Supporting Information

Mechanistic Insights into the Gold(I)-Catalyzed Annulation of Propiolates with Isoxazoles: A DFT Study

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Contents

Computational methods

All stationary points including the transition states and intermediates were optimized using the Gaussian 09 program package.[1] For all optimized geometries, the M06 density functional method[2] which includes long range correction was employed. The LANL2DZ basis set[3-4] in conjunction with the LANL2DZ pseudopotential was used to describe the Au atom and the 6-31G(d) basis set[5-6] was utilized for other atoms in the geometry optimization. Vibrational frequency analysis was performed on the optimized geometries to characterize them as minima or transition states. In addition, intrinsic reaction coordinate calculations (IRC)[7] were carried out to ensure that the optimized transition states connect to their respective reactants and products. To consider solvation effects, the optimized gas-phase structures were subjected to single-point energy (SPE) calculations at M06/SDD[8](Au)-6-311++G(d,p)(N, S, O, C, H) level of theory. The SMD solvation model[9] and 1,2-dichloroethane (DCE) as the solvent were employed for such SPE calculations. The translational entropy correction in solution was incorporated by employing the method proposed by Whitesides and co-workers.[10] Unless specified otherwise, the solvation Gibbs free energy was used for discussion and it was obtained from the addition of the solvation single-point energy and the thermal correction to the Gibbs free energy in gas phase. The Gibbs free energies were evaluated at 298.15 K and 1 atm. For description purpose, the 3D structures of some key transition states and intermediates were illustrated using the CLYview software.[11] To reduce the computational cost, the isopropyl groups of IPr ligand were replaced by methyl groups.

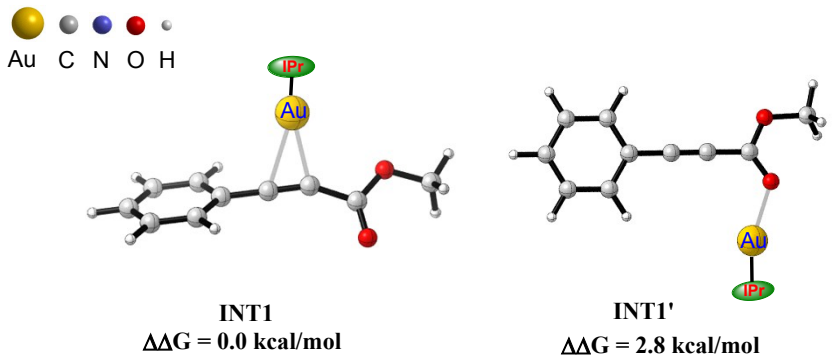


Figure S1. Diagram showing the coordination modes of Au(I)-catalyst to **1**.

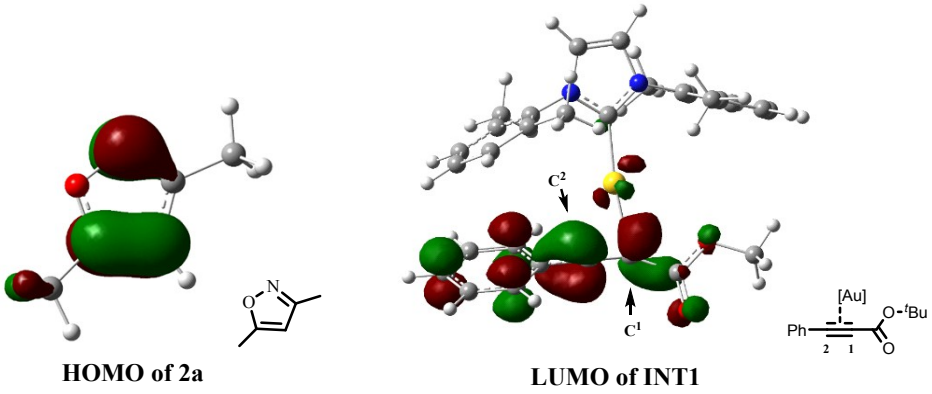


Figure S2. Diagram showing the HOMO of **2a** and the LUMO of the Au(I)-coordinated propiolate **INT1**.

For the annulation of **1** with **2a**, another molecule of **2a** could possibly undergo an intermolecular nucleophilic addition with **INT3a**. Nevertheless, the predicted energy barrier for this step via **TS9a** is substantially higher (3.8 kcal/mol) than that required for the formation of a three-membered intermediate via **TS7a** (Figure S3).

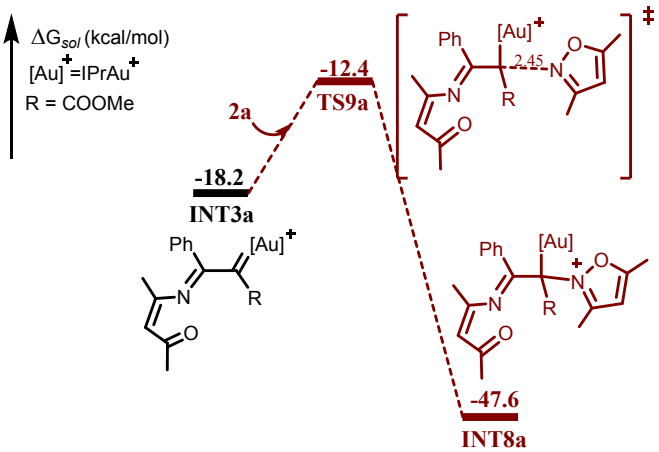


Figure S3. Energy profile showing the intermolecular nucleophilic addition of another molecule of **2a** to **INT3a**. Bond distances are given in Å.

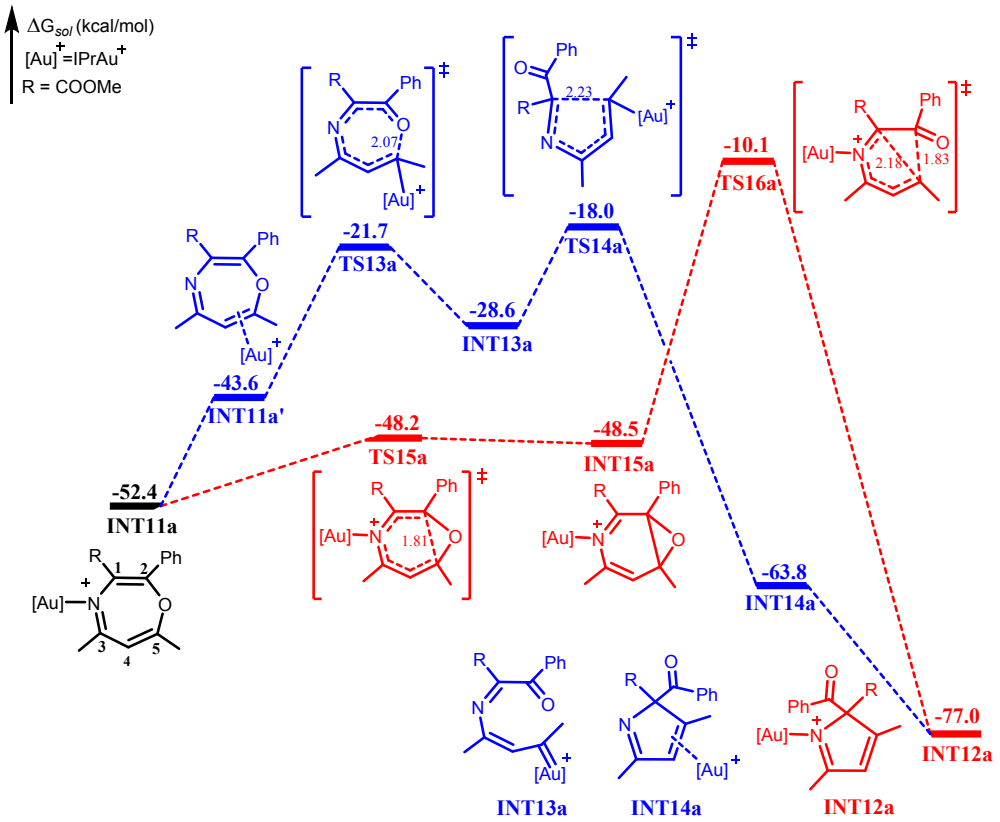


Figure S4. Energy profiles showing the alternative pathways for the formation of the five-membered azacycle **INT12a** from **INT11a**. Bond distances are given in Å.

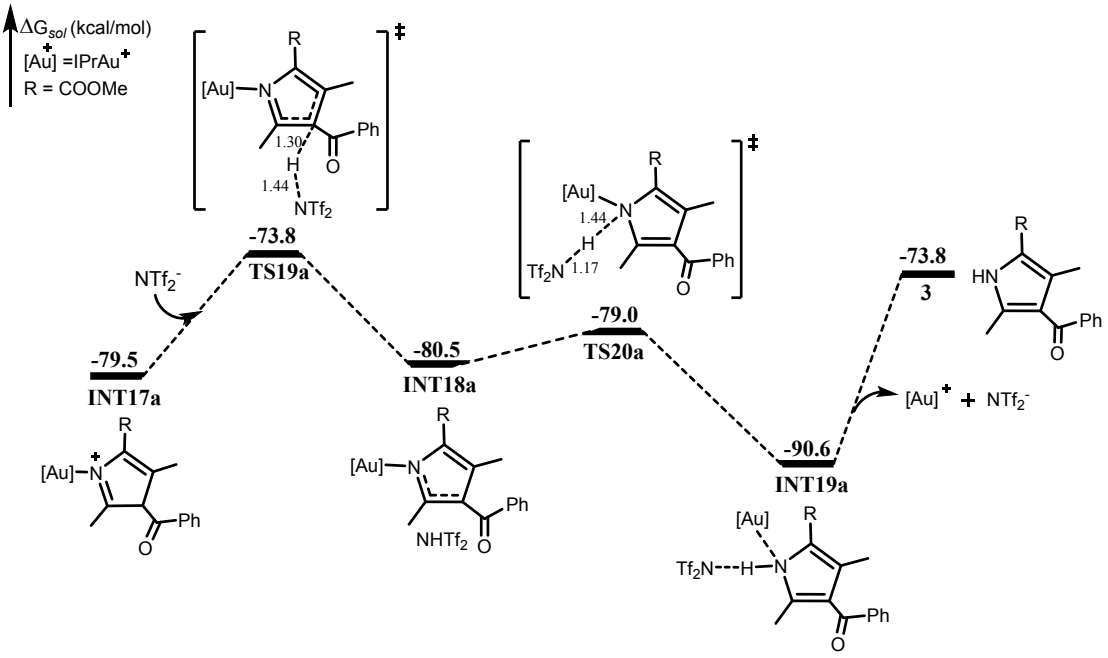


Figure S5. Energy profile showing the NTf_2 counter-ion assisted proton transfer to afford the expected product **3**. Bond distances are given in Å.

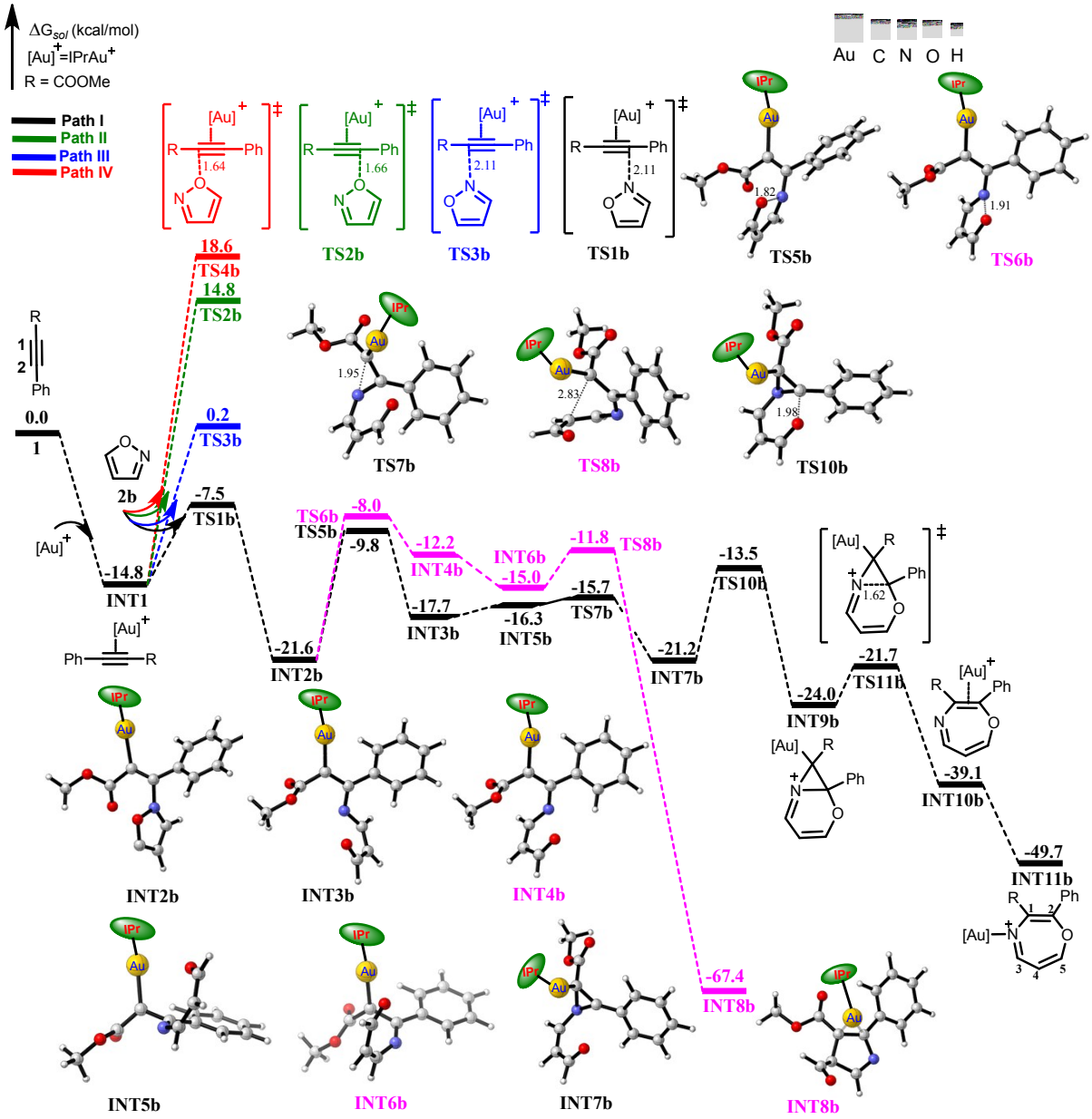


Figure S6. Energy profiles for the gold(I)-catalyzed annulation of **1** with **2b** and the subsequent formation of **INT11b** . Bond distances are given in Å.

For the annulation of **1** with **2b**, since two discrete molecules of **2b** would be required to produce product **4,** the possibility of another molecule of **2b** undergoing the intermolecular nucleophilic addition with **INT3b** were examined. The energy barrier via **TS9b** is 4.7 kcal/mol relative to **INT3b** which is 2.7 kcal/mol higher than the three-membered transition state, **TS7b** (Figure S7). Therefore this pathway is excluded.

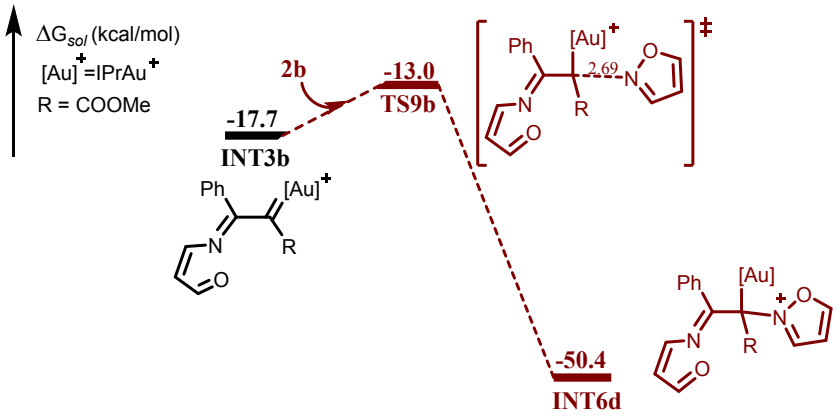


Figure S7. Energy profile showing the nucleophilic addition of another molecule of **2b** to **INT3b**. Bond distances are given in Å.

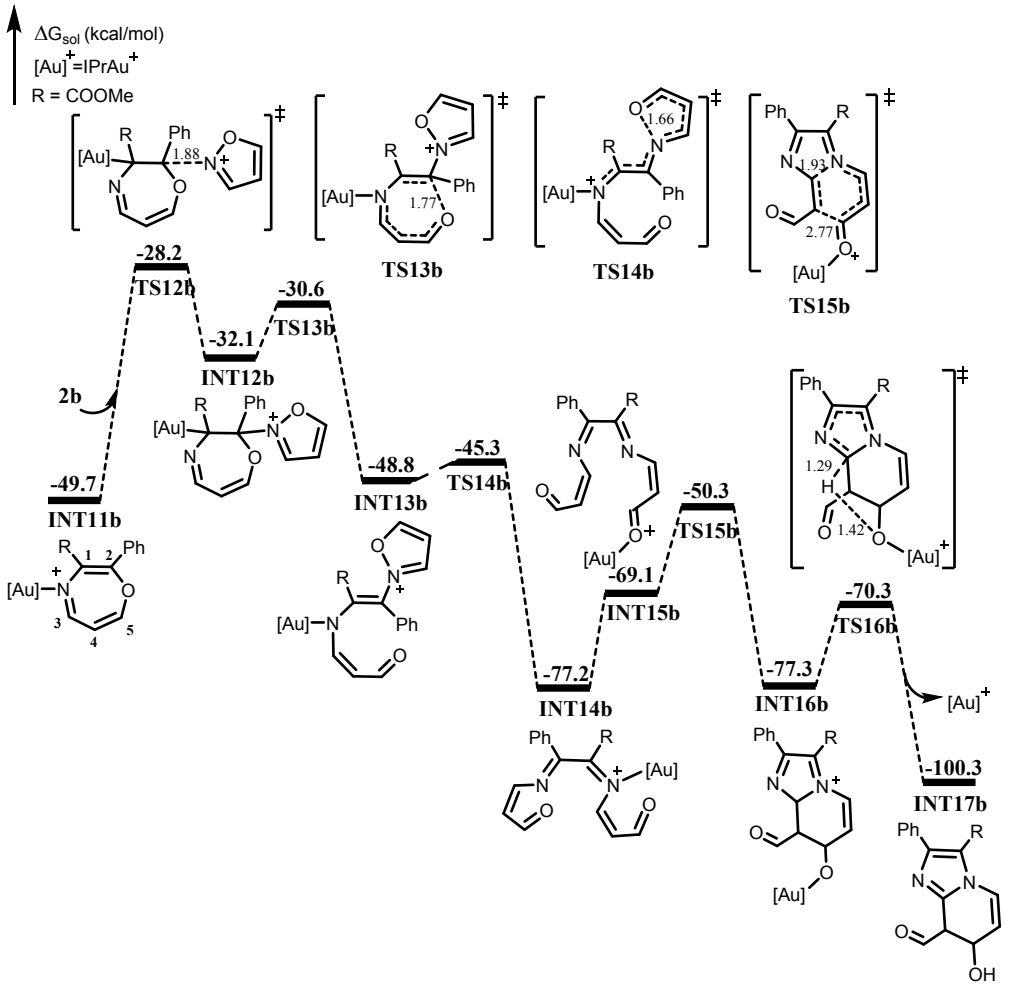


Figure S8. Energy profile showing the nucleophilic addition of the second substrate **2b** to **INT11b** and subsequent formation of **INT17b**. Bond distances are in Å

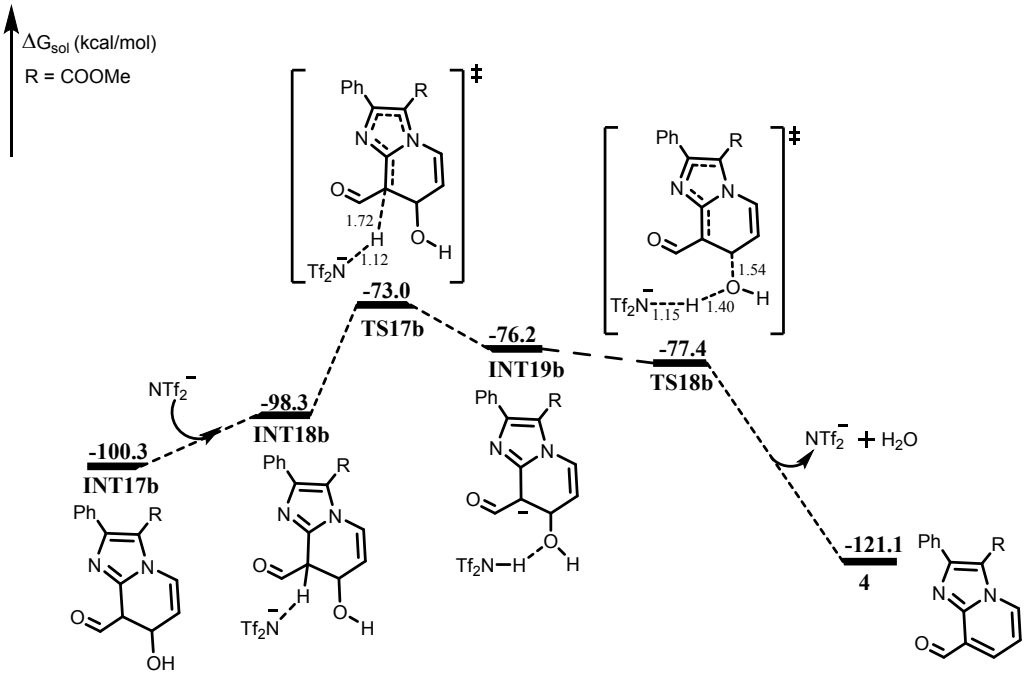


Figure S9. Energy profile showing the proton transfer step and loss of water to produce the desired imidazopyridine **4**. Bond distances are given in Å.

Due to the close energy barrier between **TS5b** and **TS6b** as shown in Figure S6, the formation of the five-membered intermediate **INT8b** might compete with formation of three-membered intermediate **INT7b**. As a result, a side product **5** would emerge from **INT8b** after counter-ion assisted proton transfer had taken place via **TS19b** and **TS20b** (Figure S10).

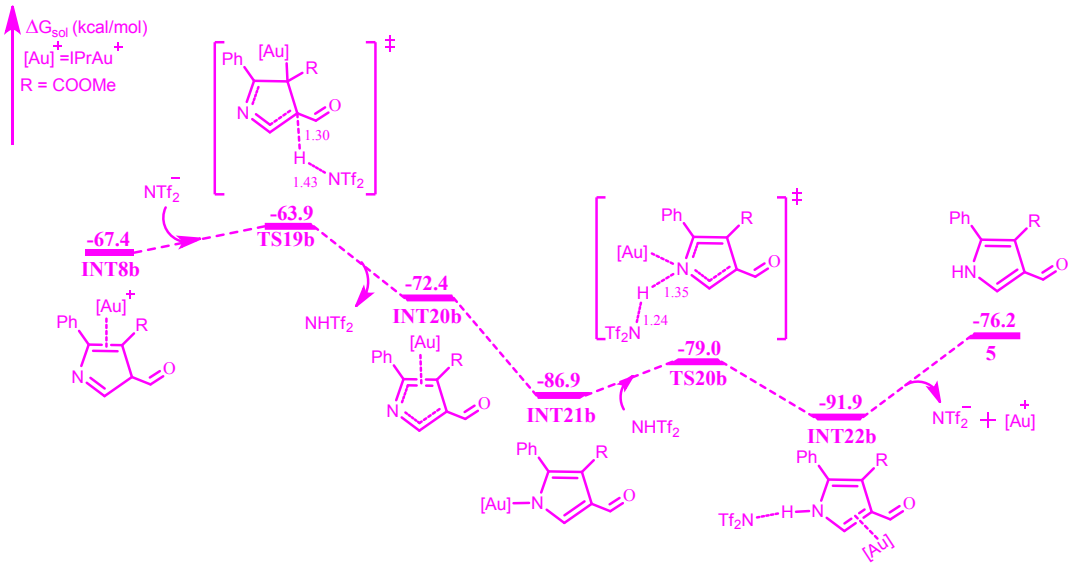


Figure S10. Energy profile showing the proton transfer step to afford pyrrole derivative **5** as side product. Bond distances are given in Å.

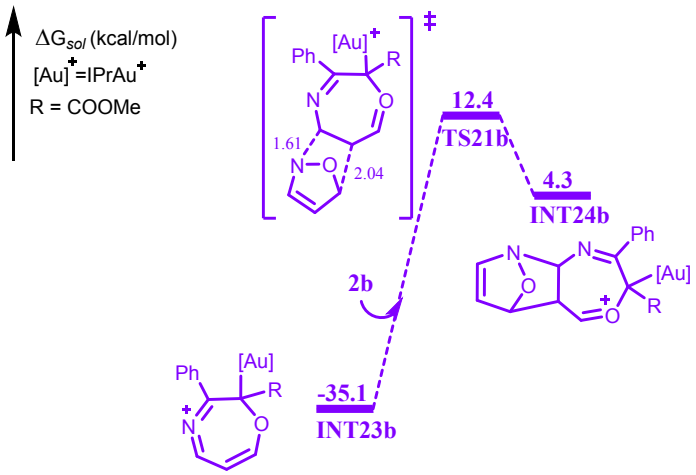


Figure S11. Energy profile showing the proposed nucleophilic addition of the second substrate **2b** to **INT23b** via cycloaddition. Bond distances are given in Å.

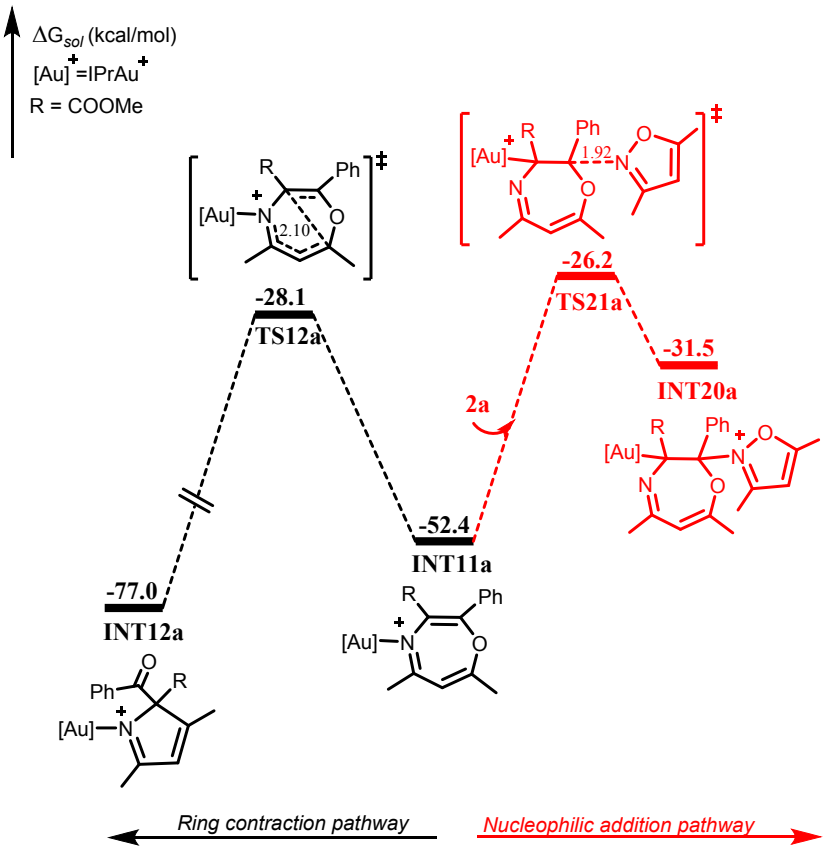


Figure S12. Energy profiles showing the preference for the ring contraction process in the annulation of **1** with **2a**, instead of the nucleophilic addition of another molecule of **2a**. Bond distances are given in Å.

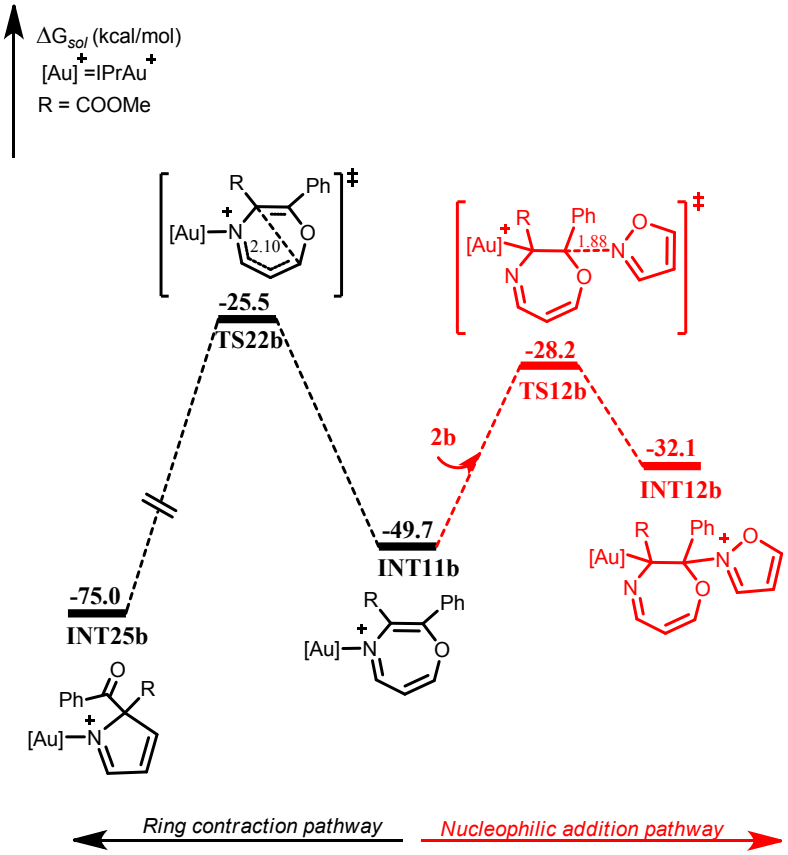
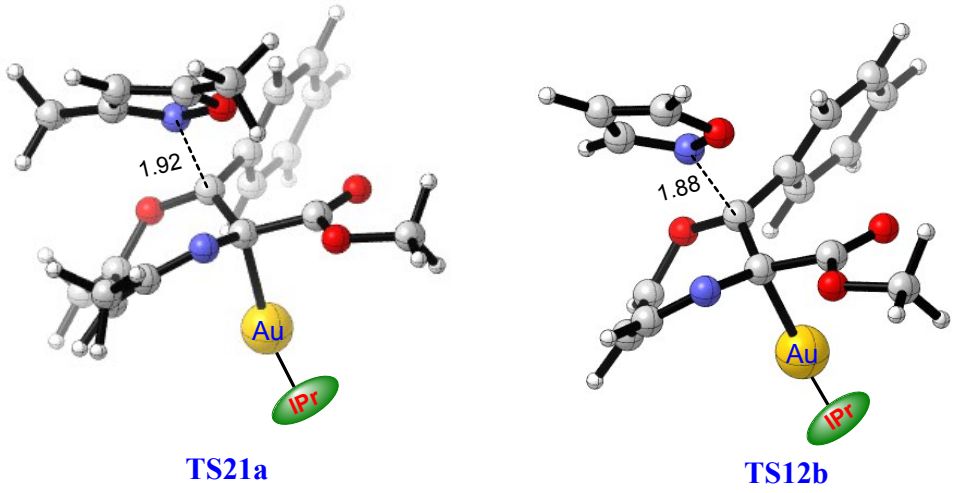


Figure S13. Energy profiles showing the preference for the nucleophilic addition of another molecule of **2b** to **INT11b** in the annulation of **1** with **2b**, instead of the ring contraction process. Bond distances are given in Å.

