804
6	1	0	-3.225023	0.135177	-3.403463
7	6	0	-1.530119	0.443763	-1.997400
8	1	0	-0.563048	0.185313	-2.435600

9	1	0	-1.681746	1.525436	-2.084539
10	6	0	-1.583602	0.056422	-0.551648
11	16	0	-4.713522	0.881164	-1.281883
12	8	0	-5.452257	0.865583	-2.538186
13	8	0	-3.998961	2.075309	-0.839339
14	6	0	-5.748541	0.316348	0.037844
15	6	0	-6.762340	-0.595494	-0.247852
16	6	0	-5.533833	0.806088	1.322489
17	6	0	-7.578341	-1.029897	0.790068
18	1	0	-6.905537	-0.945872	-1.264882
19	6	0	-6.359130	0.361861	2.350859
20	1	0	-4.739475	1.523584	1.499335
21	6	0	-7.375088	-0.553311	2.084649
22	1	0	-8.374763	-1.740165	0.588563
23	1	0	-6.208039	0.731328	3.360850
24	1	0	-8.015852	-0.897453	2.891808
25	6	0	-0.613272	0.080646	0.399585
26	1	0	-0.957210	-0.286488	1.370171
27	6	0	2.396861	2.868622	0.364568
28	6	0	4.213104	4.061697	-0.222939
29	6	0	3.755396	4.568860	0.947106
30	1	0	5.053674	4.346547	-0.837113
31	1	0	4.116351	5.383990	1.555529
32	7	0	3.370162	3.026614	-0.563005
33	7	0	2.644712	3.827825	1.288106
34	79	0	0.905295	1.481428	0.365013
35	6	0	1.855979	4.048846	2.483768
36	1	0	1.505175	5.084109	2.514131
37	1	0	0.996946	3.377252	2.456071
38	1	0	2.452557	3.837481	3.375895
39	6	0	3.532148	2.208508	-1.751906
40	1	0	3.587954	2.851836	-2.634068
41	1	0	4.443425	1.609498	-1.676149
42	1	0	2.677730	1.537421	-1.844028
43	7	0	1.063209	-1.929053	-0.308012
44	16	0	0.830886	-3.276122	0.631989
45	8	0	-0.578841	-3.352846	0.956819
46	8	0	1.589741	-4.413569	0.155974
47	6	0	1.656096	-2.716166	2.192168
48	9	0	2.947023	-2.492247	1.978005
49	9	0	1.521067	-3.669337	3.103494
50	9	0	1.089306	-1.599179	2.635896
51	16	0	1.981534	-1.855273	-1.663826
52	8	0	1.986255	-3.072904	-2.443726
53	8	0	1.656512	-0.571150	-2.276313
54	6	0	3.710616	-1.635554	-1.034242
55	9	0	4.481526	-1.280199	-2.059386
56	9	0	3.746715	-0.668732	-0.120115
57	9	0	4.165961	-2.757801	-0.507436

Zero-point correction= 0.386374 (Hartree/Particle)
Thermal correction to Energy= 0.433301
Thermal correction to Enthalpy= 0.434356
Thermal correction to Gibbs Free Energy= 0.291846
Sum of electronic and zero-point Energies= -3330.626684
Sum of electronic and thermal Energies= -3330.579757
Sum of electronic and thermal Enthalpies= -3330.578702
Sum of electronic and thermal Free Energies(333K)= -3330.721213
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.993077

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.422591	-2.051349	0.361974
2	8	0	2.829903	-1.568914	-0.844440
3	1	0	-0.254279	-1.666207	-1.930478
4	6	0	2.367321	-2.850035	1.020671
5	1	0	2.508858	-3.884776	0.695810
6	1	0	2.497907	-2.797307	2.103016
7	6	0	1.056539	-2.261667	0.509222
8	1	0	0.268550	-2.996237	0.323359
9	1	0	0.641870	-1.497544	1.177123
10	6	0	1.490281	-1.629098	-0.774927
11	16	0	3.931498	-0.653979	1.271677
12	8	0	4.380377	-1.219838	2.534090
13	8	0	2.907249	0.384418	1.216816
14	6	0	5.317856	-0.131499	0.306607
15	6	0	6.557017	-0.723975	0.539828
16	6	0	5.138997	0.863958	-0.650588
17	6	0	7.645663	-0.306091	-0.216947
18	1	0	6.658795	-1.485831	1.305990
19	6	0	6.238293	1.268877	-1.400842
20	1	0	4.159453	1.309413	-0.792406
21	6	0	7.484683	0.684517	-1.184835
22	1	0	8.621513	-0.751770	-0.048847
23	1	0	6.121345	2.043892	-2.152474
24	1	0	8.339663	1.006561	-1.772720
25	6	0	0.736755	-1.217427	-1.852824
26	1	0	1.268053	-0.977122	-2.771502
27	6	0	-0.628092	2.446656	-0.307532

28	6	0	-1.152611	4.218901	0.957075
29	6	0	-1.990766	4.217310	-0.108721
30	1	0	-1.072351	4.895402	1.793749
31	1	0	-2.786567	4.890868	-0.386448
32	7	0	-0.322183	3.131717	0.812516
33	7	0	-1.647720	3.127606	-0.875757
34	79	0	0.127833	0.685565	-0.938725
35	6	0	-2.371441	2.690943	-2.055049
36	1	0	-2.852019	3.555659	-2.517407
37	1	0	-1.669753	2.246069	-2.762260
38	1	0	-3.123941	1.948359	-1.780401
39	6	0	0.661213	2.716078	1.800056
40	1	0	1.020331	3.600763	2.330194
41	1	0	0.201798	2.007856	2.492625
42	1	0	1.494503	2.224854	1.298961
43	7	0	-2.051524	-1.097829	0.349602
44	16	0	-2.837634	-2.264778	-0.429866
45	8	0	-1.854953	-3.096747	-1.130697
46	8	0	-3.953289	-2.892333	0.258220
47	6	0	-3.598596	-1.271739	-1.792514
48	9	0	-4.366786	-0.297363	-1.301777
49	9	0	-4.342563	-2.060945	-2.555809
50	9	0	-2.653225	-0.709564	-2.556467
51	16	0	-2.265630	-0.707485	1.890882
52	8	0	-2.683234	-1.788416	2.768263
53	8	0	-1.117326	0.118953	2.268390
54	6	0	-3.679277	0.484824	1.873261
55	9	0	-3.847686	0.994034	3.089707
56	9	0	-3.426568	1.491412	1.027177
57	9	0	-4.798203	-0.115783	1.492187

Zero-point correction= 0.391394 (Hartree/Particle)
Thermal correction to Energy= 0.439124
Thermal correction to Enthalpy= 0.440179
Thermal correction to Gibbs Free Energy= 0.296311
Sum of electronic and zero-point Energies= -3330.656358
Sum of electronic and thermal Energies= -3330.608628
Sum of electronic and thermal Enthalpies= -3330.607573
Sum of electronic and thermal Free Energies(333K)= -3330.751441
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3333.031667

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.684615	-2.333055	0.919127
2	8	0	-1.425699	-1.326272	-0.993748
3	1	0	-1.542519	-0.339971	-0.693150
4	6	0	-0.460253	-3.005112	0.839977
5	1	0	0.263420	-2.496402	1.478923
6	1	0	-0.536830	-4.075746	1.076292
7	6	0	0.100689	-2.987282	-0.682940
8	1	0	1.146937	-3.293876	-0.702514
9	1	0	-0.544067	-3.682367	-1.227111
10	6	0	-0.120219	-1.597173	-1.067844
11	16	0	-3.034999	-3.286993	0.573728
12	8	0	-3.259880	-3.987146	1.840252
13	8	0	-2.878155	-4.074484	-0.648800
14	6	0	-4.252780	-2.035605	0.327609
15	6	0	-4.412158	-1.039525	1.291882
16	6	0	-5.053315	-2.102082	-0.808516
17	6	0	-5.400891	-0.083174	1.099050
18	1	0	-3.758908	-0.996676	2.157351
19	6	0	-6.048445	-1.144751	-0.977197
20	1	0	-4.884550	-2.884681	-1.540860
21	6	0	-6.218233	-0.139809	-0.029083
22	1	0	-5.517443	0.718662	1.821404
23	1	0	-6.680444	-1.175639	-1.859739
24	1	0	-6.982747	0.617459	-0.177032
25	6	0	0.836834	-0.623985	-1.255935
26	1	0	0.410212	0.336464	-1.552121
27	6	0	4.614615	-0.397098	0.101322
28	6	0	6.805212	-0.405512	0.610064
29	6	0	6.157580	0.265609	1.594438
30	1	0	7.851180	-0.637625	0.480340
31	1	0	6.529723	0.739658	2.489745
32	7	0	5.842151	-0.802208	-0.292470
33	7	0	4.820374	0.256644	1.267621
34	79	0	2.768795	-0.629367	-0.762152
35	6	0	3.778612	0.916622	2.041881
36	1	0	2.832162	0.389118	1.912036
37	1	0	4.057495	0.899795	3.097477
38	1	0	3.654186	1.950909	1.711763
39	6	0	6.113728	-1.557028	-1.499979
40	1	0	6.791016	-0.996089	-2.149796
41	1	0	6.562822	-2.521962	-1.248853
42	1	0	5.169657	-1.722152	-2.020742
43	7	0	-1.440670	1.122226	-0.026182
44	16	0	-2.630562	2.091051	-0.596021
45	8	0	-3.479332	1.277438	-1.450887
46	8	0	-3.187369	3.013362	0.377943

47	6	0	-1.664783	3.125221	-1.788112
48	9	0	-0.799450	3.907079	-1.150902
49	9	0	-2.506738	3.883111	-2.479075
50	9	0	-0.993288	2.342993	-2.633843
51	16	0	-0.851056	1.155335	1.487220
52	8	0	-1.840966	1.333028	2.534072
53	8	0	0.118474	0.060885	1.564639
54	6	0	0.237591	2.654071	1.564340
55	9	0	0.961768	2.583409	2.684230
56	9	0	1.077817	2.665178	0.527358
57	9	0	-0.463466	3.773870	1.573069

Zero-point correction= 0.388210 (Hartree/Particle)
Thermal correction to Energy= 0.427228
Thermal correction to Enthalpy= 0.428173
Thermal correction to Gibbs Free Energy= 0.310050
Sum of electronic and zero-point Energies= -3330.574112
Sum of electronic and thermal Energies= -3330.535094
Sum of electronic and thermal Enthalpies= -3330.534150
Sum of electronic and thermal Free Energies(333K)= -3330.666536
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.966099

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.264926	3.136706	0.382961
2	8	0	-0.518369	1.273138	-0.429340
3	1	0	-1.216782	0.582899	-0.485539
4	6	0	-0.452741	2.719116	1.780137
5	1	0	-0.504927	3.626867	2.392025
6	1	0	-1.369539	2.137530	1.876114
7	6	0	0.798747	1.872269	2.008516
8	1	0	1.391113	2.204467	2.872877
9	1	0	0.542164	0.822335	2.186085
10	6	0	1.614882	2.004041	0.763867
11	16	0	-1.420567	4.217158	-0.451057
12	8	0	-0.801061	4.444827	-1.739815
13	8	0	-1.638639	5.284428	0.510136
14	6	0	-2.866278	3.224636	-0.586337
15	6	0	-3.911597	3.468596	0.303513
16	6	0	-2.929526	2.235977	-1.570108
17	6	0	-5.053686	2.680512	0.208247
18	1	0	-3.825839	4.257106	1.043927
19	6	0	-4.069560	1.445474	-1.631785
20	1	0	-2.089392	2.058683	-2.231211
21	6	0	-5.124222	1.668533	-0.746575
22	1	0	-5.880826	2.848754	0.891027
23	1	0	-4.113551	0.633954	-2.350314
24	1	0	-6.007019	1.037658	-0.796671
25	6	0	0.987078	2.975166	-0.041879
26	6	0	4.182649	-0.837383	-0.487609
27	6	0	4.737474	-2.840851	-1.324065
28	6	0	5.889707	-2.153582	-1.121702
29	1	0	4.564489	-3.833720	-1.709832
30	1	0	6.919680	-2.429174	-1.288280
31	7	0	3.707147	-2.021698	-0.928386
32	7	0	5.526589	-0.927392	-0.609956
33	79	0	3.013085	0.701244	0.180671
34	1	0	1.269251	3.336099	-1.021283
35	6	0	6.464539	0.113515	-0.242110
36	1	0	5.899117	0.976823	0.110892
37	1	0	7.124606	-0.236786	0.556582
38	1	0	7.063368	0.404035	-1.109865
39	6	0	2.290892	-2.369423	-1.024145
40	1	0	2.198545	-3.452462	-1.109778
41	1	0	1.753480	-2.043668	-0.132255
42	1	0	1.844458	-1.902556	-1.904639
43	7	0	-2.044826	-1.220683	0.097074
44	16	0	-1.728670	-2.055596	-1.244380
45	8	0	-1.686066	-1.129475	-2.372807
46	8	0	-0.711021	-3.097965	-1.136942
47	6	0	-3.330305	-2.950978	-1.460212
48	9	0	-3.596814	-3.705558	-0.399727
49	9	0	-3.250210	-3.728568	-2.535877
50	9	0	-4.326319	-2.082774	-1.632283
51	16	0	-1.284949	-1.370437	1.499950
52	8	0	0.150623	-1.645443	1.417597
53	8	0	-1.725473	-0.264532	2.347351
54	6	0	-1.997519	-2.873058	2.310195
55	9	0	-1.512238	-2.962978	3.545982
56	9	0	-3.321065	-2.781662	2.371726
57	9	0	-1.666707	-3.968329	1.636392

Zero-point correction= 0.388704 (Hartree/Particle)
Thermal correction to Energy= 0.428274
Thermal correction to Enthalpy= 0.429218
Thermal correction to Gibbs Free Energy= 0.309097
Sum of electronic and zero-point Energies= -3330.552397
Sum of electronic and thermal Energies= -3330.512828
Sum of electronic and thermal Enthalpies= -3330.511883

Sum of electronic and thermal Free Energies(333K)= -3330.646587
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.950096

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.737631	0.020545	0.405810
2	8	0	-3.746837	-0.757318	1.066178
3	1	0	-4.597606	-0.723505	4.291480
4	6	0	-2.586357	1.240379	1.245809
5	1	0	-1.623105	1.708717	1.033028
6	1	0	-3.419186	1.920009	1.030112
7	6	0	-2.716437	0.648751	2.636534
8	1	0	-3.030639	1.387278	3.376916
9	6	0	-3.751456	-0.409444	2.408946
10	6	0	-4.597167	-1.000507	3.244308
11	1	0	-5.291947	-1.760249	2.905356
12	6	0	0.434743	-2.578704	-0.102260
13	6	0	1.862643	-3.988255	-1.090843
14	6	0	2.214008	-3.893551	0.215422
15	1	0	2.302536	-4.542184	-1.905355
16	1	0	3.013984	-4.359032	0.769569
17	7	0	0.761718	-3.182700	-1.263350
18	7	0	1.325601	-3.025506	0.804609
19	79	0	-1.054427	-1.288353	0.165783
20	6	0	1.340971	-2.655100	2.209436
21	1	0	0.636444	-3.276051	2.770605
22	1	0	2.350070	-2.808051	2.596287
23	1	0	1.082594	-1.599031	2.309809
24	6	0	0.139160	-2.915728	-2.547359
25	1	0	-0.896377	-2.610595	-2.386666
26	1	0	0.682550	-2.113612	-3.052097
27	1	0	0.156095	-3.827803	-3.148214
28	1	0	-1.755903	0.221850	2.951335
29	16	0	-3.521124	0.388852	-1.214742
30	8	0	-4.848393	0.889897	-0.907584
31	8	0	-3.304494	-0.821039	-1.987234
32	6	0	-2.499549	1.705543	-1.783731
33	6	0	-1.198529	1.443854	-2.214531
34	6	0	-3.038291	2.994098	-1.778893
35	6	0	-0.408558	2.512812	-2.623408
36	1	0	-0.790617	0.437951	-2.217474
37	6	0	-2.241051	4.044894	-2.214379
38	1	0	-4.060410	3.153471	-1.451261
39	6	0	-0.930246	3.804091	-2.624446
40	1	0	0.621789	2.332105	-2.909892
41	1	0	-2.641700	5.054178	-2.225067
42	1	0	-0.304483	4.633296	-2.941601
43	7	0	2.176882	0.319266	0.494035
44	16	0	2.530226	0.602315	-1.052644
45	8	0	1.733404	-0.236059	-1.955780
46	8	0	2.729669	1.998590	-1.426867
47	6	0	4.206562	-0.169211	-1.068096
48	9	0	5.017864	0.457814	-0.227761
49	9	0	4.697515	-0.074142	-2.300562
50	9	0	4.140150	-1.456719	-0.732896
51	16	0	1.320054	1.320756	1.388882
52	8	0	0.439157	2.229275	0.651846
53	8	0	0.737872	0.561297	2.500846
54	6	0	2.570837	2.409962	2.206869
55	9	0	1.940953	3.275830	2.996666
56	9	0	3.395491	1.673565	2.944538
57	9	0	3.272742	3.074620	1.300799