To further elucidate the mechanistic difference between the annulations involving **2a** and **2b**, the distortion/interaction analysis was employed. In a biomolecular reaction, the activation energy $\Delta E^{\ddagger}$ can be fragmented into two; the distortion of reactants from their ground state geometries to their geometries in the transition states (ΔE_{dist}), and the interaction energy between the deformed reactants (ΔE_{int}).[12] This can be simply represented as $\Delta E^{\ddagger} = \Delta E_{dist} + \Delta E_{int}$. The analysis results reveal that the distortion energy of the 7-membered heterocyclic complex $\Delta E_{dist}(comp)$ in **TS21a** is significantly greater than that in **TS12b** (19.2 *vs* 17.9 kcal/mol respectively). The required energy to distort the substrate into the transition state geometry $\Delta E_{dist}(sub)$ is almost the same for **TS21a** and **TS12b** (1.2 *vs* 0.9 kcal/mol respectively). This analysis indicates that the distortion of the 7-membered complex in **TS21a** is the major factor disfavouring the nucleophilic addition of the second molecule of **2a** to **INT11a**. Steric repulsion brought about by the close proximity between the

dimethylisoxazole and the 7-membered heterocyclic ring is presumed to be mainly responsible for the distortion observed in **TS21a**. However, such steric repulsion is absent in **TS12b**. In addition, the stronger interaction energy between the 7-membered heterocyclic ring and **2b** stabilizes the formation of **TS12b** relative to **TS21a** (-4.2 *vs* -0.9 kcal/mol respectively). Therefore, the distortion/interaction analysis provides explanation for the disfavoured nucleophilic addition of the second molecule of **2a** to **INT11a**, which is in agreement with the experimental report (Figure S14).[13]



TS21a

$\Delta E^{\ddagger}$ = 19.5 kcal/mol

$\Delta E_{dist}(comp)$ = 19.2 kcal/mol

$\Delta E_{dist}(sub)$ = 1.2 kcal/mol

ΔE_{int}= -0.9 kcal/mol

TS12b

$\Delta E^{\ddagger}$ = 14.6 kcal/mol

$\Delta E_{dist}(comp)$ = 17.9 kcal/mol

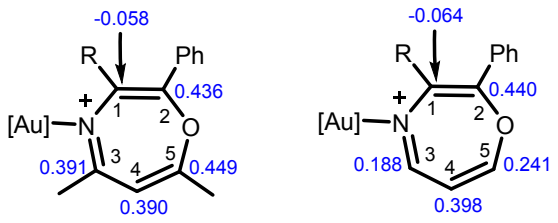
$\Delta E_{dist}(sub)$ = 0.9 kcal/mol

ΔE_{int}= -4.2 kcal/mol

Figure S14. Distortion/Interaction energy analysis of **TS21a** and **TS12b**.

In support of the disfavored formation of dicarbonylpyrroles in the annulation of **1** with **2b**, NBO analysis showed that for **INT11a**, the most electropositive carbon atom, C^5 (0.449 *e*), would readily undergo ring contraction with the most electronegative carbon atom, C^1 (-0.058*e*), affording **INT12a**, whereas this is not so in **INT11b** (0.241 *e vs* -0.064 *e* for C^5 and C^1 respectively). The most electropositive carbon atom in **INT11b** is C^2 (0.440 *e*), thus it is easier for C^5 to undergo ring contraction with C^1 to form **INT12a** than it is for **INT11b** to form **INT25b** (Figure S15). Therefore, it can be summed up that both steric and electronic effects of the methyl substituent play a crucial role in determining the mechanistic pathways

for the gold(I)-catalyzed annulation of **1** with **2a**/**2b** after the formation of the key seven-membered heterocyclic intermediate.



INT11a **INT11b**

Figure S15. NBO charges of **INT11a** and **INT11b**.

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Cartesian Coordinates and Energies

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.466899	-1.293623	-0.000035
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2a

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2b

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

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6	7	0	0.845096	-0.860936	-0.000557
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3

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4

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

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7	6	0	2.963143	0.169798	-0.648869
8	6	0	3.723457	-2.219595	0.561626
9	1	0	1.627964	-2.477737	0.997570
10	6	0	4.295624	-0.221670	-0.651906
11	1	0	2.671474	1.100285	-1.124053
12	6	0	4.681860	-1.409865	-0.040948
13	1	0	4.015442	-3.156240	1.033373
14	1	0	5.037779	0.408891	-1.138313
15	1	0	5.728987	-1.708710	-0.040256
16	8	0	1.543183	2.562618	0.152869
17	6	0	-2.778359	-1.512059	-0.061196
18	6	0	-2.915577	-2.979636	-0.006702
19	6	0	-1.516774	-0.858387	-0.051074
20	7	0	-0.302776	-1.368368	-0.026269
21	8	0	-2.021763	-3.784123	0.074644
22	1	0	-3.987166	-3.303544	-0.043046
23	7	0	-1.490370	0.543833	-0.081318
24	6	0	-2.638693	1.282752	-0.137628
25	6	0	-3.853512	0.656618	-0.153829
26	6	0	-3.921465	-0.747612	-0.113604
27	1	0	-4.753883	1.261908	-0.197572
28	1	0	-4.890198	-1.247864	-0.123871
29	1	0	-2.514031	2.357152	-0.164413
30	6	0	-0.147398	4.519929	0.346010
31	1	0	0.496952	4.819372	-0.486866
32	1	0	-1.042035	5.144874	0.381744
33	1	0	0.420240	4.608817	1.277889

Zero-point correction= 0.251195 (Hartree/Particle)
Thermal correction to Energy= 0.268501
Thermal correction to Enthalpy= 0.269446
Thermal correction to Gibbs Free Energy= 0.204090
Sum of electronic and zero-point Energies= -951.232666
Sum of electronic and thermal Energies= -951.215360
Sum of electronic and thermal Enthalpies= -951.214416
Sum of electronic and thermal Free Energies= -951.279771
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -951.73766029

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.074687	0.038987	0.044527
2	6	0	0.031190	-0.803342	0.047955
3	6	0	-1.120753	1.499049	-0.076007
4	8	0	0.089206	2.046039	-0.295578
5	6	0	1.485048	-0.611199	0.050590
6	6	0	2.103084	0.295910	0.917670
7	6	0	2.285454	-1.403126	-0.780812
8	6	0	3.485271	0.411152	0.943975
9	1	0	1.486645	0.904023	1.575797
10	6	0	3.670077	-1.287512	-0.751209
11	1	0	1.813790	-2.093129	-1.481134
12	6	0	4.273434	-0.379808	0.111431
13	1	0	3.952754	1.117806	1.627418
14	1	0	4.278470	-1.903795	-1.410767
15	1	0	5.357602	-0.286858	0.136240
16	8	0	-2.133823	2.162031	-0.006197
17	6	0	-2.248081	-0.790610	0.076213
18	6	0	-3.673667	-0.440957	0.076320
19	6	0	-1.819281	-2.096141	0.093389
20	7	0	-0.459383	-2.090018	0.066910
21	8	0	-4.545485	-1.288471	0.094740
22	6	0	0.089680	3.460397	-0.444096
23	1	0	1.133309	3.742522	-0.597656
24	1	0	-0.517829	3.759094	-1.305223

25	1	0	-0.312607	3.946637	0.451290
26	1	0	-2.403825	-3.006330	0.123967
27	1	0	-3.907752	0.641165	0.061382
28	1	0	0.135327	-2.904606	0.146919

Zero-point correction= 0.216633 (Hartree/Particle)
Thermal correction to Energy= 0.231607
Thermal correction to Enthalpy= 0.232551
Thermal correction to Gibbs Free Energy= 0.173080
Sum of electronic and zero-point Energies= -781.708862
Sum of electronic and thermal Energies= -781.693889
Sum of electronic and thermal Enthalpies= -781.692945
Sum of electronic and thermal Free Energies= -781.752415
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d) energy in DCE solvent = -782.14274841

Au(I)-catalyst

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.003649	-1.517797	-0.089552
2	6	0	-0.002427	0.485350	0.065609
3	7	0	1.080105	1.279577	0.132124
4	6	0	-0.681243	2.599260	0.238085
5	6	0	0.675112	2.599581	0.239870
6	1	0	-1.404232	3.402132	0.302708
7	1	0	1.397114	3.403112	0.307542
8	7	0	-1.085041	1.278764	0.129590
9	6	0	-2.454188	0.830646	0.055347
10	6	0	-3.128042	0.563236	1.251899
11	6	0	-3.031586	0.696461	-1.211968
12	6	0	-4.450659	0.134572	1.148715
13	6	0	-4.358019	0.269291	-1.260613
14	6	0	-5.058738	-0.009959	-0.093079
15	1	0	-5.007517	-0.082991	2.059011
16	1	0	-4.841594	0.159069	-2.230232
17	1	0	-6.093915	-0.339859	-0.150760
18	6	0	2.449642	0.831244	0.067199
19	6	0	3.053984	0.754566	-1.192806
20	6	0	3.097293	0.508168	1.263982
21	6	0	4.379106	0.322838	-1.232950
22	6	0	4.422229	0.084277	1.169838
23	6	0	5.055306	-0.008254	-0.064363
24	1	0	4.881713	0.251335	-2.196429
25	1	0	4.960269	-0.173058	2.081100
26	1	0	6.090673	-0.338672	-0.115170
27	6	0	2.314723	1.128287	-2.442380
28	1	0	2.013250	2.185162	-2.440684
29	1	0	2.938948	0.965662	-3.326929
30	1	0	1.397366	0.535664	-2.571700
31	6	0	2.399778	0.604785	2.587411
32	1	0	1.953468	1.595209	2.751309
33	1	0	1.585920	-0.130179	2.673894
34	1	0	3.099231	0.416392	3.408336
35	6	0	-2.461904	0.730322	2.584341
36	1	0	-2.127011	1.763085	2.752744
37	1	0	-3.148870	0.471636	3.396571
38	1	0	-1.575295	0.087279	2.683504
39	6	0	-2.257826	0.984608	-2.463444
40	1	0	-1.737902	1.951530	-2.420194
41	1	0	-1.490871	0.218165	-2.650658
42	1	0	-2.919733	1.001257	-3.335484

Zero-point correction= 0.344340 (Hartree/Particle)
Thermal correction to Energy= 0.365991
Thermal correction to Enthalpy= 0.366935
Thermal correction to Gibbs Free Energy= 0.291163
Sum of electronic and zero-point Energies= -979.809924
Sum of electronic and thermal Energies= -979.788273
Sum of electronic and thermal Enthalpies= -979.787329
Sum of electronic and thermal Free Energies= -979.863101
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -980.78186308

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.360769	2.377241	0.122094
2	6	0	-0.213036	2.672481	-0.246227
3	6	0	-2.682816	2.030560	0.510114
4	6	0	-3.754182	2.307232	-0.354436
5	6	0	-2.913090	1.417791	1.753916
6	6	0	-5.043183	1.970095	0.030270
7	1	0	-3.562507	2.786063	-1.312491
8	6	0	-4.205491	1.084101	2.123329
9	1	0	-2.070623	1.217545	2.414671
10	6	0	-5.268250	1.361530	1.263676
11	1	0	-5.878436	2.189135	-0.630921
12	1	0	-4.389103	0.615512	3.088234
13	1	0	-6.283512	1.104591	1.560092
14	6	0	0.872684	3.598718	-0.603180
15	8	0	0.668651	4.695237	-1.050347
16	8	0	2.062712	3.049586	-0.368903
17	6	0	3.183137	3.897294	-0.659568
18	1	0	3.187285	4.165414	-1.720627
19	1	0	3.132676	4.809521	-0.057363
20	1	0	4.066575	3.312942	-0.401413
21	79	0	0.125397	0.485178	-0.081207
22	6	0	0.657561	-1.481067	-0.059378
23	7	0	1.874112	-2.025675	0.129658
24	6	0	0.497547	-3.716793	-0.172368
25	6	0	1.797155	-3.407670	0.062679
26	1	0	-0.005441	-4.666988	-0.296925
27	1	0	2.674871	-4.028469	0.186554
28	7	0	-0.189073	-2.515834	-0.244312
29	6	0	-1.597127	-2.336742	-0.483296
30	6	0	-2.028947	-2.192021	-1.806239
31	6	0	-2.447957	-2.236575	0.622147
32	6	0	-3.383635	-1.929946	-2.008827
33	6	0	-3.793730	-1.974581	0.368959
34	6	0	-4.256182	-1.817814	-0.932350
35	1	0	-3.752916	-1.813899	-3.026980
36	1	0	-4.482969	-1.891940	1.208942
37	1	0	-5.309919	-1.609514	-1.110298
38	6	0	3.073208	-1.264197	0.362330
39	6	0	3.451117	-1.018337	1.686606
40	6	0	3.786564	-0.796994	-0.745546
41	6	0	4.612839	-0.275091	1.889981
42	6	0	4.946917	-0.065724	-0.491711
43	6	0	5.355965	0.191737	0.811712
44	1	0	4.936343	-0.068146	2.909178
45	1	0	5.535291	0.298633	-1.333245
46	1	0	6.268162	0.757990	0.990548
47	6	0	2.636810	-1.527440	2.837145
48	1	0	2.598850	-2.625321	2.862107
49	1	0	3.056200	-1.190125	3.790802
50	1	0	1.596697	-1.173540	2.784979
51	6	0	3.315860	-1.049521	-2.146060
52	1	0	3.016210	-2.094120	-2.305421
53	1	0	2.443412	-0.425114	-2.392930
54	1	0	4.102621	-0.813332	-2.870501
55	6	0	-1.071734	-2.296518	-2.954910
56	1	0	-0.555468	-3.266079	-2.974262
57	1	0	-1.594794	-2.181383	-3.910058
58	1	0	-0.291996	-1.521999	-2.907441
59	6	0	-1.934028	-2.378717	2.023256
60	1	0	-1.410648	-3.331888	2.178656
61	1	0	-1.221272	-1.579660	2.278567
62	1	0	-2.757374	-2.331097	2.744787

Zero-point correction= 0.500152 (Hartree/Particle)
Thermal correction to Energy= 0.533662
Thermal correction to Enthalpy= 0.534607
Thermal correction to Gibbs Free Energy= 0.432832
Sum of electronic and zero-point Energies= -1515.613423
Sum of electronic and thermal Energies= -1515.579913
Sum of electronic and thermal Enthalpies= -1515.578968

Sum of electronic and thermal Free Energies= -1515.680743
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1516.87839989

INT1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.188624	1.993643	0.078956
2	6	0	-2.153734	2.609594	-0.085923
3	6	0	-4.396222	1.285127	0.277796
4	6	0	-4.372072	-0.112306	0.410789
5	6	0	-5.613583	1.982464	0.348898
6	6	0	-5.558754	-0.796930	0.620205
7	1	0	-3.419317	-0.641040	0.346032
8	6	0	-6.792728	1.284469	0.554942
9	1	0	-5.615287	3.065274	0.242599
10	6	0	-6.765014	-0.101885	0.692512
11	1	0	-5.550051	-1.879496	0.731448
12	1	0	-7.737594	1.820003	0.610808
13	1	0	-7.693006	-0.645718	0.858144
14	6	0	-0.935401	3.304704	-0.263706
15	8	0	0.184393	2.762072	-0.303689
16	8	0	-1.065733	4.602649	-0.384995
17	6	0	0.136156	5.371399	-0.558316
18	1	0	0.802166	5.225087	0.296650
19	1	0	0.644806	5.070382	-1.478992
20	1	0	-0.194836	6.407942	-0.619827
21	79	0	0.627145	0.676492	-0.100391
22	6	0	1.346321	-1.192340	0.040778
23	7	0	2.659197	-1.469186	0.207777
24	6	0	1.653887	-3.417456	0.079434
25	6	0	2.867339	-2.837392	0.233216
26	1	0	1.347525	-4.454456	0.036479
27	1	0	3.858016	-3.255294	0.357177
28	7	0	0.728881	-2.389815	-0.035464
29	6	0	-0.669917	-2.625557	-0.273322
30	6	0	-1.122337	-2.620994	-1.597305
31	6	0	-1.483153	-2.936681	0.821349
32	6	0	-2.456298	-2.966251	-1.815737
33	6	0	-2.806311	-3.287103	0.551820
34	6	0	-3.284312	-3.312261	-0.754431
35	1	0	-2.838140	-2.982045	-2.835422
36	1	0	-3.460052	-3.551714	1.383379
37	1	0	-4.315313	-3.602969	-0.949390
38	6	0	3.700695	-0.479786	0.311243
39	6	0	4.063709	-0.026836	1.583516
40	6	0	4.295938	-0.027086	-0.871054
41	6	0	5.076403	0.929443	1.652802
42	6	0	5.302649	0.930082	-0.750433
43	6	0	5.688791	1.402962	0.498325
44	1	0	5.386000	1.301553	2.628418
45	1	0	5.788194	1.302062	-1.651767
46	1	0	6.479271	2.147081	0.573513
47	6	0	3.389890	-0.543223	2.818867
48	1	0	3.501226	-1.631230	2.924390
49	1	0	3.813984	-0.079501	3.715711
50	1	0	2.310680	-0.331582	2.812802
51	6	0	3.867071	-0.543786	-2.211422
52	1	0	3.935032	-1.638959	-2.274657
53	1	0	2.824175	-0.275929	-2.437215
54	1	0	4.493942	-0.127093	-3.006854
55	6	0	-0.211391	-2.269244	-2.734391
56	1	0	0.751769	-2.795071	-2.670932
57	1	0	-0.671443	-2.523247	-3.695138
58	1	0	0.015672	-1.192652	-2.750538
59	6	0	-0.952143	-2.899211	2.222428
60	1	0	-0.193286	-3.674263	2.398083
61	1	0	-0.479389	-1.932632	2.449258
62	1	0	-1.756149	-3.057492	2.949019

Zero-point correction= 0.500255 (Hartree/Particle)
Thermal correction to Energy= 0.533984
Thermal correction to Enthalpy= 0.534928
Thermal correction to Gibbs Free Energy= 0.430743

Sum of electronic and zero-point Energies= -1515.615605
Sum of electronic and thermal Energies= -1515.581876
Sum of electronic and thermal Enthalpies= -1515.580931
Sum of electronic and thermal Free Energies= -1515.685117
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1516.87187059

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.637205	-0.389756	-0.305079
2	6	0	2.109928	0.756938	-0.044320
3	79	0	-0.469154	-0.189215	-0.076459
4	6	0	2.197375	-1.698994	-0.696399
5	8	0	1.562232	-2.688119	-0.063429
6	6	0	2.102005	2.160427	0.212024
7	6	0	1.339080	2.991026	-0.626282
8	6	0	2.803588	2.709333	1.295880
9	6	0	1.280877	4.353888	-0.373180
10	1	0	0.787731	2.556505	-1.460716
11	6	0	2.738125	4.071923	1.535620
12	1	0	3.407356	2.055589	1.921208
13	6	0	1.979581	4.894321	0.702803
14	1	0	0.690089	4.995368	-1.023666
15	1	0	3.285588	4.499716	2.372553
16	1	0	1.939278	5.965332	0.892154
17	8	0	3.090916	-1.851166	-1.492539
18	6	0	6.122289	-0.821118	-0.553583
19	6	0	5.766951	-1.170603	0.711647
20	6	0	5.177351	0.165445	-0.927970
21	7	0	4.346856	0.403370	0.063721
22	8	0	4.693885	-0.451885	1.093966
23	1	0	6.935417	-1.218583	-1.146652
24	6	0	2.036675	-4.002271	-0.363213
25	1	0	1.440811	-4.677174	0.252428
26	1	0	1.895590	-4.223200	-1.426471
27	1	0	3.100653	-4.089813	-0.118520
28	6	0	-2.506249	-0.176911	0.086775
29	7	0	-3.297978	-1.263886	0.204249
30	6	0	-4.659115	0.462443	0.202593
31	6	0	-4.630735	-0.890589	0.276172
32	1	0	-5.478458	1.169322	0.219642
33	1	0	-5.420200	-1.624573	0.372622
34	7	0	-3.342265	0.882029	0.086330
35	6	0	-2.919295	2.249660	-0.049405
36	6	0	-2.766759	2.769615	-1.338633
37	6	0	-2.681999	2.989003	1.113948
38	6	0	-2.380252	4.105918	-1.446114
39	6	0	-2.294592	4.319103	0.957416
40	6	0	-2.154953	4.873982	-0.309515
41	1	0	-2.268977	4.546118	-2.436790
42	1	0	-2.107914	4.923721	1.844115
43	1	0	-1.869448	5.919978	-0.411880
44	6	0	-2.800989	-2.614062	0.218469
45	6	0	-2.460854	-3.185324	1.448098
46	6	0	-2.657391	-3.274282	-1.006250
47	6	0	-1.964282	-4.488598	1.429750
48	6	0	-2.154188	-4.574247	-0.975625
49	6	0	-1.814466	-5.176275	0.230951
50	1	0	-1.698872	-4.965911	2.372374
51	1	0	-2.037410	-5.118656	-1.912019
52	1	0	-1.435548	-6.197000	0.237279
53	6	0	-2.605462	-2.421992	2.729676
54	1	0	-3.610690	-1.995201	2.847459
55	1	0	-2.413618	-3.068295	3.592796
56	1	0	-1.894594	-1.583974	2.778113
57	6	0	-3.019238	-2.604112	-2.297371
58	1	0	-4.060735	-2.253901	-2.303360
59	1	0	-2.387002	-1.723561	-2.484888
60	1	0	-2.894085	-3.289600	-3.142247
61	6	0	-2.987160	1.921434	-2.554914
62	1	0	-3.917817	1.340723	-2.496556
63	1	0	-3.031938	2.537718	-3.459341

64	1	0	-2.169509	1.196460	-2.687458
65	6	0	-2.829180	2.369770	2.470728
66	1	0	-3.837480	1.964910	2.633215
67	1	0	-2.125245	1.536112	2.609258
68	1	0	-2.634740	3.104704	3.258939
69	6	0	5.005105	0.860212	-2.227244
70	1	0	4.590510	0.157246	-2.961023
71	1	0	4.312352	1.703348	-2.126039
72	1	0	5.960043	1.232898	-2.613728
73	6	0	6.312272	-2.123839	1.701388
74	1	0	5.544925	-2.839601	2.021313
75	1	0	7.150724	-2.679169	1.271301
76	1	0	6.666360	-1.599586	2.597681

Zero-point correction= 0.613591 (Hartree/Particle)
Thermal correction to Energy= 0.655484
Thermal correction to Enthalpy= 0.656429
Thermal correction to Gibbs Free Energy= 0.533613
Sum of electronic and zero-point Energies= -1839.964340
Sum of electronic and thermal Energies= -1839.922447
Sum of electronic and thermal Enthalpies= -1839.921503
Sum of electronic and thermal Free Energies= -1840.044319
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.42389602

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.441311	0.532451	-0.033492
2	6	0	1.617271	-0.464610	-0.249968
3	6	0	5.644004	-1.126116	0.642958
4	6	0	5.927191	-0.716406	-0.697866
5	8	0	4.018215	0.099872	-0.015028
6	6	0	4.875669	0.022778	-1.100078
7	7	0	4.501274	-0.670670	1.085424
8	1	0	6.800578	-0.970231	-1.284539
9	79	0	-0.444868	-0.182532	-0.103949
10	6	0	-2.487722	-0.081861	0.079458
11	7	0	-3.304139	-1.150556	0.215852
12	6	0	-4.626612	0.603172	0.255075
13	6	0	-4.626169	-0.749848	0.325541
14	1	0	-5.429023	1.328201	0.297310
15	1	0	-5.428651	-1.466069	0.444770
16	7	0	-3.303843	0.993258	0.103698
17	6	0	-2.862582	2.355968	-0.010793
18	6	0	-2.767396	2.917417	-1.287796
19	6	0	-2.563517	3.055156	1.162872
20	6	0	-2.382797	4.256167	-1.370237
21	6	0	-2.182776	4.390229	1.032354
22	6	0	-2.105888	4.987772	-0.220575
23	1	0	-2.315912	4.728024	-2.350095
24	1	0	-1.952504	4.964849	1.928700
25	1	0	-1.826138	6.037192	-0.302330
26	6	0	-2.836143	-2.509892	0.244637
27	6	0	-2.394021	-3.035149	1.462179
28	6	0	-2.818670	-3.227195	-0.956118
29	6	0	-1.934432	-4.352414	1.459840
30	6	0	-2.346711	-4.538166	-0.911547
31	6	0	-1.914733	-5.097174	0.286410
32	1	0	-1.595268	-4.794832	2.396064
33	1	0	-2.326906	-5.125130	-1.829117
34	1	0	-1.563682	-6.127866	0.305672
35	6	0	-2.386129	-2.210853	2.713775
36	1	0	-3.311973	-1.633537	2.840095
37	1	0	-2.259250	-2.844223	3.598487
38	1	0	-1.556843	-1.487402	2.702995
39	6	0	-3.278534	-2.602691	-2.238718
40	1	0	-4.341452	-2.325904	-2.204497
41	1	0	-2.717687	-1.683435	-2.462681
42	1	0	-3.143784	-3.291782	-3.079249
43	6	0	-3.052933	2.108473	-2.516917
44	1	0	-4.022670	1.595376	-2.460801
45	1	0	-3.060577	2.742406	-3.410128
46	1	0	-2.290109	1.329462	-2.666579

47	6	0	-2.640760	2.388279	2.502733
48	1	0	-3.629226	1.945824	2.688446
49	1	0	-1.906457	1.573298	2.584803
50	1	0	-2.437686	3.102429	3.307809
51	6	0	2.415036	1.966690	0.201392
52	6	0	1.423641	2.738192	-0.424675
53	6	0	3.344020	2.593410	1.042836
54	6	0	1.364217	4.106503	-0.201671
55	1	0	0.703983	2.259224	-1.090261
56	6	0	3.276599	3.963177	1.257520
57	1	0	4.107519	2.001582	1.544112
58	6	0	2.289240	4.722795	0.636572
59	1	0	0.591663	4.692269	-0.695593
60	1	0	3.999040	4.439315	1.917169
61	1	0	2.243979	5.797254	0.802901
62	6	0	2.080392	-1.831541	-0.585844
63	8	0	2.957865	-2.086651	-1.384683
64	8	0	1.378862	-2.755551	0.072798
65	6	0	1.744260	-4.109280	-0.195501
66	1	0	2.798223	-4.278633	0.049236
67	1	0	1.097010	-4.718897	0.437147
68	1	0	1.579649	-4.344586	-1.252441
69	6	0	4.461627	0.698973	-2.338898
70	1	0	3.580250	0.193341	-2.755138
71	1	0	4.210464	1.751909	-2.158694
72	1	0	5.272004	0.648430	-3.071552
73	6	0	6.482607	-1.972382	1.528819
74	1	0	6.655855	-2.951068	1.065743
75	1	0	7.461213	-1.505769	1.692022
76	1	0	5.994990	-2.118742	2.497009

Zero-point correction= 0.613215 (Hartree/Particle)
Thermal correction to Energy= 0.654639
Thermal correction to Enthalpy= 0.655583
Thermal correction to Gibbs Free Energy= 0.534632
Sum of electronic and zero-point Energies= -1839.941563
Sum of electronic and thermal Energies= -1839.900139
Sum of electronic and thermal Enthalpies= -1839.899195
Sum of electronic and thermal Free Energies= -1840.020146
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.39996406

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.710006	-0.142778	-0.191757
2	6	0	1.841647	-1.402524	-0.132810
3	6	0	2.479036	1.080656	-0.314926
4	6	0	3.695010	1.065786	-1.015207
5	6	0	2.032798	2.277824	0.258946
6	6	0	4.456195	2.220759	-1.115461
7	1	0	4.028845	0.139495	-1.479733
8	6	0	2.808139	3.426123	0.169485
9	1	0	1.080267	2.303780	0.791168
10	6	0	4.019123	3.401055	-0.515917
11	1	0	5.395097	2.201788	-1.665562
12	1	0	2.456109	4.346592	0.631891
13	1	0	4.620728	4.304802	-0.592704
14	79	0	-0.452341	0.011835	-0.073789
15	6	0	1.382996	-2.795379	-0.199068
16	8	0	0.188186	-2.913006	0.386865
17	6	0	6.194190	-1.639802	0.100059
18	6	0	5.061150	-2.256301	-0.489486
19	6	0	5.688221	-0.873188	1.104115
20	1	0	7.231270	-1.757929	-0.186499
21	8	0	1.982313	-3.697926	-0.724986
22	7	0	3.964863	-1.877413	0.139354
23	8	0	4.352829	-1.009903	1.139843
24	6	0	5.015835	-3.177781	-1.652753
25	1	0	5.676918	-4.036445	-1.485692
26	1	0	3.997838	-3.541721	-1.814413
27	1	0	5.369003	-2.668269	-2.558274
28	6	0	6.279449	0.049761	2.095076
29	1	0	7.368415	0.071558	1.995960

30	1	0	5.891390	1.066018	1.945470
31	1	0	6.026418	-0.255427	3.117521
32	6	0	-0.385964	-4.224197	0.316527
33	1	0	0.272534	-4.949974	0.803502
34	1	0	-1.342724	-4.148359	0.835935
35	1	0	-0.536987	-4.515538	-0.728240
36	6	0	-2.420965	0.571034	-0.007516
37	7	0	-2.839489	1.856499	-0.009364
38	6	0	-4.670126	0.645601	0.032715
39	6	0	-4.222913	1.923252	0.015496
40	1	0	-5.668666	0.228715	0.056742
41	1	0	-4.743886	2.871833	0.019882
42	7	0	-3.548226	-0.171148	0.018376
43	6	0	-3.625584	-1.606351	0.080394
44	6	0	-3.677311	-2.204587	1.343737
45	6	0	-3.728836	-2.320640	-1.117193
46	6	0	-3.879323	-3.584657	1.388604
47	6	0	-3.917916	-3.699968	-1.023137
48	6	0	-4.008660	-4.322883	0.216595
49	1	0	-3.944596	-4.078569	2.357630
50	1	0	-4.012957	-4.284183	-1.937694
51	1	0	-4.179134	-5.396675	0.270459
52	6	0	-1.967175	2.999813	0.000934
53	6	0	-1.609463	3.574173	-1.223048
54	6	0	-1.529670	3.483006	1.238770
55	6	0	-0.778882	4.693761	-1.183745
56	6	0	-0.702951	4.607053	1.228542
57	6	0	-0.336334	5.208552	0.029348
58	1	0	-0.483951	5.166655	-2.119491
59	1	0	-0.353987	5.015775	2.176530
60	1	0	0.299003	6.092810	0.040164
61	6	0	-2.099782	3.006394	-2.520510
62	1	0	-3.195243	3.046483	-2.597499
63	1	0	-1.687733	3.561177	-3.369924
64	1	0	-1.810847	1.951581	-2.636324
65	6	0	-1.916023	2.807515	2.520261
66	1	0	-3.002122	2.663378	2.602665
67	1	0	-1.456869	1.810317	2.602184
68	1	0	-1.590152	3.394484	3.385562
69	6	0	-3.516951	-1.393962	2.594304
70	1	0	-4.215366	-0.546392	2.633150
71	1	0	-3.687690	-2.008639	3.484445
72	1	0	-2.502413	-0.974619	2.667755
73	6	0	-3.652143	-1.627002	-2.443702
74	1	0	-4.436159	-0.864812	-2.553640
75	1	0	-2.689138	-1.112845	-2.576050
76	1	0	-3.765848	-2.341355	-3.265885