Zero-point correction= 0.391752 (Hartree/Particle)
Thermal correction to Energy= 0.439359
Thermal correction to Enthalpy= 0.440414
Thermal correction to Gibbs Free Energy= 0.298741
Sum of electronic and zero-point Energies= -3330.653330
Sum of electronic and thermal Energies= -3330.605723
Sum of electronic and thermal Enthalpies= -3330.604668
Sum of electronic and thermal Free Energies(333K)= -3330.746341
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3333.028505

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.401222	-0.103775	0.372439
2	8	0	-3.974931	-1.686067	1.268837
3	1	0	-6.011220	0.769235	2.047208
4	6	0	-2.553143	0.788299	1.479010
5	1	0	-1.559574	1.027054	1.873197
6	1	0	-3.059119	1.715041	1.191420
7	6	0	-3.370790	0.097763	2.649580
8	1	0	-3.763222	0.865005	3.321840
9	6	0	-4.382170	-0.685530	1.901703
10	6	0	-5.639920	-0.140563	1.582918

11	1	0	-6.303107	-0.706420	0.938517
12	6	0	0.698080	-2.662021	-0.098082
13	6	0	2.250016	-3.935323	-1.089556
14	6	0	2.598105	-3.801472	0.215158
15	1	0	2.735825	-4.451169	-1.903051
16	1	0	3.440336	-4.189657	0.766301
17	7	0	1.078082	-3.237879	-1.258879
18	7	0	1.635161	-3.018631	0.805171
19	79	0	-0.857787	-1.452501	0.162670
20	6	0	1.626377	-2.633788	2.205938
21	1	0	0.941891	-3.276039	2.767893
22	1	0	2.637542	-2.749130	2.600930
23	1	0	1.326388	-1.587732	2.304172
24	6	0	0.429727	-3.023063	-2.540243
25	1	0	-0.630250	-2.824303	-2.373730
26	1	0	0.884741	-2.162131	-3.035475
27	1	0	0.539636	-3.922216	-3.150739
28	1	0	-2.691251	-0.567685	3.185844
29	16	0	-3.324987	0.268545	-0.987818
30	8	0	-4.694898	0.614932	-0.537853
31	8	0	-3.130072	-0.805277	-1.946752
32	6	0	-2.595824	1.752887	-1.600299
33	6	0	-1.290879	1.701365	-2.098189
34	6	0	-3.312659	2.948346	-1.527168
35	6	0	-0.690149	2.882351	-2.515029
36	1	0	-0.739230	0.766328	-2.136758
37	6	0	-2.706746	4.115667	-1.976123
38	1	0	-4.325815	2.945926	-1.138956
39	6	0	-1.398664	4.081462	-2.458587
40	1	0	0.341198	2.862551	-2.851114
41	1	0	-3.250996	5.054875	-1.938011
42	1	0	-0.921347	5.001692	-2.783564
43	7	0	2.064230	0.432378	0.444461
44	16	0	2.396309	0.774702	-1.092115
45	8	0	1.689287	-0.133287	-2.000912
46	8	0	2.453082	2.188513	-1.449638
47	6	0	4.143385	0.180385	-1.121597
48	9	0	4.883764	0.864771	-0.258850
49	9	0	4.630163	0.355705	-2.347110
50	9	0	4.208784	-1.115504	-0.818211
51	16	0	1.250983	1.401229	1.415704
52	8	0	0.353099	2.354138	0.769665
53	8	0	0.705647	0.584307	2.507272
54	6	0	2.555573	2.422357	2.236892
55	9	0	1.979344	3.269415	3.086451
56	9	0	3.389349	1.636534	2.912432
57	9	0	3.243096	3.109887	1.334796

Zero-point correction= 0.388343 (Hartree/Particle)
Thermal correction to Energy= 0.427951
Thermal correction to Enthalpy= 0.428895
Thermal correction to Gibbs Free Energy= 0.309103
Sum of electronic and zero-point Energies= -3330.599218
Sum of electronic and thermal Energies= -3330.559611
Sum of electronic and thermal Enthalpies= -3330.558667
Sum of electronic and thermal Free Energies(333K)= -3330.693118
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.988091

INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.340164	0.170348	0.443152
2	8	0	5.781896	-0.043755	3.104453
3	1	0	6.365435	-0.268664	0.725873
4	6	0	2.411220	-0.593027	1.704843
5	1	0	1.420893	-0.536374	2.158484
6	1	0	2.600183	-1.655932	1.518001
7	6	0	3.440851	0.000173	2.660594
8	1	0	3.361574	-0.473316	3.645053
9	6	0	4.903297	-0.042935	2.270998
10	6	0	5.319226	0.028184	0.803665
11	1	0	5.211456	1.053612	0.426293
12	6	0	-0.700355	2.769715	-0.381983
13	6	0	-2.218925	3.953867	-1.521724
14	6	0	-2.547431	4.018651	-0.207547
15	1	0	-2.698025	4.370271	-2.393863
16	1	0	-3.362397	4.514740	0.295795
17	7	0	-1.075976	3.193980	-1.606089
18	7	0	-1.602293	3.288688	0.474715
19	79	0	0.805994	1.543161	0.029448
20	6	0	-1.584488	3.089759	1.914283
21	1	0	-0.769261	3.665022	2.362091
22	1	0	-2.535834	3.436856	2.321434
23	1	0	-1.464084	2.027215	2.139273
24	6	0	-0.457837	2.773534	-2.850567
25	1	0	0.620827	2.691812	-2.704950
26	1	0	-0.865580	1.803371	-3.143274
27	1	0	-0.662164	3.523703	-3.617535
28	1	0	3.197488	1.063830	2.806517
29	16	0	3.265322	-0.272051	-0.736067

30	8	0	4.590481	-0.891011	-0.038544
31	8	0	3.587668	0.791004	-1.672873
32	6	0	2.727179	-1.719493	-1.588090
33	6	0	1.444860	-2.199500	-1.339897
34	6	0	3.569507	-2.281765	-2.551469
35	6	0	0.990876	-3.284584	-2.087640
36	1	0	0.802441	-1.761814	-0.581249
37	6	0	3.103205	-3.371128	-3.272909
38	1	0	4.559672	-1.874656	-2.729563
39	6	0	1.816650	-3.866273	-3.043598
40	1	0	-0.018390	-3.643379	-1.914487
41	1	0	3.740074	-3.830283	-4.023235
42	1	0	1.456996	-4.711547	-3.623756
43	7	0	-2.252349	-0.255366	0.472786
44	16	0	-2.477488	-0.814204	-1.021093
45	8	0	-2.085853	0.206637	-1.991124
46	8	0	-2.076187	-2.197987	-1.259494
47	6	0	-4.323583	-0.808648	-1.092112
48	9	0	-4.831051	-1.596230	-0.149986
49	9	0	-4.709075	-1.254975	-2.284314
50	9	0	-4.789583	0.424812	-0.922553
51	16	0	-1.490109	-1.043905	1.630658
52	8	0	-0.440793	-1.966535	1.192514
53	8	0	-1.146230	-0.075075	2.673795
54	6	0	-2.760763	-2.132030	2.418960
55	9	0	-2.230100	-2.714931	3.490369
56	9	0	-3.811951	-1.411632	2.795071
57	9	0	-3.156469	-3.069087	1.566316

Zero-point correction= 0.393033 (Hartree/Particle)
Thermal correction to Energy= 0.440639
Thermal correction to Enthalpy= 0.441694
Thermal correction to Gibbs Free Energy= 0.298492
Sum of electronic and zero-point Energies= -3330.694456
Sum of electronic and thermal Energies= -3330.646850
Sum of electronic and thermal Enthalpies= -3330.645795
Sum of electronic and thermal Free Energies(333K)= -3330.788996
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3333.073854

TS13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.211975	0.840914	-0.738542
2	8	0	3.855124	-0.859403	0.113626
3	1	0	6.137401	-1.541280	-2.126397
4	6	0	3.105894	1.080363	-1.825408
5	1	0	2.747005	0.518771	-2.691756
6	1	0	3.109275	2.149310	-2.081261
7	6	0	4.596864	0.701064	-1.511523
8	1	0	5.195902	0.767144	-2.423365
9	1	0	4.965651	1.413033	-0.769684
10	6	0	4.561254	-0.666603	-0.927624
11	16	0	2.290375	1.934788	0.582128
12	8	0	3.607125	2.555955	0.630250
13	8	0	1.749930	1.181321	1.706949
14	6	0	1.116373	3.148350	0.065605
15	6	0	1.409881	4.498155	0.266687
16	6	0	-0.084030	2.730644	-0.516237
17	6	0	0.475511	5.448664	-0.128156
18	1	0	2.336957	4.784591	0.753282
19	6	0	-1.005131	3.693435	-0.906251
20	1	0	-0.292114	1.672209	-0.638676
21	6	0	-0.723925	5.047362	-0.716306
22	1	0	0.678364	6.503017	0.032681
23	1	0	-1.947364	3.390135	-1.352173
24	1	0	-1.449230	5.795377	-1.022932
25	6	0	5.344633	-1.715037	-1.404785
26	1	0	5.291578	-2.681908	-0.913502
27	6	0	0.404797	-2.631636	0.357589
28	6	0	-0.396138	-4.247680	1.686918
29	6	0	-0.763577	-4.543310	0.416173
30	1	0	-0.583876	-4.764450	2.615770
31	1	0	-1.335580	-5.367597	0.018220
32	7	0	0.317886	-3.071742	1.631568
33	7	0	-0.264738	-3.539212	-0.384468
34	79	0	1.355236	-0.963876	-0.217209
35	6	0	-0.449677	-3.484365	-1.823202
36	1	0	-0.041841	-2.542573	-2.191813
37	1	0	0.070352	-4.318309	-2.302096
38	1	0	-1.515023	-3.531937	-2.061760
39	6	0	0.908165	-2.424192	2.794274
40	1	0	1.213478	-1.410164	2.530941
41	1	0	0.166914	-2.376006	3.594952
42	1	0	1.780532	-2.988030	3.134771
43	7	0	-2.451615	-0.884284	0.213935
44	16	0	-1.410666	-0.224189	1.232695
45	8	0	-1.352332	-1.070751	2.419329
46	8	0	-0.168050	0.266140	0.645543
47	6	0	-2.256040	1.304974	1.851602
48	9	0	-2.396915	2.215111	0.891202

49	9	0	-1.532235	1.847734	2.837418
50	9	0	-3.464561	1.016334	2.337951
51	16	0	-2.659773	-0.442043	-1.313984
52	8	0	-1.994788	0.784803	-1.746617
53	8	0	-2.629211	-1.607049	-2.193429
54	6	0	-4.453203	0.009594	-1.252981
55	9	0	-4.854251	0.396428	-2.469242
56	9	0	-5.207762	-1.021655	-0.877316
57	9	0	-4.666261	1.018428	-0.406685

Zero-point correction= 0.388336 (Hartree/Particle)
Thermal correction to Energy= 0.427858
Thermal correction to Enthalpy= 0.428802
Thermal correction to Gibbs Free Energy= 0.310339
Sum of electronic and zero-point Energies= -3330.597265
Sum of electronic and thermal Energies= -3330.557744
Sum of electronic and thermal Enthalpies= -3330.556800
Sum of electronic and thermal Free Energies(333K)= -3330.68963
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3332.989056

INT15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.067791	0.521540	0.406250
2	8	0	-3.129158	-1.895116	0.766963
3	1	0	-3.948414	-2.291434	3.926197
4	6	0	-2.435683	0.765095	1.780900
5	1	0	-1.536151	0.585096	2.379002
6	1	0	-2.709565	1.829557	1.889727
7	6	0	-3.639644	-0.081543	2.292233
8	1	0	-3.760159	0.087695	3.373248
9	1	0	-4.542740	0.251277	1.771715
10	6	0	-3.383659	-1.522640	1.981139
11	16	0	-3.175854	1.037334	-0.762231
12	8	0	-4.529113	1.239918	-0.239549
13	8	0	-2.959202	0.172071	-1.920340
14	6	0	-2.443139	2.628979	-1.021406
15	6	0	-3.190985	3.778097	-0.777271
16	6	0	-1.095231	2.681805	-1.385393
17	6	0	-2.576153	5.012779	-0.927099
18	1	0	-4.231335	3.689389	-0.479796
19	6	0	-0.493130	3.920875	-1.516250
20	1	0	-0.514240	1.777956	-1.531714
21	6	0	-1.227564	5.084583	-1.289644
22	1	0	-3.138622	5.924043	-0.752891
23	1	0	0.564324	3.972454	-1.773307
24	1	0	-0.749067	6.053436	-1.387690
25	6	0	-3.536791	-2.511302	2.944699
26	1	0	-3.374624	-3.547110	2.663362
27	6	0	0.187917	-2.643851	-0.826791
28	6	0	1.368171	-3.903207	-2.248322
29	6	0	1.759171	-4.225949	-0.990341
30	1	0	1.707182	-4.257007	-3.207137
31	1	0	2.502061	-4.922214	-0.638024
32	7	0	0.394363	-2.939765	-2.124613
33	7	0	1.026199	-3.436431	-0.135513
34	79	0	-1.066900	-1.207601	-0.144922
35	6	0	1.167594	-3.441851	1.309082
36	1	0	2.211128	-3.648431	1.557869
37	1	0	0.918372	-2.454848	1.701322
38	1	0	0.527057	-4.204275	1.760048
39	6	0	-0.174694	-2.198186	-3.237651
40	1	0	-0.191710	-2.843278	-4.122056
41	1	0	-1.199689	-1.900674	-2.996079
42	1	0	0.422027	-1.302612	-3.425993
43	7	0	2.340847	-0.273803	0.544695
44	16	0	2.490553	-0.010434	-1.027542
45	8	0	3.122415	-1.183306	-1.612878
46	8	0	1.290740	0.529829	-1.676261
47	6	0	3.754255	1.336482	-1.196442
48	9	0	3.289317	2.480260	-0.702559
49	9	0	4.030528	1.505871	-2.486624
50	9	0	4.867788	1.006875	-0.554004
51	16	0	1.514569	0.636584	1.571501
52	8	0	0.940020	1.869969	1.053890
53	8	0	0.660638	-0.234710	2.399103
54	6	0	2.860659	1.156818	2.722938
55	9	0	2.334751	1.927269	3.675760
56	9	0	3.434082	0.099923	3.285197
57	9	0	3.780024	1.854667	2.064892

Zero-point correction= 0.391124 (Hartree/Particle)
Thermal correction to Energy= 0.430269
Thermal correction to Enthalpy= 0.431213
Thermal correction to Gibbs Free Energy= 0.314356
Sum of electronic and zero-point Energies= -3330.627519
Sum of electronic and thermal Energies= -3330.588375
Sum of electronic and thermal Enthalpies= -3330.587431
Sum of electronic and thermal Free Energies(333K)= -3330.718467
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3333.017032

TS14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.467506	-0.341132	0.323007
2	8	0	-5.202836	-0.660098	3.059358
3	1	0	-5.480728	-1.448961	0.490726
4	6	0	-2.422545	0.701412	1.368646
5	1	0	-1.756668	0.311535	2.142089
6	1	0	-1.937542	1.611635	0.996107
7	6	0	-3.800852	1.003071	1.967242
8	1	0	-4.376246	1.655766	1.298524
9	6	0	-4.561620	-0.276623	2.104545
10	6	0	-4.524068	-1.223563	0.949745
11	1	0	-3.842832	-2.067298	1.020508
12	6	0	0.850796	-2.699174	-0.031995
13	6	0	2.800154	-3.720431	0.370728
14	6	0	2.507391	-3.899232	-0.941521
15	1	0	3.642675	-4.048156	0.959453
16	1	0	3.050325	-4.401388	-1.726958
17	7	0	1.772242	-2.983712	0.910454
18	7	0	1.303058	-3.273998	-1.166372
19	79	0	-0.775577	-1.566488	0.148198
20	6	0	0.690142	-3.122374	-2.474456
21	1	0	1.103893	-2.240709	-2.968841
22	1	0	0.880193	-4.022671	-3.063200
23	1	0	-0.385581	-2.988207	-2.350616
24	6	0	1.693859	-2.556001	2.296982
25	1	0	1.385624	-1.508718	2.341285
26	1	0	0.984351	-3.182440	2.845269
27	1	0	2.684212	-2.654505	2.745367
28	1	0	-3.721474	1.493553	2.940882
29	16	0	-3.208710	0.018352	-1.102295
30	8	0	-4.658821	0.103231	-0.709913
31	8	0	-2.849964	-0.990990	-2.087014
32	6	0	-2.718222	1.638784	-1.610953
33	6	0	-1.383298	1.824659	-1.970530
34	6	0	-3.644040	2.681685	-1.614195
35	6	0	-0.962491	3.102601	-2.320878
36	1	0	-0.678396	0.997319	-1.971222
37	6	0	-3.208907	3.948283	-1.989643
38	1	0	-4.677193	2.493919	-1.341113
39	6	0	-1.873788	4.156675	-2.332566
40	1	0	0.085505	3.262098	-2.553090
41	1	0	-3.914111	4.774129	-2.007731
42	1	0	-1.538484	5.153295	-2.605459
43	7	0	1.972915	0.483843	0.406394
44	16	0	2.264406	0.851388	-1.130213
45	8	0	1.603392	-0.110675	-2.017563
46	8	0	2.207261	2.264231	-1.493038
47	6	0	4.048444	0.383183	-1.204687
48	9	0	4.755791	1.106597	-0.345482
49	9	0	4.500335	0.604152	-2.435590
50	9	0	4.205099	-0.908374	-0.916868
51	16	0	1.266356	1.462038	1.453661
52	8	0	0.341265	2.439071	0.884243
53	8	0	0.803592	0.637554	2.573428
54	6	0	2.649674	2.459227	2.168807
55	9	0	2.162375	3.295942	3.080351
56	9	0	3.534918	1.655387	2.751067
57	9	0	3.258193	3.155985	1.217624

Zero-point correction= 0.389346 (Hartree/Particle)
Thermal correction to Energy= 0.428848
Thermal correction to Enthalpy= 0.429792
Thermal correction to Gibbs Free Energy= 0.309883
Sum of electronic and zero-point Energies= -3330.623536
Sum of electronic and thermal Energies= -3330.584034
Sum of electronic and thermal Enthalpies= -3330.583089
Sum of electronic and thermal Free Energies (333K)= -3330.717522
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3333.004917

TS15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.446778	0.362049	0.527287
2	8	0	-2.247163	-2.186533	1.694620
3	1	0	-4.690902	-1.853934	1.044521
4	6	0	-2.298762	1.006611	1.834214
5	1	0	-1.369343	1.584261	1.883732
6	1	0	-3.145280	1.686860	1.986586
7	6	0	-2.325629	-0.117444	2.901629
8	1	0	-1.311870	-0.409188	3.187976
9	1	0	-2.863804	0.215932	3.794234
10	6	0	-2.993137	-1.273621	2.201740
11	16	0	-3.062142	1.273103	-0.728931
12	8	0	-4.479551	1.505464	-0.458649

13	8	0	-2.644945	0.548501	-1.931776
14	6	0	-2.260500	2.862646	-0.700588
15	6	0	-0.904110	2.958860	-1.005995
16	6	0	-3.024021	3.985142	-0.384294
17	6	0	-0.305967	4.214203	-0.990079
18	1	0	-0.327043	2.071023	-1.241103
19	6	0	-2.411822	5.234541	-0.379425
20	1	0	-4.079786	3.867902	-0.163814
21	6	0	-1.056682	5.347579	-0.681249
22	1	0	0.751712	4.300779	-1.218603
23	1	0	-2.995817	6.119778	-0.142249
24	1	0	-0.582386	6.325098	-0.675282
25	6	0	-4.306128	-1.161629	1.784643
26	1	0	-4.980535	-0.416773	2.196266
27	6	0	-0.190080	-2.862454	-0.585738
28	6	0	0.997161	-4.750664	-0.594707
29	6	0	0.683193	-4.457829	-1.881421
30	1	0	1.558735	-5.568500	-0.170913
31	1	0	0.921227	-4.965344	-2.803051
32	7	0	0.445401	-3.762051	0.186331
33	7	0	-0.055005	-3.298453	-1.853792
34	79	0	-1.129841	-1.150400	-0.031915
35	6	0	-0.489756	-2.579164	-3.038509
36	1	0	-1.246102	-1.842665	-2.758263
37	1	0	0.366409	-2.062209	-3.481665
38	1	0	-0.919817	-3.286658	-3.754014
39	6	0	0.613056	-3.654157	1.628775
40	1	0	0.755060	-4.657474	2.036812
41	1	0	1.475237	-3.022691	1.855889
42	1	0	-0.284194	-3.205585	2.055739
43	7	0	2.563247	-0.442488	0.311813
44	16	0	2.191228	-0.201397	-1.209427
45	8	0	2.694472	-1.312525	-2.005883
46	8	0	0.776945	0.217417	-1.446428
47	6	0	3.132451	1.283077	-1.809598
48	9	0	2.716146	2.382981	-1.191171
49	9	0	2.935136	1.413490	-3.112863
50	9	0	4.423508	1.113285	-1.574470
51	16	0	2.000110	0.428727	1.555767
52	8	0	1.165667	1.571740	1.193657
53	8	0	1.541263	-0.472851	2.607034
54	6	0	3.580630	1.144369	2.194089
55	9	0	3.300288	1.964965	3.201627
56	9	0	4.377734	0.179609	2.624871
57	9	0	4.193611	1.826846	1.232778

Zero-point correction= 0.389708 (Hartree/Particle)
Thermal correction to Energy= 0.428647
Thermal correction to Enthalpy= 0.429591
Thermal correction to Gibbs Free Energy= 0.314111
Sum of electronic and zero-point Energies= -3330.608688
Sum of electronic and thermal Energies= -3330.569749
Sum of electronic and thermal Enthalpies= -3330.568805
Sum of electronic and thermal Free Energies(333K)= -3330.698299
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3332.996924

INT16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.720339	-0.180374	-0.501277
2	8	0	5.600856	-0.025512	-2.602718
3	1	0	4.346234	-1.583501	-0.708229
4	6	0	2.504482	1.117819	-1.242784
5	1	0	1.764240	0.897512	-2.017159
6	1	0	2.043112	1.850134	-0.579987
7	6	0	3.852054	1.504835	-1.836947
8	1	0	4.442208	2.147491	-1.175246
9	6	0	4.581482	0.182730	-1.999980
10	6	0	3.748055	-0.897588	-1.311589
11	1	0	3.229136	-1.481889	-2.080168
12	6	0	-0.637894	-2.586115	-0.144262
13	6	0	-2.524995	-3.705049	-0.567603
14	6	0	-2.180345	-3.955330	0.719701
15	1	0	-3.364360	-4.043404	-1.154687
16	1	0	-2.666328	-4.543271	1.482521
17	7	0	-1.566014	-2.864083	-1.080635
18	7	0	-1.012735	-3.268738	0.956988
19	79	0	0.947550	-1.399139	-0.306223
20	6	0	-0.374758	-3.169541	2.257210
21	1	0	-0.854054	-2.373769	2.832340
22	1	0	-0.468081	-4.126989	2.774582
23	1	0	0.682524	-2.935719	2.119857
24	6	0	-1.559824	-2.351891	-2.440194
25	1	0	-1.170272	-1.331813	-2.442209
26	1	0	-0.953423	-2.996203	-3.083956
27	1	0	-2.587335	-2.333303	-2.808139
28	1	0	3.761721	2.009391	-2.802817
29	16	0	3.444594	0.061551	1.131394
30	8	0	4.798669	0.550012	0.897106
31	8	0	3.223159	-1.208062	1.806976

32	6	0	2.475938	1.345907	1.851145
33	6	0	1.181153	1.081817	2.297468
34	6	0	3.066304	2.604715	1.980607
35	6	0	0.450400	2.121212	2.861968
36	1	0	0.735023	0.096980	2.197976
37	6	0	2.325447	3.625948	2.562660
38	1	0	4.085281	2.764018	1.643502
39	6	0	1.021473	3.385060	2.991761
40	1	0	-0.573745	1.944105	3.170768
41	1	0	2.766303	4.611949	2.675023
42	1	0	0.439710	4.192135	3.427330
43	7	0	-2.077861	0.425512	-0.437356
44	16	0	-2.519925	0.610091	1.098833
45	8	0	-1.859320	-0.381417	1.955493
46	8	0	-2.618026	1.978784	1.593746
47	6	0	-4.258884	0.008662	0.954974
48	9	0	-4.952316	0.790878	0.138124
49	9	0	-4.817458	0.033375	2.161413
50	9	0	-4.293611	-1.241118	0.493977
51	16	0	-1.248813	1.511098	-1.263261
52	8	0	-0.402972	2.402232	-0.473381
53	8	0	-0.643358	0.822440	-2.409877
54	6	0	-2.535198	2.596539	-2.029588
55	9	0	-1.937325	3.534653	-2.758368
56	9	0	-3.323863	1.873643	-2.819246
57	9	0	-3.272711	3.174330	-1.091591

Zero-point correction= 0.393092 (Hartree/Particle)
Thermal correction to Energy= 0.440469
Thermal correction to Enthalpy= 0.441524
Thermal correction to Gibbs Free Energy= 0.300567
Sum of electronic and zero-point Energies= -3330.726274
Sum of electronic and thermal Energies= -3330.678897
Sum of electronic and thermal Enthalpies= -3330.677842
Sum of electronic and thermal Free Energies(333K)= -3330.818799
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3333.106164

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.088200	0.399109	1.006106
2	8	0	4.205703	-0.558112	-0.450356
3	1	0	2.588788	1.616274	0.044380
4	6	0	1.094065	-1.097378	1.207973
5	1	0	1.367198	-1.255449	2.255611
6	1	0	0.084306	-1.486491	1.065795
7	6	0	2.152606	-1.669008	0.273990
8	1	0	1.748109	-1.961190	-0.699941
9	6	0	3.123665	-0.518404	0.064378
10	6	0	2.511952	0.737470	0.688871
11	1	0	3.036002	0.956920	1.625995
12	1	0	2.673928	-2.532054	0.696580
13	16	0	0.121438	0.900570	-0.440573
14	8	0	0.741669	0.243012	-1.578051
15	8	0	0.079062	2.348808	-0.317749
16	6	0	-1.476898	0.208535	-0.155378
17	6	0	-2.408081	0.922268	0.600457
18	6	0	-1.794610	-1.002349	-0.773913
19	6	0	-3.678071	0.382220	0.770215
20	1	0	-2.150017	1.890712	1.016864
21	6	0	-3.070065	-1.525951	-0.593466
22	1	0	-1.064803	-1.502400	-1.403090
23	6	0	-4.003801	-0.838986	0.181009
24	1	0	-4.420856	0.924221	1.347315
25	1	0	-3.338625	-2.463495	-1.070139
26	1	0	-5.000484	-1.250097	0.311487

Zero-point correction= 0.203648 (Hartree/Particle)
Thermal correction to Energy= 0.216640
Thermal correction to Enthalpy= 0.217585
Thermal correction to Gibbs Free Energy= 0.162299
Sum of electronic and zero-point Energies= -1065.123229
Sum of electronic and thermal Energies= -1065.110237
Sum of electronic and thermal Enthalpies= -1065.109293
Sum of electronic and thermal Free Energies(333K)= -1065.171238
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1065.891332

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.677471	0.525619	0.784132
2	8	0	-2.421043	0.631105	-0.584369
3	1	0	-1.828830	1.420374	-0.658704
4	6	0	-2.297150	-0.798835	1.247559
5	1	0	-2.672524	-0.896290	2.269038
6	1	0	-2.738678	-1.589368	0.622372
7	6	0	-0.767452	-0.926951	1.284950

8	1	0	-0.344366	-0.008596	1.706741
9	1	0	-0.495860	-1.769748	1.932640
10	6	0	-0.182076	-1.141300	-0.037017
11	16	0	-4.313420	0.945854	1.076704
12	8	0	-4.486457	2.279481	0.535034
13	8	0	-4.534228	0.635426	2.485101
14	6	0	-5.278112	-0.185747	0.100715
15	6	0	-5.847510	-1.297308	0.719111
16	6	0	-5.424575	0.045060	-1.266706
17	6	0	-6.580259	-2.196141	-0.051011
18	1	0	-5.731403	-1.430232	1.790461
19	6	0	-6.155198	-0.864129	-2.024737
20	1	0	-4.978176	0.926080	-1.713974
21	6	0	-6.729786	-1.981097	-1.419591
22	1	0	-7.040221	-3.060625	0.419688
23	1	0	-6.281176	-0.696985	-3.090695
24	1	0	-7.303912	-2.684193	-2.017684
25	6	0	0.207116	-1.354819	-1.184893
26	6	0	4.052649	-0.362666	0.164774
27	6	0	5.945000	0.766838	0.543647
28	6	0	6.232184	-0.555411	0.656382
29	1	0	6.573021	1.637668	0.650970
30	1	0	7.157561	-1.064090	0.877281
31	7	0	4.609833	0.863492	0.242115
32	7	0	5.058028	-1.231480	0.420644
33	79	0	2.123834	-0.763860	-0.248058
34	1	0	0.233154	-1.515550	-2.244169
35	6	0	4.931515	-2.675035	0.448472
36	1	0	5.603461	-3.123495	-0.288031
37	1	0	5.173850	-3.054420	1.444707
38	1	0	3.900948	-2.933061	0.202947
39	6	0	3.885577	2.115661	0.039862
40	1	0	3.136764	2.249511	0.820210
41	1	0	4.604596	2.936029	0.065333
42	1	0	3.370035	2.095246	-0.919546
43	9	0	-0.686556	2.597770	-0.899319
44	5	0	0.674749	2.381895	-0.600493
45	9	0	1.344647	3.578371	-0.448282
46	9	0	1.264348	1.624412	-1.637518
47	9	0	0.763055	1.628703	0.602755

Zero-point correction= 0.349214 (Hartree/Particle)
Thermal correction to Energy= 0.379487
Thermal correction to Enthalpy= 0.380431
Thermal correction to Gibbs Free Energy= 0.283220
Sum of electronic and zero-point Energies= -1928.837888
Sum of electronic and thermal Energies= -1928.807616
Sum of electronic and thermal Enthalpies= -1928.806671
Sum of electronic and thermal Free Energies(333K)= -1928.915652
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.520492

TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.857045	-0.718706	1.085099
2	8	0	-2.215289	-0.147001	-0.021895
3	1	0	-1.849015	0.738378	0.299014
4	6	0	-1.856542	-1.498741	1.827115
5	1	0	-1.323351	-0.794769	2.469985
6	1	0	-2.377500	-2.234807	2.443777
7	6	0	-0.876070	-2.155681	0.847976
8	1	0	-0.003486	-2.518821	1.403949
9	1	0	-1.335314	-3.008038	0.333350
10	6	0	-0.392752	-1.194977	-0.134849
11	16	0	-4.145045	-1.679578	0.443392
12	8	0	-4.702000	-2.338398	1.618036
13	8	0	-3.681444	-2.456346	-0.701396
14	6	0	-5.243523	-0.414349	-0.123163
15	6	0	-6.227867	0.051479	0.744968
16	6	0	-5.105211	0.075560	-1.419512
17	6	0	-7.095838	1.041333	0.297061
18	1	0	-6.308831	-0.366070	1.743355
19	6	0	-5.977519	1.069744	-1.849788
20	1	0	-4.329877	-0.317644	-2.067864
21	6	0	-6.967584	1.549614	-0.994474
22	1	0	-7.873121	1.415563	0.956817
23	1	0	-5.882512	1.470047	-2.854705
24	1	0	-7.646303	2.325447	-1.337952
25	6	0	0.362627	-0.593408	-0.956218
26	1	0	0.056958	0.179134	-1.658979
27	6	0	4.274104	-0.188036	0.100208
28	6	0	5.980777	0.873694	1.089726
29	6	0	6.501141	-0.160283	0.381423
30	1	0	6.459466	1.622682	1.701525
31	1	0	7.520455	-0.490265	0.252736
32	7	0	4.619180	0.840196	0.904611
33	7	0	5.437329	-0.798383	-0.217860
34	79	0	2.372409	-0.582679	-0.464170
35	6	0	5.557317	-1.959406	-1.076450
36	1	0	4.558028	-2.244733	-1.407522