Zero-point correction= 0.612762 (Hartree/Particle)
Thermal correction to Energy= 0.654865
Thermal correction to Enthalpy= 0.655809
Thermal correction to Gibbs Free Energy= 0.531562
Sum of electronic and zero-point Energies= -1839.957816
Sum of electronic and thermal Energies= -1839.915713
Sum of electronic and thermal Enthalpies= -1839.914769
Sum of electronic and thermal Free Energies= -1840.039016
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.41451721

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495587	0.687509	-0.087581
2	6	0	2.332341	-0.318884	-0.015475
3	6	0	1.750173	2.125554	-0.139310
4	6	0	2.859072	2.661436	-0.817255
5	6	0	0.842381	3.009827	0.467285
6	6	0	3.056065	4.034599	-0.865491
7	1	0	3.541607	1.999615	-1.346392
8	6	0	1.064488	4.379613	0.445079
9	1	0	-0.047388	2.612579	0.959335
10	6	0	2.170906	4.896383	-0.222454
11	1	0	3.906847	4.436183	-1.412670
12	1	0	0.354032	5.045268	0.932383

13	1	0	2.335417	5.971661	-0.257280
14	79	0	-0.515721	0.030705	-0.082967
15	6	0	2.274095	-1.789057	0.006386
16	8	0	3.419073	-2.360187	0.390886
17	6	0	6.012669	-0.071208	0.876422
18	6	0	5.994149	-0.270441	-0.542241
19	6	0	4.731880	0.131954	1.241062
20	8	0	1.265282	-2.396237	-0.266958
21	7	0	4.791078	-0.194024	-1.044613
22	8	0	3.977796	0.096348	0.085259
23	1	0	6.880817	-0.073457	1.523232
24	6	0	7.149345	-0.530260	-1.437945
25	1	0	7.861937	0.302135	-1.397747
26	1	0	7.681785	-1.435721	-1.123509
27	1	0	6.813390	-0.657293	-2.471169
28	6	0	4.014166	0.391875	2.500704
29	1	0	3.414309	1.308426	2.427189
30	1	0	3.336179	-0.437003	2.743518
31	1	0	4.731905	0.504739	3.318249
32	6	0	3.391641	-3.791279	0.408274
33	1	0	2.602965	-4.149920	1.077150
34	1	0	3.208058	-4.176994	-0.599473
35	1	0	4.374708	-4.100736	0.765639
36	6	0	-2.525494	-0.377732	-0.060485
37	7	0	-3.158961	-1.569042	-0.091682
38	6	0	-4.755602	-0.056375	-0.046078
39	6	0	-4.534053	-1.393007	-0.084461
40	1	0	-5.669278	0.523307	-0.028063
41	1	0	-5.212333	-2.235910	-0.109521
42	7	0	-3.509115	0.549086	-0.030130
43	6	0	-3.260817	1.963255	0.033171
44	6	0	-3.158052	2.673140	-1.167377
45	6	0	-3.096091	2.551044	1.291224
46	6	0	-2.886444	4.038256	-1.082516
47	6	0	-2.829324	3.920333	1.327863
48	6	0	-2.727305	4.656278	0.152596
49	1	0	-2.802196	4.618840	-2.000263
50	1	0	-2.707712	4.409767	2.294024
51	1	0	-2.526443	5.725393	0.199276
52	6	0	-2.486979	-2.840542	-0.104641
53	6	0	-2.287942	-3.488839	1.118251
54	6	0	-2.055800	-3.356301	-1.329060
55	6	0	-1.641430	-4.723109	1.089992
56	6	0	-1.414095	-4.594421	-1.308593
57	6	0	-1.212146	-5.272050	-0.113050
58	1	0	-1.478466	-5.256699	2.025897
59	1	0	-1.070809	-5.026087	-2.248023
60	1	0	-0.716028	-6.241022	-0.118453
61	6	0	-2.742896	-2.870639	2.405893
62	1	0	-3.835086	-2.755376	2.447644
63	1	0	-2.443873	-3.485695	3.261543
64	1	0	-2.312306	-1.867777	2.543605
65	6	0	-2.242068	-2.596912	-2.607173
66	1	0	-3.247374	-2.162559	-2.693596
67	1	0	-1.525385	-1.764325	-2.675978
68	1	0	-2.078169	-3.245006	-3.475049
69	6	0	-3.317231	1.985047	-2.489054
70	1	0	-4.300617	1.504763	-2.586795
71	1	0	-3.209632	2.695429	-3.315539
72	1	0	-2.562845	1.195694	-2.623522
73	6	0	-3.163763	1.737654	2.548593
74	1	0	-4.026399	1.058034	2.561632
75	1	0	-2.265311	1.111723	2.663165
76	1	0	-3.231147	2.384549	3.430122

Zero-point correction= 0.612713 (Hartree/Particle)
Thermal correction to Energy= 0.654313
Thermal correction to Enthalpy= 0.655257
Thermal correction to Gibbs Free Energy= 0.533609
Sum of electronic and zero-point Energies= -1839.935548
Sum of electronic and thermal Energies= -1839.893948
Sum of electronic and thermal Enthalpies= -1839.893004
Sum of electronic and thermal Free Energies= -1840.014652
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.39274606

TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.240152	-1.216631	-0.047569
2	6	0	2.426303	-0.607669	-0.466048
3	79	0	-0.592892	-0.323061	0.029568
4	6	0	1.344355	-2.635964	0.351636
5	8	0	1.339399	-2.816270	1.664938
6	6	0	2.511424	0.759827	-1.034621
7	6	0	1.656413	1.156034	-2.068726
8	6	0	3.501371	1.639893	-0.588405
9	6	0	1.798319	2.410491	-2.651237
10	1	0	0.898395	0.462318	-2.436519
11	6	0	3.630404	2.899217	-1.162887
12	1	0	4.156280	1.337380	0.228347
13	6	0	2.785428	3.283114	-2.200325
14	1	0	1.146837	2.699904	-3.474398
15	1	0	4.397937	3.581684	-0.802637
16	1	0	2.900521	4.261849	-2.663305
17	8	0	1.375619	-3.503651	-0.491811
18	6	0	5.859465	-1.385425	-0.403011
19	6	0	5.647305	-1.193357	0.983523
20	6	0	4.658497	-1.411107	-1.063331
21	7	0	3.539505	-1.338976	-0.315148
22	8	0	4.455475	-0.993651	1.343571
23	1	0	6.820789	-1.569232	-0.868666
24	6	0	1.383343	-4.182823	2.094419
25	1	0	1.374707	-4.150236	3.184315
26	1	0	0.511971	-4.726498	1.715992
27	1	0	2.294990	-4.666235	1.729796
28	6	0	-2.388487	0.687753	0.252268
29	7	0	-3.655652	0.259738	0.071213
30	6	0	-3.829900	2.358704	0.704432
31	6	0	-4.559411	1.274474	0.342359
32	1	0	-4.120987	3.358620	0.998939
33	1	0	-5.626652	1.121624	0.247544
34	7	0	-2.500535	1.976974	0.642086
35	6	0	-1.365389	2.814506	0.921756
36	6	0	-0.804225	3.535430	-0.136869
37	6	0	-0.851730	2.828619	2.221895
38	6	0	0.326776	4.301438	0.140344
39	6	0	0.281030	3.609124	2.451413
40	6	0	0.866112	4.334963	1.420749
41	1	0	0.787662	4.874023	-0.663789
42	1	0	0.704474	3.643229	3.454543
43	1	0	1.750465	4.938241	1.618478
44	6	0	-4.008306	-1.059827	-0.379026
45	6	0	-4.314997	-2.028158	0.581652
46	6	0	-4.019312	-1.307570	-1.755004
47	6	0	-4.658682	-3.298157	0.120400
48	6	0	-4.370379	-2.592127	-2.169193
49	6	0	-4.688068	-3.576613	-1.241250
50	1	0	-4.905999	-4.074599	0.843348
51	1	0	-4.393473	-2.816630	-3.234885
52	1	0	-4.962226	-4.572733	-1.583106
53	6	0	-4.260583	-1.713978	2.046264
54	1	0	-4.952019	-0.905887	2.322239
55	1	0	-4.523566	-2.593272	2.643884
56	1	0	-3.254747	-1.389580	2.350927
57	6	0	-3.645947	-0.244142	-2.743920
58	1	0	-4.140211	0.714206	-2.533110
59	1	0	-2.561835	-0.052480	-2.733104
60	1	0	-3.916423	-0.545685	-3.761679
61	6	0	-1.379849	3.461503	-1.518670
62	1	0	-2.456095	3.681600	-1.534336
63	1	0	-0.883567	4.175319	-2.185838
64	1	0	-1.253524	2.456230	-1.950590
65	6	0	-1.475263	2.017180	3.317066
66	1	0	-2.557525	2.187111	3.395425
67	1	0	-1.332325	0.939528	3.148269
68	1	0	-1.027347	2.261493	4.286259
69	6	0	6.724147	-1.285424	2.012991
70	1	0	6.706552	-2.287715	2.460646

71	1	0	7.711511	-1.123660	1.569393
72	1	0	6.549418	-0.562564	2.815673
73	6	0	4.446480	-1.619395	-2.526397
74	1	0	3.712314	-2.417772	-2.690702
75	1	0	4.046504	-0.699264	-2.974678
76	1	0	5.387735	-1.877497	-3.019258

Zero-point correction= 0.612739 (Hartree/Particle)
Thermal correction to Energy= 0.654582
Thermal correction to Enthalpy= 0.655526
Thermal correction to Gibbs Free Energy= 0.532260
Sum of electronic and zero-point Energies= -1839.970203
Sum of electronic and thermal Energies= -1839.928360
Sum of electronic and thermal Enthalpies= -1839.927416
Sum of electronic and thermal Free Energies= -1840.050682
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43335940

TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.444737	-0.910009	-0.375168
2	6	0	2.507165	-0.113695	-0.849764
3	79	0	-0.477057	-0.279440	-0.093144
4	6	0	1.738170	-2.287000	0.061132
5	8	0	1.958165	-2.392049	1.363357
6	6	0	2.316535	1.286837	-1.303493
7	6	0	1.275098	1.618503	-2.175431
8	6	0	3.231461	2.270508	-0.919860
9	6	0	1.158436	2.914756	-2.663947
10	1	0	0.578489	0.847939	-2.510266
11	6	0	3.099911	3.569471	-1.395471
12	1	0	4.044294	2.006410	-0.245357
13	6	0	2.069378	3.892140	-2.274262
14	1	0	0.364217	3.155521	-3.368976
15	1	0	3.813548	4.331288	-1.087210
16	1	0	1.982092	4.905247	-2.663981
17	8	0	1.721568	-3.203378	-0.733457
18	6	0	5.261661	-2.122193	0.062642
19	6	0	5.265490	-1.221742	1.162216
20	6	0	4.412594	-1.704851	-0.932924
21	7	0	3.763530	-0.541602	-0.773582
22	8	0	4.483475	-0.245671	1.108379
23	1	0	5.918201	-2.979871	-0.034578
24	6	0	2.203233	-3.722705	1.839211
25	1	0	2.350606	-3.627584	2.915481
26	1	0	1.346835	-4.367925	1.620576
27	1	0	3.097777	-4.134378	1.359497
28	6	0	-2.355630	0.465445	0.360392
29	7	0	-3.569668	-0.116132	0.267285
30	6	0	-3.941275	1.900512	1.062498
31	6	0	-4.561462	0.752003	0.693728
32	1	0	-4.324925	2.833477	1.454449
33	1	0	-5.604947	0.464907	0.688944
34	7	0	-2.588172	1.703025	0.849686
35	6	0	-1.541491	2.660694	1.085980
36	6	0	-1.239607	3.566485	0.064496
37	6	0	-0.847575	2.604437	2.298349
38	6	0	-0.186141	4.450851	0.287095
39	6	0	0.201251	3.506910	2.473982
40	6	0	0.531029	4.417333	1.477246
41	1	0	0.076110	5.167636	-0.490084
42	1	0	0.761920	3.490015	3.407828
43	1	0	1.354691	5.112313	1.630596
44	6	0	-3.791671	-1.450476	-0.220675
45	6	0	-3.874688	-2.488146	0.713002
46	6	0	-3.902155	-1.643227	-1.600934
47	6	0	-4.090039	-3.774252	0.220202
48	6	0	-4.118765	-2.946884	-2.046867
49	6	0	-4.212958	-4.000802	-1.145910
50	1	0	-4.162404	-4.604683	0.921500
51	1	0	-4.214820	-3.130936	-3.116225
52	1	0	-4.384693	-5.010886	-1.512677
53	6	0	-3.728935	-2.224820	2.181595

54	1	0	-4.541423	-1.594966	2.570176
55	1	0	-3.739927	-3.161823	2.748546
56	1	0	-2.787115	-1.703781	2.408120
57	6	0	-3.770898	-0.501432	-2.563938
58	1	0	-4.359550	0.373665	-2.256264
59	1	0	-2.724769	-0.168843	-2.649250
60	1	0	-4.103585	-0.795469	-3.565294
61	6	0	-2.010806	3.570005	-1.220473
62	1	0	-3.076312	3.787405	-1.061997
63	1	0	-1.619026	4.327519	-1.908323
64	1	0	-1.958269	2.593370	-1.725962
65	6	0	-1.195612	1.598848	3.354441
66	1	0	-2.278102	1.537506	3.530166
67	1	0	-0.859606	0.589511	3.072144
68	1	0	-0.714354	1.850828	4.305686
69	6	0	6.201802	-1.365184	2.320547
70	1	0	5.689494	-1.109772	3.253495
71	1	0	6.613253	-2.377455	2.382443
72	1	0	7.033037	-0.658868	2.198391
73	6	0	4.265269	-2.374931	-2.266467
74	1	0	3.212933	-2.608023	-2.462435
75	1	0	4.631605	-1.710653	-3.057920
76	1	0	4.845654	-3.301475	-2.281835

Zero-point correction= 0.612815 (Hartree/Particle)
Thermal correction to Energy= 0.654492
Thermal correction to Enthalpy= 0.655436
Thermal correction to Gibbs Free Energy= 0.532865
Sum of electronic and zero-point Energies= -1839.966813
Sum of electronic and thermal Energies= -1839.925136
Sum of electronic and thermal Enthalpies= -1839.924192
Sum of electronic and thermal Free Energies= -1840.046762
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.42835775

TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.314974	-0.992365	1.285324
2	6	0	-2.511924	-1.047749	0.470465
3	79	0	0.360103	-0.080031	0.544320
4	6	0	-1.434387	-1.401647	2.696322
5	8	0	-1.266311	-2.669752	2.993584
6	6	0	-3.398618	-0.005335	0.019671
7	6	0	-4.478506	-0.300992	-0.824152
8	6	0	-3.186208	1.303911	0.469981
9	6	0	-5.335494	0.711721	-1.218981
10	1	0	-4.640382	-1.324528	-1.160561
11	6	0	-4.050094	2.312827	0.067781
12	1	0	-2.350331	1.523873	1.137150
13	6	0	-5.120110	2.016925	-0.772480
14	1	0	-6.177485	0.490463	-1.870898
15	1	0	-3.889930	3.330643	0.416647
16	1	0	-5.800639	2.808974	-1.079401
17	8	0	-1.648092	-0.484043	3.460025
18	6	0	-2.254486	-2.995592	-2.082042
19	6	0	-1.448683	-1.893166	-2.614365
20	6	0	-2.679598	-3.157383	-0.803394
21	7	0	-2.388363	-2.298210	0.237800
22	8	0	-1.095992	-0.926326	-1.944534
23	1	0	-2.503440	-3.797023	-2.777800
24	6	0	-1.350345	-2.981655	4.395643
25	1	0	-0.597035	-2.415464	4.951430
26	1	0	-2.346007	-2.736035	4.776694
27	1	0	-1.161491	-4.052712	4.467694
28	6	0	1.962544	0.991571	-0.190367
29	7	0	1.965732	2.318006	-0.439892
30	6	0	3.956410	1.602291	-1.033669
31	6	0	3.186601	2.715472	-0.960952
32	1	0	4.969977	1.446687	-1.379677
33	1	0	3.380374	3.745880	-1.228915
34	7	0	3.185963	0.554835	-0.553324
35	6	0	3.595817	-0.822532	-0.507897
36	6	0	3.264277	-1.641584	-1.592052

37	6	0	4.293199	-1.273636	0.616440
38	6	0	3.674542	-2.973140	-1.532562
39	6	0	4.680299	-2.613105	0.631813
40	6	0	4.376474	-3.453296	-0.433209
41	1	0	3.440603	-3.636639	-2.364467
42	1	0	5.227997	-2.995727	1.492173
43	1	0	4.692051	-4.494534	-0.406445
44	6	0	0.827118	3.173269	-0.241263
45	6	0	0.736065	3.887430	0.958376
46	6	0	-0.137802	3.232951	-1.252463
47	6	0	-0.374170	4.713753	1.127737
48	6	0	-1.227489	4.078432	-1.039788
49	6	0	-1.341485	4.814218	0.133829
50	1	0	-0.471494	5.287849	2.048277
51	1	0	-1.992323	4.156209	-1.812454
52	1	0	-2.191574	5.480639	0.274748
53	6	0	1.784878	3.757124	2.020967
54	1	0	2.771335	4.089924	1.669670
55	1	0	1.526624	4.356922	2.900018
56	1	0	1.898448	2.713378	2.348269
57	6	0	-0.030374	2.405128	-2.497613
58	1	0	0.996711	2.370397	-2.885949
59	1	0	-0.344360	1.363927	-2.316315
60	1	0	-0.674011	2.810405	-3.286599
61	6	0	2.483272	-1.113964	-2.758238
62	1	0	2.899423	-0.172745	-3.143744
63	1	0	2.480731	-1.837945	-3.581332
64	1	0	1.435362	-0.910574	-2.483299
65	6	0	4.599670	-0.354752	1.760231
66	1	0	5.249077	0.478211	1.457098
67	1	0	3.684297	0.090813	2.176258
68	1	0	5.107738	-0.892610	2.567670
69	6	0	-3.441153	-4.364295	-0.358010
70	1	0	-3.617271	-5.057698	-1.185740
71	1	0	-2.888869	-4.882359	0.436298
72	1	0	-4.409505	-4.069288	0.069336
73	6	0	-1.059514	-2.019904	-4.061662
74	1	0	-0.409376	-2.894612	-4.204769
75	1	0	-1.944400	-2.180493	-4.692094
76	1	0	-0.533642	-1.118803	-4.391438

Zero-point correction= 0.612754 (Hartree/Particle)
Thermal correction to Energy= 0.654575
Thermal correction to Enthalpy= 0.655519
Thermal correction to Gibbs Free Energy= 0.534176
Sum of electronic and zero-point Energies= -1839.979637
Sum of electronic and thermal Energies= -1839.937815
Sum of electronic and thermal Enthalpies= -1839.936871
Sum of electronic and thermal Free Energies= -1840.058214
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43856720

TS8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.031685	1.681325	-0.517242
2	6	0	-2.449820	1.488874	-0.152348
3	79	0	0.284807	0.177059	-0.178737
4	6	0	-0.697982	2.798714	-1.401773
5	8	0	-0.234780	3.921679	-0.917632
6	6	0	-3.195997	0.372465	-0.746289
7	6	0	-2.803063	-0.194472	-1.965506
8	6	0	-4.347169	-0.091665	-0.098168
9	6	0	-3.565619	-1.205638	-2.536024
10	1	0	-1.927174	0.185997	-2.491299
11	6	0	-5.100597	-1.103736	-0.672478
12	1	0	-4.635215	0.357421	0.849885
13	6	0	-4.714870	-1.656278	-1.893254
14	1	0	-3.271234	-1.629646	-3.494233
15	1	0	-5.998043	-1.460602	-0.170904
16	1	0	-5.317690	-2.441570	-2.346826
17	8	0	-0.871417	2.497917	-2.568221
18	6	0	-1.210475	3.049423	2.220091
19	6	0	-0.704454	1.761811	2.711834

20	6	0	-2.255620	3.251088	1.371007
21	7	0	-2.969350	2.246836	0.743958
22	8	0	-1.160138	0.673333	2.375301
23	6	0	-2.832927	4.610389	1.139290
24	1	0	-3.860551	4.642771	1.524902
25	1	0	-2.242662	5.389074	1.631659
26	1	0	-2.895397	4.829110	0.064523
27	6	0	0.461277	1.860542	3.660070
28	1	0	1.331063	2.273340	3.125940
29	1	0	0.249297	2.543127	4.493161
30	1	0	0.715694	0.871753	4.054168
31	6	0	0.103247	4.924437	-1.900164
32	1	0	0.466611	5.777380	-1.327742
33	1	0	0.880482	4.542926	-2.568159
34	1	0	-0.784864	5.192743	-2.479714
35	6	0	1.519198	-1.461690	0.051194
36	7	0	1.081759	-2.712158	0.309719
37	6	0	3.268913	-2.864875	0.173439
38	6	0	2.143140	-3.593057	0.389248
39	1	0	4.314436	-3.143771	0.148579
40	1	0	1.993669	-4.644771	0.596066
41	7	0	2.862722	-1.559217	-0.036225
42	6	0	3.739358	-0.443881	-0.272029
43	6	0	4.206938	0.268146	0.837291
44	6	0	4.068862	-0.123359	-1.592042
45	6	0	5.052377	1.349086	0.590600
46	6	0	4.919750	0.964148	-1.789128
47	6	0	5.406957	1.691595	-0.709493
48	1	0	5.439653	1.921578	1.432651
49	1	0	5.202806	1.236462	-2.805210
50	1	0	6.074281	2.533667	-0.882984
51	6	0	-0.305795	-3.036897	0.516860
52	6	0	-1.059310	-3.448602	-0.588441
53	6	0	-0.834569	-2.884011	1.801553
54	6	0	-2.406518	-3.724985	-0.371763
55	6	0	-2.192348	-3.162914	1.965371
56	6	0	-2.968428	-3.578928	0.892253
57	1	0	-3.019697	-4.055893	-1.209238
58	1	0	-2.636454	-3.050623	2.953626
59	1	0	-4.024911	-3.796308	1.040799
60	6	0	-0.446521	-3.568455	-1.951230
61	1	0	0.403776	-4.264207	-1.965929
62	1	0	-1.182686	-3.930629	-2.677445
63	1	0	-0.070248	-2.599362	-2.313072
64	6	0	-0.006400	-2.397726	2.951348
65	1	0	1.043789	-2.710602	2.882755
66	1	0	-0.038824	-1.297994	2.989776
67	1	0	-0.407616	-2.769277	3.901218
68	6	0	3.814891	-0.121191	2.231091
69	1	0	4.193867	-1.117567	2.499564
70	1	0	4.213710	0.590196	2.962564
71	1	0	2.721964	-0.156583	2.353558
72	6	0	3.517687	-0.905925	-2.745635
73	1	0	3.700893	-1.983863	-2.640154
74	1	0	2.429185	-0.775552	-2.836652
75	1	0	3.969603	-0.581474	-3.688959
76	1	0	-0.781061	3.940920	2.678393

Zero-point correction= 0.612994 (Hartree/Particle)
Thermal correction to Energy= 0.654539
Thermal correction to Enthalpy= 0.655483
Thermal correction to Gibbs Free Energy= 0.535268
Sum of electronic and zero-point Energies= -1839.975957
Sum of electronic and thermal Energies= -1839.934411
Sum of electronic and thermal Enthalpies= -1839.933467
Sum of electronic and thermal Free Energies= -1840.053682
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43838736

TS9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.365782	1.319380	1.314571
2	6	0	-0.228068	2.521661	0.463102

3	79	0	0.363864	-0.481142	0.637651
4	6	0	-0.716454	1.623383	2.706363
5	8	0	-1.960262	1.549497	3.120190
6	6	0	1.115344	3.112614	0.297567
7	6	0	1.192106	4.511583	0.260409
8	6	0	2.297931	2.363621	0.244157
9	6	0	2.417555	5.149740	0.146591
10	1	0	0.280501	5.100190	0.349919
11	6	0	3.521966	3.007807	0.129431
12	1	0	2.269750	1.273214	0.264000
13	6	0	3.586786	4.396977	0.080295
14	1	0	2.461827	6.236495	0.122884
15	1	0	4.431708	2.412270	0.081458
16	1	0	4.550990	4.895266	-0.000556
17	8	0	0.256376	1.952161	3.354262
18	6	0	-1.160857	3.338091	-2.337403
19	6	0	-0.456451	2.111564	-2.684418
20	6	0	-1.538490	3.748827	-1.088555
21	7	0	-1.332787	3.017682	0.045961
22	8	0	0.103431	1.364332	-1.879004
23	1	0	-1.530961	3.930851	-3.174729
24	7	0	-2.453331	0.355293	0.471438
25	6	0	-3.613639	-0.069307	0.929400
26	6	0	-4.626431	0.130879	-0.042951
27	6	0	-3.973954	0.678279	-1.104075
28	1	0	-5.678228	-0.112760	0.039583
29	8	0	-2.671201	0.800667	-0.811079
30	6	0	-2.151401	1.879235	4.507500
31	1	0	-1.830481	2.907388	4.697852
32	1	0	-3.221536	1.770577	4.688428
33	1	0	-1.578472	1.194927	5.140557
34	6	0	1.007433	-2.242075	-0.201904
35	7	0	0.220593	-3.255315	-0.623068
36	6	0	2.270648	-3.840696	-1.156898
37	6	0	0.981112	-4.252200	-1.215913
38	1	0	3.190395	-4.296837	-1.499138
39	1	0	0.526534	-5.147272	-1.620046
40	7	0	2.264396	-2.603331	-0.531815
41	6	0	3.414326	-1.755030	-0.370943
42	6	0	4.173095	-1.870206	0.797974
43	6	0	3.704884	-0.848718	-1.396676
44	6	0	5.285021	-1.038452	0.922350
45	6	0	4.835324	-0.046880	-1.232809
46	6	0	5.617663	-0.142327	-0.087588
47	1	0	5.898177	-1.104742	1.820101
48	1	0	5.096860	0.662134	-2.018273
49	1	0	6.499631	0.487585	0.019231
50	6	0	-1.215227	-3.245053	-0.558417
51	6	0	-1.918521	-2.581952	-1.571944
52	6	0	-1.836382	-3.903505	0.506841
53	6	0	-3.311043	-2.629289	-1.511165
54	6	0	-3.231265	-3.918363	0.526710
55	6	0	-3.961093	-3.295028	-0.478566
56	1	0	-3.891452	-2.144023	-2.296463
57	1	0	-3.743507	-4.436038	1.337524
58	1	0	-5.049767	-3.326633	-0.456868
59	6	0	-1.215593	-1.834343	-2.665210
60	1	0	-0.356766	-2.390591	-3.066027
61	1	0	-1.900630	-1.635550	-3.498868
62	1	0	-0.832173	-0.863629	-2.308246
63	6	0	-1.031584	-4.556441	1.589439
64	1	0	-0.383965	-5.353745	1.199859
65	1	0	-0.373835	-3.831879	2.091727
66	1	0	-1.684183	-5.001372	2.348209
67	6	0	3.796080	-2.840911	1.875613
68	1	0	3.768923	-3.875402	1.506382
69	1	0	4.511407	-2.801733	2.703895
70	1	0	2.798799	-2.620761	2.283291
71	6	0	2.824065	-0.708099	-2.601641
72	1	0	2.488284	-1.679357	-2.990200
73	1	0	1.921578	-0.118738	-2.367268
74	1	0	3.354954	-0.189810	-3.408347
75	6	0	-3.740718	-0.701561	2.267165
76	1	0	-2.754911	-0.948316	2.676587
77	1	0	-4.257347	-0.038712	2.972584

78	1	0	-4.325697	-1.626041	2.186663
79	6	0	-4.375719	1.124598	-2.455331
80	1	0	-5.465273	1.169828	-2.542182
81	1	0	-3.957413	2.118209	-2.668634
82	1	0	-3.998178	0.437747	-3.225695
83	6	0	-2.431409	4.935291	-0.901625
84	1	0	-2.578903	5.483202	-1.837357
85	1	0	-3.408256	4.605045	-0.522458
86	1	0	-2.022470	5.623728	-0.149881
87	6	0	-0.476325	1.753135	-4.150208
88	1	0	-1.500950	1.509393	-4.467287
89	1	0	-0.147675	2.597143	-4.770825
90	1	0	0.169047	0.888033	-4.335810

Zero-point correction= 0.728082 (Hartree/Particle)
Thermal correction to Energy= 0.777620
Thermal correction to Enthalpy= 0.778564
Thermal correction to Gibbs Free Energy= 0.642984
Sum of electronic and zero-point Energies= -2164.335329
Sum of electronic and thermal Energies= -2164.285792
Sum of electronic and thermal Enthalpies= -2164.284848
Sum of electronic and thermal Free Energies= -2164.420428
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2165.99804128

TS10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.298502	-1.325521	-0.754269
2	6	0	2.429477	-1.175535	0.104156
3	79	0	-0.430485	-0.206692	-0.316705
4	6	0	1.557009	-1.433671	-2.221854
5	8	0	1.509964	-2.691199	-2.653442
6	6	0	3.732440	-0.591120	0.137200
7	6	0	4.773654	-1.197102	0.853370
8	6	0	3.930472	0.607452	-0.560480
9	6	0	6.024823	-0.606237	0.854969
10	1	0	4.586826	-2.128487	1.388359
11	6	0	5.187391	1.194209	-0.545694
12	1	0	3.098106	1.046135	-1.112499
13	6	0	6.226643	0.587734	0.157466
14	1	0	6.848504	-1.067451	1.394903
15	1	0	5.363584	2.119918	-1.089023
16	1	0	7.212752	1.048635	0.161524
17	8	0	1.737991	-0.458686	-2.915425
18	6	0	1.084937	-2.587101	2.374467
19	6	0	1.412003	-1.220551	2.729735
20	6	0	1.221970	-3.095687	1.126354
21	7	0	1.916022	-2.425461	0.120001
22	8	0	1.861079	-0.388775	1.921598
23	1	0	0.590714	-3.192740	3.131790
24	6	0	1.703440	-2.856539	-4.062343
25	1	0	0.935346	-2.308683	-4.617500
26	1	0	2.690364	-2.486042	-4.356712
27	1	0	1.624117	-3.928180	-4.249525
28	6	0	-1.916072	1.165486	0.053917
29	7	0	-1.645443	2.483700	0.179846
30	6	0	-3.816726	2.301787	0.453135
31	6	0	-2.803720	3.202330	0.427431
32	1	0	-4.880893	2.417595	0.612531
33	1	0	-2.790604	4.276653	0.556935
34	7	0	-3.249673	1.056801	0.221060
35	6	0	-3.971076	-0.185095	0.175692
36	6	0	-4.032076	-0.958550	1.338445
37	6	0	-4.564579	-0.562639	-1.032428
38	6	0	-4.745438	-2.154889	1.274353
39	6	0	-5.265412	-1.768220	-1.050283
40	6	0	-5.358631	-2.554019	0.092446
41	1	0	-4.820710	-2.775626	2.166626
42	1	0	-5.742092	-2.089253	-1.975638
43	1	0	-5.915604	-3.488490	0.061363
44	6	0	-0.313364	3.017905	0.076107
45	6	0	0.162869	3.388310	-1.184935
46	6	0	0.463624	3.073242	1.238572