37	1	0	6.172618	-1.720639	-1.948318
38	1	0	6.008356	-2.789831	-0.526100
39	6	0	3.666334	1.775308	1.496859
40	1	0	4.222137	2.529161	2.056142
41	1	0	3.075071	2.263628	0.719446
42	1	0	2.992692	1.246765	2.173972
43	9	0	0.868341	2.292817	-0.348952
44	5	0	-0.205825	3.176604	0.094545
45	9	0	-0.894998	3.726834	-1.069022
46	9	0	-1.153051	2.420704	0.908779
47	9	0	0.356408	4.266061	0.887374

Zero-point correction= 0.348616 (Hartree/Particle)
Thermal correction to Energy= 0.377947
Thermal correction to Enthalpy= 0.378891
Thermal correction to Gibbs Free Energy= 0.282466
Sum of electronic and zero-point Energies= -1928.829069
Sum of electronic and thermal Energies= -1928.799738
Sum of electronic and thermal Enthalpies= -1928.798793
Sum of electronic and thermal Free Energies(333K)= -1928.906886
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.499373

INT6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.839233	0.156585	0.982701
2	8	0	-2.091857	-0.002629	-0.214787
3	1	0	-1.716912	0.961801	-0.365432
4	6	0	-1.833747	0.016537	2.066691
5	1	0	-1.345777	0.988694	2.161033
6	1	0	-2.352741	-0.244652	2.992653
7	6	0	-0.841540	-1.021288	1.565361
8	1	0	0.134920	-0.900044	2.041859
9	1	0	-1.213468	-2.043757	1.735716
10	6	0	-0.675659	-0.747088	0.110296
11	16	0	-4.086033	-1.067288	1.021307
12	8	0	-4.583062	-0.958671	2.386344
13	8	0	-3.587870	-2.326280	0.487177
14	6	0	-5.265073	-0.385050	-0.104396
15	6	0	-6.113704	0.632903	0.344782
16	6	0	-5.345605	-0.900210	-1.390031
17	6	0	-7.054953	1.145135	-0.537847
18	1	0	-6.030391	1.000898	1.362697
19	6	0	-6.293914	-0.377927	-2.261593
20	1	0	-4.680068	-1.704754	-1.691933
21	6	0	-7.142583	0.643851	-1.836468
22	1	0	-7.722141	1.934150	-0.210679
23	1	0	-6.375565	-0.765994	-3.273388
24	1	0	-7.886484	1.047666	-2.520516
25	6	0	0.229784	-0.744972	-0.846267
26	1	0	-0.097849	-0.366485	-1.823185
27	6	0	4.174054	-0.205561	-0.031747
28	6	0	5.965631	1.039068	0.514792
29	6	0	6.401553	-0.227428	0.298043
30	1	0	6.502236	1.932533	0.794598
31	1	0	7.390785	-0.655672	0.348177
32	7	0	4.606641	1.030721	0.306787
33	7	0	5.290913	-0.970799	-0.035941
34	79	0	2.245369	-0.679956	-0.446374
35	6	0	5.312736	-2.384344	-0.352621
36	1	0	4.294064	-2.696779	-0.584254
37	1	0	5.955740	-2.563221	-1.222695
38	1	0	5.689826	-2.954518	0.501114
39	6	0	3.736286	2.193963	0.448728
40	1	0	4.363771	3.075741	0.598238
41	1	0	3.125712	2.317455	-0.445383
42	1	0	3.060930	2.068679	1.299589
43	9	0	0.960295	2.102894	-1.123381
44	5	0	0.246230	2.536684	-0.011473
45	9	0	0.418716	3.875143	0.220019
46	9	0	-1.183975	2.289567	-0.295025
47	9	0	0.564863	1.776565	1.121803

Zero-point correction= 0.348359 (Hartree/Particle)
Thermal correction to Energy= 0.377797
Thermal correction to Enthalpy= 0.378741
Thermal correction to Gibbs Free Energy= 0.280790
Sum of electronic and zero-point Energies= -1928.841472
Sum of electronic and thermal Energies= -1928.812034
Sum of electronic and thermal Enthalpies= -1928.811090
Sum of electronic and thermal Free Energies(333K)= -1928.920887
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1930.503915

TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.578252	-0.210235	-1.095424

2	8	0	2.163934	0.565943	0.016984
3	1	0	1.825586	1.438964	-0.378421
4	6	0	2.255025	-1.618230	-0.852609
5	1	0	2.832176	-2.185023	-1.587048
6	1	0	2.564252	-1.916501	0.159914
7	6	0	0.765390	-1.875553	-1.047648
8	1	0	0.484286	-1.685438	-2.090333
9	1	0	0.551941	-2.931323	-0.845403
10	6	0	-0.045379	-0.996130	-0.156629
11	16	0	4.266263	0.101791	-1.324394
12	8	0	4.362532	1.541745	-1.460116
13	8	0	4.658035	-0.824759	-2.377521
14	6	0	5.064620	-0.378695	0.186576
15	6	0	5.659981	-1.636435	0.269326
16	6	0	5.069072	0.507587	1.263315
17	6	0	6.270328	-2.013405	1.461655
18	1	0	5.662463	-2.288576	-0.598459
19	6	0	5.678580	0.114278	2.449951
20	1	0	4.615545	1.487222	1.159787
21	6	0	6.275143	-1.141725	2.548768
22	1	0	6.748966	-2.985460	1.538662
23	1	0	5.693028	0.793694	3.297113
24	1	0	6.753961	-1.439961	3.477434
25	6	0	0.316146	0.023018	0.509621
26	6	0	-4.111056	-0.475853	0.189233
27	6	0	-6.091076	0.546164	0.445539
28	6	0	-6.341299	-0.753039	0.149860
29	1	0	-6.761420	1.368483	0.643122
30	1	0	-7.271277	-1.286809	0.028053
31	7	0	-4.723516	0.697439	0.461168
32	7	0	-5.115240	-1.362549	-0.000749
33	79	0	-2.111182	-0.781805	0.078745
34	1	0	0.180869	0.919495	1.104687
35	6	0	-4.938959	-2.757624	-0.350297
36	1	0	-5.492501	-3.389280	0.349640
37	1	0	-5.292588	-2.941928	-1.368835
38	1	0	-3.876525	-2.996575	-0.288882
39	6	0	-4.047433	1.946269	0.790743
40	1	0	-3.072950	1.998709	0.299442
41	1	0	-4.663064	2.777457	0.440653
42	1	0	-3.915772	2.023549	1.873711
43	9	0	0.941508	2.841045	-0.837742
44	5	0	-0.226827	3.265964	-0.103675
45	9	0	-0.398850	4.611174	-0.234342
46	9	0	-0.020754	2.891759	1.244489
47	9	0	-1.325972	2.540868	-0.601427

Zero-point correction= 0.349167 (Hartree/Particle)
Thermal correction to Energy= 0.378324
Thermal correction to Enthalpy= 0.379268
Thermal correction to Gibbs Free Energy= 0.283292
Sum of electronic and zero-point Energies= -1928.815223
Sum of electronic and thermal Energies= -1928.786067
Sum of electronic and thermal Enthalpies= -1928.785123
Sum of electronic and thermal Free Energies(333K)= -1928.892711
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.492481

INT7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.215288	-0.786367	-1.290470
2	8	0	1.806654	0.290394	-0.436045
3	1	0	2.181834	1.634133	-0.974340
4	6	0	1.653269	-2.041819	-0.782128
5	1	0	2.119963	-2.837716	-1.368000
6	1	0	1.903299	-2.175592	0.280301
7	6	0	0.144585	-1.987876	-0.979597
8	1	0	-0.094342	-2.099735	-2.045085
9	1	0	-0.303712	-2.848543	-0.468092
10	6	0	-0.430460	-0.698795	-0.449904
11	16	0	3.938212	-0.719169	-1.322984
12	8	0	4.237511	0.657172	-1.675322
13	8	0	4.305390	-1.850611	-2.159300
14	6	0	4.501634	-1.021178	0.331520
15	6	0	4.921963	-2.306381	0.672656
16	6	0	4.501502	0.025158	1.254199
17	6	0	5.353322	-2.547359	1.972934
18	1	0	4.927824	-3.088106	-0.080342
19	6	0	4.930955	-0.236251	2.551472
20	1	0	4.178733	1.019956	0.966741
21	6	0	5.354373	-1.514920	2.909181
22	1	0	5.694127	-3.540088	2.252789
23	1	0	4.937643	0.567236	3.282019
24	1	0	5.692647	-1.707347	3.923752
25	6	0	0.401522	0.312635	-0.211595
26	6	0	-4.412394	-0.113830	0.244139
27	6	0	-6.392051	0.909117	0.588860
28	6	0	-6.612057	-0.426895	0.632893
29	1	0	-7.068509	1.742056	0.705508
30	1	0	-7.518572	-0.990454	0.792870

31	7	0	-5.045579	1.079023	0.349376
32	7	0	-5.392010	-1.032565	0.421068
33	79	0	-2.414606	-0.430404	-0.102825
34	1	0	0.168721	1.288383	0.196429
35	6	0	-5.192058	-2.467353	0.387151
36	1	0	-5.513797	-2.914377	1.332120
37	1	0	-5.757765	-2.909224	-0.438270
38	1	0	-4.128568	-2.659753	0.240120
39	6	0	-4.397984	2.372603	0.239825
40	1	0	-3.352933	2.213728	-0.028432
41	1	0	-4.883780	2.968871	-0.537277
42	1	0	-4.448437	2.903069	1.194876
43	9	0	2.228509	2.612001	-1.196858
44	5	0	2.134838	3.581964	0.202526
45	9	0	2.516656	4.768589	-0.281953
46	9	0	2.999866	2.940921	1.026742
47	9	0	0.825734	3.444593	0.528346

Zero-point correction= 0.349992 (Hartree/Particle)
Thermal correction to Energy= 0.379631
Thermal correction to Enthalpy= 0.380576
Thermal correction to Gibbs Free Energy= 0.282517
Sum of electronic and zero-point Energies= -1928.834781
Sum of electronic and thermal Energies= -1928.805142
Sum of electronic and thermal Enthalpies= -1928.804198
Sum of electronic and thermal Free Energies(333K)= -1928.914116
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.498501

INT8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.432198	-0.004226	-0.083883
2	8	0	-2.717630	1.320128	-0.403127
3	1	0	-1.979402	1.834876	0.010329
4	6	0	-2.099589	-0.797184	-1.260792
5	1	0	-2.972688	-1.312893	-1.683187
6	1	0	-1.742741	-0.064543	-1.983840
7	6	0	-0.980816	-1.830416	-0.976267
8	1	0	-1.395266	-2.722746	-0.494647
9	1	0	-0.509515	-2.131814	-1.914365
10	6	0	-0.044643	-1.183131	-0.041154
11	16	0	-3.602685	-0.618059	0.978228
12	8	0	-3.535803	0.196981	2.177704
13	8	0	-3.349613	-2.058036	1.003630
14	6	0	-5.155599	-0.329071	0.174832
15	6	0	-5.773722	-1.382053	-0.493833
16	6	0	-5.705635	0.952190	0.203993
17	6	0	-6.979270	-1.143447	-1.148050
18	1	0	-5.323904	-2.369704	-0.470588
19	6	0	-6.907992	1.175108	-0.458934
20	1	0	-5.199351	1.747433	0.739052
21	6	0	-7.539665	0.130810	-1.130594
22	1	0	-7.483554	-1.956793	-1.664373
23	1	0	-7.352522	2.164756	-0.446390
24	1	0	-8.482937	0.313303	-1.644021
25	6	0	-0.123441	-0.322813	0.870959
26	6	0	4.011926	-0.321972	-0.181957
27	6	0	6.253886	-0.447645	-0.119210
28	6	0	5.917324	0.818191	-0.474310
29	1	0	7.216576	-0.917110	0.015384
30	1	0	6.533409	1.673900	-0.701645
31	7	0	5.070728	-1.130033	0.055929
32	7	0	4.544262	0.874936	-0.511545
33	79	0	2.040847	-0.735537	-0.010414
34	1	0	-0.088462	0.468728	1.593857
35	6	0	3.788916	2.091190	-0.801173
36	1	0	3.641650	2.669829	0.112650
37	1	0	4.346822	2.675475	-1.535266
38	1	0	2.807286	1.834961	-1.196836
39	6	0	4.987541	-2.523993	0.444908
40	1	0	5.483777	-2.674694	1.404716
41	1	0	3.933881	-2.790402	0.539103
42	1	0	5.454817	-3.155572	-0.314461
43	9	0	-0.737481	2.692824	0.693906
44	5	0	0.602410	2.700200	0.197943
45	9	0	1.400727	2.032867	1.161956
46	9	0	0.632343	1.965096	-1.002352
47	9	0	1.056149	3.979935	0.003850

Zero-point correction= 0.348908 (Hartree/Particle)
Thermal correction to Energy= 0.379332
Thermal correction to Enthalpy= 0.380276
Thermal correction to Gibbs Free Energy= 0.282454
Sum of electronic and zero-point Energies= -1928.838490
Sum of electronic and thermal Energies= -1928.808067
Sum of electronic and thermal Enthalpies= -1928.807122
Sum of electronic and thermal Free Energies(333K)= -1928.916787
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1930.519457

TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.575618	-0.166082	-0.332138
2	8	0	-2.896961	1.153798	-0.564318
3	1	0	-2.022157	1.642863	-0.560367
4	6	0	-2.451058	-0.988642	-1.560366
5	1	0	-3.350255	-1.564648	-1.799994
6	1	0	-2.244632	-0.274192	-2.358526
7	6	0	-1.212425	-1.808696	-1.195674
8	1	0	-1.482012	-2.770672	-0.748972
9	1	0	-0.520716	-1.972795	-2.029283
10	6	0	-0.638013	-0.896475	-0.186873
11	16	0	-3.638211	-0.782370	0.902954
12	8	0	-3.390593	0.025598	2.077661
13	8	0	-3.408351	-2.221616	0.871128
14	6	0	-5.263526	-0.449772	0.282724
15	6	0	-5.986234	-1.492207	-0.295900
16	6	0	-5.782066	0.840958	0.386639
17	6	0	-7.260496	-1.229333	-0.788753
18	1	0	-5.558219	-2.489058	-0.331303
19	6	0	-7.054750	1.086796	-0.115803
20	1	0	-5.195730	1.625171	0.851997
21	6	0	-7.789188	0.056844	-0.702209
22	1	0	-7.842416	-2.030774	-1.234501
23	1	0	-7.475617	2.085394	-0.045834
24	1	0	-8.784463	0.257601	-1.089048
25	6	0	0.193210	-0.244233	0.508734
26	6	0	4.228208	-0.478130	-0.052474
27	6	0	6.373613	-1.088610	-0.341269
28	6	0	6.342836	0.259099	-0.199418
29	1	0	7.197473	-1.765983	-0.505906
30	1	0	7.137088	0.989698	-0.209061
31	7	0	5.068788	-1.521305	-0.247046
32	7	0	5.023368	0.614290	-0.030322
33	79	0	2.217611	-0.478538	0.193006
34	1	0	-0.001275	0.630548	1.132681
35	6	0	4.661787	-2.907598	-0.351400
36	1	0	4.892543	-3.295544	-1.346944
37	1	0	5.177002	-3.507176	0.403474
38	1	0	3.586694	-2.960198	-0.180992
39	6	0	4.584635	1.981529	0.219157
40	1	0	3.537584	2.099074	-0.068903
41	1	0	4.708530	2.223565	1.278018
42	1	0	5.192484	2.662397	-0.381908
43	9	0	-0.681135	2.343557	-1.036845
44	5	0	0.334828	2.929671	-0.199217
45	9	0	0.047556	2.597571	1.128276
46	9	0	0.360254	4.285755	-0.382985
47	9	0	1.569583	2.338570	-0.589023