47	6	0	1.471780	3.868455	-1.256871
48	6	0	1.768073	3.547710	1.117184
49	6	0	2.264048	3.950393	-0.118226
50	1	0	1.866870	4.177128	-2.224094
51	1	0	2.396938	3.601461	2.005027
52	1	0	3.280663	4.333332	-0.192799
53	6	0	-0.669806	3.225767	-2.420136
54	1	0	-1.718245	3.510968	-2.263744
55	1	0	-0.272693	3.831371	-3.242015
56	1	0	-0.664222	2.176809	-2.754622
57	6	0	-0.074806	2.596695	2.552995
58	1	0	-1.030736	3.072195	2.811805
59	1	0	-0.251288	1.509626	2.529571
60	1	0	0.634121	2.804291	3.362470
61	6	0	-3.333035	-0.532367	2.594558
62	1	0	-3.519514	0.522323	2.839605
63	1	0	-3.657058	-1.139297	3.447333
64	1	0	-2.241683	-0.646596	2.494238
65	6	0	-4.435894	0.289025	-2.259105
66	1	0	-4.901677	1.275606	-2.128006
67	1	0	-3.381231	0.466534	-2.516266
68	1	0	-4.914655	-0.190557	-3.119419
69	6	0	0.641530	-4.380945	0.669416
70	1	0	0.087739	-4.888060	1.464561
71	1	0	-0.038179	-4.181063	-0.172959
72	1	0	1.427399	-5.043021	0.284380
73	6	0	1.114114	-0.786888	4.130291
74	1	0	0.028471	-0.811073	4.302631
75	1	0	1.564557	-1.482558	4.850334
76	1	0	1.484666	0.226323	4.306540

Zero-point correction= 0.613323 (Hartree/Particle)
Thermal correction to Energy= 0.654708
Thermal correction to Enthalpy= 0.655652
Thermal correction to Gibbs Free Energy= 0.535235
Sum of electronic and zero-point Energies= -1839.985536
Sum of electronic and thermal Energies= -1839.944151
Sum of electronic and thermal Enthalpies= -1839.943207
Sum of electronic and thermal Free Energies= -1840.063625
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.44519491

TS11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.835519	0.019989	0.427068
2	6	0	-2.667732	-1.028290	-0.098563
3	79	0	0.273515	0.082785	0.104570
4	6	0	-2.257472	1.432296	0.170005
5	8	0	-2.469523	2.122307	1.292063
6	6	0	-4.057899	-0.928734	-0.562550
7	6	0	-4.909911	0.045085	-0.026204
8	6	0	-4.533644	-1.794185	-1.554028
9	6	0	-6.214136	0.151932	-0.484112
10	1	0	-4.562881	0.692547	0.776945
11	6	0	-5.836291	-1.669401	-2.017373
12	1	0	-3.879881	-2.554244	-1.973990
13	6	0	-6.678447	-0.698788	-1.484005
14	1	0	-6.874265	0.903011	-0.055948
15	1	0	-6.195644	-2.337087	-2.797393
16	1	0	-7.700879	-0.607611	-1.844905
17	8	0	-2.294918	1.896781	-0.946772
18	6	0	-1.001387	-2.533240	1.593447
19	6	0	-1.079233	-2.742506	0.241034
20	6	0	-1.889518	-1.645009	2.229231
21	7	0	-2.488613	-0.628317	1.594521
22	8	0	-2.063244	-2.197151	-0.479467
23	1	0	-0.354092	-3.186195	2.174881
24	6	0	-2.740758	3.511269	1.094823
25	1	0	-2.909835	3.925743	2.089886
26	1	0	-1.885015	3.998488	0.611875
27	1	0	-3.628585	3.641105	0.466196
28	6	0	2.268846	0.442665	-0.258799
29	7	0	3.318878	-0.396285	-0.391881

30	6	0	4.142961	1.623400	-0.671961
31	6	0	4.485123	0.313048	-0.646004
32	1	0	4.729371	2.517727	-0.837362
33	1	0	5.435022	-0.187763	-0.780707
34	7	0	2.779734	1.681415	-0.433275
35	6	0	1.998436	2.886790	-0.342344
36	6	0	2.011047	3.581797	0.872874
37	6	0	1.246564	3.286318	-1.451256
38	6	0	1.249737	4.746118	0.951783
39	6	0	0.496570	4.456322	-1.323634
40	6	0	0.505963	5.183315	-0.139770
41	1	0	1.245100	5.313978	1.881493
42	1	0	-0.098690	4.795019	-2.170488
43	1	0	-0.074887	6.101364	-0.065021
44	6	0	3.249962	-1.825810	-0.277945
45	6	0	3.191000	-2.580159	-1.454947
46	6	0	3.277394	-2.396291	0.998963
47	6	0	3.192311	-3.969692	-1.328309
48	6	0	3.266653	-3.790350	1.077850
49	6	0	3.238727	-4.569308	-0.074161
50	1	0	3.162003	-4.583365	-2.228121
51	1	0	3.307243	-4.264504	2.058271
52	1	0	3.255750	-5.654895	0.006039
53	6	0	3.104571	-1.915612	-2.795933
54	1	0	3.998898	-1.319392	-3.022797
55	1	0	2.991518	-2.656933	-3.594202
56	1	0	2.246598	-1.227852	-2.846563
57	6	0	3.314283	-1.544785	2.231925
58	1	0	4.083442	-0.762755	2.169450
59	1	0	2.353719	-1.030885	2.391615
60	1	0	3.522668	-2.150473	3.120650
61	6	0	2.800131	3.081580	2.045451
62	1	0	3.883558	3.129056	1.867144
63	1	0	2.589061	3.677928	2.939514
64	1	0	2.560094	2.032546	2.275259
65	6	0	1.213632	2.484625	-2.716834
66	1	0	2.198972	2.076699	-2.979535
67	1	0	0.519685	1.634882	-2.623358
68	1	0	0.864601	3.096524	-3.555628
69	6	0	-2.256372	-1.815941	3.661636
70	1	0	-3.325199	-2.057589	3.734431
71	1	0	-1.682462	-2.612376	4.145165
72	1	0	-2.114500	-0.872289	4.202722
73	6	0	-0.259366	-3.697325	-0.531890
74	1	0	0.312504	-3.146444	-1.293533
75	1	0	0.450121	-4.225882	0.111705
76	1	0	-0.896655	-4.418044	-1.059667

Zero-point correction= 0.614897 (Hartree/Particle)
Thermal correction to Energy= 0.655338
Thermal correction to Enthalpy= 0.656282
Thermal correction to Gibbs Free Energy= 0.538874
Sum of electronic and zero-point Energies= -1839.999348
Sum of electronic and thermal Energies= -1839.958907
Sum of electronic and thermal Enthalpies= -1839.957963
Sum of electronic and thermal Free Energies= -1840.075370
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.45984842

TS12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225260	-1.425985	-0.705798
2	6	0	3.040259	-1.405939	0.479003
3	79	0	-0.542794	-0.372779	-0.158091
4	6	0	2.507644	-0.435461	-1.759814
5	8	0	1.510848	-0.287399	-2.642539
6	6	0	3.503609	-0.342931	1.318613
7	6	0	4.439465	-0.620320	2.331447
8	6	0	2.989920	0.958703	1.172162
9	6	0	4.851668	0.388052	3.185392
10	1	0	4.838573	-1.627626	2.427481
11	6	0	3.409340	1.958080	2.031543
12	1	0	2.259315	1.179328	0.392448

13	6	0	4.337601	1.675281	3.034145
14	1	0	5.578702	0.177816	3.966163
15	1	0	3.010462	2.964150	1.918028
16	1	0	4.666237	2.468028	3.703679
17	8	0	3.587120	0.111813	-1.850808
18	6	0	1.782474	-4.016360	-0.478790
19	6	0	0.678294	-3.170540	-0.289703
20	6	0	3.002724	-3.360729	-0.441518
21	1	0	1.660182	-5.009662	-0.907365
22	6	0	-0.703921	-3.657942	-0.023504
23	1	0	-1.453181	-3.087033	-0.590503
24	1	0	-0.794024	-4.720613	-0.275287
25	1	0	-0.948704	-3.551061	1.042496
26	8	0	3.265836	-2.646350	0.819281
27	7	0	0.896581	-1.867868	-0.473162
28	6	0	4.286012	-3.793246	-1.044897
29	1	0	4.873062	-4.394902	-0.337382
30	1	0	4.094876	-4.389496	-1.943261
31	1	0	4.893237	-2.923426	-1.329116
32	6	0	1.820451	0.555472	-3.752296
33	1	0	2.714547	0.193947	-4.270322
34	1	0	0.951766	0.513241	-4.412625
35	1	0	2.000930	1.582076	-3.411993
36	6	0	-1.953183	1.043583	0.132476
37	7	0	-1.835019	2.384487	0.032011
38	6	0	-3.950685	2.008771	0.505965
39	6	0	-3.059283	2.998440	0.256678
40	1	0	-5.009439	2.031751	0.728881
41	1	0	-3.169961	4.073982	0.211304
42	7	0	-3.251028	0.814984	0.426093
43	6	0	-3.801756	-0.503448	0.595234
44	6	0	-3.840785	-1.045177	1.883850
45	6	0	-4.232811	-1.190863	-0.544021
46	6	0	-4.347188	-2.337649	2.018134
47	6	0	-4.731980	-2.480523	-0.360617
48	6	0	-4.788614	-3.047931	0.907342
49	1	0	-4.396205	-2.786234	3.009641
50	1	0	-5.082910	-3.039928	-1.227067
51	1	0	-5.186211	-4.053353	1.031999
52	6	0	-0.617328	3.067298	-0.308697
53	6	0	-0.240302	3.124239	-1.654845
54	6	0	0.128713	3.647654	0.723015
55	6	0	0.934717	3.812972	-1.961332
56	6	0	1.286321	4.339121	0.365086
57	6	0	1.688395	4.419170	-0.963678
58	1	0	1.244790	3.892418	-3.003322
59	1	0	1.869237	4.833561	1.142643
60	1	0	2.592361	4.965638	-1.224658
61	6	0	-1.048430	2.456525	-2.726162
62	1	0	-2.129038	2.583683	-2.575864
63	1	0	-0.795049	2.858065	-3.714093
64	1	0	-0.852323	1.372012	-2.745081
65	6	0	-0.287159	3.507924	2.156085
66	1	0	-1.262629	3.971704	2.355803
67	1	0	-0.373409	2.449051	2.443160
68	1	0	0.443800	3.978271	2.823269
69	6	0	-3.342827	-0.272384	3.067530
70	1	0	-3.888784	0.671349	3.203283
71	1	0	-3.453893	-0.854431	3.988541
72	1	0	-2.279270	-0.013104	2.960218
73	6	0	-4.134960	-0.579319	-1.909163
74	1	0	-4.559239	0.433483	-1.942846
75	1	0	-3.086527	-0.497302	-2.235256
76	1	0	-4.664628	-1.188854	-2.649102

Zero-point correction= 0.615806 (Hartree/Particle)
Thermal correction to Energy= 0.655795
Thermal correction to Enthalpy= 0.656740
Thermal correction to Gibbs Free Energy= 0.542219
Sum of electronic and zero-point Energies= -1840.005386
Sum of electronic and thermal Energies= -1839.965397
Sum of electronic and thermal Enthalpies= -1839.964452
Sum of electronic and thermal Free Energies= -1840.078973
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.46563894

TS13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.936423	-1.278741	0.438943
2	6	0	-2.853277	-0.641610	-0.579332
3	79	0	0.609429	-0.131112	-0.867449
4	6	0	-1.777338	-0.488563	1.709157
5	8	0	-1.486594	-1.245458	2.757360
6	6	0	-4.249951	-0.440801	-0.185717
7	6	0	-4.774248	-1.012987	0.983338
8	6	0	-5.083131	0.308637	-1.028878
9	6	0	-6.111697	-0.833801	1.302617
10	1	0	-4.147207	-1.623029	1.634636
11	6	0	-6.414797	0.494711	-0.697759
12	1	0	-4.663248	0.741750	-1.933936
13	6	0	-6.928591	-0.076310	0.466250
14	1	0	-6.520616	-1.285929	2.203255
15	1	0	-7.059287	1.083670	-1.346412
16	1	0	-7.976471	0.068184	0.722058
17	8	0	-1.915823	0.713009	1.712549
18	6	0	-0.968331	-2.559884	-2.012656
19	6	0	-0.616375	-1.181356	-2.184415
20	6	0	-1.364800	-3.151171	-0.843723
21	7	0	-1.440097	-2.455868	0.339845
22	8	0	-2.467767	-0.388941	-1.725064
23	1	0	-0.891929	-3.207792	-2.891334
24	6	0	3.187298	2.558363	1.236802
25	6	0	3.896377	1.412881	1.383463
26	1	0	3.380386	3.572592	1.560922
27	1	0	4.845227	1.207389	1.861542
28	7	0	2.041101	2.227372	0.533354
29	7	0	3.161877	0.412002	0.767476
30	6	0	2.017832	0.907438	0.245496
31	6	0	-1.657406	-4.608528	-0.737774
32	1	0	-1.074684	-5.042044	0.084592
33	1	0	-2.716005	-4.779482	-0.500241
34	1	0	-1.423934	-5.134949	-1.668379
35	6	0	-0.614368	-0.696592	-3.593007
36	1	0	-1.410562	-1.136087	-4.209275
37	1	0	-0.661633	0.395921	-3.650923
38	1	0	0.355480	-0.998025	-4.022420
39	6	0	-1.303234	-0.543479	3.991203
40	1	0	-1.167819	-1.313062	4.752232
41	1	0	-0.416618	0.097933	3.932860
42	1	0	-2.179533	0.074614	4.212139
43	6	0	0.975521	3.137019	0.211845
44	6	0	0.907816	3.665032	-1.081510
45	6	0	0.046671	3.432267	1.214118
46	6	0	-0.149551	4.529847	-1.361300
47	6	0	-0.998381	4.294427	0.885378
48	6	0	-1.094121	4.839345	-0.389065
49	1	0	-0.226516	4.965451	-2.356975
50	1	0	-1.743419	4.534516	1.642817
51	1	0	-1.913097	5.515175	-0.628018
52	6	0	3.558023	-0.967068	0.683426
53	6	0	3.020513	-1.873461	1.601965
54	6	0	4.456634	-1.335248	-0.323719
55	6	0	3.427724	-3.203880	1.501298
56	6	0	4.833274	-2.675855	-0.387083
57	6	0	4.326401	-3.600764	0.518921
58	1	0	3.032552	-3.932230	2.208679
59	1	0	5.533664	-2.992758	-1.158906
60	1	0	4.636819	-4.642152	0.458643
61	6	0	2.019332	-1.448312	2.633311
62	1	0	2.251262	-0.461541	3.057830
63	1	0	1.008559	-1.392590	2.197977
64	1	0	1.976227	-2.170841	3.456719
65	6	0	4.981495	-0.328562	-1.302740
66	1	0	4.165145	0.221699	-1.793435
67	1	0	5.624709	0.420867	-0.820843
68	1	0	5.574669	-0.816710	-2.083356
69	6	0	0.175775	2.853053	2.590196
70	1	0	0.920593	3.395314	3.190541

71	1	0	-0.782014	2.897265	3.119985
72	1	0	0.487726	1.799208	2.553656
73	6	0	1.916601	3.307350	-2.131551
74	1	0	2.944880	3.332139	-1.746010
75	1	0	1.747725	2.290901	-2.521151
76	1	0	1.857795	3.998638	-2.979451

Zero-point correction= 0.613694 (Hartree/Particle)
Thermal correction to Energy= 0.654712
Thermal correction to Enthalpy= 0.655656
Thermal correction to Gibbs Free Energy= 0.537574
Sum of electronic and zero-point Energies= -1839.990791
Sum of electronic and thermal Energies= -1839.949773
Sum of electronic and thermal Enthalpies= -1839.948829
Sum of electronic and thermal Free Energies= -1840.066911
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.45088538

TS14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.141528	0.683023	0.568510
2	6	0	-2.949805	0.640907	-0.748052
3	79	0	0.319329	-0.368749	0.141634
4	6	0	-1.245031	1.928104	0.667609
5	8	0	-0.784167	2.052593	1.909624
6	6	0	-4.417815	0.445184	-0.690518
7	6	0	-5.220626	0.793969	0.402917
8	6	0	-5.014923	-0.074152	-1.847117
9	6	0	-6.596381	0.610715	0.339134
10	1	0	-4.777537	1.233545	1.295107
11	6	0	-6.385720	-0.273960	-1.897943
12	1	0	-4.381362	-0.311631	-2.699885
13	6	0	-7.177826	0.068451	-0.803766
14	1	0	-7.219072	0.900906	1.182878
15	1	0	-6.841749	-0.688996	-2.794295
16	1	0	-8.255258	-0.079544	-0.845904
17	8	0	-1.053134	2.705915	-0.231425
18	6	0	-2.381502	-1.855336	0.947814
19	6	0	-1.574508	-1.388907	-0.035955
20	6	0	-2.912488	-0.957481	1.935065
21	7	0	-2.660109	0.302739	1.743775
22	8	0	-2.352115	0.777538	-1.794678
23	1	0	-2.727706	-2.891669	0.941025
24	6	0	4.393867	0.499397	-0.867890
25	6	0	4.403339	-0.850481	-0.761965
26	1	0	5.158127	1.203611	-1.169045
27	1	0	5.177217	-1.584045	-0.946477
28	7	0	3.125137	0.925652	-0.504161
29	7	0	3.138823	-1.217688	-0.336995
30	6	0	2.348850	-0.129744	-0.177819
31	6	0	-3.767206	-1.414710	3.060024
32	1	0	-4.783030	-1.613359	2.687354
33	1	0	-3.393038	-2.344188	3.504370
34	1	0	-3.835058	-0.638354	3.827568
35	6	0	2.671153	-2.565389	-0.158990
36	6	0	2.679958	-3.108890	1.129342
37	6	0	2.191540	-3.249194	-1.282566
38	6	0	2.169729	-4.398467	1.281214
39	6	0	1.689788	-4.535223	-1.080955
40	6	0	1.676302	-5.102646	0.188972
41	1	0	2.167004	-4.852499	2.271406
42	1	0	1.313380	-5.096458	-1.935911
43	1	0	1.286320	-6.109366	0.326551
44	6	0	2.739636	2.312375	-0.478427
45	6	0	1.881398	2.805183	-1.465709
46	6	0	3.292510	3.113742	0.531942
47	6	0	1.579098	4.168556	-1.419922
48	6	0	2.977193	4.470358	0.520559
49	6	0	2.126832	4.993655	-0.449338
50	1	0	0.900180	4.576880	-2.167185
51	1	0	3.395882	5.117485	1.290719
52	1	0	1.887009	6.055180	-0.443111
53	6	0	1.278055	1.941377	-2.531778

54	1	0	0.284675	1.576359	-2.224850
55	1	0	1.130150	2.518251	-3.452104
56	1	0	1.903039	1.072575	-2.776182
57	6	0	4.149703	2.528288	1.615583
58	1	0	4.292517	3.250779	2.426515
59	1	0	3.693185	1.623915	2.045940
60	1	0	5.148477	2.241514	1.258579
61	6	0	2.208835	-2.624429	-2.645700
62	1	0	1.736087	-1.630892	-2.649715
63	1	0	3.232507	-2.489195	-3.021487
64	1	0	1.675724	-3.252056	-3.368501
65	6	0	3.199429	-2.330727	2.300252
66	1	0	2.535766	-1.490408	2.552121
67	1	0	3.278549	-2.967475	3.187767
68	1	0	4.192066	-1.904035	2.102633
69	6	0	0.034925	3.199489	2.147945
70	1	0	-0.452617	4.105663	1.774561
71	1	0	0.169214	3.246321	3.229533
72	1	0	0.999493	3.077463	1.641591
73	6	0	-1.487820	-2.068203	-1.371894
74	1	0	-1.276133	-1.342898	-2.167323
75	1	0	-0.654018	-2.788879	-1.359913
76	1	0	-2.412411	-2.605640	-1.623407

Zero-point correction= 0.613715 (Hartree/Particle)
Thermal correction to Energy= 0.654399
Thermal correction to Enthalpy= 0.655344
Thermal correction to Gibbs Free Energy= 0.538916
Sum of electronic and zero-point Energies= -1839.984905
Sum of electronic and thermal Energies= -1839.944221
Sum of electronic and thermal Enthalpies= -1839.943276
Sum of electronic and thermal Free Energies= -1840.059704
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.44627534

TS15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281290	-0.566792	-0.124191
2	6	0	-3.514517	-1.111920	0.265255
3	79	0	0.699434	-0.286962	-0.168329
4	6	0	-2.103700	0.925301	-0.235404
5	8	0	-1.980639	1.298204	-1.508682
6	6	0	-4.765626	-0.343427	0.320779
7	6	0	-5.628010	-0.490516	1.412392
8	6	0	-5.108126	0.526413	-0.721350
9	6	0	-6.802410	0.247952	1.472281
10	1	0	-5.364448	-1.180896	2.211304
11	6	0	-6.282248	1.264913	-0.653405
12	1	0	-4.461204	0.607134	-1.594882
13	6	0	-7.128466	1.128759	0.443823
14	1	0	-7.466616	0.137658	2.326935
15	1	0	-6.547228	1.936658	-1.467335
16	1	0	-8.051090	1.703637	0.493057
17	8	0	-2.035653	1.654554	0.722859
18	6	0	-2.431578	-3.263005	-0.884992
19	6	0	-3.603326	-2.854490	-0.231908
20	6	0	-1.227198	-2.597970	-0.745038
21	7	0	-1.180924	-1.288047	-0.377269
22	8	0	-3.441807	-2.282154	1.020092
23	1	0	-2.486885	-4.111000	-1.566869
24	6	0	4.668535	0.744699	0.737384
25	6	0	4.147597	1.995327	0.734006
26	1	0	5.666715	0.378960	0.939863
27	1	0	4.591112	2.961539	0.935677
28	7	0	3.633222	-0.114920	0.409842
29	7	0	2.806339	1.871247	0.403967
30	6	0	2.489445	0.574486	0.207062
31	6	0	0.060520	-3.231018	-1.164624
32	1	0	0.570968	-2.637777	-1.936661
33	1	0	0.746575	-3.317685	-0.308569
34	1	0	-0.107690	-4.240512	-1.554512
35	6	0	-4.953194	-3.401540	-0.541001

36	1	0	-4.984868	-3.828981	-1.548266
37	1	0	-5.208530	-4.182696	0.187296
38	1	0	-5.723594	-2.624552	-0.464773
39	6	0	-1.705850	2.688868	-1.716634
40	1	0	-1.808658	2.854970	-2.789770
41	1	0	-2.413681	3.305601	-1.152860
42	1	0	-0.685271	2.916765	-1.386488
43	6	0	1.896256	2.979289	0.282630
44	6	0	1.971036	3.758400	-0.879016
45	6	0	1.005701	3.239353	1.328732
46	6	0	1.123128	4.861658	-0.965087
47	6	0	0.164108	4.344467	1.188354
48	6	0	0.230900	5.154333	0.062271
49	1	0	1.165825	5.493817	-1.851474
50	1	0	-0.546231	4.567082	1.983213
51	1	0	-0.422247	6.021268	-0.019647
52	6	0	3.727274	-1.547342	0.316908
53	6	0	3.520765	-2.297694	1.479640
54	6	0	3.991244	-2.116163	-0.932921
55	6	0	3.590331	-3.685908	1.363377
56	6	0	4.053720	-3.508230	-0.999682
57	6	0	3.855720	-4.284755	0.136390
58	1	0	3.439149	-4.299242	2.250811
59	1	0	4.265546	-3.982811	-1.957160
60	1	0	3.914295	-5.369284	0.066418
61	6	0	3.225420	-1.634342	2.790983
62	1	0	4.036599	-0.962295	3.103512
63	1	0	2.310277	-1.025655	2.740643
64	1	0	3.088267	-2.378192	3.582847
65	6	0	4.172379	-1.267412	-2.155116
66	1	0	3.225236	-0.797388	-2.460982
67	1	0	4.891813	-0.453481	-1.992609
68	1	0	4.530998	-1.867759	-2.998070
69	6	0	0.933784	2.368507	2.545753
70	1	0	0.318686	1.476298	2.353635
71	1	0	1.924483	2.023398	2.871547
72	1	0	0.469420	2.905558	3.379871
73	6	0	2.912455	3.408904	-1.992586
74	1	0	3.964316	3.558174	-1.712141
75	1	0	2.809097	2.355185	-2.291513
76	1	0	2.719247	4.029116	-2.874363

Zero-point correction= 0.615763 (Hartree/Particle)
Thermal correction to Energy= 0.656097
Thermal correction to Enthalpy= 0.657041
Thermal correction to Gibbs Free Energy= 0.540911
Sum of electronic and zero-point Energies= -1840.038506
Sum of electronic and thermal Energies= -1839.998171
Sum of electronic and thermal Enthalpies= -1839.997227
Sum of electronic and thermal Free Energies= -1840.113357
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.49631910

TS16a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.304997	-0.798920	-0.119598
2	6	0	-3.502506	-1.323169	0.533544
3	79	0	0.676471	-0.294642	-0.003098
4	6	0	-2.252429	0.591868	-0.708120
5	8	0	-2.344443	1.493246	0.260160
6	6	0	-4.738033	-0.468209	0.515865
7	6	0	-5.519263	-0.486725	1.671251
8	6	0	-5.140610	0.307503	-0.576433
9	6	0	-6.670389	0.288373	1.749724
10	1	0	-5.208834	-1.116330	2.502550
11	6	0	-6.296417	1.075155	-0.497503
12	1	0	-4.574335	0.297609	-1.509054
13	6	0	-7.059189	1.071798	0.667623
14	1	0	-7.269229	0.275819	2.658173
15	1	0	-6.610898	1.666144	-1.355574
16	1	0	-7.964756	1.672487	0.726462
17	8	0	-2.076158	0.816587	-1.880002
18	6	0	-2.296593	-3.252285	-1.007389

19	6	0	-3.435236	-2.522539	-0.843766
20	6	0	-1.093445	-2.726306	-0.520029
21	7	0	-1.116700	-1.435429	-0.165670
22	8	0	-3.466184	-2.344925	1.284621
23	1	0	-2.331383	-4.232704	-1.479017
24	6	0	4.709041	0.828099	0.248762
25	6	0	4.187982	2.075892	0.173499
26	1	0	5.729081	0.474316	0.323542
27	1	0	4.652263	3.053409	0.164108
28	7	0	3.637988	-0.049070	0.212456
29	7	0	2.810059	1.932302	0.094102
30	6	0	2.471475	0.627295	0.116413
31	6	0	0.177858	-3.492910	-0.463543
32	1	0	0.947156	-3.031218	-1.100834
33	1	0	0.577878	-3.507580	0.559941
34	1	0	0.031185	-4.526186	-0.792749
35	6	0	-4.818263	-2.905858	-1.197741
36	1	0	-5.317123	-2.136725	-1.799952
37	1	0	-4.779120	-3.840532	-1.772687
38	1	0	-5.424810	-3.080188	-0.302642
39	6	0	-2.261395	2.856687	-0.171250
40	1	0	-2.304045	3.458823	0.736912
41	1	0	-1.319776	3.026469	-0.706878
42	1	0	-3.107189	3.083753	-0.830179
43	6	0	3.732439	-1.484262	0.250720
44	6	0	3.850226	-2.171298	-0.962454
45	6	0	3.683986	-2.118903	1.496367
46	6	0	3.926389	-3.563300	-0.902627
47	6	0	3.759370	-3.511994	1.505506
48	6	0	3.881180	-4.226479	0.318807
49	1	0	4.028538	-4.127742	-1.828912
50	1	0	3.730423	-4.036690	2.459664
51	1	0	3.949228	-5.312352	0.346912
52	6	0	1.907547	3.045207	-0.036578
53	6	0	1.518414	3.438996	-1.321192
54	6	0	1.522176	3.718643	1.128121
55	6	0	0.733571	4.589419	-1.423353
56	6	0	0.732573	4.857964	0.975985
57	6	0	0.354240	5.296962	-0.288347
58	1	0	0.426992	4.932476	-2.410921
59	1	0	0.424913	5.410567	1.862996
60	1	0	-0.245448	6.199766	-0.390009
61	6	0	1.946762	3.233967	2.481598
62	1	0	1.650225	2.188024	2.646860
63	1	0	3.036766	3.280567	2.613190
64	1	0	1.493350	3.839744	3.273149
65	6	0	1.897501	2.650030	-2.537943
66	1	0	1.809201	3.260404	-3.443214
67	1	0	2.924760	2.264504	-2.487111
68	1	0	1.231302	1.782221	-2.662791
69	6	0	3.542302	-1.335848	2.766564
70	1	0	4.315707	-0.561740	2.862727
71	1	0	2.570280	-0.823469	2.818773
72	1	0	3.617402	-1.992226	3.639851
73	6	0	3.863463	-1.443817	-2.273370
74	1	0	2.884790	-0.987941	-2.489668
75	1	0	4.601669	-0.630630	-2.291090
76	1	0	4.099138	-2.126212	-3.096946

Zero-point correction= 0.613919 (Hartree/Particle)
Thermal correction to Energy= 0.654657
Thermal correction to Enthalpy= 0.655601
Thermal correction to Gibbs Free Energy= 0.538245
Sum of electronic and zero-point Energies= -1839.967596
Sum of electronic and thermal Energies= -1839.926859
Sum of electronic and thermal Enthalpies= -1839.925914
Sum of electronic and thermal Free Energies= -1840.043270
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43291285

TS17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.800650	-0.958504	-0.985035

2	6	0	3.866010	-0.468283	0.716759
3	6	0	3.091592	0.197695	-1.863612
4	8	0	2.045316	1.020366	-2.010909
5	6	0	2.868242	-0.382184	1.799549
6	6	0	2.576204	-1.407861	2.696804
7	6	0	2.229187	0.859732	1.902895
8	6	0	1.624108	-1.194687	3.689733
9	1	0	3.103958	-2.356707	2.634497
10	6	0	1.284129	1.060384	2.897418
11	1	0	2.469901	1.658677	1.199896
12	6	0	0.971456	0.030910	3.783350
13	1	0	1.402503	-1.988905	4.399651
14	1	0	0.796076	2.029576	2.978324
15	1	0	0.228648	0.193538	4.563078
16	8	0	4.171207	0.370650	-2.374742
17	6	0	2.997244	-2.983607	-0.001771
18	6	0	1.672642	-2.574639	-0.007823
19	6	0	3.765436	-1.976316	-0.627726
20	1	0	3.381234	-3.920865	0.389559
21	6	0	0.494023	-3.284073	0.552903
22	1	0	0.752561	-4.315022	0.818904
23	1	0	0.123902	-2.780176	1.458028
24	1	0	-0.336237	-3.308074	-0.167603
25	8	0	4.863522	0.141870	0.560393
26	7	0	1.561250	-1.346618	-0.592139
27	6	0	5.151184	-2.144534	-1.147769
28	1	0	5.653269	-2.972007	-0.634272
29	1	0	5.111903	-2.372384	-2.220152
30	1	0	5.743895	-1.231676	-1.042017
31	79	0	-0.229696	-0.231880	-0.383605
32	6	0	2.300052	2.138233	-2.868506
33	1	0	3.090198	2.767555	-2.446102
34	1	0	2.609365	1.794505	-3.860380
35	1	0	1.359143	2.687642	-2.925796
36	6	0	-2.047273	0.625003	-0.140258
37	7	0	-3.220689	-0.045358	-0.136241
38	6	0	-3.752830	2.071952	0.116695
39	6	0	-4.284014	0.829312	0.019623
40	1	0	-4.211232	3.043987	0.243589
41	1	0	-5.307588	0.478704	0.044107
42	7	0	-2.377430	1.925171	0.017195
43	6	0	-1.411370	2.979009	0.148728
44	6	0	-0.836305	3.509755	-1.008965
45	6	0	-1.081095	3.403952	1.439685
46	6	0	0.127380	4.505331	-0.842932
47	6	0	-0.110730	4.399101	1.556958
48	6	0	0.490264	4.941784	0.426169
49	1	0	0.585736	4.952742	-1.724860
50	1	0	0.166966	4.756204	2.548713
51	1	0	1.240282	5.722730	0.535230
52	6	0	-3.318489	-1.476974	-0.231460
53	6	0	-3.213362	-2.222544	0.947223
54	6	0	-3.480090	-2.051041	-1.496080
55	6	0	-3.284297	-3.610876	0.833071
56	6	0	-3.542345	-3.443035	-1.561524
57	6	0	-3.447785	-4.214933	-0.408818
58	1	0	-3.213720	-4.220614	1.733352
59	1	0	-3.670648	-3.921611	-2.531539
60	1	0	-3.505913	-5.299425	-0.478995
61	6	0	-3.002667	-1.558639	2.275095
62	1	0	-3.727907	-0.753589	2.457362
63	1	0	-3.095860	-2.282724	3.091943
64	1	0	-2.000661	-1.104978	2.341874
65	6	0	-3.571262	-1.203016	-2.728421
66	1	0	-4.441066	-0.532085	-2.701413
67	1	0	-2.681487	-0.567393	-2.848494
68	1	0	-3.661375	-1.825150	-3.625049
69	6	0	-1.237972	3.021482	-2.368330
70	1	0	-2.329067	2.957417	-2.476977
71	1	0	-0.865796	3.691651	-3.152061
72	1	0	-0.840958	2.012677	-2.566620
73	6	0	-1.749601	2.810373	2.644193
74	1	0	-2.805570	3.106384	2.713633
75	1	0	-1.728128	1.709820	2.620226
76	1	0	-1.262483	3.143072	3.568608

Zero-point correction= 0.615214 (Hartree/Particle)
Thermal correction to Energy= 0.655752
Thermal correction to Enthalpy= 0.656696
Thermal correction to Gibbs Free Energy= 0.540757
Sum of electronic and zero-point Energies= -1840.052136
Sum of electronic and thermal Energies= -1840.011598
Sum of electronic and thermal Enthalpies= -1840.010653
Sum of electronic and thermal Free Energies= -1840.126592
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.51696915

TS18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.755252	-0.792563	-1.132114
2	6	0	4.094298	-1.206418	1.108038
3	6	0	2.817508	0.426406	-1.961425
4	8	0	1.653414	0.703898	-2.556764
5	6	0	3.142244	-0.225557	1.690926
6	6	0	2.360546	-0.612773	2.778428
7	6	0	3.100232	1.082537	1.208878
8	6	0	1.494003	0.307207	3.358784
9	1	0	2.433445	-1.629629	3.164778
10	6	0	2.231942	1.996393	1.794564
11	1	0	3.744246	1.380154	0.382142
12	6	0	1.427195	1.606411	2.861536
13	1	0	0.880373	0.012168	4.208226
14	1	0	2.182105	3.016503	1.416931
15	1	0	0.753179	2.328948	3.319376
16	8	0	3.823954	1.087189	-2.091529
17	6	0	3.284803	-2.627340	0.067034
18	6	0	1.904614	-2.404782	0.114277
19	6	0	3.866958	-1.576366	-0.756415
20	1	0	3.814720	-3.502003	0.431892
21	6	0	0.867947	-3.174934	0.846090
22	1	0	1.270467	-4.128928	1.203889
23	1	0	0.490851	-2.614459	1.714728
24	1	0	0.004240	-3.383175	0.197871
25	8	0	5.162162	-1.531174	1.512693
26	7	0	1.614649	-1.282737	-0.588599
27	6	0	5.220966	-1.607193	-1.384188
28	1	0	5.207377	-2.269538	-2.258915
29	1	0	5.529401	-0.609114	-1.707429
30	1	0	5.959031	-2.002748	-0.677917
31	79	0	-0.254267	-0.304304	-0.347093
32	6	0	1.663419	1.875621	-3.377860
33	1	0	2.529830	1.867570	-4.045298
34	1	0	0.734992	1.846497	-3.950608
35	1	0	1.701551	2.772079	-2.747577
36	6	0	-2.113055	0.437777	-0.043841
37	7	0	-3.226044	-0.325890	0.024579
38	6	0	-3.921510	1.747639	0.232494
39	6	0	-4.351844	0.463536	0.193825
40	1	0	-4.453493	2.683147	0.346837
41	1	0	-5.341365	0.031688	0.268491
42	7	0	-2.542511	1.711308	0.087365
43	6	0	-1.676100	2.856068	0.147836
44	6	0	-1.202908	3.402955	-1.048176
45	6	0	-1.352994	3.364712	1.409818
46	6	0	-0.352851	4.505369	-0.953191
47	6	0	-0.506748	4.472795	1.455694
48	6	0	-0.008869	5.035689	0.285498
49	1	0	0.023326	4.964632	-1.867188
50	1	0	-0.243220	4.899760	2.423518
51	1	0	0.644620	5.904420	0.338594
52	6	0	-3.205088	-1.763897	-0.013917
53	6	0	-3.008179	-2.449210	1.189613
54	6	0	-3.345972	-2.400920	-1.250506
55	6	0	-2.959883	-3.842008	1.131338
56	6	0	-3.286172	-3.794481	-1.260312
57	6	0	-3.097273	-4.507786	-0.081803
58	1	0	-2.816320	-4.406071	2.052458
59	1	0	-3.395065	-4.321666	-2.207230

60	1	0	-3.061616	-5.595197	-0.108734
61	6	0	-2.824798	-1.715166	2.483952
62	1	0	-3.613525	-0.969778	2.655587
63	1	0	-2.831460	-2.409482	3.331257
64	1	0	-1.866424	-1.172179	2.502479
65	6	0	-3.541063	-1.616123	-2.512261
66	1	0	-4.448923	-0.998406	-2.475283
67	1	0	-2.698219	-0.934208	-2.698715
68	1	0	-3.628629	-2.282385	-3.376844
69	6	0	-1.608011	2.833446	-2.374052
70	1	0	-2.699890	2.752251	-2.466150
71	1	0	-1.250957	3.464358	-3.196021
72	1	0	-1.201896	1.820241	-2.520263
73	6	0	-1.897081	2.738736	2.658832
74	1	0	-2.989674	2.832517	2.725962
75	1	0	-1.666309	1.663219	2.704416
76	1	0	-1.477788	3.216038	3.552138

Zero-point correction= 0.615080 (Hartree/Particle)
Thermal correction to Energy= 0.655723
Thermal correction to Enthalpy= 0.656668
Thermal correction to Gibbs Free Energy= 0.540230
Sum of electronic and zero-point Energies= -1840.052528
Sum of electronic and thermal Energies= -1840.011885
Sum of electronic and thermal Enthalpies= -1840.010941
Sum of electronic and thermal Free Energies= -1840.127378
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.51787570

TS19a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.648590	1.131091	2.125012
2	6	0	-3.473821	2.624868	0.317223
3	6	0	0.007886	0.567359	3.300035
4	8	0	1.211079	-0.003225	3.042564
5	6	0	-3.315167	3.829804	-0.540038
6	6	0	-4.328591	4.126208	-1.454165
7	6	0	-2.227803	4.694837	-0.403484
8	6	0	-4.238838	5.263401	-2.245052
9	1	0	-5.168491	3.438713	-1.536190
10	6	0	-2.153448	5.848313	-1.176134
11	1	0	-1.448967	4.473543	0.328178
12	6	0	-3.153956	6.126435	-2.103764
13	1	0	-5.018610	5.482646	-2.972329
14	1	0	-1.314611	6.531763	-1.055040
15	1	0	-3.089195	7.022856	-2.718785
16	8	0	-0.468308	0.582003	4.414241
17	6	0	-2.259771	1.841648	0.720188
18	6	0	-0.991363	1.737731	0.023552
19	6	0	-1.961215	1.525949	2.115063
20	1	0	-2.617357	0.630149	0.408733
21	6	0	-0.735113	1.983039	-1.419625
22	1	0	-1.616504	1.734101	-2.023260
23	1	0	-0.514943	3.044625	-1.599678
24	1	0	0.121612	1.392682	-1.768775
25	8	0	-4.576258	2.274291	0.697580
26	7	0	-0.085025	1.234775	0.843180
27	6	0	-2.936789	1.517894	3.233918
28	1	0	-2.876250	0.572957	3.786019
29	1	0	-2.701221	2.307869	3.959379
30	1	0	-3.954339	1.661679	2.859378
31	79	0	1.683761	0.301081	0.179533
32	6	0	4.721159	-2.390749	-0.969394
33	6	0	5.491819	-1.303172	-0.731775
34	1	0	4.971952	-3.402991	-1.257159
35	1	0	6.562828	-1.153088	-0.766311
36	7	0	4.626897	-0.272909	-0.392098
37	7	0	3.407257	-2.001504	-0.770349
38	6	0	3.342911	-0.698554	-0.410484
39	7	0	-2.984020	-0.690345	-0.018102
40	16	0	-3.559886	-0.730559	-1.552037
41	8	0	-4.623487	-1.685255	-1.776832
42	8	0	-3.701035	0.666733	-1.935939

43	16	0	-2.647712	-2.043458	0.831718
44	8	0	-2.574262	-3.226542	-0.010738
45	8	0	-1.587124	-1.741400	1.781576
46	6	0	-4.172086	-2.244964	1.847136
47	6	0	-2.093485	-1.337270	-2.550762
48	9	0	-2.068648	-0.668780	-3.694955
49	9	0	-2.193924	-2.624682	-2.806775
50	9	0	-0.962026	-1.099308	-1.895491
51	9	0	-4.016123	-3.305080	2.625940
52	9	0	-4.351866	-1.171010	2.597767
53	9	0	-5.214756	-2.418796	1.061912
54	6	0	5.039591	1.070957	-0.099446
55	6	0	5.224686	1.442454	1.234665
56	6	0	5.228936	1.947442	-1.172710
57	6	0	5.649173	2.747639	1.483762
58	6	0	5.652718	3.242097	-0.877171
59	6	0	5.865708	3.636959	0.438588
60	1	0	5.803913	3.064840	2.514563
61	1	0	5.809854	3.946604	-1.693335
62	1	0	6.198380	4.651279	0.651700
63	6	0	2.255553	-2.829595	-1.013629
64	6	0	1.520851	-3.323243	0.067514
65	6	0	1.897981	-3.053431	-2.350048
66	6	0	0.383175	-4.076094	-0.225842
67	6	0	0.764977	-3.825197	-2.591477
68	6	0	0.007474	-4.323911	-1.537439
69	1	0	-0.234277	-4.439448	0.594345
70	1	0	0.452431	-4.001321	-3.620680
71	1	0	-0.904794	-4.882340	-1.736509
72	6	0	4.921943	0.494104	2.353668
73	1	0	3.832316	0.395425	2.479565
74	1	0	5.318117	-0.514090	2.169104
75	1	0	5.336670	0.857045	3.300891
76	6	0	4.945023	1.519821	-2.580850
77	1	0	5.506199	0.619808	-2.867660
78	1	0	3.878452	1.283705	-2.710989
79	1	0	5.200214	2.314977	-3.289897
80	6	0	1.869256	-3.027917	1.494577
81	1	0	1.655622	-3.895413	2.131138
82	1	0	2.924482	-2.753087	1.628054
83	1	0	1.255812	-2.192523	1.867193
84	6	0	2.675995	-2.444158	-3.478685
85	1	0	2.831843	-1.365835	-3.323212
86	1	0	3.671187	-2.895274	-3.599727
87	1	0	2.142101	-2.571034	-4.426991
88	6	0	1.802582	-0.638865	4.169800
89	1	0	2.722580	-1.105880	3.805790
90	1	0	2.028345	0.091462	4.955019
91	1	0	1.128402	-1.399157	4.579556

Zero-point correction= 0.670579 (Hartree/Particle)
Thermal correction to Energy= 0.725972
Thermal correction to Enthalpy= 0.726917
Thermal correction to Gibbs Free Energy= 0.578134
Sum of electronic and zero-point Energies= -3666.928774
Sum of electronic and thermal Energies= -3666.873380
Sum of electronic and thermal Enthalpies= -3666.872436
Sum of electronic and thermal Free Energies= -3667.021219
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3668.76811136

TS20a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.185588	-1.360382	0.851956
2	6	0	-3.651934	-2.186977	-1.762963
3	6	0	-0.707042	-1.151399	2.207398
4	8	0	0.029156	-0.007415	2.313437
5	6	0	-5.039322	-2.171558	-1.210860
6	6	0	-6.028807	-2.893681	-1.884365
7	6	0	-5.391488	-1.388307	-0.106649
8	6	0	-7.344132	-2.859847	-1.444064
9	1	0	-5.737371	-3.473264	-2.758572
10	6	0	-6.713288	-1.339125	0.321102

11	1	0	-4.632046	-0.801233	0.410551
12	6	0	-7.687870	-2.080136	-0.340906
13	1	0	-8.108210	-3.435643	-1.964063
14	1	0	-6.981926	-0.716553	1.172953
15	1	0	-8.721685	-2.046505	0.000234
16	8	0	-0.956312	-1.854101	3.165015
17	6	0	-2.536513	-1.786687	-0.885908
18	6	0	-1.558176	-0.894030	-1.297264
19	6	0	-2.283538	-2.107145	0.486190
20	6	0	-1.347033	-0.252382	-2.620272
21	1	0	-0.863564	0.728174	-2.500223
22	1	0	-0.699638	-0.868384	-3.260115
23	1	0	-2.293203	-0.130267	-3.158871
24	8	0	-3.464067	-2.450480	-2.944387
25	7	0	-0.746908	-0.569526	-0.231367
26	6	0	-3.045753	-3.032414	1.372481
27	1	0	-3.783605	-3.617300	0.812708
28	1	0	-2.367139	-3.716615	1.893830
29	1	0	-3.576997	-2.472112	2.155691
30	79	0	1.382611	-0.676013	-0.405017
31	1	0	-0.971169	0.822828	0.066193
32	7	0	-1.238751	1.932534	0.337205
33	16	0	0.096148	2.914013	0.359482
34	8	0	0.488714	3.347273	1.685439
35	8	0	1.037855	2.277636	-0.543627
36	16	0	-2.593648	2.095427	1.291743
37	8	0	-2.937993	0.804471	1.854196
38	8	0	-2.550352	3.302266	2.086804
39	6	0	-3.823979	2.360635	-0.059437
40	6	0	-0.467455	4.422959	-0.552256
41	9	0	-0.978701	4.064599	-1.715691
42	9	0	0.604890	5.173557	-0.748581
43	9	0	-1.361216	5.096465	0.140234
44	9	0	-5.030522	2.374744	0.476669
45	9	0	-3.739851	1.371695	-0.933872
46	9	0	-3.583997	3.509903	-0.664523
47	6	0	0.256349	0.443221	3.643342
48	1	0	-0.684036	0.447176	4.206228
49	1	0	0.976344	-0.202699	4.162896
50	1	0	0.646122	1.461231	3.549534
51	6	0	3.374340	-0.974093	-0.220564
52	7	0	4.402081	-0.098141	-0.246518
53	6	0	5.283674	-2.020428	0.365244
54	6	0	5.587269	-0.724651	0.111029
55	1	0	5.895463	-2.858226	0.672737
56	1	0	6.521659	-0.180388	0.150078
57	7	0	3.920862	-2.154315	0.156764
58	6	0	3.136454	-3.341800	0.363894
59	6	0	3.014844	-4.246141	-0.694436
60	6	0	2.462475	-3.487661	1.581465
61	6	0	2.186653	-5.350744	-0.502178
62	6	0	1.632744	-4.599586	1.723387
63	6	0	1.497035	-5.521656	0.692647
64	1	0	2.069281	-6.071310	-1.310975
65	1	0	1.075571	-4.724063	2.651207
66	1	0	0.840522	-6.380571	0.819366
67	6	0	4.268482	1.310904	-0.504453
68	6	0	3.914166	2.146479	0.557826
69	6	0	4.475779	1.770341	-1.807405
70	6	0	3.813167	3.511829	0.291944
71	6	0	4.351592	3.140397	-2.030072
72	6	0	4.031148	4.003501	-0.988236
73	1	0	3.527006	4.185354	1.099549
74	1	0	4.505272	3.528546	-3.036612
75	1	0	3.939690	5.071132	-1.180295
76	6	0	3.576717	1.591433	1.907308
77	1	0	4.300653	0.838542	2.249926
78	1	0	3.522983	2.388175	2.657715
79	1	0	2.588852	1.103000	1.876206
80	6	0	4.794908	0.818555	-2.920509
81	1	0	5.723754	0.260569	-2.735962
82	1	0	3.996051	0.073225	-3.047490
83	1	0	4.909056	1.352587	-3.870304
84	6	0	3.712580	-4.007214	-1.999152
85	1	0	3.505560	-4.817690	-2.706522

86	1	0	3.378550	-3.065789	-2.460240
87	1	0	4.802652	-3.934406	-1.881201
88	6	0	2.585749	-2.469434	2.674601
89	1	0	3.634489	-2.238981	2.910049
90	1	0	2.103742	-1.521553	2.386879
91	1	0	2.093395	-2.819393	3.588765

Zero-point correction= 0.672448 (Hartree/Particle)
Thermal correction to Energy= 0.727324
Thermal correction to Enthalpy= 0.728269
Thermal correction to Gibbs Free Energy= 0.581667
Sum of electronic and zero-point Energies= -3666.941951
Sum of electronic and thermal Energies= -3666.887075
Sum of electronic and thermal Enthalpies= -3666.886131
Sum of electronic and thermal Free Energies= -3667.032732
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3668.77994444

TS21a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.543274	-0.054479	-0.475715
2	6	0	-2.136443	-0.052518	0.870063
3	79	0	0.631890	-0.002814	-0.142202
4	6	0	-1.551653	-1.384884	-1.189975
5	8	0	-1.491797	-1.220524	-2.523709
6	6	0	-2.195717	-1.266644	1.747914
7	6	0	-3.180199	-2.248881	1.660218
8	6	0	-1.170687	-1.408087	2.686114
9	6	0	-3.136457	-3.355090	2.495692
10	1	0	-3.977459	-2.159530	0.927948
11	6	0	-1.121934	-2.523740	3.514333
12	1	0	-0.401254	-0.639773	2.766737
13	6	0	-2.107428	-3.499024	3.422392
14	1	0	-3.912150	-4.114237	2.419145
15	1	0	-0.317843	-2.621219	4.241741
16	1	0	-2.079518	-4.369352	4.075249
17	8	0	-1.505766	-2.477279	-0.668655
18	6	0	-1.085124	2.724849	0.162790
19	6	0	-1.162340	2.140494	1.365459
20	6	0	-1.741547	2.245172	-1.051757
21	7	0	-1.952282	1.016322	-1.342393
22	8	0	-1.928838	1.031297	1.671132
23	1	0	-0.498684	3.644212	0.104632
24	6	0	-1.232704	-2.419504	-3.244727
25	1	0	-1.161525	-2.127349	-4.294598
26	1	0	-0.291144	-2.870805	-2.903207
27	1	0	-2.037316	-3.149134	-3.103059
28	6	0	2.677403	0.007600	-0.123434
29	7	0	3.511713	1.066400	-0.058288
30	6	0	4.806287	-0.699519	-0.277266
31	6	0	4.833091	0.650512	-0.150949
32	1	0	5.599527	-1.428330	-0.380746
33	1	0	5.654509	1.354345	-0.121178
34	7	0	3.472045	-1.073368	-0.258278
35	6	0	2.937498	-2.403734	-0.383996
36	6	0	2.615851	-2.868719	-1.663060
37	6	0	2.679018	-3.124924	0.785235
38	6	0	2.031952	-4.131950	-1.753758
39	6	0	2.085359	-4.378473	0.645167
40	6	0	1.764665	-4.876988	-0.611331
41	1	0	1.783206	-4.530385	-2.737430
42	1	0	1.865395	-4.962468	1.537755
43	1	0	1.300531	-5.856889	-0.702211
44	6	0	3.057327	2.423009	0.069064
45	6	0	3.048708	2.998302	1.344091
46	6	0	2.614259	3.092188	-1.076986
47	6	0	2.602846	4.315843	1.452276
48	6	0	2.174868	4.408031	-0.920431
49	6	0	2.174471	5.016736	0.329423
50	1	0	2.598100	4.793519	2.432130
51	1	0	1.840737	4.960328	-1.798672
52	1	0	1.842285	6.048603	0.429662
53	6	0	3.481156	2.218884	2.548747

54	1	0	4.558513	2.002830	2.537298
55	1	0	3.266557	2.772494	3.469777
56	1	0	2.965933	1.248172	2.604953
57	6	0	2.564264	2.421372	-2.416071
58	1	0	3.435985	1.778985	-2.599412
59	1	0	1.671352	1.780280	-2.497106
60	1	0	2.512382	3.162255	-3.221664
61	6	0	2.840931	-2.025176	-2.881506
62	1	0	3.865037	-1.631551	-2.938400
63	1	0	2.652371	-2.601558	-3.794223
64	1	0	2.163413	-1.156141	-2.893027
65	6	0	2.993403	-2.558604	2.136690
66	1	0	4.042933	-2.245666	2.224175
67	1	0	2.376335	-1.672655	2.351676
68	1	0	2.798420	-3.297154	2.922000
69	7	0	-3.978015	0.253401	0.436371
70	6	0	-4.670279	1.383791	0.457833
71	6	0	-5.416542	1.499210	-0.735751
72	6	0	-5.086251	0.394635	-1.464891
73	1	0	-6.086990	2.301807	-1.014295
74	8	0	-4.243241	-0.368638	-0.757755
75	6	0	-2.175183	3.295661	-2.027646
76	1	0	-2.642649	2.826698	-2.899391
77	1	0	-2.884867	4.000193	-1.569441
78	1	0	-1.310955	3.891194	-2.359065
79	6	0	-0.531536	2.657289	2.608100
80	1	0	0.084908	1.876056	3.074642
81	1	0	0.101774	3.524607	2.391251
82	1	0	-1.296800	2.941968	3.343825
83	6	0	-5.400100	-0.085651	-2.822396
84	1	0	-5.825008	-1.096082	-2.799163
85	1	0	-6.106802	0.585507	-3.317509
86	1	0	-4.468426	-0.125949	-3.404626
87	6	0	-4.629072	2.322708	1.607622
88	1	0	-4.182867	1.856494	2.489646
89	1	0	-4.044281	3.215832	1.348166
90	1	0	-5.643403	2.655821	1.854480

Zero-point correction= 0.734288 (Hartree/Particle)
Thermal correction to Energy= 0.780785
Thermal correction to Enthalpy= 0.781729
Thermal correction to Gibbs Free Energy= 0.656079
Sum of electronic and zero-point Energies= -2164.361688
Sum of electronic and thermal Energies= -2164.315191
Sum of electronic and thermal Enthalpies= -2164.314246
Sum of electronic and thermal Free Energies= -2164.439896
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2166.03306842

INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.657260	-0.429372	-0.218433
2	6	0	2.564583	0.554964	-0.071117
3	79	0	-0.400389	-0.199899	-0.094845
4	6	0	2.146883	-1.808495	-0.474016
5	8	0	1.438326	-2.721432	0.200378
6	6	0	2.354430	2.006824	0.054567
7	6	0	1.325798	2.641105	-0.653676
8	6	0	3.196275	2.781613	0.862024
9	6	0	1.127062	4.009262	-0.530424
10	1	0	0.690401	2.052523	-1.315873
11	6	0	2.992594	4.150299	0.986485
12	1	0	4.002930	2.302362	1.417851
13	6	0	1.954975	4.767143	0.293355
14	1	0	0.323519	4.486051	-1.088358
15	1	0	3.645582	4.737699	1.629134
16	1	0	1.799605	5.840366	0.386559
17	8	0	3.054292	-2.101966	-1.230940
18	6	0	5.994909	-0.540304	-0.543073
19	6	0	5.670025	-0.934518	0.724039
20	6	0	4.873788	0.154446	-1.025086
21	7	0	3.971245	0.188428	-0.055203
22	8	0	4.437953	-0.499692	1.039102

23	1	0	6.910837	-0.746842	-1.080429
24	6	0	1.820655	-4.076723	-0.023683
25	1	0	1.212517	-4.674190	0.657229
26	1	0	1.620058	-4.360831	-1.062683
27	1	0	2.886727	-4.219853	0.182992
28	6	0	-2.456621	-0.133015	0.091633
29	7	0	-3.252541	-1.223990	0.179457
30	6	0	-4.611230	0.494353	0.324484
31	6	0	-4.581578	-0.859475	0.323702
32	1	0	-5.427259	1.199613	0.414103
33	1	0	-5.366756	-1.598901	0.413136
34	7	0	-3.298236	0.920394	0.180028
35	6	0	-2.904429	2.300985	0.122883
36	6	0	-2.934731	2.944739	-1.118563
37	6	0	-2.542988	2.940899	1.312248
38	6	0	-2.615395	4.302239	-1.144164
39	6	0	-2.225641	4.297262	1.237788
40	6	0	-2.273582	4.973896	0.024825
41	1	0	-2.645479	4.834456	-2.094654
42	1	0	-1.947817	4.825721	2.149076
43	1	0	-2.038971	6.036677	-0.010584
44	6	0	-2.763284	-2.574208	0.122539
45	6	0	-2.411263	-3.201643	1.321056
46	6	0	-2.640992	-3.183392	-1.130347
47	6	0	-1.932549	-4.509079	1.241311
48	6	0	-2.151698	-4.488946	-1.161998
49	6	0	-1.807778	-5.147800	0.012686
50	1	0	-1.660983	-5.028880	2.159807
51	1	0	-2.051635	-4.991936	-2.123294
52	1	0	-1.441585	-6.172436	-0.029817
53	6	0	-2.518016	-2.485506	2.632760
54	1	0	-3.526173	-2.085334	2.807236
55	1	0	-2.275519	-3.155395	3.464724
56	1	0	-1.824195	-1.632432	2.675852
57	6	0	-3.010858	-2.457125	-2.388113
58	1	0	-4.050206	-2.101053	-2.369174
59	1	0	-2.374351	-1.573957	-2.545361
60	1	0	-2.899246	-3.108642	-3.261484
61	6	0	-3.284808	2.198626	-2.370404
62	1	0	-4.281539	1.739649	-2.315356
63	1	0	-3.273925	2.865317	-3.239450
64	1	0	-2.570422	1.383949	-2.561485
65	6	0	-2.476859	2.193739	2.609096
66	1	0	-3.379266	1.594688	2.792397
67	1	0	-1.624518	1.498484	2.617633
68	1	0	-2.352242	2.883474	3.450763
69	6	0	4.581989	0.723026	-2.356280
70	1	0	3.854705	0.066198	-2.853256
71	1	0	4.139326	1.722962	-2.274694
72	1	0	5.488252	0.774298	-2.965002
73	6	0	6.381217	-1.694631	1.768522
74	1	0	5.787274	-2.559090	2.088218
75	1	0	7.342609	-2.048947	1.387060
76	1	0	6.561756	-1.069993	2.651907

Zero-point correction= 0.617774 (Hartree/Particle)
Thermal correction to Energy= 0.658458
Thermal correction to Enthalpy= 0.659402
Thermal correction to Gibbs Free Energy= 0.542295
Sum of electronic and zero-point Energies= -1839.996997
Sum of electronic and thermal Energies= -1839.956314
Sum of electronic and thermal Enthalpies= -1839.955370
Sum of electronic and thermal Free Energies= -1840.072476
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.46228533

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.168662	-1.324640	-0.085313
2	6	0	2.382813	-0.763484	-0.606371
3	79	0	-0.608492	-0.357798	0.031161
4	6	0	1.262258	-2.720701	0.371708
5	8	0	1.485670	-2.887414	1.655912