Zero-point correction= 0.348049 (Hartree/Particle)
Thermal correction to Energy= 0.377624
Thermal correction to Enthalpy= 0.378568
Thermal correction to Gibbs Free Energy= 0.281210
Sum of electronic and zero-point Energies= -1928.812810
Sum of electronic and thermal Energies= -1928.783235
Sum of electronic and thermal Enthalpies= -1928.782291
Sum of electronic and thermal Free Energies(333K)= -1928.891427
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.490626

INT9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.258242	0.027449	0.323711
2	8	0	2.609317	0.923390	-0.653821
3	1	0	1.782829	1.495071	-0.844932
4	6	0	2.308559	0.494767	1.761977
5	1	0	3.150812	0.068998	2.308603
6	1	0	2.332369	1.582276	1.731764
7	6	0	0.904960	-0.080597	1.999698
8	1	0	0.893764	-0.986932	2.611619
9	1	0	0.184912	0.652578	2.366838
10	6	0	0.807926	-0.334491	0.518843
11	16	0	3.302097	-1.469070	-0.039840
12	8	0	2.874379	-1.895650	-1.354214
13	8	0	3.155994	-2.286306	1.151788
14	6	0	4.927500	-0.786711	-0.105871
15	6	0	5.747281	-0.916940	1.014747
16	6	0	5.357333	-0.164066	-1.277740
17	6	0	7.035675	-0.396681	0.957136
18	1	0	5.383937	-1.435286	1.896280
19	6	0	6.646848	0.351655	-1.314140
20	1	0	4.690570	-0.087183	-2.128916
21	6	0	7.479736	0.237633	-0.201379
22	1	0	7.693821	-0.492177	1.815435
23	1	0	7.002444	0.844231	-2.213913
24	1	0	8.486679	0.643506	-0.239869

25	6	0	-0.071012	-0.550017	-0.447993
26	6	0	-4.104947	-0.442893	0.029055
27	6	0	-6.300812	-0.947838	0.080666
28	6	0	-6.169571	0.353833	0.434097
29	1	0	-7.176664	-1.569896	-0.023264
30	1	0	-6.909201	1.092042	0.704098
31	7	0	-5.027970	-1.416389	-0.161882
32	7	0	-4.823735	0.643361	0.394861
33	79	0	-2.073565	-0.563187	-0.191712
34	1	0	0.344709	-0.570151	-1.456549
35	6	0	-4.725368	-2.769502	-0.581808
36	1	0	-5.094236	-3.484901	0.158875
37	1	0	-5.186788	-2.976891	-1.551746
38	1	0	-3.642204	-2.864821	-0.669125
39	6	0	-4.267635	1.943539	0.736087
40	1	0	-4.839800	2.723014	0.226481
41	1	0	-4.325439	2.099972	1.817394
42	1	0	-3.226481	2.003903	0.415104
43	5	0	-0.022120	3.076876	-0.219250
44	9	0	0.625703	2.719965	0.976090
45	9	0	-1.342302	2.625547	-0.203717
46	9	0	0.060807	4.422361	-0.453748
47	9	0	0.669188	2.366860	-1.286664

Zero-point correction= 0.350103 (Hartree/Particle)
Thermal correction to Energy= 0.379444
Thermal correction to Enthalpy= 0.380388
Thermal correction to Gibbs Free Energy= 0.284512
Sum of electronic and zero-point Energies= -1928.836221
Sum of electronic and thermal Energies= -1928.806881
Sum of electronic and thermal Enthalpies= -1928.805937
Sum of electronic and thermal Free Energies(333K)= -1928.920356
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.505201

TS8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.408719	-0.029512	-0.179842
2	8	0	-2.796611	1.242496	-0.592062
3	1	0	-1.983307	1.799108	-0.469374
4	6	0	-2.079170	-0.906050	-1.303871
5	1	0	-2.943059	-1.494324	-1.635823
6	1	0	-1.780748	-0.223708	-2.101309
7	6	0	-0.897291	-1.840896	-0.966786
8	1	0	-1.243195	-2.736238	-0.440068
9	1	0	-0.402287	-2.153190	-1.890196
10	6	0	0.003979	-1.088613	-0.060384
11	16	0	-3.551157	-0.615475	0.956970
12	8	0	-3.500114	0.291002	2.087461
13	8	0	-3.227197	-2.033121	1.077967
14	6	0	-5.129334	-0.460992	0.162209
15	6	0	-5.701548	-1.591827	-0.417696
16	6	0	-5.757721	0.783140	0.125209
17	6	0	-6.932833	-1.469242	-1.054346
18	1	0	-5.193377	-2.548122	-0.343753
19	6	0	-6.985571	0.889798	-0.518308
20	1	0	-5.287947	1.639798	0.595092
21	6	0	-7.569352	-0.231150	-1.107052
22	1	0	-7.397209	-2.342200	-1.503928
23	1	0	-7.489815	1.850913	-0.557791
24	1	0	-8.530405	-0.139257	-1.605673
25	6	0	-0.234066	-0.165415	0.754949
26	6	0	4.072224	-0.457417	-0.189988
27	6	0	6.303505	-0.597967	-0.004000
28	6	0	6.019860	0.427989	-0.846682
29	1	0	7.246531	-0.988836	0.345795
30	1	0	6.669612	1.110136	-1.372848
31	7	0	5.095329	-1.128654	0.386038
32	7	0	4.652248	0.495095	-0.949469
33	79	0	2.079928	-0.751913	-0.000309
34	1	0	-0.253484	0.648642	1.465411
35	6	0	3.919113	1.485865	-1.732617
36	1	0	4.637850	2.075265	-2.303673
37	1	0	3.238212	0.985309	-2.422814
38	1	0	3.343818	2.139991	-1.074813
39	6	0	4.953840	-2.246581	1.298071
40	1	0	5.409440	-2.003119	2.261668
41	1	0	3.890760	-2.442344	1.442287
42	1	0	5.432880	-3.136134	0.879758
43	9	0	-0.737596	2.940883	-0.521072
44	5	0	0.391354	3.186871	0.371432
45	9	0	0.090563	2.650869	1.695753
46	9	0	1.583220	2.531785	-0.159526
47	9	0	0.629227	4.623947	0.470570

Zero-point correction= 0.348571 (Hartree/Particle)
Thermal correction to Energy= 0.378177
Thermal correction to Enthalpy= 0.379122
Thermal correction to Gibbs Free Energy= 0.282276
Sum of electronic and zero-point Energies= -1928.822788

Sum of electronic and thermal Energies= -1928.793182
Sum of electronic and thermal Enthalpies= -1928.792238
Sum of electronic and thermal Free Energies(333K)= -1928.900803
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1930.500356

INT10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.346699	-0.006171	-0.057504
2	8	0	-2.672086	1.302801	-0.383353
3	1	0	-1.934716	1.853156	0.000879
4	6	0	-2.071829	-0.810009	-1.258243
5	1	0	-2.979087	-1.301381	-1.626688
6	1	0	-1.744045	-0.072852	-1.996338
7	6	0	-0.943142	-1.817589	-0.981006
8	1	0	-1.333048	-2.724670	-0.509301
9	1	0	-0.465178	-2.104597	-1.923073
10	6	0	-0.003771	-1.139171	-0.034895
11	16	0	-3.598705	-0.629570	0.993121
12	8	0	-3.534102	0.196492	2.182021
13	8	0	-3.355139	-2.064436	1.015136
14	6	0	-5.130370	-0.321840	0.151926
15	6	0	-5.757003	-1.380608	-0.506886
16	6	0	-5.690934	0.954242	0.189100
17	6	0	-6.966563	-1.147993	-1.153298
18	1	0	-5.306855	-2.368074	-0.487072
19	6	0	-6.897283	1.171163	-0.466003
20	1	0	-5.185830	1.750120	0.724330
21	6	0	-7.532458	0.126069	-1.137837
22	1	0	-7.469695	-1.961955	-1.664774
23	1	0	-7.347203	2.160657	-0.450025
24	1	0	-8.474954	0.302788	-1.642974
25	6	0	-0.439321	-0.243231	0.776064
26	6	0	4.012706	-0.311628	-0.159729
27	6	0	6.254623	-0.446424	-0.113166
28	6	0	5.923181	0.818991	-0.469875
29	1	0	7.217267	-0.915421	0.018412
30	1	0	6.539328	1.674736	-0.701907
31	7	0	5.071420	-1.124101	0.070585
32	7	0	4.550152	0.880198	-0.499430
33	79	0	2.041518	-0.745789	-0.011092
34	1	0	-0.380832	0.553932	1.498375
35	6	0	3.794837	2.090929	-0.791322
36	1	0	3.640849	2.675275	0.116767
37	1	0	4.348745	2.674805	-1.529983
38	1	0	2.813959	1.829006	-1.188391
39	6	0	4.983109	-2.517769	0.455587
40	1	0	5.477811	-2.672482	1.421341
41	1	0	3.929398	-2.784492	0.543262
42	1	0	5.456875	-3.149808	-0.302476
43	9	0	-0.749242	2.697125	0.685752
44	5	0	0.606462	2.699589	0.197014
45	9	0	1.388434	2.033353	1.157891
46	9	0	0.623654	1.973489	-1.007631
47	9	0	1.050043	3.984330	0.007592

Zero-point correction= 0.351548 (Hartree/Particle)
Thermal correction to Energy= 0.380648
Thermal correction to Enthalpy= 0.381592
Thermal correction to Gibbs Free Energy= 0.286237
Sum of electronic and zero-point Energies= -1928.863173
Sum of electronic and thermal Energies= -1928.834073
Sum of electronic and thermal Enthalpies= -1928.833129
Sum of electronic and thermal Free Energies(333K)= -1928.940025
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.534724

INT11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.420035	-1.240593	-0.879972
2	8	0	1.337259	-1.174744	-1.796013
3	1	0	-1.772167	-2.292688	-1.571726
4	6	0	2.084495	-2.365776	0.012921
5	1	0	2.509032	-3.265248	-0.442894
6	1	0	2.545374	-2.211841	0.990440
7	6	0	0.559527	-2.399432	0.047397
8	1	0	0.124518	-3.400272	0.048168
9	1	0	0.123091	-1.878734	0.904308
10	6	0	0.215731	-1.692678	-1.229767
11	16	0	2.525326	0.307434	-0.056047
12	8	0	1.723786	0.333294	1.164398
13	8	0	2.328015	1.305590	-1.096444
14	6	0	4.236192	0.222839	0.401552
15	6	0	4.566388	0.192585	1.753429
16	6	0	5.208402	0.229020	-0.598149
17	6	0	5.911593	0.162259	2.111205
18	1	0	3.778017	0.199875	2.499598

19	6	0	6.546254	0.195881	-0.225043
20	1	0	4.915076	0.259042	-1.642622
21	6	0	6.895279	0.162219	1.125489
22	1	0	6.189595	0.139887	3.160784
23	1	0	7.318909	0.197915	-0.988087
24	1	0	7.943495	0.137157	1.410010
25	6	0	-0.974052	-1.637749	-1.915696
26	1	0	-0.965197	-1.287437	-2.945238
27	6	0	-1.964802	1.900842	0.146406
28	6	0	-3.018834	3.384353	1.449151
29	6	0	-2.145093	4.073235	0.671083
30	1	0	-3.703968	3.720722	2.211785
31	1	0	-1.921059	5.127378	0.618522
32	7	0	-2.892866	2.058147	1.112970
33	7	0	-1.507134	3.145124	-0.118530
34	79	0	-1.403841	0.174816	-0.725968
35	6	0	-0.503787	3.460968	-1.120266
36	1	0	-0.042907	4.417559	-0.864914
37	1	0	0.263141	2.684426	-1.129880
38	1	0	-0.964271	3.532182	-2.109834
39	6	0	-3.642315	0.966819	1.726619
40	1	0	-4.216059	1.376236	2.559676
41	1	0	-4.308351	0.508055	0.995043
42	1	0	-2.953536	0.195974	2.074797
43	9	0	-1.915787	-1.626118	1.626460
44	5	0	-2.888815	-2.449238	0.973418
45	9	0	-2.199617	-3.428611	0.230981
46	9	0	-3.728084	-3.009563	1.903717
47	9	0	-3.603512	-1.627665	0.070887

Zero-point correction= 0.351528 (Hartree/Particle)
Thermal correction to Energy= 0.380677
Thermal correction to Enthalpy= 0.381621
Thermal correction to Gibbs Free Energy= 0.287238
Sum of electronic and zero-point Energies= -1928.892109
Sum of electronic and thermal Energies= -1928.862960
Sum of electronic and thermal Enthalpies= -1928.862015
Sum of electronic and thermal Free Energies(333K)= -1928.967809
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1930.556020

INT17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.351879	-0.106490	-1.905862
2	8	0	2.990981	1.161510	-1.426890
3	1	0	3.682718	1.734067	-1.798775
4	6	0	2.218835	-0.860566	-2.395667
5	1	0	1.793060	-0.272919	-3.214684
6	1	0	2.635462	-1.776448	-2.823436
7	6	0	1.106610	-1.265853	-1.405953
8	1	0	0.407937	-1.910344	-1.950367
9	1	0	1.522339	-1.872135	-0.591998
10	6	0	0.395234	-0.121309	-0.811338
11	16	0	4.518537	-0.825914	-0.888598
12	8	0	5.552551	0.189496	-0.798046
13	8	0	4.726820	-2.143763	-1.468008
14	6	0	3.821010	-1.034641	0.734418
15	6	0	3.511770	-2.323726	1.167646
16	6	0	3.636139	0.078508	1.555244
17	6	0	2.989879	-2.496790	2.446244
18	1	0	3.710246	-3.170001	0.516117
19	6	0	3.105903	-0.109684	2.827337
20	1	0	3.922213	1.065097	1.208362
21	6	0	2.783466	-1.391857	3.270887
22	1	0	2.765647	-3.496917	2.806004
23	1	0	2.965779	0.745490	3.482414
24	1	0	2.389105	-1.532776	4.273464
25	6	0	0.221245	0.985751	-0.277661
26	6	0	-3.683975	-0.746937	-0.029499
27	6	0	-5.552269	-1.698240	0.759084
28	6	0	-5.897629	-0.938293	-0.309925
29	1	0	-6.152232	-2.312948	1.413003
30	1	0	-6.858122	-0.759264	-0.769148
31	7	0	-4.192837	-1.565985	0.916628
32	7	0	-4.739631	-0.365577	-0.780631
33	79	0	-1.755911	-0.213174	-0.280926
34	6	0	-4.692905	0.527021	-1.926835
35	1	0	-5.292778	1.418594	-1.727955
36	1	0	-3.657879	0.821060	-2.103124
37	1	0	-5.077564	0.013094	-2.811352
38	6	0	-3.435617	-2.234903	1.961256
39	1	0	-2.390464	-1.933492	1.886281
40	1	0	-3.825046	-1.948557	2.941461
41	1	0	-3.509141	-3.318415	1.838120
42	6	0	0.175646	2.319669	0.233343
43	6	0	0.451771	3.390243	-0.632730
44	6	0	-0.102274	2.562612	1.587962
45	6	0	0.451406	4.688075	-0.140347
46	1	0	0.676443	3.188401	-1.675297
47	6	0	-0.106633	3.866217	2.066018

48	1	0	-0.305802	1.727048	2.251472
49	6	0	0.169367	4.927363	1.204363
50	1	0	0.670980	5.516977	-0.806756
51	1	0	-0.320762	4.056895	3.113457
52	1	0	0.167649	5.945353	1.582996

Zero-point correction= 0.414826 (Hartree/Particle)
Thermal correction to Energy= 0.444726
Thermal correction to Enthalpy= 0.445670
Thermal correction to Gibbs Free Energy= 0.344822
Sum of electronic and zero-point Energies= -1735.321246
Sum of electronic and thermal Energies= -1735.291346
Sum of electronic and thermal Enthalpies= -1735.290401
Sum of electronic and thermal Free Energies(333K)= -1735.403447
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -1736.858887