6	6	0	2.414938	0.600261	-1.186016
7	6	0	1.569906	0.947552	-2.245667
8	6	0	3.334425	1.531669	-0.695846
9	6	0	1.667113	2.206480	-2.826669
10	1	0	0.858730	0.216682	-2.634843
11	6	0	3.411159	2.797098	-1.266106
12	1	0	3.965864	1.260877	0.149520
13	6	0	2.587684	3.130941	-2.337637
14	1	0	1.028553	2.463975	-3.670034
15	1	0	4.119188	3.524847	-0.873960
16	1	0	2.663174	4.116056	-2.795648
17	8	0	1.069421	-3.573955	-0.467319
18	6	0	5.795304	-1.163544	-0.347769
19	6	0	5.641153	-1.027490	1.089985
20	6	0	4.662653	-1.341457	-1.068871
21	7	0	3.442754	-1.512737	-0.458637
22	8	0	4.510908	-0.939480	1.571034
23	1	0	6.771110	-1.166812	-0.827044
24	6	0	1.547611	-4.252001	2.102257
25	1	0	1.726011	-4.200397	3.176191
26	1	0	0.603435	-4.761852	1.887680
27	1	0	2.367541	-4.772179	1.598525
28	6	0	-2.355908	0.731189	0.267648
29	7	0	-3.636988	0.348527	0.086797
30	6	0	-3.733314	2.451562	0.721707
31	6	0	-4.502454	1.394465	0.359502
32	1	0	-3.987896	3.460489	1.019291
33	1	0	-5.574671	1.281002	0.265822
34	7	0	-2.418958	2.022835	0.657305
35	6	0	-1.256310	2.815282	0.956030
36	6	0	-0.693172	3.571791	-0.076659
37	6	0	-0.728236	2.759298	2.249250
38	6	0	0.453525	4.304998	0.222574
39	6	0	0.422263	3.507168	2.500087
40	6	0	1.007300	4.270525	1.497154
41	1	0	0.915198	4.907318	-0.559255
42	1	0	0.858001	3.487323	3.498247
43	1	0	1.903562	4.849735	1.712476
44	6	0	-4.033593	-0.963371	-0.349791
45	6	0	-4.385202	-1.904166	0.623123
46	6	0	-4.035444	-1.232968	-1.721753
47	6	0	-4.766321	-3.169179	0.178081
48	6	0	-4.426537	-2.511252	-2.119145
49	6	0	-4.789410	-3.468528	-1.179295
50	1	0	-5.047630	-3.925200	0.910135
51	1	0	-4.444370	-2.752891	-3.181156
52	1	0	-5.093009	-4.460327	-1.508468
53	6	0	-4.344207	-1.565314	2.082871
54	1	0	-5.087873	-0.801288	2.349667
55	1	0	-4.549468	-2.450443	2.694284
56	1	0	-3.361671	-1.170470	2.380220
57	6	0	-3.611444	-0.200924	-2.723742
58	1	0	-4.056345	0.783529	-2.523886
59	1	0	-2.518549	-0.064288	-2.718313
60	1	0	-3.898579	-0.500752	-3.737424
61	6	0	-1.292317	3.575379	-1.450293
62	1	0	-2.337058	3.915875	-1.445520
63	1	0	-0.730593	4.237218	-2.119103
64	1	0	-1.287180	2.567190	-1.892635
65	6	0	-1.355082	1.912092	3.315502
66	1	0	-2.443182	2.050921	3.371481
67	1	0	-1.178156	0.841473	3.132518
68	1	0	-0.935363	2.149789	4.298845
69	6	0	6.870938	-1.032088	1.950311
70	1	0	7.390168	-1.995351	1.859710
71	1	0	7.573663	-0.258862	1.613403
72	1	0	6.604143	-0.861017	2.996066
73	6	0	4.635385	-1.509808	-2.559059
74	1	0	4.155918	-2.458081	-2.830186
75	1	0	4.054392	-0.699435	-3.020433
76	1	0	5.651285	-1.493189	-2.963877

Zero-point correction= 0.612496 (Hartree/Particle)
Thermal correction to Energy= 0.655324
Thermal correction to Enthalpy= 0.656268

Thermal correction to Gibbs Free Energy= 0.530554
Sum of electronic and zero-point Energies= -1839.973153
Sum of electronic and thermal Energies= -1839.930324
Sum of electronic and thermal Enthalpies= -1839.929380
Sum of electronic and thermal Free Energies= -1840.055094
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43825427

INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.456253	-0.934751	-0.476922
2	6	0	2.494440	-0.121513	-1.048352
3	79	0	-0.440941	-0.300098	-0.112833
4	6	0	1.788019	-2.286155	-0.002354
5	8	0	1.984375	-2.380260	1.299317
6	6	0	2.190373	1.248060	-1.529591
7	6	0	1.106321	1.494081	-2.378183
8	6	0	3.049620	2.293544	-1.181063
9	6	0	0.895229	2.771313	-2.884520
10	1	0	0.453085	0.674732	-2.684029
11	6	0	2.820493	3.572914	-1.671107
12	1	0	3.889785	2.086401	-0.520145
13	6	0	1.748971	3.812031	-2.528034
14	1	0	0.071707	2.950062	-3.573970
15	1	0	3.487230	4.386021	-1.390310
16	1	0	1.583238	4.811718	-2.927164
17	8	0	1.783491	-3.195275	-0.806498
18	6	0	5.108809	-1.968166	0.229104
19	6	0	5.050913	-1.018988	1.321200
20	6	0	4.410055	-1.647583	-0.893576
21	7	0	3.753909	-0.465573	-1.012275
22	8	0	4.384674	0.010430	1.199330
23	1	0	5.730371	-2.859540	0.265549
24	6	0	2.305467	-3.693216	1.782422
25	1	0	2.395013	-3.593727	2.864626
26	1	0	1.512372	-4.399932	1.520792
27	1	0	3.252556	-4.026362	1.342295
28	6	0	-2.292315	0.454067	0.428153
29	7	0	-3.510203	-0.121113	0.350793
30	6	0	-3.849875	1.871387	1.217192
31	6	0	-4.485646	0.737063	0.830370
32	1	0	-4.218109	2.793161	1.648478
33	1	0	-5.530372	0.454790	0.844526
34	7	0	-2.504107	1.676529	0.960902
35	6	0	-1.450250	2.627599	1.196212
36	6	0	-1.176057	3.562127	0.192660
37	6	0	-0.729071	2.542813	2.390921
38	6	0	-0.124048	4.448105	0.416485
39	6	0	0.317624	3.447633	2.567682
40	6	0	0.618097	4.388521	1.590199
41	1	0	0.114929	5.189120	-0.345413
42	1	0	0.899754	3.408809	3.487533
43	1	0	1.439037	5.085994	1.746083
44	6	0	-3.749862	-1.434576	-0.184507
45	6	0	-3.817144	-2.509225	0.707860
46	6	0	-3.891607	-1.570276	-1.569015
47	6	0	-4.048134	-3.773357	0.167384
48	6	0	-4.122991	-2.853896	-2.062897
49	6	0	-4.201461	-3.943459	-1.203858
50	1	0	-4.109033	-4.631570	0.835495
51	1	0	-4.243962	-2.993741	-3.136393
52	1	0	-4.385280	-4.937142	-1.607620
53	6	0	-3.639473	-2.306868	2.182565
54	1	0	-4.438781	-1.687555	2.612980
55	1	0	-3.646450	-3.266006	2.711193
56	1	0	-2.689127	-1.802373	2.411078
57	6	0	-3.779758	-0.391137	-2.488763
58	1	0	-4.351489	0.475117	-2.128664
59	1	0	-2.734083	-0.062335	-2.594082
60	1	0	-4.145304	-0.642309	-3.490310
61	6	0	-1.971907	3.593966	-1.076760
62	1	0	-3.035437	3.801939	-0.893881
63	1	0	-1.594175	4.368711	-1.753355

64	1	0	-1.920756	2.631019	-1.607835
65	6	0	-1.049284	1.508851	3.428408
66	1	0	-2.125214	1.453633	3.642570
67	1	0	-0.735436	0.504752	3.105341
68	1	0	-0.531079	1.727641	4.368270
69	6	0	5.828334	-1.311624	2.572101
70	1	0	5.639458	-0.544339	3.326737
71	1	0	5.552733	-2.299054	2.966167
72	1	0	6.902772	-1.345521	2.348660
73	6	0	4.449803	-2.462766	-2.156579
74	1	0	3.435696	-2.671183	-2.514973
75	1	0	4.987062	-1.910406	-2.936802
76	1	0	4.964479	-3.410001	-1.971742

Zero-point correction= 0.612611 (Hartree/Particle)
Thermal correction to Energy= 0.655064
Thermal correction to Enthalpy= 0.656008
Thermal correction to Gibbs Free Energy= 0.531935
Sum of electronic and zero-point Energies= -1839.967549
Sum of electronic and thermal Energies= -1839.925096
Sum of electronic and thermal Enthalpies= -1839.924152
Sum of electronic and thermal Free Energies= -1840.048225
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43130950

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.084213	-1.373484	-1.211201
2	6	0	2.336152	-1.354965	-0.461054
3	79	0	-0.394078	-0.138411	-0.557498
4	6	0	1.020007	-2.184517	-2.431325
5	8	0	0.636972	-3.433686	-2.353461
6	6	0	3.226009	-0.217000	-0.322893
7	6	0	4.175968	-0.148745	0.704702
8	6	0	3.151147	0.801111	-1.283082
9	6	0	5.039231	0.933650	0.768638
10	1	0	4.225243	-0.936651	1.454692
11	6	0	4.029347	1.873460	-1.220269
12	1	0	2.420048	0.733037	-2.090334
13	6	0	4.970042	1.939132	-0.195835
14	1	0	5.775197	0.994337	1.567392
15	1	0	3.981544	2.656979	-1.973333
16	1	0	5.659438	2.780545	-0.147915
17	8	0	1.309215	-1.549327	-3.426031
18	6	0	2.340951	-2.766092	2.510629
19	6	0	1.327013	-1.767674	2.842884
20	6	0	2.783101	-3.048207	1.258469
21	7	0	2.267764	-2.495123	0.107027
22	8	0	0.853450	-0.997343	2.010194
23	1	0	2.751529	-3.361093	3.325775
24	6	0	0.554314	-4.129751	-3.612016
25	1	0	-0.159555	-3.626468	-4.270587
26	1	0	1.537804	-4.159006	-4.089936
27	1	0	0.212868	-5.134772	-3.365329
28	6	0	-1.792448	1.210203	0.143767
29	7	0	-1.567341	2.518751	0.387578
30	6	0	-3.658742	2.162687	0.959893
31	6	0	-2.706555	3.125333	0.890249
32	1	0	-4.687146	2.187428	1.296061
33	1	0	-2.721761	4.175838	1.149897
34	7	0	-3.076849	0.994901	0.494506
35	6	0	-3.715253	-0.293268	0.464547
36	6	0	-3.526804	-1.143860	1.558789
37	6	0	-4.481086	-0.630642	-0.655295
38	6	0	-4.160351	-2.385701	1.513915
39	6	0	-5.092764	-1.883555	-0.655312
40	6	0	-4.936222	-2.750668	0.419993
41	1	0	-4.042046	-3.070141	2.353191
42	1	0	-5.699358	-2.176416	-1.511402
43	1	0	-5.426200	-3.722388	0.405676
44	6	0	-0.294390	3.163186	0.207014
45	6	0	-0.047539	3.817066	-1.004435
46	6	0	0.632917	3.094000	1.252684

47	6	0	1.188884	4.444904	-1.150533
48	6	0	1.855809	3.736518	1.059615
49	6	0	2.127451	4.409819	-0.125207
50	1	0	1.407799	4.972969	-2.078117
51	1	0	2.600329	3.705118	1.854789
52	1	0	3.084018	4.915699	-0.251042
53	6	0	-1.071537	3.837480	-2.098910
54	1	0	-1.996290	4.342666	-1.787334
55	1	0	-0.689914	4.362102	-2.981260
56	1	0	-1.353745	2.820560	-2.408284
57	6	0	0.336776	2.347791	2.518635
58	1	0	-0.677590	2.548123	2.890479
59	1	0	0.419090	1.258841	2.370781
60	1	0	1.044046	2.630658	3.306593
61	6	0	-2.665212	-0.746308	2.720257
62	1	0	-2.900156	0.264196	3.083398
63	1	0	-2.800841	-1.441202	3.557182
64	1	0	-1.596169	-0.749542	2.451569
65	6	0	-4.625293	0.313459	-1.810582
66	1	0	-5.129588	1.245844	-1.520932
67	1	0	-3.646756	0.596675	-2.225221
68	1	0	-5.211440	-0.142035	-2.615772
69	6	0	3.805835	-4.105396	0.983604
70	1	0	4.157182	-4.569598	1.910019
71	1	0	3.386758	-4.879294	0.328686
72	1	0	4.666241	-3.669544	0.456221
73	6	0	0.875130	-1.730272	4.276932
74	1	0	0.249214	-2.608449	4.491347
75	1	0	1.725176	-1.770994	4.969874
76	1	0	0.288498	-0.824544	4.462531

Zero-point correction= 0.613137 (Hartree/Particle)
Thermal correction to Energy= 0.655681
Thermal correction to Enthalpy= 0.656625
Thermal correction to Gibbs Free Energy= 0.533829
Sum of electronic and zero-point Energies= -1839.979602
Sum of electronic and thermal Energies= -1839.937059
Sum of electronic and thermal Enthalpies= -1839.936115
Sum of electronic and thermal Free Energies= -1840.058910
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43950943

INT6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.061887	1.556069	-0.770070
2	6	0	-2.401987	1.376489	-0.214172
3	79	0	0.306831	0.146797	-0.305671
4	6	0	-0.829367	2.663028	-1.697875
5	8	0	-0.536618	3.841462	-1.203089
6	6	0	-3.284419	0.299610	-0.659878
7	6	0	-3.012077	-0.378863	-1.853586
8	6	0	-4.418023	-0.026162	0.092024
9	6	0	-3.874760	-1.373869	-2.293873
10	1	0	-2.138780	-0.108840	-2.449817
11	6	0	-5.271995	-1.023989	-0.350781
12	1	0	-4.612229	0.511450	1.018293
13	6	0	-5.002843	-1.695154	-1.543824
14	1	0	-3.669274	-1.894978	-3.227161
15	1	0	-6.155195	-1.279399	0.231169
16	1	0	-5.681127	-2.472604	-1.891736
17	8	0	-0.928352	2.337658	-2.862812
18	6	0	-1.138797	3.196806	2.352431
19	6	0	-0.444118	2.002358	2.804861
20	6	0	-2.098923	3.233363	1.391062
21	7	0	-2.655113	2.133941	0.783992
22	8	0	-0.573286	0.903610	2.260831
23	6	0	-2.815142	4.505518	1.047817
24	1	0	-3.868222	4.439527	1.349712
25	1	0	-2.356895	5.362990	1.549808
26	1	0	-2.801599	4.676528	-0.036516
27	6	0	0.465079	2.176001	3.992185
28	1	0	1.293641	2.853358	3.740267
29	1	0	-0.071003	2.633545	4.833966

30	1	0	0.871813	1.208053	4.302073
31	6	0	-0.313270	4.887091	-2.172968
32	1	0	-0.085611	5.778452	-1.588687
33	1	0	0.526744	4.619949	-2.820110
34	1	0	-1.213673	5.034498	-2.776512
35	6	0	1.551686	-1.459396	0.050682
36	7	0	1.122944	-2.698655	0.369741
37	6	0	3.316671	-2.819134	0.334247
38	6	0	2.195072	-3.553559	0.548044
39	1	0	4.366610	-3.078562	0.374102
40	1	0	2.054159	-4.592847	0.814971
41	7	0	2.897987	-1.536232	0.026791
42	6	0	3.759741	-0.411767	-0.217405
43	6	0	4.016656	0.460349	0.845831
44	6	0	4.278070	-0.237722	-1.503753
45	6	0	4.855922	1.544227	0.590161
46	6	0	5.110794	0.861451	-1.711457
47	6	0	5.399969	1.740411	-0.674135
48	1	0	5.085849	2.237715	1.398318
49	1	0	5.534299	1.024625	-2.701705
50	1	0	6.057290	2.589163	-0.853216
51	6	0	-0.264821	-3.028458	0.565822
52	6	0	-1.006477	-3.467895	-0.535861
53	6	0	-0.805841	-2.851954	1.843598
54	6	0	-2.353341	-3.753493	-0.322915
55	6	0	-2.160507	-3.145793	2.004402
56	6	0	-2.925286	-3.591258	0.933990
57	1	0	-2.957753	-4.105559	-1.158371
58	1	0	-2.612733	-3.022206	2.987692
59	1	0	-3.980248	-3.817874	1.079530
60	6	0	-0.386963	-3.598477	-1.894602
61	1	0	0.507280	-4.236592	-1.885792
62	1	0	-1.097781	-4.033178	-2.606330
63	1	0	-0.074782	-2.619913	-2.290860
64	6	0	0.015016	-2.330688	2.984017
65	1	0	1.035805	-2.735682	2.988082
66	1	0	0.088507	-1.233060	2.931325
67	1	0	-0.450717	-2.584739	3.942855
68	6	0	3.398636	0.248382	2.196028
69	1	0	3.538712	-0.779316	2.559931
70	1	0	3.836427	0.928090	2.935892
71	1	0	2.311581	0.429127	2.176288
72	6	0	3.939127	-1.186417	-2.613712
73	1	0	4.351604	-2.189968	-2.439371
74	1	0	2.851464	-1.303833	-2.727051
75	1	0	4.339376	-0.828495	-3.568163
76	1	0	-0.907440	4.135801	2.854040

Zero-point correction= 0.612847 (Hartree/Particle)
Thermal correction to Energy= 0.655418
Thermal correction to Enthalpy= 0.656362
Thermal correction to Gibbs Free Energy= 0.533198
Sum of electronic and zero-point Energies= -1839.977562
Sum of electronic and thermal Energies= -1839.934991
Sum of electronic and thermal Enthalpies= -1839.934046
Sum of electronic and thermal Free Energies= -1840.057210
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.43756120

INT7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.327401	-1.169554	1.241164
2	6	0	-2.188337	-1.460011	0.137768
3	79	0	0.254676	0.066470	0.615955
4	6	0	-1.930284	-0.985015	2.592264
5	8	0	-1.931528	-2.105847	3.312636
6	6	0	-3.181775	-0.947796	-0.724592
7	6	0	-3.795421	-1.738676	-1.711075
8	6	0	-3.549157	0.396176	-0.535074
9	6	0	-4.783597	-1.181646	-2.499816
10	1	0	-3.487560	-2.775784	-1.837187
11	6	0	-4.534476	0.944224	-1.339847
12	1	0	-3.057730	0.980170	0.245628

13	6	0	-5.147636	0.155898	-2.313168
14	1	0	-5.275884	-1.777379	-3.264597
15	1	0	-4.834518	1.980971	-1.203464
16	1	0	-5.926902	0.587349	-2.938943
17	8	0	-2.340690	0.089171	2.963174
18	6	0	-0.164441	-3.695248	-1.052550
19	6	0	-0.210547	-2.739863	-2.172015
20	6	0	-0.717441	-3.571662	0.171973
21	7	0	-1.571380	-2.528683	0.553375
22	8	0	-0.742611	-1.638713	-2.096719
23	1	0	0.460518	-4.576183	-1.202245
24	6	0	-2.481734	-1.977197	4.629160
25	1	0	-1.919969	-1.233173	5.202517
26	1	0	-3.530473	-1.668890	4.574251
27	1	0	-2.394267	-2.963660	5.086338
28	6	0	1.636728	1.404107	-0.112952
29	7	0	1.371149	2.693554	-0.414526
30	6	0	3.490731	2.397529	-0.915491
31	6	0	2.501732	3.324507	-0.910340
32	1	0	4.527744	2.451044	-1.220522
33	1	0	2.487036	4.364447	-1.209433
34	7	0	2.937602	1.224772	-0.422480
35	6	0	3.597892	-0.049421	-0.348581
36	6	0	3.504478	-0.895974	-1.458529
37	6	0	4.269757	-0.391712	0.827715
38	6	0	4.131369	-2.138442	-1.368123
39	6	0	4.879728	-1.645561	0.872857
40	6	0	4.812327	-2.509376	-0.213818
41	1	0	4.096802	-2.813925	-2.223292
42	1	0	5.415933	-1.940562	1.774019
43	1	0	5.302606	-3.479825	-0.163064
44	6	0	0.058108	3.272015	-0.311525
45	6	0	-0.285805	3.942337	0.866829
46	6	0	-0.824434	3.095245	-1.382521
47	6	0	-1.574591	4.467995	0.951918
48	6	0	-2.097770	3.652100	-1.257649
49	6	0	-2.470191	4.329897	-0.102640
50	1	0	-1.872584	4.993436	1.858134
51	1	0	-2.799468	3.548536	-2.085619
52	1	0	-3.467160	4.760588	-0.023311
53	6	0	0.686926	4.067570	1.999615
54	1	0	1.605937	4.588677	1.698127
55	1	0	0.245979	4.624167	2.833164
56	1	0	0.988469	3.080150	2.378762
57	6	0	-0.445076	2.303359	-2.597506
58	1	0	0.573776	2.526594	-2.941958
59	1	0	-0.488284	1.220760	-2.396121
60	1	0	-1.132655	2.509263	-3.425629
61	6	0	2.749383	-0.486119	-2.687450
62	1	0	3.032094	0.517879	-3.032072
63	1	0	2.939728	-1.182833	-3.512399
64	1	0	1.662565	-0.464754	-2.506425
65	6	0	4.318753	0.547878	1.994094
66	1	0	4.779090	1.509222	1.727731
67	1	0	3.310797	0.772268	2.372612
68	1	0	4.898198	0.118553	2.818285
69	6	0	-0.444751	-4.502799	1.300905
70	1	0	0.233887	-5.307354	1.004073
71	1	0	0.005483	-3.943021	2.133066
72	1	0	-1.378127	-4.934474	1.684338
73	6	0	0.487994	-3.190720	-3.423249
74	1	0	1.545671	-3.402832	-3.210465
75	1	0	0.049636	-4.128361	-3.792183
76	1	0	0.415013	-2.420858	-4.196383

Zero-point correction= 0.614386 (Hartree/Particle)
Thermal correction to Energy= 0.656364
Thermal correction to Enthalpy= 0.657308
Thermal correction to Gibbs Free Energy= 0.535958
Sum of electronic and zero-point Energies= -1839.989400
Sum of electronic and thermal Energies= -1839.947423
Sum of electronic and thermal Enthalpies= -1839.946479
Sum of electronic and thermal Free Energies= -1840.067828
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.45163502

INT8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.538570	-1.739419	-0.729762
2	6	0	1.677163	-1.859877	0.226118
3	79	0	-0.286616	0.235745	-0.441635
4	6	0	1.052250	-1.959610	-2.146285
5	8	0	1.350676	-3.254012	-2.353293
6	6	0	2.904260	-1.099216	-0.168003
7	6	0	3.938575	-1.818258	-0.775528
8	6	0	3.058073	0.267319	0.069648
9	6	0	5.110622	-1.174652	-1.156713
10	1	0	3.813279	-2.887602	-0.954374
11	6	0	4.236887	0.903327	-0.305679
12	1	0	2.265738	0.826722	0.572072
13	6	0	5.258835	0.188597	-0.922870
14	1	0	5.909579	-1.739476	-1.633441
15	1	0	4.352455	1.967954	-0.110818
16	1	0	6.176263	0.694645	-1.217586
17	8	0	1.220310	-1.094727	-2.966763
18	6	0	2.439340	-1.561739	3.301397
19	6	0	1.479122	-0.470736	3.366246
20	6	0	2.500970	-2.513637	2.329094
21	7	0	1.609680	-2.559149	1.286562
22	8	0	0.640701	-0.217486	2.496656
23	1	0	3.124900	-1.664788	4.142455
24	7	0	-0.597765	-2.644083	-0.455883
25	6	0	-1.645330	-2.981893	-1.213254
26	6	0	-2.671957	-3.411346	-0.358757
27	6	0	-2.187055	-3.258910	0.908122
28	1	0	-3.649547	-3.766398	-0.656519
29	8	0	-0.936153	-2.784250	0.856755
30	6	0	1.924894	-3.539213	-3.633074
31	1	0	2.862967	-2.987148	-3.755080
32	1	0	2.102566	-4.615605	-3.649036
33	1	0	1.238669	-3.246103	-4.436339
34	6	0	-1.282458	1.997810	-0.135010
35	7	0	-2.613736	2.101977	0.076906
36	6	0	-1.847291	4.159108	0.151923
37	6	0	-2.982221	3.427908	0.257178
38	1	0	-1.664624	5.223283	0.225486
39	1	0	-4.009601	3.712176	0.443785
40	7	0	-0.816488	3.261999	-0.089061
41	6	0	0.572010	3.621573	-0.184909
42	6	0	1.107358	3.899422	-1.445678
43	6	0	1.312107	3.681738	1.000846
44	6	0	2.444839	4.291757	-1.498105
45	6	0	2.643876	4.085230	0.899736
46	6	0	3.200052	4.398211	-0.336072
47	1	0	2.890473	4.523418	-2.464596
48	1	0	3.244876	4.158522	1.805814
49	1	0	4.237272	4.725172	-0.394441
50	6	0	-3.500422	0.978667	0.186892
51	6	0	-3.638830	0.368181	1.438470
52	6	0	-4.184211	0.553076	-0.956953
53	6	0	-4.552512	-0.683321	1.534948
54	6	0	-5.067420	-0.518034	-0.817187
55	6	0	-5.262286	-1.119203	0.421881
56	1	0	-4.717496	-1.149764	2.506712
57	1	0	-5.624873	-0.861555	-1.688507
58	1	0	-5.982103	-1.931199	0.522555
59	6	0	-2.823076	0.803288	2.618501
60	1	0	-2.795684	1.896562	2.723837
61	1	0	-3.232083	0.388717	3.547469
62	1	0	-1.775734	0.467053	2.530383
63	6	0	-3.968557	1.224663	-2.279301
64	1	0	-4.246934	2.287025	-2.248951
65	1	0	-2.911879	1.185375	-2.583420
66	1	0	-4.566760	0.748529	-3.063875
67	6	0	0.281821	3.761940	-2.688719
68	1	0	-0.669886	4.305918	-2.616412
69	1	0	0.822494	4.144472	-3.560963
70	1	0	0.036944	2.707434	-2.885635

71	6	0	0.706949	3.296820	2.317061
72	1	0	-0.249409	3.806138	2.500939
73	1	0	0.510063	2.212152	2.361876
74	1	0	1.382366	3.549139	3.142808
75	6	0	-1.701497	-2.805969	-2.682280
76	1	0	-1.443807	-1.773472	-2.959432
77	1	0	-1.008091	-3.480261	-3.197999
78	1	0	-2.716102	-3.015797	-3.033326
79	6	0	-2.711996	-3.533231	2.258008
80	1	0	-3.783427	-3.748697	2.209005
81	1	0	-2.200413	-4.395772	2.703825
82	1	0	-2.543384	-2.670231	2.913937
83	6	0	3.462268	-3.655125	2.399479
84	1	0	4.023158	-3.659095	3.339282
85	1	0	2.930205	-4.609025	2.293396
86	1	0	4.176069	-3.591514	1.565417
87	6	0	1.557142	0.380364	4.611636
88	1	0	1.628823	-0.232794	5.518875
89	1	0	2.462996	1.003040	4.578357
90	1	0	0.681069	1.033939	4.676870

Zero-point correction= 0.731286 (Hartree/Particle)
Thermal correction to Energy= 0.780682
Thermal correction to Enthalpy= 0.781626
Thermal correction to Gibbs Free Energy= 0.644905
Sum of electronic and zero-point Energies= -2164.384951
Sum of electronic and thermal Energies= -2164.335554
Sum of electronic and thermal Enthalpies= -2164.334610
Sum of electronic and thermal Free Energies= -2164.471331
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2166.05607817

INT9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.698472	-0.136833	-0.597439
2	6	0	2.665211	-0.425893	0.502904
3	79	0	-0.348208	0.126868	-0.244000
4	6	0	2.260269	0.648971	-1.736943
5	8	0	2.977283	-0.074288	-2.594996
6	6	0	4.070781	0.048428	0.512910
7	6	0	5.121276	-0.867645	0.468071
8	6	0	4.328237	1.418156	0.592086
9	6	0	6.433457	-0.412535	0.503073
10	1	0	4.905929	-1.933860	0.392162
11	6	0	5.642296	1.867950	0.628544
12	1	0	3.496560	2.122584	0.609437
13	6	0	6.692102	0.953559	0.584603
14	1	0	7.256732	-1.122743	0.462757
15	1	0	5.849010	2.934537	0.685246
16	1	0	7.720627	1.308414	0.609056
17	8	0	2.060308	1.838880	-1.830353
18	6	0	1.668400	-2.830074	1.452142
19	6	0	1.825853	-1.738903	2.288668
20	6	0	1.698160	-2.596635	0.070269
21	7	0	2.313110	-1.494403	-0.370995
22	8	0	2.160987	-0.541455	1.855397
23	1	0	1.318628	-3.773478	1.860295
24	6	0	3.577436	0.674948	-3.654356
25	1	0	2.813141	1.209701	-4.226960
26	1	0	4.289223	1.399876	-3.244436
27	1	0	4.091751	-0.054426	-4.281649
28	6	0	-2.373265	0.349948	0.073646
29	7	0	-3.057297	1.489664	0.306549
30	6	0	-4.570453	-0.105699	0.299895
31	6	0	-4.411704	1.231870	0.447585
32	1	0	-5.450482	-0.735191	0.327132
33	1	0	-5.123571	2.025793	0.631978
34	7	0	-3.305971	-0.629360	0.072091
35	6	0	-3.007489	-2.012569	-0.171094
36	6	0	-2.696015	-2.830488	0.919971
37	6	0	-3.025427	-2.470504	-1.492861
38	6	0	-2.408536	-4.170170	0.657632
39	6	0	-2.733150	-3.818554	-1.708144

40	6	0	-2.434495	-4.661502	-0.643335
41	1	0	-2.175615	-4.833721	1.490299
42	1	0	-2.751391	-4.206922	-2.725785
43	1	0	-2.222035	-5.712929	-0.829936
44	6	0	-2.443143	2.788301	0.382577
45	6	0	-2.161782	3.464224	-0.807863
46	6	0	-2.133052	3.295816	1.649186
47	6	0	-1.557762	4.717409	-0.701044
48	6	0	-1.530382	4.550749	1.705830
49	6	0	-1.248124	5.256024	0.541084
50	1	0	-1.327082	5.270640	-1.610559
51	1	0	-1.279087	4.974267	2.677522
52	1	0	-0.779420	6.236182	0.603733
53	6	0	-2.455556	2.863139	-2.149179
54	1	0	-3.393450	2.291701	-2.158947
55	1	0	-2.525628	3.641276	-2.917270
56	1	0	-1.651248	2.175890	-2.454190
57	6	0	-2.422228	2.509586	2.892344
58	1	0	-3.500244	2.370789	3.055064
59	1	0	-1.975770	1.504753	2.845264
60	1	0	-2.019070	3.016519	3.775669
61	6	0	-2.659051	-2.280887	2.313509
62	1	0	-3.628193	-1.861934	2.617377
63	1	0	-2.394942	-3.062188	3.035116
64	1	0	-1.924082	-1.466515	2.403668
65	6	0	-3.330566	-1.545174	-2.631432
66	1	0	-4.287457	-1.023564	-2.493212
67	1	0	-2.558496	-0.768133	-2.736472
68	1	0	-3.383047	-2.094136	-3.577627
69	6	0	1.014811	-3.457364	-0.917148
70	1	0	0.878505	-4.476702	-0.541569
71	1	0	0.010175	-3.037048	-1.102639
72	1	0	1.552199	-3.465309	-1.870793
73	6	0	1.560822	-1.770374	3.743384
74	1	0	0.819582	-1.002103	3.998213
75	1	0	1.207219	-2.750892	4.072339
76	1	0	2.479560	-1.513756	4.287354

Zero-point correction= 0.618336 (Hartree/Particle)
Thermal correction to Energy= 0.658287
Thermal correction to Enthalpy= 0.659232
Thermal correction to Gibbs Free Energy= 0.543626
Sum of electronic and zero-point Energies= -1840.006355
Sum of electronic and thermal Energies= -1839.966404
Sum of electronic and thermal Enthalpies= -1839.965459
Sum of electronic and thermal Free Energies= -1840.081065
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.47196943

INT10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.450759	-1.989876	0.780788
2	6	0	-0.131157	-2.368725	0.527762
3	79	0	-0.090529	0.020217	0.203089
4	6	0	-2.400132	-1.795583	-0.382674
5	8	0	-3.472368	-2.559544	-0.253929
6	6	0	0.399686	-2.902049	-0.741779
7	6	0	-0.392460	-3.683431	-1.589302
8	6	0	1.738398	-2.661526	-1.077792
9	6	0	0.137670	-4.186618	-2.770350
10	1	0	-1.415551	-3.931444	-1.307412
11	6	0	2.261054	-3.162232	-2.261047
12	1	0	2.364114	-2.065522	-0.412176
13	6	0	1.460507	-3.921481	-3.111575
14	1	0	-0.480642	-4.803767	-3.418618
15	1	0	3.300929	-2.966826	-2.518365
16	1	0	1.873148	-4.320223	-4.036172
17	8	0	-2.200803	-1.041929	-1.312358
18	6	0	-0.179070	-1.203862	3.278205
19	6	0	0.862697	-1.648792	2.559612
20	6	0	-1.530700	-1.740618	3.127292
21	7	0	-2.067127	-2.080279	2.008402
22	8	0	0.709713	-2.627871	1.588384

23	1	0	0.016616	-0.503181	4.089815
24	6	0	-4.439256	-2.429969	-1.301860
25	1	0	-5.267981	-3.080166	-1.020188
26	1	0	-4.769877	-1.389439	-1.383354
27	1	0	-4.004890	-2.745996	-2.256756
28	6	0	0.528326	1.899798	-0.304608
29	7	0	1.792576	2.349153	-0.447489
30	6	0	0.491607	4.044121	-0.970478
31	6	0	1.790529	3.673612	-0.861398
32	1	0	0.030287	4.978071	-1.264068
33	1	0	2.712505	4.211925	-1.038831
34	7	0	-0.268911	2.939029	-0.623476
35	6	0	-1.707160	2.866266	-0.647297
36	6	0	-2.409432	3.270355	0.493789
37	6	0	-2.324283	2.369302	-1.798900
38	6	0	-3.798463	3.167755	0.457642
39	6	0	-3.717060	2.287652	-1.787982
40	6	0	-4.446094	2.680592	-0.673081
41	1	0	-4.374982	3.477005	1.328625
42	1	0	-4.227599	1.909216	-2.672945
43	1	0	-5.532307	2.613535	-0.685763
44	6	0	2.966443	1.544768	-0.243667
45	6	0	3.398289	0.724268	-1.291721
46	6	0	3.611974	1.613339	0.995795
47	6	0	4.537711	-0.050478	-1.066485
48	6	0	4.751648	0.827945	1.170165
49	6	0	5.210325	0.002738	0.149186
50	1	0	4.907017	-0.689865	-1.868018
51	1	0	5.277682	0.864639	2.123789
52	1	0	6.103036	-0.600620	0.301273
53	6	0	2.660516	0.655025	-2.594676
54	1	0	2.368396	1.648054	-2.961439
55	1	0	3.278186	0.179926	-3.365131
56	1	0	1.737745	0.059899	-2.502486
57	6	0	3.076198	2.462854	2.108013
58	1	0	3.020609	3.525111	1.834581
59	1	0	2.057669	2.154160	2.390461
60	1	0	3.709844	2.384364	2.998351
61	6	0	-1.696305	3.781279	1.709026
62	1	0	-1.107468	4.683769	1.494294
63	1	0	-2.409812	4.033716	2.500629
64	1	0	-0.997926	3.033509	2.112961
65	6	0	-1.534034	1.910925	-2.986121
66	1	0	-0.677403	2.564199	-3.199541
67	1	0	-1.144879	0.894379	-2.826598
68	1	0	-2.164103	1.880277	-3.881852
69	6	0	-2.332849	-1.891269	4.376554
70	1	0	-1.811656	-2.534744	5.097819
71	1	0	-2.464649	-0.914193	4.863313
72	1	0	-3.314850	-2.315775	4.151896
73	6	0	2.286504	-1.286900	2.755348
74	1	0	2.714147	-0.881999	1.826230
75	1	0	2.404963	-0.542771	3.550519
76	1	0	2.868161	-2.182048	3.013988

Zero-point correction= 0.617689 (Hartree/Particle)
Thermal correction to Energy= 0.657857
Thermal correction to Enthalpy= 0.658801
Thermal correction to Gibbs Free Energy= 0.544090
Sum of electronic and zero-point Energies= -1840.028537
Sum of electronic and thermal Energies= -1839.988368
Sum of electronic and thermal Enthalpies= -1839.987424
Sum of electronic and thermal Free Energies= -1840.102135
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.48963507

INT11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.079713	1.028739	0.681498
2	6	0	3.090078	1.265876	-0.197918
3	79	0	-0.737590	0.355045	0.134793
4	6	0	2.188719	0.019702	1.766123
5	8	0	1.104704	0.053271	2.568172

6	6	0	4.178680	0.380041	-0.593710
7	6	0	5.429344	0.912034	-0.930989
8	6	0	3.954136	-0.995351	-0.739068
9	6	0	6.452678	0.078388	-1.357690
10	1	0	5.597611	1.984413	-0.852402
11	6	0	4.974670	-1.822363	-1.178107
12	1	0	2.967168	-1.403949	-0.522722
13	6	0	6.227225	-1.289799	-1.478687
14	1	0	7.426724	0.496513	-1.602125
15	1	0	4.797863	-2.890265	-1.294283
16	1	0	7.027515	-1.943320	-1.820613
17	8	0	3.133896	-0.702688	1.974083
18	6	0	1.873443	3.893051	0.533929
19	6	0	0.723683	3.009130	0.582220
20	6	0	2.955876	3.623079	-0.213315
21	1	0	1.787752	4.880795	0.982591
22	6	0	-0.624329	3.647482	0.554133
23	1	0	-1.413408	2.949299	0.858953
24	1	0	-0.644908	4.525851	1.211250
25	1	0	-0.848957	4.003933	-0.461095
26	8	0	3.094289	2.444709	-0.914246
27	7	0	0.831616	1.719849	0.589519
28	6	0	4.078391	4.556739	-0.465880
29	1	0	4.223274	4.684976	-1.546456
30	1	0	3.901265	5.534457	-0.008196
31	1	0	5.014439	4.145049	-0.062746
32	6	0	1.187167	-0.806983	3.702895
33	1	0	2.046281	-0.537834	4.325920
34	1	0	0.254758	-0.664851	4.253249
35	1	0	1.298701	-1.850723	3.385236
36	6	0	-2.115860	-1.034990	-0.366885
37	7	0	-1.878883	-2.357921	-0.499398
38	6	0	-4.016669	-2.087634	-0.937438
39	6	0	-3.041543	-3.025573	-0.851491
40	1	0	-5.068864	-2.160954	-1.179745
41	1	0	-3.056545	-4.097096	-1.002054
42	7	0	-3.426870	-0.869750	-0.635753
43	6	0	-4.102607	0.397764	-0.554686
44	6	0	-4.171701	1.194065	-1.701957
45	6	0	-4.622857	0.783077	0.685277
46	6	0	-4.803687	2.431461	-1.580872
47	6	0	-5.246206	2.028441	0.757599
48	6	0	-5.334836	2.844616	-0.364372
49	1	0	-4.879066	3.073221	-2.457855
50	1	0	-5.666613	2.355605	1.707784
51	1	0	-5.828421	3.811856	-0.290792
52	6	0	-0.595908	-2.957045	-0.246283
53	6	0	-0.249296	-3.238938	1.079626
54	6	0	0.255139	-3.191718	-1.331343
55	6	0	1.016910	-3.780226	1.307220
56	6	0	1.507151	-3.741159	-1.054468
57	6	0	1.886986	-4.027713	0.252242
58	1	0	1.314577	-4.025015	2.326753
59	1	0	2.188859	-3.939870	-1.881289
60	1	0	2.869615	-4.451613	0.452010
61	6	0	-1.182943	-2.947312	2.216079
62	1	0	-2.226428	-3.194600	1.979256
63	1	0	-0.897361	-3.514517	3.109513
64	1	0	-1.159118	-1.878459	2.482193
65	6	0	-0.155840	-2.852064	-2.731596
66	1	0	-1.033156	-3.428456	-3.055803
67	1	0	-0.419080	-1.788709	-2.827963
68	1	0	0.655060	-3.060469	-3.437376
69	6	0	-3.579423	0.744306	-3.002994
70	1	0	-3.998699	-0.213378	-3.340513
71	1	0	-3.765127	1.482651	-3.790358
72	1	0	-2.491046	0.606924	-2.924811
73	6	0	-4.495826	-0.097676	1.891535
74	1	0	-4.831356	-1.124656	1.692226
75	1	0	-3.450968	-0.164653	2.230481
76	1	0	-5.089621	0.293023	2.724736

Zero-point correction= 0.620021 (Hartree/Particle)
Thermal correction to Energy= 0.659496
Thermal correction to Enthalpy= 0.660440

Thermal correction to Gibbs Free Energy= 0.547943
Sum of electronic and zero-point Energies= -1840.041926
Sum of electronic and thermal Energies= -1840.002451
Sum of electronic and thermal Enthalpies= -1840.001507
Sum of electronic and thermal Free Energies= -1840.114004
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.51017188

INT11a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.454616	-2.237023	0.697576
2	6	0	-2.263474	-1.806869	-0.303489
3	79	0	0.693364	-0.295026	-0.700944
4	6	0	-1.548866	-1.641938	2.069846
5	8	0	-0.462993	-1.966242	2.781514
6	6	0	-3.500825	-1.025217	-0.297890
7	6	0	-4.540995	-1.298831	0.597922
8	6	0	-3.691061	-0.057878	-1.293413
9	6	0	-5.741964	-0.611275	0.501151
10	1	0	-4.407410	-2.061704	1.360324
11	6	0	-4.895767	0.622487	-1.390586
12	1	0	-2.878660	0.175447	-1.983971
13	6	0	-5.924727	0.345204	-0.494828
14	1	0	-6.548079	-0.836989	1.195943
15	1	0	-5.030762	1.374670	-2.166351
16	1	0	-6.875263	0.869474	-0.577222
17	8	0	-2.440382	-0.939731	2.486661
18	6	0	0.400987	-2.339858	-1.484976
19	6	0	-0.789726	-2.146711	-2.190543
20	6	0	0.343830	-3.309953	-0.342072
21	7	0	-0.531553	-3.272156	0.579536
22	8	0	-1.985483	-2.180510	-1.638262
23	1	0	1.265646	-2.460521	-2.145632
24	6	0	1.485968	3.488900	1.098491
25	6	0	2.723257	2.936403	1.122094
26	1	0	1.113608	4.440656	1.454801
27	1	0	3.669371	3.300832	1.500760
28	7	0	0.648306	2.569513	0.487272
29	7	0	2.611409	1.690773	0.526571
30	6	0	1.337126	1.464181	0.138628
31	6	0	1.357059	-4.404501	-0.378549
32	1	0	1.196913	-5.095886	0.452755
33	1	0	1.317759	-4.956099	-1.327418
34	1	0	2.366439	-3.972843	-0.301021
35	6	0	-0.857472	-1.942742	-3.658484
36	1	0	-1.306983	-2.831244	-4.123720
37	1	0	-1.512613	-1.095891	-3.895864
38	1	0	0.135046	-1.784721	-4.089264
39	6	0	-0.465987	-1.541129	4.143142
40	1	0	0.393187	-2.029036	4.607547
41	1	0	-0.365795	-0.451956	4.210928
42	1	0	-1.394344	-1.844312	4.637432
43	6	0	-0.771555	2.739296	0.323600
44	6	0	-1.247363	3.282190	-0.874148
45	6	0	-1.598393	2.369878	1.389035
46	6	0	-2.624285	3.473352	-0.980419
47	6	0	-2.971127	2.553471	1.226180
48	6	0	-3.474571	3.116781	0.060508
49	1	0	-3.028214	3.910558	-1.893523
50	1	0	-3.643790	2.253888	2.028748
51	1	0	-4.547063	3.272235	-0.040868
52	6	0	3.683914	0.748060	0.349335
53	6	0	3.837262	-0.277653	1.288245
54	6	0	4.506761	0.892850	-0.774231
55	6	0	4.875200	-1.186388	1.075385
56	6	0	5.528066	-0.040234	-0.944751
57	6	0	5.711206	-1.069787	-0.028172
58	1	0	5.027466	-1.989371	1.795943
59	1	0	6.185955	0.047013	-1.808488
60	1	0	6.517388	-1.786302	-0.173343
61	6	0	2.914835	-0.426904	2.461043
62	1	0	2.631556	0.540083	2.898164
63	1	0	1.982690	-0.939688	2.173343

64	1	0	3.384357	-1.027592	3.248361
65	6	0	4.289511	1.997791	-1.763534
66	1	0	3.267768	1.982805	-2.170381
67	1	0	4.438467	2.989968	-1.315500
68	1	0	4.986266	1.908968	-2.603618
69	6	0	-1.028524	1.833258	2.665665
70	1	0	-0.550648	2.627955	3.256960
71	1	0	-1.811921	1.370855	3.274684
72	1	0	-0.262614	1.066747	2.475176
73	6	0	-0.316693	3.647671	-1.990968
74	1	0	0.467288	4.345119	-1.664587
75	1	0	0.195032	2.762959	-2.397705
76	1	0	-0.861998	4.124639	-2.812523

Zero-point correction= 0.619499 (Hartree/Particle)
Thermal correction to Energy= 0.659084
Thermal correction to Enthalpy= 0.660029
Thermal correction to Gibbs Free Energy= 0.547737
Sum of electronic and zero-point Energies= -1840.027761
Sum of electronic and thermal Energies= -1839.988176
Sum of electronic and thermal Enthalpies= -1839.987232
Sum of electronic and thermal Free Energies= -1840.099523
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.49587171

INT12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.900745	-1.356831	-0.108544
2	6	0	3.189941	-0.765074	1.309294
3	79	0	-0.204439	-0.412617	-0.069622
4	6	0	3.366706	-0.438478	-1.233558
5	8	0	2.475656	-0.328086	-2.218018
6	6	0	2.731871	0.603036	1.644334
7	6	0	2.782700	0.962601	2.998007
8	6	0	2.264507	1.535772	0.710064
9	6	0	2.364934	2.218817	3.409975
10	1	0	3.158686	0.232969	3.711809
11	6	0	1.861419	2.798101	1.122398
12	1	0	2.214268	1.311319	-0.354036
13	6	0	1.905655	3.139836	2.470439
14	1	0	2.406429	2.485236	4.464000
15	1	0	1.521700	3.519558	0.383171
16	1	0	1.590190	4.133606	2.786809
17	8	0	4.452064	0.084767	-1.213438
18	6	0	2.677602	-3.620034	-0.454495
19	6	0	1.385501	-2.992539	-0.338231
20	6	0	3.624927	-2.671490	-0.300619
21	1	0	2.837135	-4.683395	-0.606827
22	6	0	0.085117	-3.699898	-0.436657
23	1	0	-0.350039	-3.543488	-1.434644
24	1	0	0.205739	-4.777614	-0.286055
25	1	0	-0.632791	-3.312077	0.297336
26	8	0	3.708260	-1.489485	2.130237
27	7	0	1.481325	-1.700044	-0.147637
28	6	0	5.093011	-2.817268	-0.255071
29	1	0	5.407955	-3.798210	-0.624843
30	1	0	5.600208	-2.028116	-0.823257
31	1	0	5.422762	-2.712755	0.788539
32	6	0	2.876286	0.527584	-3.296415
33	1	0	3.840216	0.207598	-3.702261
34	1	0	2.090021	0.443114	-4.047914
35	1	0	2.961365	1.560829	-2.938743
36	6	0	-1.990145	0.559178	-0.108527
37	7	0	-2.323921	1.845968	-0.353875
38	6	0	-4.235513	0.772307	-0.154983
39	6	0	-3.704148	1.993309	-0.391044
40	1	0	-5.259996	0.429063	-0.092676
41	1	0	-4.161156	2.955634	-0.581650
42	7	0	-3.169267	-0.095016	0.015427
43	6	0	-3.306940	-1.504894	0.265032
44	6	0	-3.345306	-1.943340	1.593004
45	6	0	-3.417683	-2.363575	-0.834091
46	6	0	-3.508512	-3.312281	1.808946

47	6	0	-3.581616	-3.723207	-0.568534
48	6	0	-3.630176	-4.192702	0.739593
49	1	0	-3.548043	-3.684379	2.831863
50	1	0	-3.679870	-4.417051	-1.402904
51	1	0	-3.768932	-5.255676	0.927671
52	6	0	-1.430944	2.952190	-0.570921
53	6	0	-0.814922	3.086726	-1.819645
54	6	0	-1.297265	3.892684	0.457231
55	6	0	-0.048080	4.233661	-2.033175
56	6	0	-0.545746	5.036087	0.187105
57	6	0	0.068554	5.208648	-1.048447
58	1	0	0.435789	4.371481	-2.999660
59	1	0	-0.436488	5.792991	0.963646
60	1	0	0.647668	6.108750	-1.245352
61	6	0	-0.980583	2.054269	-2.893982
62	1	0	-2.033119	1.769088	-3.032191
63	1	0	-0.604175	2.426830	-3.853308
64	1	0	-0.433519	1.128765	-2.653282
65	6	0	-1.896374	3.654091	1.810151
66	1	0	-2.988890	3.548647	1.778539
67	1	0	-1.496752	2.727899	2.251284
68	1	0	-1.661735	4.478608	2.492001
69	6	0	-3.209038	-0.982845	2.735286
70	1	0	-3.962883	-0.184661	2.694534
71	1	0	-3.323287	-1.498995	3.694313
72	1	0	-2.224317	-0.493027	2.734814
73	6	0	-3.345669	-1.847083	-2.239646
74	1	0	-4.124817	-1.100937	-2.448224
75	1	0	-2.379184	-1.360926	-2.444440
76	1	0	-3.469152	-2.661992	-2.961199

Zero-point correction= 0.619916 (Hartree/Particle)
Thermal correction to Energy= 0.659481
Thermal correction to Enthalpy= 0.660425
Thermal correction to Gibbs Free Energy= 0.548197
Sum of electronic and zero-point Energies= -1840.080642
Sum of electronic and thermal Energies= -1840.041077
Sum of electronic and thermal Enthalpies= -1840.040132
Sum of electronic and thermal Free Energies= -1840.152360
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.54962512

INT13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.429564	-0.229958	0.925526
2	6	0	-2.942553	-0.300680	-0.510228
3	79	0	0.864505	-0.736088	0.045309
4	6	0	-2.447004	1.123874	1.580750
5	8	0	-1.559487	1.240519	2.552169
6	6	0	-4.312128	-0.765077	-0.747058
7	6	0	-5.242116	-0.857098	0.296076
8	6	0	-4.690277	-1.090130	-2.055455
9	6	0	-6.536798	-1.283847	0.033040
10	1	0	-4.963416	-0.567495	1.310241
11	6	0	-5.981612	-1.522575	-2.312051
12	1	0	-3.952707	-0.996651	-2.850238
13	6	0	-6.902220	-1.620319	-1.268791
14	1	0	-7.265628	-1.346085	0.838011
15	1	0	-6.277487	-1.783268	-3.325828
16	1	0	-7.916865	-1.956283	-1.473794
17	8	0	-3.276279	1.936167	1.248677
18	6	0	-0.944242	-3.250296	0.743822
19	6	0	0.182233	-2.683597	0.173621
20	6	0	-1.999810	-2.566305	1.356817
21	7	0	-2.027667	-1.247823	1.553492
22	8	0	-2.134681	-0.022546	-1.374813
23	1	0	-1.055140	-4.339704	0.746668
24	6	0	2.932652	2.943547	-0.896486
25	6	0	3.941423	2.049454	-0.770726
26	1	0	2.925747	3.989097	-1.175608
27	1	0	5.010918	2.142953	-0.907471
28	7	0	1.758810	2.267257	-0.594922
29	7	0	3.357110	0.851228	-0.399318

30	6	0	2.010557	0.974983	-0.291357
31	6	0	-3.154545	-3.312241	1.941704
32	1	0	-4.059102	-3.098475	1.352161
33	1	0	-2.976276	-4.390766	1.936895
34	1	0	-3.349899	-2.977865	2.967210
35	6	0	4.063173	-0.382653	-0.182729
36	6	0	4.442045	-0.710686	1.122945
37	6	0	4.309140	-1.208669	-1.285160
38	6	0	5.096612	-1.927635	1.313060
39	6	0	4.968461	-2.414593	-1.047016
40	6	0	5.358390	-2.771149	0.239341
41	1	0	5.407048	-2.208571	2.318775
42	1	0	5.178350	-3.076820	-1.886316
43	1	0	5.875647	-3.714245	0.405768
44	6	0	0.461951	2.882895	-0.645801
45	6	0	-0.345622	2.652263	-1.762547
46	6	0	0.099336	3.735086	0.404405
47	6	0	-1.574296	3.314010	-1.808618
48	6	0	-1.127167	4.389211	0.303044
49	6	0	-1.957945	4.178562	-0.792820
50	1	0	-2.227635	3.149092	-2.664447
51	1	0	-1.429841	5.078071	1.092306
52	1	0	-2.916102	4.690748	-0.849906
53	6	0	0.082234	1.733877	-2.865153
54	1	0	0.002868	0.682816	-2.549917
55	1	0	-0.559572	1.860198	-3.743902
56	1	0	1.121557	1.914507	-3.173160
57	6	0	0.997629	3.926530	1.590104
58	1	0	0.528709	4.578032	2.336633
59	1	0	1.234589	2.965590	2.072829
60	1	0	1.957907	4.384357	1.316235
61	6	0	3.863369	-0.824355	-2.663601
62	1	0	2.777218	-0.653595	-2.706306
63	1	0	4.342671	0.101307	-3.011194
64	1	0	4.107154	-1.611792	-3.384986
65	6	0	4.136297	0.199403	2.273547
66	1	0	3.055665	0.238912	2.476181
67	1	0	4.634089	-0.144914	3.186400
68	1	0	4.461628	1.230595	2.079783
69	6	0	-1.669456	2.440437	3.330091
70	1	0	-2.631667	2.458370	3.852259
71	1	0	-0.844860	2.407384	4.042931
72	1	0	-1.593981	3.317001	2.678227
73	6	0	1.141133	-3.640327	-0.445722
74	1	0	1.306888	-3.368451	-1.500156
75	1	0	2.131727	-3.527259	0.024402
76	1	0	0.834035	-4.695226	-0.392555

Zero-point correction= 0.616466 (Hartree/Particle)
Thermal correction to Energy= 0.657360
Thermal correction to Enthalpy= 0.658304
Thermal correction to Gibbs Free Energy= 0.541993
Sum of electronic and zero-point Energies= -1840.001626
Sum of electronic and thermal Energies= -1839.960731
Sum of electronic and thermal Enthalpies= -1839.959787
Sum of electronic and thermal Free Energies= -1840.076098
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.46617531

INT14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.434395	-0.565067	0.074558
2	6	0	3.793371	-1.367278	0.005574
3	79	0	-0.722263	-0.070610	-0.614604
4	6	0	1.922757	-0.726647	1.506922
5	8	0	2.887497	-0.467913	2.371207
6	6	0	5.094480	-0.716319	-0.232850
7	6	0	5.391068	0.615388	0.086028
8	6	0	6.105321	-1.548411	-0.740868
9	6	0	6.675506	1.102819	-0.119336
10	1	0	4.622230	1.254488	0.508849
11	6	0	7.376656	-1.047803	-0.965417
12	1	0	5.868227	-2.587891	-0.957041

13	6	0	7.663029	0.280269	-0.653175
14	1	0	6.908136	2.133044	0.142405
15	1	0	8.150342	-1.692915	-1.376311
16	1	0	8.664314	0.673056	-0.820925
17	8	0	0.781417	-1.008803	1.798730
18	6	0	1.209705	-0.088270	-1.826769
19	6	0	1.505235	-1.141333	-0.983943
20	6	0	1.871616	1.114712	-1.265929
21	7	0	2.526455	0.863227	-0.185340
22	8	0	3.684204	-2.567443	0.152460
23	1	0	0.792902	-0.171422	-2.831762
24	6	0	-4.231950	1.527458	1.093429
25	6	0	-4.623241	0.231023	1.004668
26	1	0	-4.734536	2.406881	1.474364
27	1	0	-5.540091	-0.266026	1.293790
28	7	0	-2.948674	1.590725	0.575934
29	7	0	-3.570767	-0.465855	0.434138
30	6	0	-2.546980	0.368291	0.173732
31	6	0	1.725876	2.474329	-1.842334
32	1	0	2.050142	2.496964	-2.891008
33	1	0	0.668469	2.782328	-1.821573
34	1	0	2.311602	3.196681	-1.266626
35	6	0	-3.523663	-1.881159	0.174094
36	6	0	-4.001819	-2.342238	-1.056786
37	6	0	-2.960665	-2.711242	1.148537
38	6	0	-3.906975	-3.710893	-1.304042
39	6	0	-2.888814	-4.073569	0.855162
40	6	0	-3.355079	-4.567308	-0.357390
41	1	0	-4.273540	-4.104610	-2.251221
42	1	0	-2.463582	-4.750898	1.594848
43	1	0	-3.292999	-5.633681	-0.565775
44	6	0	-2.119118	2.761541	0.468961
45	6	0	-1.157174	2.984160	1.460088
46	6	0	-2.281198	3.585283	-0.650398
47	6	0	-0.331732	4.098645	1.306116
48	6	0	-1.436523	4.690163	-0.757561
49	6	0	-0.471672	4.944017	0.211751
50	1	0	0.424493	4.304001	2.062747
51	1	0	-1.542671	5.356488	-1.612840
52	1	0	0.176736	5.812689	0.113572
53	6	0	-1.002880	2.058033	2.629418
54	1	0	-0.510287	1.115580	2.341269
55	1	0	-0.394669	2.524682	3.412503
56	1	0	-1.970245	1.786768	3.073745
57	6	0	-3.311156	3.282607	-1.696733
58	1	0	-3.228709	3.978249	-2.538479
59	1	0	-3.201272	2.261440	-2.091017
60	1	0	-4.333988	3.362297	-1.303351
61	6	0	-2.435977	-2.163114	2.441374
62	1	0	-1.469407	-1.656541	2.300421
63	1	0	-3.123161	-1.434736	2.892953
64	1	0	-2.280263	-2.968848	3.167117
65	6	0	-4.579509	-1.400295	-2.069823
66	1	0	-3.856270	-0.623878	-2.360473
67	1	0	-4.875533	-1.936907	-2.977397
68	1	0	-5.468760	-0.879529	-1.688459
69	6	0	2.530936	-0.537107	3.757426
70	1	0	2.156527	-1.536024	4.000103
71	1	0	3.447537	-0.323874	4.307702
72	1	0	1.761305	0.207779	3.984788
73	6	0	1.133859	-2.569732	-1.142685
74	1	0	0.658980	-2.948272	-0.227089
75	1	0	0.444851	-2.707548	-1.984201
76	1	0	2.031782	-3.180789	-1.295042

Zero-point correction= 0.616348 (Hartree/Particle)
Thermal correction to Energy= 0.657321
Thermal correction to Enthalpy= 0.658265
Thermal correction to Gibbs Free Energy= 0.539840
Sum of electronic and zero-point Energies= -1840.056157
Sum of electronic and thermal Energies= -1840.015184
Sum of electronic and thermal Enthalpies= -1840.014240
Sum of electronic and thermal Free Energies= -1840.132665
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.52012013

INT15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.256023	-0.677540	-0.035417
2	6	0	-3.544700	-1.284401	0.303578
3	79	0	0.707192	-0.292979	-0.131323
4	6	0	-2.144781	0.821394	-0.127058
5	8	0	-2.074300	1.226636	-1.387797
6	6	0	-4.773371	-0.471236	0.117714
7	6	0	-5.568812	-0.127550	1.210467
8	6	0	-5.120289	-0.042450	-1.165086
9	6	0	-6.703913	0.651155	1.017856
10	1	0	-5.291647	-0.476051	2.203733
11	6	0	-6.256513	0.736590	-1.352287
12	1	0	-4.506225	-0.331583	-2.019355
13	6	0	-7.047398	1.083661	-0.260538
14	1	0	-7.323666	0.922393	1.870142
15	1	0	-6.532264	1.062362	-2.353241
16	1	0	-7.939529	1.689219	-0.407456
17	8	0	-2.087102	1.514282	0.858400
18	6	0	-2.317425	-3.440083	-0.232347
19	6	0	-3.566653	-2.820740	0.193951
20	6	0	-1.155808	-2.754379	-0.285204
21	7	0	-1.151887	-1.352734	-0.182070
22	8	0	-3.478275	-2.131453	1.427373
23	1	0	-2.330447	-4.494247	-0.507654
24	6	0	4.671370	0.916840	0.547828
25	6	0	4.084727	2.135172	0.633097
26	1	0	5.698407	0.599373	0.672415
27	1	0	4.488198	3.115403	0.850445
28	7	0	3.665810	0.015014	0.242120
29	7	0	2.734576	1.950258	0.377112
30	6	0	2.477314	0.647008	0.138506
31	6	0	0.166767	-3.390535	-0.552683
32	1	0	0.665760	-2.950881	-1.428931
33	1	0	0.843791	-3.259924	0.305461
34	1	0	0.052088	-4.466190	-0.723851
35	6	0	-4.857351	-3.528758	-0.081912
36	1	0	-4.993681	-3.675362	-1.160488
37	1	0	-4.851860	-4.514388	0.400319
38	1	0	-5.709456	-2.962703	0.305907
39	6	0	-1.863009	2.633601	-1.572353
40	1	0	-2.029140	2.821632	-2.633652
41	1	0	-2.561431	3.208149	-0.956083
42	1	0	-0.834365	2.887369	-1.288875
43	6	0	1.759839	3.008806	0.352552
44	6	0	1.739076	3.847507	-0.768778
45	6	0	0.898491	3.159784	1.444580
46	6	0	0.823105	4.899094	-0.763876
47	6	0	-0.014710	4.214227	1.393219
48	6	0	-0.043138	5.082491	0.309621
49	1	0	0.791254	5.575278	-1.617643
50	1	0	-0.705310	4.351213	2.223943
51	1	0	-0.750662	5.909588	0.297914
52	6	0	3.830002	-1.403575	0.069923
53	6	0	3.759151	-2.221321	1.203023
54	6	0	4.020269	-1.893069	-1.226335
55	6	0	3.898041	-3.595449	1.005763
56	6	0	4.153689	-3.273755	-1.373586
57	6	0	4.095025	-4.115584	-0.268869
58	1	0	3.855369	-4.259540	1.868219
59	1	0	4.310671	-3.687249	-2.369155
60	1	0	4.208379	-5.189835	-0.401739
61	6	0	3.528926	-1.645387	2.567811
62	1	0	4.344373	-0.976384	2.875691
63	1	0	2.600664	-1.055700	2.611109
64	1	0	3.453947	-2.439527	3.318172
65	6	0	4.055100	-0.974703	-2.410427
66	1	0	3.062446	-0.544946	-2.614220
67	1	0	4.741271	-0.130289	-2.259175
68	1	0	4.374520	-1.510461	-3.310621
69	6	0	0.934502	2.234055	2.622222
70	1	0	0.387355	1.301629	2.413826