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.668516	0.302371	0.117285
2	8	0	-0.879383	1.694913	0.082721
3	1	0	-0.315060	2.009010	0.806238
4	6	0	-0.525865	-0.218095	-1.245714
5	1	0	-1.488903	-0.536933	-1.669135
6	1	0	-0.167053	0.626766	-1.836736
7	6	0	0.480236	-1.370067	-1.297589
8	1	0	0.146623	-2.165950	-0.622542
9	1	0	0.467175	-1.785975	-2.314150
10	6	0	1.834696	-0.953840	-0.955988
11	16	0	-1.899946	-0.399282	1.074907
12	8	0	-1.834072	0.305461	2.344232
13	8	0	-1.685307	-1.836334	0.960348
14	6	0	-3.446199	-0.006870	0.292088
15	6	0	-4.063041	-0.971381	-0.503059
16	6	0	-4.004275	1.258278	0.472117
17	6	0	-5.262716	-0.656561	-1.134152
18	1	0	-3.614352	-1.955505	-0.595385
19	6	0	-5.200970	1.559692	-0.167824
20	1	0	-3.510444	1.979881	1.112879
21	6	0	-5.826541	0.606263	-0.969610
22	1	0	-5.760208	-1.401076	-1.749001
23	1	0	-5.650663	2.539394	-0.034707
24	1	0	-6.763977	0.847529	-1.463195
25	6	0	2.954904	-0.594248	-0.687045
26	6	0	4.385672	-0.151736	-0.328317
27	6	0	5.076685	-0.793308	0.699962
28	6	0	4.991123	0.888993	-1.032260
29	6	0	6.372957	-0.393458	1.024534
30	1	0	4.599325	-1.614107	1.254541
31	6	0	6.287759	1.289375	-0.707231
32	1	0	4.446754	1.394317	-1.843189
33	6	0	6.978369	0.648226	0.321128
34	1	0	6.917662	-0.898890	1.835068
35	1	0	6.764908	2.110016	-1.262365
36	1	0	8.000281	0.963548	0.577533

Zero-point correction= 0.282636 (Hartree/Particle)
Thermal correction to Energy= 0.301831
Thermal correction to Enthalpy= 0.302775
Thermal correction to Gibbs Free Energy= 0.230969
Sum of electronic and zero-point Energies= -1295.702754
Sum of electronic and thermal Energies= -1295.683559
Sum of electronic and thermal Enthalpies= -1295.682615
Sum of electronic and thermal Free Energies(333K)= -1295.763095
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1296.729750

INT18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.023735	0.162928	-1.340059
2	8	0	2.395564	0.159054	-0.102864
3	1	0	1.959505	1.045408	-0.023201
4	6	0	2.043671	-0.111075	-2.380243
5	1	0	1.533750	0.834762	-2.583969
6	1	0	2.568426	-0.429812	-3.283962
7	6	0	0.981767	-1.155805	-1.968300
8	1	0	0.108037	-0.973813	-2.610235
9	1	0	1.341221	-2.174910	-2.169926
10	6	0	0.521648	-1.112846	-0.571493
11	16	0	4.408046	-0.811804	-1.210302
12	8	0	5.174592	-0.265247	-0.110267
13	8	0	4.905741	-0.891501	-2.576355
14	6	0	3.862495	-2.441576	-0.733837
15	6	0	3.791905	-3.437547	-1.704123
16	6	0	3.517756	-2.691180	0.594000
17	6	0	3.356787	-4.709129	-1.340283
18	1	0	4.100293	-3.212887	-2.720807

19	6	0	3.074075	-3.964923	0.944276
20	1	0	3.604546	-1.905533	1.333489
21	6	0	2.994716	-4.968504	-0.019467
22	1	0	3.311407	-5.501134	-2.082665
23	1	0	2.797847	-4.172776	1.976392
24	1	0	2.657044	-5.963061	0.262719
25	6	0	0.009916	-1.411359	0.543354
26	6	0	-3.886259	-1.221324	-0.803800
27	6	0	-5.794646	-0.171589	-1.314882
28	6	0	-6.041562	-1.505541	-1.344813
29	1	0	-6.439325	0.671205	-1.502600
30	1	0	-6.944974	-2.054731	-1.564673
31	7	0	-4.468206	-0.018615	-0.980910
32	7	0	-4.857937	-2.130567	-1.028934
33	79	0	-1.953297	-1.453113	-0.273052
34	6	0	-4.687633	-3.571309	-0.951490
35	1	0	-5.337444	-3.986123	-0.179577
36	1	0	-4.928096	-4.026912	-1.917997
37	1	0	-3.646745	-3.779532	-0.704915
38	6	0	-3.782135	1.264438	-0.835574
39	1	0	-4.455966	2.057510	-1.157046
40	1	0	-3.497319	1.426014	0.206085
41	1	0	-2.881488	1.282635	-1.451240
42	7	0	0.847866	2.366884	0.138819
43	16	0	1.030515	3.136679	1.565115
44	8	0	2.113735	2.433191	2.239290
45	8	0	1.024610	4.587322	1.475005
46	6	0	-0.509953	2.692798	2.534412
47	9	0	-1.369111	3.698964	2.534366
48	9	0	-0.154829	2.425466	3.785388
49	9	0	-1.108497	1.611527	2.025039
50	16	0	-0.256126	2.793006	-0.944202
51	8	0	-0.503658	1.644224	-1.825018
52	8	0	-1.402871	3.506548	-0.391423
53	6	0	0.616182	3.992554	-2.051770
54	9	0	-0.215344	4.344165	-3.031182
55	9	0	0.991111	5.069278	-1.392195
56	9	0	1.685773	3.406958	-2.588129
57	6	0	0.193562	-1.496982	1.979587
58	6	0	-0.584162	-2.398179	2.718507
59	6	0	1.140654	-0.699161	2.640286
60	6	0	-0.407197	-2.517621	4.091091
61	1	0	-1.319075	-3.011968	2.206168
62	6	0	1.301622	-0.816214	4.015810
63	1	0	1.741723	0.012058	2.090079
64	6	0	0.535221	-1.726556	4.742968
65	1	0	-1.008571	-3.225484	4.652683
66	1	0	2.025662	-0.179687	4.514492
67	1	0	0.668648	-1.809974	5.817808

Zero-point correction= 0.471540 (Hartree/Particle)
Thermal correction to Energy= 0.517060
Thermal correction to Enthalpy= 0.518004
Thermal correction to Gibbs Free Energy= 0.381824
Sum of electronic and zero-point Energies= -3561.299932
Sum of electronic and thermal Energies= -3561.254412
Sum of electronic and thermal Enthalpies= -3561.253468
Sum of electronic and thermal Free Energies(333K)= -3561.406163
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.936186

TS16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.820550	0.355876	-1.389478
2	8	0	2.209014	0.207763	-0.145543
3	1	0	1.660152	1.055625	-0.006399
4	6	0	1.940765	-0.228163	-2.399726
5	1	0	1.219771	0.545140	-2.673194
6	1	0	2.538489	-0.487423	-3.275901
7	6	0	1.201041	-1.439979	-1.830630
8	1	0	0.352488	-1.669115	-2.482657
9	1	0	1.849638	-2.325651	-1.813604
10	6	0	0.704082	-1.222547	-0.460812
11	16	0	4.441179	-0.186746	-1.286042
12	8	0	5.085932	0.675886	-0.317718
13	8	0	4.867134	-0.276175	-2.676877
14	6	0	4.394529	-1.832099	-0.610240
15	6	0	4.557318	-2.920081	-1.466963
16	6	0	4.186167	-2.002516	0.757776
17	6	0	4.493336	-4.206479	-0.939488
18	1	0	4.750737	-2.746400	-2.521133
19	6	0	4.112647	-3.294469	1.268993
20	1	0	4.092585	-1.135935	1.402882
21	6	0	4.262989	-4.391876	0.422978
22	1	0	4.631295	-5.064376	-1.591577
23	1	0	3.941427	-3.441774	2.331270
24	1	0	4.210585	-5.398147	0.829596
25	6	0	0.091352	-1.523285	0.607305
26	6	0	-3.743393	-1.514212	-0.935734
27	6	0	-5.736534	-0.635054	-1.455663

28	6	0	-5.844810	-1.983240	-1.568657
29	1	0	-6.460703	0.148218	-1.618516
30	1	0	-6.679652	-2.606669	-1.849434
31	7	0	-4.445520	-0.368878	-1.068331
32	7	0	-4.612080	-2.503563	-1.244024
33	79	0	-1.819837	-1.622684	-0.337059
34	6	0	-4.300274	-3.919086	-1.243763
35	1	0	-4.952100	-4.446612	-0.542035
36	1	0	-4.431484	-4.333131	-2.247323
37	1	0	-3.261571	-4.041943	-0.934984
38	6	0	-3.896124	0.963631	-0.838338
39	1	0	-4.656628	1.703059	-1.092099
40	1	0	-3.612183	1.082192	0.209034
41	1	0	-3.014244	1.117694	-1.461331
42	7	0	0.536320	2.277267	0.187217
43	16	0	0.593185	3.084354	1.609972
44	8	0	1.687441	2.474093	2.349876
45	8	0	0.479980	4.526851	1.494281
46	6	0	-0.962749	2.544021	2.507782
47	9	0	-1.899047	3.473214	2.422540
48	9	0	-0.659510	2.347989	3.785764
49	9	0	-1.440577	1.402287	2.003734
50	16	0	-0.524401	2.647324	-0.966985
51	8	0	-0.691386	1.465105	-1.820237
52	8	0	-1.718472	3.337955	-0.491961
53	6	0	0.372082	3.840022	-2.061890
54	9	0	-0.431338	4.172308	-3.069865
55	9	0	0.718439	4.927634	-1.398807
56	9	0	1.459999	3.251676	-2.551657
57	6	0	0.164144	-1.484028	2.059784
58	6	0	-0.709769	-2.268487	2.827200
59	6	0	1.103513	-0.674211	2.715653
60	6	0	-0.646472	-2.246868	4.215392
61	1	0	-1.433117	-2.903102	2.321588
62	6	0	1.149513	-0.643253	4.104022
63	1	0	1.776736	-0.047097	2.144435
64	6	0	0.280722	-1.429938	4.858009
65	1	0	-1.327043	-2.863952	4.795742
66	1	0	1.862360	0.014053	4.593133
67	1	0	0.321964	-1.401040	5.943465

Zero-point correction= 0.471085 (Hartree/Particle)
Thermal correction to Energy= 0.515022
Thermal correction to Enthalpy= 0.515966
Thermal correction to Gibbs Free Energy= 0.386579
Sum of electronic and zero-point Energies= -3561.283993
Sum of electronic and thermal Energies= -3561.240056
Sum of electronic and thermal Enthalpies= -3561.239111
Sum of electronic and thermal Free Energies(333K)= -3561.384208
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.905565

TS17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.203988	1.531802	-1.306705
2	8	0	-1.069384	1.058392	0.008016
3	1	0	-1.761254	-0.375817	0.055394
4	6	0	-0.124720	2.462878	-1.628136
5	1	0	-0.416528	2.998653	-2.534990
6	1	0	0.018838	3.180938	-0.805070
7	6	0	1.157335	1.683284	-1.872001
8	1	0	1.010171	0.986801	-2.708380
9	1	0	1.943845	2.383414	-2.173916
10	6	0	1.604237	0.907453	-0.665106
11	16	0	-2.761715	2.230479	-1.455467
12	8	0	-3.699821	1.173030	-1.114453
13	8	0	-2.777115	2.879305	-2.763808
14	6	0	-2.866648	3.486358	-0.202519
15	6	0	-2.702041	4.819786	-0.572485
16	6	0	-3.065246	3.111453	1.127529
17	6	0	-2.745435	5.802707	0.412644
18	1	0	-2.565283	5.070916	-1.620278
19	6	0	-3.099405	4.106453	2.100948
20	1	0	-3.202930	2.066800	1.388041
21	6	0	-2.940122	5.445408	1.746160
22	1	0	-2.632942	6.847890	0.137380
23	1	0	-3.260551	3.833030	3.140599
24	1	0	-2.975071	6.215707	2.512849
25	6	0	0.834046	0.520228	0.303592
26	6	0	5.492197	-0.245052	-0.056196
27	6	0	7.393892	-1.452088	-0.096161
28	6	0	7.643526	-0.293311	0.606987
29	1	0	8.033302	-2.295087	-0.345036
30	1	0	8.544907	0.077395	1.086998
31	7	0	6.075842	-1.401755	-0.497417
32	7	0	6.469204	0.429922	0.618455
33	79	0	3.558519	0.327644	-0.359410
34	6	0	6.315665	1.748993	1.254198
35	1	0	5.275383	2.058314	1.146603
36	1	0	6.561696	1.686516	2.332501

37	1	0	6.970118	2.496141	0.758849
38	6	0	5.404497	-2.473254	-1.253303
39	1	0	5.218770	-3.350719	-0.599870
40	1	0	4.449422	-2.096039	-1.622698
41	1	0	6.027307	-2.771950	-2.116674
42	7	0	-2.242029	-1.340636	0.115346
43	16	0	-1.738612	-2.507119	-0.970459
44	8	0	-0.353939	-2.251076	-1.330365
45	8	0	-2.199145	-3.810573	-0.538921
46	16	0	-3.072942	-1.603071	1.545713
47	8	0	-2.664863	-2.832831	2.194855
48	8	0	-3.052087	-0.322376	2.231782
49	6	0	-2.736340	-2.055226	-2.476442
50	6	0	-4.829303	-1.866712	1.002969
51	9	0	-5.557242	-1.991739	2.112209
52	9	0	-4.922562	-2.977076	0.286017
53	9	0	-5.267551	-0.838404	0.301620
54	9	0	-2.254551	-0.959011	-3.030410
55	9	0	-2.627944	-3.067396	-3.338471
56	9	0	-4.011501	-1.888066	-2.150353
57	6	0	0.683929	-0.165732	1.562871
58	6	0	0.133975	0.491827	2.672764
59	6	0	1.106845	-1.499738	1.685897
60	6	0	0.024211	-0.171659	3.886715
61	1	0	-0.228543	1.507266	2.555538
62	6	0	1.003775	-2.150301	2.909066
63	1	0	1.473431	-2.017152	0.805135
64	6	0	0.463998	-1.487935	4.010187
65	1	0	-0.421635	0.335390	4.737342
66	1	0	1.315809	-3.187074	2.995720
67	1	0	0.363603	-2.005794	4.959597

Zero-point correction= 0.470680 (Hartree/Particle)
Thermal correction to Energy= 0.514839
Thermal correction to Enthalpy= 0.515784
Thermal correction to Gibbs Free Energy= 0.384807
Sum of electronic and zero-point Energies= -3561.286021
Sum of electronic and thermal Energies= -3561.241862
Sum of electronic and thermal Enthalpies= -3561.240918
Sum of electronic and thermal Free Energies(333K)= -3561.387789
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.908282

INT19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.024199	0.003988	0.351671
2	8	0	2.178001	-1.191463	1.095082
3	1	0	2.051747	-0.875918	2.007799
4	6	0	1.831379	-0.361176	-1.047550
5	1	0	2.770166	-0.607720	-1.564171
6	1	0	1.218038	-1.266579	-1.031127
7	6	0	1.105003	0.751367	-1.809318
8	1	0	1.743936	1.641593	-1.868342
9	1	0	0.897561	0.413965	-2.831675
10	6	0	-0.130877	1.192031	-1.168489
11	16	0	3.377902	1.029226	0.695338
12	8	0	3.390536	1.049762	2.149599
13	8	0	3.133539	2.213369	-0.116851
14	6	0	4.830790	0.213256	0.105466
15	6	0	5.354392	0.579870	-1.135372
16	6	0	5.415853	-0.785105	0.885712
17	6	0	6.487437	-0.077374	-1.603973
18	1	0	4.899221	1.389092	-1.697707
19	6	0	6.545427	-1.433809	0.400629
20	1	0	5.006649	-1.026723	1.860186
21	6	0	7.076553	-1.082999	-0.839988
22	1	0	6.917360	0.205190	-2.560155
23	1	0	7.020068	-2.206582	0.997624
24	1	0	7.964226	-1.589096	-1.208237
25	6	0	-1.118673	1.707443	-0.640396
26	6	0	-2.475033	-2.172845	0.139195
27	6	0	-3.818969	-3.961461	0.203626
28	6	0	-2.909945	-4.092433	1.203551
29	1	0	-4.628895	-4.605164	-0.104308
30	1	0	-2.777454	-4.870994	1.939267
31	7	0	-3.535425	-2.778755	-0.436649
32	7	0	-2.093858	-2.988721	1.145526
33	79	0	-1.639825	-0.406059	-0.348761
34	6	0	-4.284998	-2.282392	-1.579345
35	1	0	-3.867689	-1.322714	-1.884458
36	1	0	-4.209266	-2.989926	-2.408681
37	1	0	-5.333734	-2.148836	-1.303419
38	6	0	-1.012668	-2.715185	2.081200
39	1	0	-0.147092	-2.319227	1.545864
40	1	0	-1.341316	-1.997675	2.837752
41	1	0	-0.729875	-3.649783	2.567737
42	6	0	-2.094582	2.764758	-0.091500
43	6	0	-3.309733	2.994412	-0.737362
44	6	0	-1.763757	3.492729	1.051374
45	6	0	-4.193502	3.952317	-0.240781

46	1	0	-3.569916	2.420870	-1.638802
47	6	0	-2.648118	4.450268	1.548803
48	1	0	-0.806148	3.311727	1.560641
49	6	0	-3.862787	4.680256	0.902876
50	1	0	-5.151040	4.133831	-0.750163
51	1	0	-2.387189	5.023799	2.450164
52	1	0	-4.559792	5.435436	1.294260

Zero-point correction= 0.415510 (Hartree/Particle)
Thermal correction to Energy= 0.444974
Thermal correction to Enthalpy= 0.445918
Thermal correction to Gibbs Free Energy= 0.349068
Sum of electronic and zero-point Energies= -1735.329353
Sum of electronic and thermal Energies= -1735.299889
Sum of electronic and thermal Enthalpies= -1735.298945
Sum of electronic and thermal Free Energies(333K)= -1735.407521
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1736.861688

INT20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.676320	0.837946	-0.272270
2	8	0	2.577507	-0.547993	-0.124942
3	1	0	1.681254	-0.700684	0.245023
4	6	0	2.689795	1.177566	-1.685356
5	1	0	3.013350	2.217289	-1.772660
6	1	0	3.376359	0.525199	-2.243135
7	6	0	1.267763	1.002683	-2.235586
8	1	0	1.238841	1.282449	-3.295006
9	1	0	0.963645	-0.045903	-2.153529
10	6	0	0.323530	1.827497	-1.469174
11	16	0	3.972659	1.404872	0.680668
12	8	0	3.656675	1.030873	2.045688
13	8	0	4.150218	2.795386	0.274670
14	6	0	5.395834	0.478124	0.158179
15	6	0	6.306313	1.069913	-0.715194
16	6	0	5.563942	-0.827450	0.618183
17	6	0	7.410899	0.335038	-1.135526
18	1	0	6.152395	2.096211	-1.033325
19	6	0	6.669386	-1.551418	0.184641
20	1	0	4.840384	-1.255357	1.303033
21	6	0	7.588797	-0.972669	-0.688881
22	1	0	8.135771	0.786231	-1.807235
23	1	0	6.815118	-2.569690	0.533305
24	1	0	8.452585	-1.543167	-1.019547
25	6	0	-0.109815	2.694542	-0.699311
26	6	0	-3.531918	0.178437	-0.922761
27	6	0	-5.287022	-1.168452	-1.254405
28	6	0	-5.541690	-0.428665	-0.146558
29	1	0	-5.870161	-1.930139	-1.748156
30	1	0	-6.393244	-0.414816	0.515627
31	7	0	-4.051902	-0.776338	-1.717751
32	7	0	-4.455736	0.395908	0.035831
33	79	0	-1.751005	1.097430	-1.061226
34	6	0	-4.247970	1.251908	1.191309
35	1	0	-3.847434	2.214539	0.867573
36	1	0	-5.206125	1.410197	1.689214
37	1	0	-3.538993	0.780272	1.875597
38	6	0	-3.349307	-1.409984	-2.822817
39	1	0	-2.688187	-0.677521	-3.288530
40	1	0	-2.758011	-2.250706	-2.449119
41	1	0	-4.081615	-1.754928	-3.556100
42	7	0	-0.175941	-1.420317	0.285881
43	16	0	-0.618937	-1.377550	1.845050
44	8	0	0.295841	-2.092178	2.721238
45	8	0	-0.960208	0.018307	2.126465
46	6	0	-2.238780	-2.273190	2.063066
47	9	0	-3.113999	-1.956591	1.108933
48	9	0	-2.748342	-1.881284	3.231200
49	9	0	-2.065619	-3.582175	2.083155
50	16	0	-0.200683	-2.680069	-0.721324
51	8	0	-1.466949	-3.412241	-0.726599
52	8	0	0.338834	-2.204745	-1.993449
53	6	0	1.039457	-3.911757	-0.098211
54	9	0	1.247888	-4.819997	-1.045823
55	9	0	2.186027	-3.310912	0.189264
56	9	0	0.569548	-4.513481	0.985712
57	6	0	-0.477296	3.723554	0.226713
58	6	0	-0.752736	5.022390	-0.225919
59	6	0	-0.532293	3.422837	1.598170
60	6	0	-1.073900	6.015442	0.690060
61	1	0	-0.704839	5.240528	-1.288484
62	6	0	-0.854516	4.427869	2.501740
63	1	0	-0.326785	2.409722	1.935967
64	6	0	-1.124326	5.719688	2.052111
65	1	0	-1.282039	7.022957	0.341868
66	1	0	-0.888458	4.200481	3.563183
67	1	0	-1.371966	6.500707	2.765770

Zero-point correction= 0.471994 (Hartree/Particle)

Thermal correction to Energy= 0.517358
Thermal correction to Enthalpy= 0.518302
Thermal correction to Gibbs Free Energy= 0.384500
Sum of electronic and zero-point Energies= -3561.304955
Sum of electronic and thermal Energies= -3561.259591
Sum of electronic and thermal Enthalpies= -3561.258647
Sum of electronic and thermal Free Energies(333K)= -3561.408686
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3563.937399

TS18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.205973	-1.721460	-0.520129
2	8	0	-1.603028	-1.370564	0.760710
3	1	0	-1.760552	-0.384328	0.782697
4	6	0	-1.111651	-0.625235	-1.521142
5	1	0	-1.885736	-0.687189	-2.290073
6	1	0	-1.198138	0.327290	-1.000539
7	6	0	0.307422	-0.875609	-2.010187
8	1	0	0.316620	-1.574120	-2.854949
9	1	0	0.859673	0.029395	-2.284839
10	6	0	0.865308	-1.527358	-0.806694
11	16	0	-2.204074	-3.059700	-1.057111
12	8	0	-2.089740	-4.070159	-0.021452
13	8	0	-1.742754	-3.299582	-2.420467
14	6	0	-3.853813	-2.424443	-1.094488
15	6	0	-4.452896	-2.200535	-2.334880
16	6	0	-4.507272	-2.144226	0.106185
17	6	0	-5.743986	-1.685926	-2.367819
18	1	0	-3.914594	-2.446674	-3.244766
19	6	0	-5.790826	-1.611960	0.051698
20	1	0	-4.015588	-2.319931	1.055416
21	6	0	-6.406202	-1.387637	-1.177877
22	1	0	-6.231903	-1.515472	-3.323160
23	1	0	-6.299581	-1.358381	0.976009
24	1	0	-7.410106	-0.973256	-1.209450
25	6	0	1.678694	-1.846167	0.114381
26	6	0	4.637411	0.943546	-0.673540
27	6	0	6.611647	1.928430	-1.095795
28	6	0	5.741400	2.895780	-0.714430
29	1	0	7.651372	1.982264	-1.380192
30	1	0	5.871590	3.961519	-0.604273
31	7	0	5.916540	0.740277	-1.065273
32	7	0	4.540599	2.274283	-0.458786
33	79	0	3.177468	-0.433396	-0.410260
34	6	0	6.495021	-0.548425	-1.394116
35	1	0	5.707311	-1.301529	-1.352195
36	1	0	6.916541	-0.521233	-2.402459
37	1	0	7.278472	-0.804562	-0.675488
38	6	0	3.337249	2.978150	-0.040181
39	1	0	2.550207	2.260021	0.195351
40	1	0	3.553370	3.572595	0.850964
41	1	0	2.992707	3.635304	-0.842524
42	7	0	-1.967587	1.372279	0.916451
43	16	0	-3.454775	1.759532	1.463771
44	8	0	-4.084254	0.551079	1.975219
45	8	0	-3.538284	3.014865	2.189576
46	16	0	-0.628527	2.224913	1.190463
47	8	0	-0.482416	2.793623	2.516965
48	8	0	0.459748	1.431922	0.608487
49	6	0	-4.289497	2.056134	-0.160421
50	6	0	-0.719832	3.673541	0.040173
51	9	0	0.467394	4.292992	0.048288
52	9	0	-1.651802	4.538249	0.399044
53	9	0	-0.962360	3.254124	-1.202441
54	9	0	-3.819973	3.161075	-0.732066
55	9	0	-4.084912	1.030134	-0.987491
56	9	0	-5.596006	2.192079	0.037856
57	6	0	1.773409	-2.690535	1.297420
58	6	0	0.819848	-3.693766	1.522068
59	6	0	2.811248	-2.520800	2.224145
60	6	0	0.908782	-4.500109	2.649427
61	1	0	0.004997	-3.838671	0.822153
62	6	0	2.892232	-3.327917	3.352541
63	1	0	3.549611	-1.739364	2.062103
64	6	0	1.941512	-4.322478	3.567616
65	1	0	0.158149	-5.268686	2.810727
66	1	0	3.698171	-3.177376	4.065600
67	1	0	2.003901	-4.954939	4.449107

Zero-point correction= 0.470221 (Hartree/Particle)
Thermal correction to Energy= 0.514853
Thermal correction to Enthalpy= 0.515797
Thermal correction to Gibbs Free Energy= 0.384073
Sum of electronic and zero-point Energies= -3561.272497
Sum of electronic and thermal Energies= -3561.227865
Sum of electronic and thermal Enthalpies= -3561.226921
Sum of electronic and thermal Free Energies(333K)= -3561.374632
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3563.898461

TS19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.233565	-1.134316	-0.380900
2	8	0	-2.524258	0.045644	0.293175
3	1	0	-1.662541	0.524036	0.431887
4	6	0	-1.988354	-0.918517	-1.801814
5	1	0	-2.154491	-1.874764	-2.304035
6	1	0	-2.669561	-0.151302	-2.183677
7	6	0	-0.525227	-0.481358	-1.980735
8	1	0	-0.203399	-0.668720	-3.010143
9	1	0	-0.421572	0.593917	-1.800767
10	6	0	0.322023	-1.217834	-0.995062
11	16	0	-3.465719	-2.273017	0.032732
12	8	0	-3.501122	-2.312912	1.480610
13	8	0	-3.144942	-3.448501	-0.768633
14	6	0	-4.969503	-1.557425	-0.576088
15	6	0	-5.541277	-2.085756	-1.731769
16	6	0	-5.537092	-0.478761	0.102634
17	6	0	-6.715638	-1.519237	-2.216829
18	1	0	-5.074784	-2.933613	-2.223103
19	6	0	-6.705781	0.081116	-0.401733
20	1	0	-5.064043	-0.089203	0.996915
21	6	0	-7.292527	-0.437410	-1.555090
22	1	0	-7.180277	-1.923873	-3.111339
23	1	0	-7.159079	0.925748	0.108518
24	1	0	-8.207072	0.005274	-1.940059
25	6	0	-0.087886	-1.851273	0.033873
26	6	0	4.368273	-0.759968	-0.527882
27	6	0	6.570199	-0.441124	-0.844000
28	6	0	6.319507	-0.300801	0.481060
29	1	0	7.488199	-0.356657	-1.404925
30	1	0	6.978841	-0.077093	1.305525
31	7	0	5.362453	-0.724527	-1.443254
32	7	0	4.968504	-0.496817	0.653652
33	79	0	2.384213	-1.068631	-0.800302
34	6	0	4.286659	-0.458078	1.939219
35	1	0	4.205205	-1.467297	2.352298
36	1	0	4.865204	0.168845	2.620555
37	1	0	3.291983	-0.023984	1.819221
38	6	0	5.186244	-0.917865	-2.868804
39	1	0	4.153332	-1.217964	-3.049211
40	1	0	5.390465	0.012940	-3.405492
41	1	0	5.859715	-1.702230	-3.224587
42	7	0	-0.554037	1.994203	0.385529
43	16	0	0.752937	2.276999	1.293944
44	8	0	0.664960	3.396377	2.216950
45	8	0	1.184997	0.968552	1.797219
46	6	0	2.104569	2.755442	0.085115
47	9	0	1.843306	2.288058	-1.135523
48	9	0	3.253740	2.206473	0.502617
49	9	0	2.265123	4.061863	0.031663
50	16	0	-1.301945	3.192865	-0.424457
51	8	0	-0.465150	4.366375	-0.634427
52	8	0	-2.004035	2.577823	-1.543567
53	6	0	-2.644564	3.730547	0.730692
54	9	0	-3.406037	4.626473	0.108674
55	9	0	-3.397939	2.688699	1.074206
56	9	0	-2.132185	4.274767	1.823160
57	6	0	-0.149938	-2.610087	1.230952
58	6	0	-0.353029	-4.001350	1.168614
59	6	0	-0.038870	-1.965967	2.477546
60	6	0	-0.431011	-4.737785	2.340399
61	1	0	-0.467459	-4.477742	0.200421
62	6	0	-0.116948	-2.717243	3.641413
63	1	0	0.121969	-0.892193	2.504929
64	6	0	-0.313487	-4.096379	3.573883
65	1	0	-0.593285	-5.810628	2.296327
66	1	0	-0.032349	-2.225559	4.606159
67	1	0	-0.381416	-4.676655	4.490405

Zero-point correction= 0.471197 (Hartree/Particle)
Thermal correction to Energy= 0.515697
Thermal correction to Enthalpy= 0.516642
Thermal correction to Gibbs Free Energy= 0.382356
Sum of electronic and zero-point Energies= -3561.296905
Sum of electronic and thermal Energies= -3561.252405
Sum of electronic and thermal Enthalpies= -3561.251460
Sum of electronic and thermal Free Energies(333K)= -3561.401966
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.922066

INT21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.224694	-1.117295	-0.383905
2	8	0	-2.485473	0.075956	0.281173

3	1	0	-1.611928	0.553645	0.392155
4	6	0	-2.010489	-0.912863	-1.814431
5	1	0	-2.185616	-1.873737	-2.304845
6	1	0	-2.700888	-0.147598	-2.184402
7	6	0	-0.546359	-0.482847	-2.006735
8	1	0	-0.227277	-0.693890	-3.031469
9	1	0	-0.436852	0.595465	-1.847339
10	6	0	0.291213	-1.213569	-1.004717
11	16	0	-3.502655	-2.217439	0.057546
12	8	0	-3.527179	-2.225995	1.503692
13	8	0	-3.212221	-3.414095	-0.727344
14	6	0	-4.992783	-1.481930	-0.558909
15	6	0	-5.591115	-2.032495	-1.690635
16	6	0	-5.546560	-0.389700	0.110486
17	6	0	-6.774215	-1.475196	-2.163899
18	1	0	-5.138647	-2.892992	-2.170051
19	6	0	-6.724427	0.163794	-0.381462
20	1	0	-5.054253	0.017841	0.988037
21	6	0	-7.334184	-0.377123	-1.510933
22	1	0	-7.258027	-1.898164	-3.038249
23	1	0	-7.167041	1.017680	0.120554
24	1	0	-8.257218	0.056669	-1.884244
25	6	0	-0.217913	-1.819514	0.019395
26	6	0	4.335780	-0.807687	-0.540929
27	6	0	6.536384	-0.479466	-0.851551
28	6	0	6.291888	-0.389088	0.479083
29	1	0	7.452108	-0.372863	-1.412990
30	1	0	6.952234	-0.198085	1.308358
31	7	0	5.325297	-0.736676	-1.459047
32	7	0	4.941345	-0.591423	0.647046
33	79	0	2.347520	-1.092691	-0.819684
34	6	0	4.261832	-0.593844	1.934622
35	1	0	4.157416	-1.616182	2.303970
36	1	0	4.852687	-0.007961	2.639734
37	1	0	3.275172	-0.134493	1.833230
38	6	0	5.142573	-0.875207	-2.890254
39	1	0	4.104690	-1.142706	-3.078713
40	1	0	5.369366	0.068404	-3.392632
41	1	0	5.796522	-1.662579	-3.273594
42	7	0	-0.498801	1.994818	0.385313
43	16	0	0.798407	2.243806	1.318085
44	8	0	0.714235	3.355311	2.249011
45	8	0	1.199799	0.925012	1.817017
46	6	0	2.178570	2.713150	0.133349
47	9	0	1.921989	2.277750	-1.099021
48	9	0	3.306828	2.129177	0.553474
49	9	0	2.368440	4.015756	0.110288
50	16	0	-1.206075	3.215189	-0.426852
51	8	0	-0.335139	4.368782	-0.615299
52	8	0	-1.906956	2.626537	-1.559765
53	6	0	-2.553624	3.779759	0.709051
54	9	0	-3.274786	4.704624	0.084558
55	9	0	-3.341565	2.757804	1.025924
56	9	0	-2.048100	4.297285	1.817784
57	6	0	-0.248156	-2.596005	1.211097
58	6	0	-0.442186	-3.988128	1.129701
59	6	0	-0.100103	-1.977036	2.464964
60	6	0	-0.484925	-4.750405	2.290096
61	1	0	-0.581412	-4.447939	0.156233
62	6	0	-0.138709	-2.751554	3.620107
63	1	0	0.064667	-0.904051	2.510218
64	6	0	-0.336214	-4.131258	3.533763
65	1	0	-0.642219	-5.821402	2.231069
66	1	0	-0.024026	-2.278803	4.590396
67	1	0	-0.379888	-4.728908	4.440628

Zero-point correction= 0.473178 (Hartree/Particle)
Thermal correction to Energy= 0.517334
Thermal correction to Enthalpy= 0.518278
Thermal correction to Gibbs Free Energy= 0.387117
Sum of electronic and zero-point Energies= -3561.325476
Sum of electronic and thermal Energies= -3561.281320
Sum of electronic and thermal Enthalpies= -3561.280376
Sum of electronic and thermal Free Energies(333K)= -3561.427456
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.940823

TS20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.679204	0.009673	0.260756
2	8	0	1.677332	-0.221455	0.986179
3	1	0	3.097222	-0.578777	0.271315
4	6	0	0.828161	0.380282	-1.159539
5	1	0	1.501605	1.233788	-1.234568
6	1	0	1.289562	-0.483978	-1.653689
7	6	0	-0.614425	0.599298	-1.588674
8	1	0	-0.852610	1.669047	-1.644566
9	1	0	-0.834806	0.165004	-2.568685
10	6	0	-1.450569	-0.016811	-0.499753
11	16	0	-0.231025	2.542652	1.016038

12	8	0	0.144866	2.663721	2.452624
13	8	0	-1.684230	2.260123	0.685490
14	6	0	0.014488	4.192803	0.308892
15	6	0	-0.755841	4.621341	-0.767465
16	6	0	1.039540	4.982252	0.820852
17	6	0	-0.495844	5.864582	-1.337746
18	1	0	-1.569499	3.995647	-1.123244
19	6	0	1.293639	6.223791	0.243644
20	1	0	1.609570	4.625806	1.673708
21	6	0	0.530606	6.663225	-0.836369
22	1	0	-1.101310	6.215577	-2.169687
23	1	0	2.087676	6.850894	0.640569
24	1	0	0.733099	7.631953	-1.285525
25	6	0	-0.607057	-0.357632	0.550747
26	6	0	-5.420061	-0.844344	-0.624810
27	6	0	-7.600680	-0.935055	-1.180381
28	6	0	-7.431636	-1.685041	-0.064070
29	1	0	-8.485266	-0.714419	-1.758051
30	1	0	-8.139247	-2.253054	0.520339
31	7	0	-6.360516	-0.431816	-1.506457
32	7	0	-6.095144	-1.614332	0.260443
33	79	0	-3.417975	-0.418572	-0.593162
34	6	0	-5.492765	-2.310047	1.383928
35	1	0	-6.126952	-2.192045	2.265943
36	1	0	-5.377725	-3.373421	1.155104
37	1	0	-4.511801	-1.877813	1.587963
38	6	0	-6.109478	0.445232	-2.633164
39	1	0	-5.040357	0.657049	-2.670070
40	1	0	-6.416027	-0.041750	-3.563016
41	1	0	-6.658908	1.382918	-2.511395
42	7	0	4.000820	-0.908463	-0.174157
43	16	0	4.301772	-2.548424	-0.080291
44	8	0	5.720723	-2.808859	-0.067347
45	8	0	3.380281	-3.067061	0.907629
46	6	0	3.658150	-3.118680	-1.720861
47	9	0	2.356834	-2.844271	-1.797384
48	9	0	3.835327	-4.427355	-1.805490
49	9	0	4.292190	-2.511886	-2.707391
50	16	0	4.995490	0.285045	-0.792484
51	8	0	5.934637	-0.285425	-1.728494
52	8	0	4.118716	1.391235	-1.118879
53	6	0	5.944796	0.793277	0.715982
54	9	0	6.787476	1.753239	0.366381
55	9	0	5.099106	1.244084	1.627077
56	9	0	6.612439	-0.241896	1.193507
57	6	0	-0.950352	-0.940713	1.854732
58	6	0	-2.043401	-0.427266	2.564640
59	6	0	-0.224090	-2.014821	2.382095
60	6	0	-2.420506	-1.004006	3.773827
61	1	0	-2.546669	0.455882	2.180750
62	6	0	-0.613033	-2.590180	3.587050
63	1	0	0.645315	-2.395052	1.855030
64	6	0	-1.712356	-2.090843	4.282594
65	1	0	-3.253855	-0.585454	4.332444
66	1	0	-0.047892	-3.427072	3.987921
67	1	0	-2.004093	-2.536665	5.230106

Zero-point correction= 0.470515 (Hartree/Particle)
Thermal correction to Energy= 0.515128
Thermal correction to Enthalpy= 0.516072
Thermal correction to Gibbs Free Energy= 0.380620
Sum of electronic and zero-point Energies= -3561.301672
Sum of electronic and thermal Energies= -3561.257059
Sum of electronic and thermal Enthalpies= -3561.256115
Sum of electronic and thermal Free Energies(333K)= -3561.407987
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.912105

INT22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.015153	-1.823259	-0.580644
2	8	0	-0.872533	-2.538229	0.139133
3	1	0	-1.724471	-1.976323	0.145100
4	6	0	-0.357447	-1.359851	-1.916706
5	1	0	-0.791095	-2.191269	-2.475195
6	1	0	-1.121260	-0.580670	-1.803174
7	6	0	0.965911	-0.813343	-2.432697
8	1	0	1.530392	-1.622860	-2.917688
9	1	0	0.837309	-0.004005	-3.153660
10	6	0	1.669338	-0.377642	-1.138952
11	16	0	3.924468	-1.613829	-1.818065
12	8	0	3.369072	-2.836479	-1.179128
13	8	0	3.071416	-0.241016	-1.209209
14	6	0	5.416660	-1.184330	-0.920621
15	6	0	6.175841	-0.089844	-1.327472
16	6	0	5.808047	-1.996032	0.137598
17	6	0	7.347759	0.207079	-0.638712
18	1	0	5.853221	0.525505	-2.163584
19	6	0	6.984812	-1.691723	0.816153
20	1	0	5.185863	-2.843802	0.411382

21	6	0	7.750638	-0.593357	0.429807
22	1	0	7.949840	1.060276	-0.938402
23	1	0	7.305795	-2.314367	1.646660
24	1	0	8.670903	-0.362317	0.959399
25	6	0	1.136464	-1.322611	-0.122012
26	6	0	0.095514	3.191092	0.320681
27	6	0	-0.933849	5.180850	0.486650
28	6	0	-0.771737	4.694451	1.742182
29	1	0	-1.378794	6.098352	0.133831
30	1	0	-1.049262	5.104556	2.700827
31	7	0	-0.389735	4.248245	-0.367144
32	7	0	-0.135327	3.481594	1.618343
33	79	0	0.894736	1.467056	-0.408681
34	6	0	0.133583	2.575279	2.724205
35	1	0	0.177488	3.153689	3.649196
36	1	0	-0.656220	1.822115	2.777376
37	1	0	1.092544	2.080997	2.560542
38	6	0	-0.452473	4.324599	-1.813448
39	1	0	0.379791	3.757999	-2.233361
40	1	0	-1.393938	3.897172	-2.169667
41	1	0	-0.376326	5.368233	-2.126287
42	7	0	-3.070774	-1.054607	-0.031250
43	16	0	-4.240095	-1.726095	-0.949467
44	8	0	-5.341510	-0.824675	-1.245229
45	8	0	-3.557942	-2.449931	-2.012656
46	6	0	-4.921572	-3.046035	0.152187
47	9	0	-3.935065	-3.847028	0.547099
48	9	0	-5.811219	-3.757165	-0.531820
49	9	0	-5.505618	-2.516645	1.215563
50	16	0	-3.289664	0.215538	0.945954
51	8	0	-4.529011	0.235662	1.702427
52	8	0	-2.009468	0.408594	1.624815
53	6	0	-3.408546	1.680982	-0.197052
54	9	0	-3.051125	2.771376	0.490004
55	9	0	-2.568703	1.552448	-1.232226
56	9	0	-4.631464	1.853493	-0.657578
57	6	0	1.695377	-1.593033	1.202862
58	6	0	2.666264	-0.721245	1.723584
59	6	0	1.318605	-2.717702	1.952687
60	6	0	3.225003	-0.955276	2.972622
61	1	0	2.990676	0.130938	1.136661
62	6	0	1.891882	-2.949480	3.197355
63	1	0	0.583405	-3.406886	1.558860
64	6	0	2.838157	-2.069375	3.715131
65	1	0	3.973256	-0.270379	3.361885
66	1	0	1.592209	-3.824910	3.766280
67	1	0	3.277139	-2.253545	4.692166

Zero-point correction= 0.473122 (Hartree/Particle)
Thermal correction to Energy= 0.517331
Thermal correction to Enthalpy= 0.518275
Thermal correction to Gibbs Free Energy= 0.387943
Sum of electronic and zero-point Energies= -3561.368783
Sum of electronic and thermal Energies= -3561.324574
Sum of electronic and thermal Enthalpies= -3561.323630
Sum of electronic and thermal Free Energies(333K)= -3561.469787
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-3563.964342

INT23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.498448	0.389277	-0.781869
2	8	0	-1.417303	1.285375	-1.164709
3	1	0	-2.341384	0.839683	-1.027508
4	6	0	-0.512619	-0.941702	-1.388995
5	1	0	-1.353629	-1.496805	-0.965781
6	1	0	-0.693458	-0.820290	-2.458919
7	6	0	0.863380	-1.488635	-1.025923
8	1	0	0.808127	-2.501508	-0.620972
9	1	0	1.498527	-1.539174	-1.912869
10	6	0	1.454839	-0.489936	0.011101
11	16	0	1.597741	-1.272583	1.646957
12	8	0	1.931556	-0.242377	2.631211
13	8	0	2.485378	-2.431051	1.460363
14	6	0	-0.027173	-1.911477	2.012952
15	6	0	-0.283707	-3.269016	1.821521
16	6	0	-1.024601	-1.034799	2.439579
17	6	0	-1.571640	-3.747641	2.042258
18	1	0	0.524720	-3.928136	1.520377
19	6	0	-2.311265	-1.523926	2.644353
20	1	0	-0.798663	0.011765	2.619449
21	6	0	-2.583821	-2.875115	2.438487
22	1	0	-1.786161	-4.802775	1.897930
23	1	0	-3.098047	-0.840083	2.945513
24	1	0	-3.593883	-3.247286	2.583336
25	6	0	0.502511	0.654128	0.016363
26	6	0	5.460300	0.098705	-0.853520
27	6	0	7.459611	0.733239	-1.661500
28	6	0	7.673657	-0.279316	-0.786190
29	1	0	8.148266	1.309524	-2.260263

30	1	0	8.587034	-0.759411	-0.469726
31	7	0	6.098800	0.949048	-1.688537
32	7	0	6.439482	-0.654682	-0.303585
33	79	0	3.481164	-0.079789	-0.445737
34	6	0	0.581439	1.899573	0.786555
35	6	0	-0.590676	2.513413	1.263697
36	6	0	1.822759	2.466175	1.109370
37	6	0	-0.509163	3.664686	2.034975
38	1	0	-1.564981	2.084464	1.063259
39	6	0	1.893600	3.631645	1.859586
40	1	0	2.737055	1.989898	0.770650
41	6	0	0.728183	4.234372	2.325703
42	1	0	-1.424230	4.114066	2.408950
43	1	0	2.863618	4.060643	2.093833
44	1	0	0.784645	5.141164	2.921996
45	6	0	6.235777	-1.710307	0.676305
46	1	0	5.165450	-1.852486	0.837823
47	1	0	6.671371	-2.642411	0.307105
48	1	0	6.706944	-1.434041	1.623352
49	6	0	5.448105	1.953937	-2.506943
50	1	0	4.373066	1.894696	-2.333115
51	1	0	5.804651	2.950777	-2.233385
52	1	0	5.654148	1.768372	-3.564616
53	7	0	-3.761626	0.213877	-0.685369
54	16	0	-4.610883	0.997685	0.464561
55	8	0	-5.897992	0.411024	0.786399
56	8	0	-3.659907	1.322446	1.526077
57	6	0	-4.956350	2.630637	-0.333954
58	9	0	-3.801408	3.217971	-0.647008
59	9	0	-5.614300	3.401144	0.525005
60	9	0	-5.677879	2.478569	-1.432254
61	16	0	-4.438221	-0.727528	-1.833583
62	8	0	-5.805723	-0.393664	-2.183371
63	8	0	-3.416873	-0.894223	-2.860466
64	6	0	-4.528394	-2.383016	-1.003128
65	9	0	-5.181339	-3.223685	-1.796205
66	9	0	-3.297168	-2.861552	-0.798510
67	9	0	-5.151506	-2.307463	0.164025

Zero-point correction= 0.474027 (Hartree/Particle)
Thermal correction to Energy= 0.518159
Thermal correction to Enthalpy= 0.519103
Thermal correction to Gibbs Free Energy= 0.387636
Sum of electronic and zero-point Energies= -3561.371781
Sum of electronic and thermal Energies= -3561.327649
Sum of electronic and thermal Enthalpies= -3561.326705
Sum of electronic and thermal Free Energies(333K)= -3561.474156
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy = -3563.985460

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.416362	0.674283	1.967380
2	8	0	-1.105186	1.737841	2.401222
3	6	0	0.864328	0.355580	2.598704
4	1	0	1.602527	1.082357	2.250273
5	1	0	0.747934	0.484120	3.676717
6	6	0	1.112896	-1.078134	2.143722
7	1	0	2.127140	-1.217420	1.763120
8	1	0	0.994100	-1.768780	2.981299
9	6	0	0.046424	-1.364178	1.046699
10	16	0	0.835795	-1.560975	-0.580306
11	8	0	-0.207513	-1.592992	-1.605975
12	8	0	1.767650	-2.690793	-0.439158
13	6	0	1.823340	-0.093365	-0.811297
14	6	0	3.196767	-0.153191	-0.575738
15	6	0	1.198492	1.098423	-1.178238
16	6	0	3.950011	1.011326	-0.690197
17	1	0	3.654571	-1.104834	-0.323801
18	6	0	1.961156	2.258308	-1.276679
19	1	0	0.134705	1.119357	-1.394144
20	6	0	3.331353	2.214465	-1.025646
21	1	0	5.020921	0.979865	-0.510422
22	1	0	1.474548	3.194278	-1.530720
23	1	0	3.917993	3.126480	-1.087290
24	6	0	-0.863662	-0.187072	1.091464
25	6	0	-2.069257	0.061203	0.294307
26	6	0	-2.398114	1.369161	-0.104962
27	6	0	-2.879435	-1.001145	-0.131310
28	6	0	-3.512346	1.594440	-0.901630
29	1	0	-1.775767	2.210096	0.176027
30	6	0	-4.005940	-0.763835	-0.906445
31	1	0	-2.624235	-2.018535	0.146718
32	6	0	-4.325785	0.534415	-1.295016
33	1	0	-3.739915	2.609148	-1.214246
34	1	0	-4.626237	-1.598248	-1.220821
35	1	0	-5.202115	0.718615	-1.910760
36	1	0	-0.385324	-2.331730	1.196150

Zero-point correction= 0.286471 (Hartree/Particle)

Thermal correction to Energy= 0.303881
Thermal correction to Enthalpy= 0.304826
Thermal correction to Gibbs Free Energy= 0.239030
Sum of electronic and zero-point Energies= -1295.778507
Sum of electronic and thermal Energies= -1295.761097
Sum of electronic and thermal Enthalpies= -1295.760153
Sum of electronic and thermal Free Energies(333K)= -1295.833902
B2PLYP/def2-TZVP/SMD // PBE0/6-31G(d)-LANL2DZ energy =-1296.787027