71	1	0	1.959940	1.956896	2.902805
72	1	0	0.457547	2.698143	3.492203
73	6	0	2.652186	3.614486	-1.935164
74	1	0	3.695131	3.874895	-1.706596
75	1	0	2.648208	2.559571	-2.247345
76	1	0	2.347971	4.221832	-2.794402

Zero-point correction= 0.619397 (Hartree/Particle)
Thermal correction to Energy= 0.659015
Thermal correction to Enthalpy= 0.659959
Thermal correction to Gibbs Free Energy= 0.546753
Sum of electronic and zero-point Energies= -1840.039950
Sum of electronic and thermal Energies= -1840.000332
Sum of electronic and thermal Enthalpies= -1839.999388
Sum of electronic and thermal Free Energies= -1840.112594
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.50275235

INT16a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.711751	0.430372	-1.132006
2	6	0	4.577632	-0.139298	0.345784
3	6	0	2.571863	1.885613	-0.888138
4	8	0	1.365669	2.348875	-1.195806
5	6	0	3.594119	-0.378958	1.443524
6	6	0	2.978974	-1.611758	1.672132
7	6	0	3.274585	0.718887	2.249253
8	6	0	2.017836	-1.732325	2.670286
9	1	0	3.264137	-2.485747	1.089759
10	6	0	2.302802	0.594518	3.236059
11	1	0	3.782256	1.667765	2.082781
12	6	0	1.667724	-0.627834	3.442767
13	1	0	1.553796	-2.701278	2.852065
14	1	0	2.054846	1.452031	3.859227
15	1	0	0.915843	-0.727086	4.225055
16	8	0	3.490079	2.545752	-0.458398
17	6	0	3.613311	-1.649374	-1.407903
18	6	0	2.265204	-1.720640	-1.386331
19	6	0	4.032162	-0.246235	-1.165738
20	1	0	4.304645	-2.474951	-1.549188
21	6	0	1.356901	-2.888079	-1.473598
22	1	0	1.914099	-3.791460	-1.744004
23	1	0	0.857215	-3.071459	-0.507793
24	1	0	0.568322	-2.728867	-2.222489
25	8	0	5.712982	0.199590	0.524747
26	7	0	1.727538	-0.420925	-1.195820
27	6	0	5.079400	0.324216	-2.110754
28	1	0	6.014420	-0.234283	-2.000656
29	1	0	4.739258	0.247523	-3.149657
30	1	0	5.281094	1.371444	-1.865001
31	79	0	-0.282854	-0.125805	-0.576561
32	6	0	1.168375	3.745746	-0.942910
33	1	0	1.366668	3.966762	0.110888
34	1	0	1.842340	4.338384	-1.569391
35	1	0	0.124604	3.945515	-1.190219
36	6	0	-2.198406	-0.053954	0.069007
37	7	0	-2.965582	-1.147402	0.278621
38	6	0	-4.251135	0.573182	0.737705
39	6	0	-4.235656	-0.780575	0.691730
40	1	0	-5.026839	1.277814	1.007840
41	1	0	-4.996101	-1.519104	0.909924
42	7	0	-2.989488	1.002001	0.351084
43	6	0	-2.589927	2.384010	0.320285
44	6	0	-2.895650	3.139944	-0.816399
45	6	0	-1.964829	2.914176	1.454498
46	6	0	-2.570881	4.497026	-0.787273
47	6	0	-1.661613	4.275899	1.437792
48	6	0	-1.969442	5.061250	0.332760
49	1	0	-2.808517	5.114986	-1.652425
50	1	0	-1.189273	4.722744	2.312091
51	1	0	-1.738371	6.124865	0.344274
52	6	0	-2.484639	-2.497286	0.149493
53	6	0	-1.881738	-3.084288	1.267758

54	6	0	-2.619854	-3.144034	-1.082467
55	6	0	-1.389144	-4.380884	1.122009
56	6	0	-2.119557	-4.443193	-1.178462
57	6	0	-1.508741	-5.054432	-0.089526
58	1	0	-0.918651	-4.868163	1.975710
59	1	0	-2.214972	-4.976633	-2.123487
60	1	0	-1.127212	-6.069377	-0.183795
61	6	0	-1.764386	-2.340929	2.563501
62	1	0	-2.739624	-1.989091	2.927673
63	1	0	-1.330771	-2.978737	3.342013
64	1	0	-1.123414	-1.452468	2.457743
65	6	0	-3.255494	-2.463819	-2.256581
66	1	0	-4.284266	-2.144139	-2.041841
67	1	0	-2.696483	-1.563214	-2.551672
68	1	0	-3.290728	-3.132629	-3.123056
69	6	0	-3.548731	2.518144	-2.013364
70	1	0	-4.560795	2.154235	-1.788378
71	1	0	-3.635018	3.242442	-2.830107
72	1	0	-2.974849	1.657329	-2.385468
73	6	0	-1.626982	2.056923	2.637203
74	1	0	-2.460609	1.402421	2.927446
75	1	0	-0.766015	1.404662	2.424285
76	1	0	-1.367661	2.674806	3.504030

Zero-point correction= 0.619219 (Hartree/Particle)
Thermal correction to Energy= 0.659091
Thermal correction to Enthalpy= 0.660036
Thermal correction to Gibbs Free Energy= 0.546021
Sum of electronic and zero-point Energies= -1840.065319
Sum of electronic and thermal Energies= -1840.025447
Sum of electronic and thermal Enthalpies= -1840.024502
Sum of electronic and thermal Free Energies= -1840.138517
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.53611804

INT17a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.309647	2.656291	-0.552663
2	6	0	4.478413	1.027423	-0.880806
3	6	0	0.262750	3.491708	0.064407
4	8	0	-0.960623	2.996303	-0.169076
5	6	0	4.424804	0.383279	0.454377
6	6	0	5.504370	-0.438373	0.807839
7	6	0	3.366680	0.551822	1.355834
8	6	0	5.530702	-1.068692	2.042490
9	1	0	6.317492	-0.559868	0.095378
10	6	0	3.403058	-0.069647	2.598429
11	1	0	2.522407	1.193002	1.108628
12	6	0	4.483403	-0.877362	2.943625
13	1	0	6.375998	-1.698068	2.312855
14	1	0	2.590873	0.088100	3.306012
15	1	0	4.514954	-1.354277	3.922000
16	8	0	0.478299	4.495815	0.701363
17	6	0	3.247913	1.809564	-1.421871
18	6	0	2.088034	0.897994	-1.655895
19	6	0	2.633928	2.930126	-0.638092
20	1	0	3.608675	2.198096	-2.389228
21	6	0	2.206966	-0.425850	-2.302506
22	1	0	2.924777	-0.391602	-3.131597
23	1	0	2.590967	-1.160221	-1.574376
24	1	0	1.238510	-0.787946	-2.666687
25	8	0	5.431527	0.905297	-1.618543
26	7	0	1.001143	1.398234	-1.152460
27	6	0	3.411248	4.088208	-0.141581
28	1	0	4.017547	4.524518	-0.946950
29	1	0	2.759602	4.854867	0.283634
30	1	0	4.118099	3.762554	0.637244
31	79	0	-0.626756	0.145249	-0.579836
32	6	0	-2.046199	3.715409	0.419012
33	1	0	-2.027471	4.761944	0.100014
34	1	0	-2.952856	3.214650	0.071288
35	1	0	-1.979627	3.672687	1.512463
36	6	0	-1.861833	-1.300383	0.105785

37	7	0	-1.451935	-2.571986	0.319490
38	6	0	-3.558303	-2.513180	0.940905
39	6	0	-2.486257	-3.335583	0.835206
40	1	0	-4.567543	-2.685203	1.292054
41	1	0	-2.354678	-4.382657	1.074960
42	7	0	-3.154129	-1.265424	0.488341
43	6	0	-3.990949	-0.094055	0.470642
44	6	0	-4.714437	0.189933	-0.691947
45	6	0	-4.050536	0.690372	1.627498
46	6	0	-5.545286	1.310600	-0.668537
47	6	0	-4.902896	1.794300	1.607092
48	6	0	-5.646089	2.099156	0.472106
49	1	0	-6.126495	1.556322	-1.556346
50	1	0	-4.977412	2.420103	2.495984
51	1	0	-6.309662	2.961812	0.475776
52	6	0	-0.098618	-3.007986	0.092176
53	6	0	0.855240	-2.736098	1.079902
54	6	0	0.210087	-3.625438	-1.124520
55	6	0	2.178465	-3.089060	0.809977
56	6	0	1.541540	-3.980605	-1.341563
57	6	0	2.517066	-3.710109	-0.386934
58	1	0	2.947086	-2.873045	1.553203
59	1	0	1.811201	-4.471190	-2.276215
60	1	0	3.552264	-3.988662	-0.577107
61	6	0	0.481512	-2.063890	2.366300
62	1	0	-0.470224	-2.435232	2.769859
63	1	0	1.256859	-2.219978	3.125086
64	1	0	0.367480	-0.976950	2.228594
65	6	0	-0.842274	-3.866488	-2.163688
66	1	0	-1.632220	-4.539745	-1.804074
67	1	0	-1.335807	-2.929744	-2.463270
68	1	0	-0.408180	-4.318393	-3.061839
69	6	0	-4.599858	-0.671468	-1.912890
70	1	0	-4.833175	-1.723677	-1.699231
71	1	0	-5.286507	-0.330743	-2.694894
72	1	0	-3.582182	-0.647011	-2.328954
73	6	0	-3.216904	0.373504	2.832018
74	1	0	-3.421107	-0.629730	3.231223
75	1	0	-2.142742	0.409298	2.595552
76	1	0	-3.404643	1.093687	3.635732

Zero-point correction= 0.619074 (Hartree/Particle)
Thermal correction to Energy= 0.659162
Thermal correction to Enthalpy= 0.660106
Thermal correction to Gibbs Free Energy= 0.545322
Sum of electronic and zero-point Energies= -1840.079814
Sum of electronic and thermal Energies= -1840.039726
Sum of electronic and thermal Enthalpies= -1840.038782
Sum of electronic and thermal Free Energies= -1840.153566
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1841.55063331

NTf_2 counter-ion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000039	0.000115	0.838950
2	16	0	1.144027	0.837784	0.085234
3	8	0	0.883543	1.211448	-1.299133
4	8	0	1.663768	1.842233	1.003872
5	6	0	2.526263	-0.382960	-0.030864
6	16	0	-1.143939	-0.837669	0.085106
7	8	0	-0.883365	-1.211106	-1.299307
8	8	0	-1.663567	-1.842301	1.003609
9	6	0	-2.526353	0.382863	-0.030906
10	9	0	3.570184	0.198724	-0.621544
11	9	0	2.906361	-0.792071	1.174034
12	9	0	2.177251	-1.443269	-0.746880
13	9	0	-2.177597	1.443115	-0.747127
14	9	0	-3.570281	-0.199056	-0.621345
15	9	0	-2.906321	0.792083	1.173995

Zero-point correction= 0.055863 (Hartree/Particle)
Thermal correction to Energy= 0.069904

Thermal correction to Enthalpy= 0.070848
Thermal correction to Gibbs Free Energy= 0.012497
Sum of electronic and zero-point Energies= -1826.762563
Sum of electronic and thermal Energies= -1826.748522
Sum of electronic and thermal Enthalpies= -1826.747578
Sum of electronic and thermal Free Energies= -1826.805929
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -1827.21703786

$NHTf_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000057	0.000166	0.822546
2	16	0	1.246165	0.886130	0.097995
3	8	0	0.833241	1.297875	-1.217515
4	8	0	1.722434	1.777332	1.129173
5	6	0	2.542550	-0.422371	-0.107089
6	16	0	-1.245874	-0.885832	0.097734
7	8	0	-0.832527	-1.297256	-1.217747
8	8	0	-1.721842	-1.777411	1.128723
9	6	0	-2.542858	0.422143	-0.107218
10	9	0	3.606926	0.154188	-0.625444
11	9	0	2.828817	-0.921870	1.080612
12	9	0	2.099957	-1.370216	-0.901038
13	9	0	-2.101096	1.369993	-0.901614
14	9	0	-3.607232	-0.154951	-0.624979
15	9	0	-2.828891	0.921859	1.080449
16	1	0	0.000011	0.000090	1.843391

Zero-point correction= 0.068161 (Hartree/Particle)
Thermal correction to Energy= 0.082572
Thermal correction to Enthalpy= 0.083517
Thermal correction to Gibbs Free Energy= 0.025429
Sum of electronic and zero-point Energies= -1827.238890
Sum of electronic and thermal Energies= -1827.224479
Sum of electronic and thermal Enthalpies= -1827.223535
Sum of electronic and thermal Free Energies= -1827.281622
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -1827.64277558

INT18a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.897918	0.756814	2.131164
2	6	0	-3.490756	2.817841	0.574171
3	6	0	-0.374845	-0.157895	3.136413
4	8	0	0.930954	-0.499364	2.954950
5	6	0	-3.385455	4.018409	-0.308275
6	6	0	-4.414960	4.271044	-1.217255
7	6	0	-2.327185	4.922356	-0.197554
8	6	0	-4.369301	5.397253	-2.028628
9	1	0	-5.239724	3.562388	-1.272278
10	6	0	-2.294211	6.063033	-0.991688
11	1	0	-1.535788	4.730969	0.527568
12	6	0	-3.310318	6.295939	-1.914284
13	1	0	-5.164615	5.581306	-2.749402
14	1	0	-1.474863	6.773353	-0.890517
15	1	0	-3.280086	7.183851	-2.544523
16	8	0	-1.013683	-0.605156	4.067904
17	6	0	-2.269291	2.106975	0.972687
18	6	0	-1.080519	1.898711	0.242897
19	6	0	-2.154992	1.361106	2.178792
20	1	0	-2.481956	-0.136445	0.611067
21	6	0	-0.733259	2.335235	-1.142312
22	1	0	-1.628106	2.602750	-1.715020
23	1	0	-0.062810	3.207503	-1.146161
24	1	0	-0.216623	1.524936	-1.677227
25	8	0	-4.593044	2.451730	0.963048
26	7	0	-0.260099	1.088205	0.941820
27	6	0	-3.184063	1.282831	3.256254
28	1	0	-4.010753	0.623307	2.959776
29	1	0	-2.756430	0.897362	4.184822

30	1	0	-3.638575	2.265550	3.429435
31	79	0	1.528401	0.325734	0.187356
32	6	0	4.784268	-1.859558	-1.402248
33	6	0	5.459406	-0.793525	-0.912381
34	1	0	5.120092	-2.763666	-1.892625
35	1	0	6.515157	-0.558801	-0.879515
36	7	0	4.508685	0.069008	-0.386707
37	7	0	3.439216	-1.622242	-1.165006
38	6	0	3.262112	-0.438338	-0.532563
39	7	0	-2.737793	-0.992639	0.082106
40	16	0	-3.466852	-0.742016	-1.420987
41	8	0	-4.488637	-1.730744	-1.651919
42	8	0	-3.694379	0.681247	-1.501846
43	16	0	-2.183604	-2.466043	0.650698
44	8	0	-2.345587	-3.436870	-0.409019
45	8	0	-0.930032	-2.276116	1.347754
46	6	0	-3.453387	-2.830918	1.941838
47	6	0	-2.062910	-1.104112	-2.616820
48	9	0	-2.119437	-0.195369	-3.572225
49	9	0	-2.213316	-2.302367	-3.133334
50	9	0	-0.896402	-1.016297	-2.000502
51	9	0	-3.150294	-4.001835	2.472705
52	9	0	-3.416904	-1.891203	2.860369
53	9	0	-4.641048	-2.881669	1.378797
54	6	0	4.808912	1.328913	0.233638
55	6	0	4.890535	1.387146	1.627447
56	6	0	4.993932	2.442574	-0.591950
57	6	0	5.204959	2.619915	2.199769
58	6	0	5.305674	3.653725	0.023001
59	6	0	5.414924	3.740480	1.406278
60	1	0	5.276265	2.695044	3.284370
61	1	0	5.455286	4.538200	-0.595501
62	1	0	5.659383	4.694149	1.870751
63	6	0	2.372029	-2.503168	-1.554866
64	6	0	1.771375	-3.306656	-0.581591
65	6	0	1.966691	-2.487607	-2.893963
66	6	0	0.727390	-4.134815	-0.993517
67	6	0	0.928603	-3.341161	-3.261175
68	6	0	0.310519	-4.153571	-2.317483
69	1	0	0.220897	-4.753753	-0.254030
70	1	0	0.583325	-3.342289	-4.295145
71	1	0	-0.523479	-4.789826	-2.607919
72	6	0	4.591612	0.190736	2.477606
73	1	0	3.502015	0.043995	2.549230
74	1	0	5.016486	-0.735206	2.065857
75	1	0	4.978301	0.324353	3.494373
76	6	0	4.819358	2.342155	-2.077126
77	1	0	5.480915	1.589614	-2.527792
78	1	0	3.788788	2.053554	-2.331463
79	1	0	5.026688	3.303219	-2.560444
80	6	0	2.174085	-3.233992	0.858397
81	1	0	1.828898	-4.118748	1.406188
82	1	0	3.262020	-3.144875	0.988906
83	1	0	1.708687	-2.354641	1.330446
84	6	0	2.585090	-1.542787	-3.880143
85	1	0	2.481658	-0.500141	-3.543293
86	1	0	3.658965	-1.724576	-4.025741
87	1	0	2.098967	-1.628527	-4.858284
88	6	0	1.397944	-1.471975	3.879004
89	1	0	2.440098	-1.673356	3.609726
90	1	0	1.336536	-1.097632	4.906794
91	1	0	0.803509	-2.391062	3.805079

Zero-point correction= 0.676969 (Hartree/Particle)
Thermal correction to Energy= 0.732439
Thermal correction to Enthalpy= 0.733383
Thermal correction to Gibbs Free Energy= 0.584131
Sum of electronic and zero-point Energies= -3666.942301
Sum of electronic and thermal Energies= -3666.886830
Sum of electronic and thermal Enthalpies= -3666.885886
Sum of electronic and thermal Free Energies= -3667.035138
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3668.78479926

INT19a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.680557	0.716254	0.965646
2	6	0	-4.101350	0.690470	-1.837860
3	6	0	-1.118344	0.636472	2.312277
4	8	0	0.228895	0.610381	2.270746
5	6	0	-5.351318	1.435584	-1.528351
6	6	0	-6.534018	1.042119	-2.161877
7	6	0	-5.358611	2.550164	-0.684841
8	6	0	-7.714155	1.732951	-1.929386
9	1	0	-6.498657	0.188410	-2.836276
10	6	0	-6.537841	3.252728	-0.466373
11	1	0	-4.431178	2.880430	-0.216999
12	6	0	-7.716393	2.838843	-1.080632
13	1	0	-8.636056	1.416050	-2.414045
14	1	0	-6.536400	4.127313	0.181547
15	1	0	-8.641528	3.384969	-0.902737
16	8	0	-1.766610	0.583803	3.335096
17	6	0	-2.965058	0.771534	-0.890861
18	6	0	-1.660352	0.929664	-1.296918
19	6	0	-2.982154	0.635313	0.546850
20	6	0	-1.064145	1.253228	-2.615997
21	1	0	-0.621654	2.260172	-2.597620
22	1	0	-0.254206	0.556811	-2.869530
23	1	0	-1.822420	1.203999	-3.401646
24	8	0	-4.003105	0.039401	-2.869318
25	7	0	-0.837695	0.846949	-0.170783
26	6	0	-4.170454	0.390588	1.412115
27	1	0	-4.943581	-0.174129	0.876381
28	1	0	-3.880407	-0.153598	2.316579
29	1	0	-4.626466	1.335065	1.738914
30	79	0	0.119117	-1.183087	-0.252146
31	1	0	-0.017099	1.493286	-0.112112
32	7	0	1.500701	2.491137	0.008882
33	16	0	2.723640	1.460995	-0.145415
34	8	0	3.334604	0.992724	1.092569
35	8	0	2.295422	0.478753	-1.144239
36	16	0	1.303883	3.563344	1.216455
37	8	0	-0.066034	3.458333	1.703919
38	8	0	2.406051	3.673235	2.157092
39	6	0	1.310864	5.119870	0.231198
40	6	0	4.056425	2.409140	-0.999680
41	9	0	3.590182	2.942518	-2.116170
42	9	0	5.046616	1.575844	-1.295751
43	9	0	4.516506	3.364502	-0.212367
44	9	0	1.130132	6.141208	1.053398
45	9	0	0.331028	5.098778	-0.659999
46	9	0	2.467002	5.263291	-0.397323
47	6	0	0.899580	0.783394	3.518980
48	1	0	0.565469	1.713950	3.990471
49	1	0	0.693687	-0.061014	4.187999
50	1	0	1.962080	0.845014	3.269629
51	6	0	0.660321	-3.105475	0.003255
52	7	0	1.847192	-3.710813	-0.198431
53	6	0	0.547509	-5.237088	0.711846
54	6	0	1.798239	-5.027184	0.232990
55	1	0	0.076666	-6.110285	1.143742
56	1	0	2.660893	-5.675894	0.157533
57	7	0	-0.138518	-4.042590	0.561887
58	6	0	-1.482806	-3.771474	0.994778
59	6	0	-2.530404	-4.023465	0.104804
60	6	0	-1.666536	-3.201001	2.259181
61	6	0	-3.820523	-3.707613	0.529461
62	6	0	-2.973843	-2.903505	2.642459
63	6	0	-4.039749	-3.158932	1.787630
64	1	0	-4.657651	-3.890770	-0.143375
65	1	0	-3.146907	-2.449940	3.618117
66	1	0	-5.053444	-2.915220	2.102279
67	6	0	3.016120	-3.038550	-0.701075
68	6	0	3.776057	-2.284635	0.196767
69	6	0	3.303558	-3.140272	-2.064821
70	6	0	4.891196	-1.622344	-0.315818
71	6	0	4.429247	-2.464733	-2.530408
72	6	0	5.213723	-1.712239	-1.663418

73	1	0	5.489068	-1.006034	0.354318
74	1	0	4.679501	-2.520025	-3.589466
75	1	0	6.079797	-1.175021	-2.046153
76	6	0	3.382071	-2.145395	1.635578
77	1	0	3.069921	-3.101327	2.079726
78	1	0	4.209908	-1.740089	2.227283
79	1	0	2.545852	-1.435816	1.738177
80	6	0	2.416347	-3.920558	-2.987491
81	1	0	2.368503	-4.985535	-2.719071
82	1	0	1.384316	-3.540089	-2.965821
83	1	0	2.774702	-3.854172	-4.020632
84	6	0	-2.268390	-4.575522	-1.263356
85	1	0	-3.206129	-4.733209	-1.806896
86	1	0	-1.650924	-3.885885	-1.857564
87	1	0	-1.733140	-5.534462	-1.227960
88	6	0	-0.504458	-2.870531	3.145690
89	1	0	0.188723	-3.715462	3.260308
90	1	0	0.078326	-2.033068	2.728620
91	1	0	-0.847700	-2.567842	4.141204

Zero-point correction= 0.676866 (Hartree/Particle)
Thermal correction to Energy= 0.732566
Thermal correction to Enthalpy= 0.733510
Thermal correction to Gibbs Free Energy= 0.583300
Sum of electronic and zero-point Energies= -3666.952455
Sum of electronic and thermal Energies= -3666.896756
Sum of electronic and thermal Enthalpies= -3666.895812
Sum of electronic and thermal Free Energies= -3667.046022
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3668.80002576

INT20a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.439168	0.010118	-0.729315
2	6	0	-2.300715	0.021025	0.535342
3	79	0	0.667919	-0.024035	-0.202252
4	6	0	-1.539051	-1.272081	-1.517338
5	8	0	-0.830822	-1.176117	-2.660028
6	6	0	-2.407983	-1.268796	1.338741
7	6	0	-3.556098	-2.055642	1.371403
8	6	0	-1.304710	-1.643756	2.107609
9	6	0	-3.594518	-3.210015	2.143773
10	1	0	-4.424317	-1.800467	0.765110
11	6	0	-1.338650	-2.805061	2.869127
12	1	0	-0.418202	-1.009296	2.118012
13	6	0	-2.484999	-3.592441	2.889624
14	1	0	-4.495844	-3.819616	2.153117
15	1	0	-0.466371	-3.085971	3.458050
16	1	0	-2.516414	-4.499512	3.490041
17	8	0	-2.106841	-2.293996	-1.196374
18	6	0	-1.136756	2.797071	0.089911
19	6	0	-1.263573	2.146663	1.259389
20	6	0	-1.515065	2.341755	-1.240641
21	7	0	-1.647613	1.122156	-1.620117
22	8	0	-1.929885	0.975567	1.498599
23	1	0	-0.635554	3.765983	0.147535
24	6	0	-0.691936	-2.395092	-3.375894
25	1	0	-0.162493	-2.143386	-4.297590
26	1	0	-0.108818	-3.114064	-2.784899
27	1	0	-1.667362	-2.837825	-3.603317
28	6	0	2.702839	0.034853	0.056356
29	7	0	3.477711	1.136692	0.163437
30	6	0	4.872408	-0.564080	0.156802
31	6	0	4.819956	0.788115	0.227034
32	1	0	5.706304	-1.253645	0.169721
33	1	0	5.598326	1.534929	0.313378
34	7	0	3.561688	-1.006157	0.052782
35	6	0	3.127750	-2.371340	-0.065783
36	6	0	3.033088	-2.928085	-1.345257
37	6	0	2.758019	-3.052439	1.097401
38	6	0	2.568260	-4.239602	-1.439000
39	6	0	2.298075	-4.360850	0.954784
40	6	0	2.206204	-4.950016	-0.300333

41	1	0	2.490063	-4.703142	-2.422268
42	1	0	2.005391	-4.918904	1.843624
43	1	0	1.844941	-5.972335	-0.392951
44	6	0	2.958767	2.475893	0.194583
45	6	0	2.814982	3.096288	1.440357
46	6	0	2.598569	3.088122	-1.010743
47	6	0	2.324963	4.402087	1.459075
48	6	0	2.114229	4.395904	-0.943390
49	6	0	1.985403	5.050353	0.276121
50	1	0	2.218092	4.912479	2.416484
51	1	0	1.848907	4.906865	-1.869079
52	1	0	1.621348	6.075968	0.304753
53	6	0	3.152204	2.371703	2.708324
54	1	0	4.228808	2.171739	2.799444
55	1	0	2.851042	2.957291	3.584414
56	1	0	2.644522	1.396228	2.759022
57	6	0	2.681370	2.368288	-2.322443
58	1	0	3.577363	1.738190	-2.400255
59	1	0	1.808371	1.708319	-2.458544
60	1	0	2.690850	3.077999	-3.157387
61	6	0	3.384539	-2.134935	-2.567478
62	1	0	4.425493	-1.783229	-2.550249
63	1	0	3.251797	-2.736937	-3.473206
64	1	0	2.746795	-1.242769	-2.662619
65	6	0	2.807252	-2.388859	2.440533
66	1	0	3.754674	-1.860932	2.614466
67	1	0	2.003612	-1.641164	2.540963
68	1	0	2.679417	-3.124433	3.242790
69	7	0	-3.725529	0.450245	0.139126
70	6	0	-4.723286	1.061415	0.770017
71	6	0	-5.844687	1.012782	-0.077128
72	6	0	-5.441430	0.333894	-1.194008
73	1	0	-6.822169	1.431303	0.124055
74	8	0	-4.156713	-0.019588	-1.061129
75	6	0	-1.661011	3.420619	-2.273684
76	1	0	-1.933711	2.984264	-3.238871
77	1	0	-2.412052	4.168455	-1.983710
78	1	0	-0.707416	3.960177	-2.386154
79	6	0	-0.754677	2.668153	2.558946
80	1	0	-0.050814	1.945058	2.996136
81	1	0	-0.241246	3.625810	2.427121
82	1	0	-1.569779	2.792677	3.285813
83	6	0	-6.097699	-0.059737	-2.453431
84	1	0	-6.033340	-1.144655	-2.598332
85	1	0	-7.149397	0.237867	-2.442492
86	1	0	-5.600850	0.417610	-3.306916
87	6	0	-4.620188	1.660304	2.121320
88	1	0	-4.165779	0.958236	2.829027
89	1	0	-3.989107	2.557252	2.091718
90	1	0	-5.616432	1.943417	2.472573

Zero-point correction= 0.737442 (Hartree/Particle)
Thermal correction to Energy= 0.783486
Thermal correction to Enthalpy= 0.784430
Thermal correction to Gibbs Free Energy= 0.660307
Sum of electronic and zero-point Energies= -2164.366128
Sum of electronic and thermal Energies= -2164.320084
Sum of electronic and thermal Enthalpies= -2164.319140
Sum of electronic and thermal Free Energies= -2164.443263
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2166.04581428

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.548321	-1.220936	-0.231969
2	6	0	2.458681	-0.352150	-0.022282
3	79	0	-0.305679	-0.199637	-0.116665

4	6	0	1.585989	-2.676730	-0.491815
5	8	0	0.547782	-3.286563	0.084685
6	6	0	2.942295	0.994985	0.058272
7	6	0	2.679276	1.861701	-1.015255
8	6	0	3.645458	1.459833	1.178692
9	6	0	3.115103	3.177931	-0.960354
10	1	0	2.129159	1.489581	-1.878863
11	6	0	4.075436	2.776973	1.222751
12	1	0	3.858512	0.773379	1.995540
13	6	0	3.814748	3.633733	0.153812
14	1	0	2.913082	3.848136	-1.793382
15	1	0	4.624048	3.137875	2.090086
16	1	0	4.162870	4.664780	0.189979
17	8	0	2.427328	-3.228177	-1.158568
18	6	0	5.917983	-2.709649	-0.582736
19	6	0	5.253708	-3.331930	0.426581
20	6	0	5.252541	-1.470637	-0.687397
21	7	0	4.294151	-1.374305	0.204463
22	8	0	4.280821	-2.549911	0.905814
23	1	0	6.748653	-3.077505	-1.167509
24	6	0	0.488386	-4.700793	-0.112667
25	1	0	-0.404624	-5.035084	0.416860
26	1	0	0.415070	-4.932084	-1.180330
27	1	0	1.382585	-5.182079	0.296720
28	6	0	-2.136694	0.689840	0.080684
29	7	0	-3.326260	0.066461	0.212632
30	6	0	-3.766747	2.215352	0.358132
31	6	0	-4.345210	0.990070	0.385404
32	1	0	-4.180552	3.210491	0.455871
33	1	0	-5.374823	0.680861	0.510059
34	7	0	-2.408415	2.009381	0.169417
35	6	0	-1.417779	3.046602	0.073540
36	6	0	-1.242547	3.674945	-1.164015
37	6	0	-0.674200	3.369484	1.213273
38	6	0	-0.291344	4.691811	-1.236360
39	6	0	0.268922	4.389709	1.091823
40	6	0	0.452497	5.048858	-0.117477
41	1	0	-0.140093	5.208281	-2.183911
42	1	0	0.861423	4.668227	1.962916
43	1	0	1.185513	5.851404	-0.189178
44	6	0	-3.487659	-1.362420	0.174752
45	6	0	-3.391933	-2.071444	1.376062
46	6	0	-3.705181	-1.970131	-1.065480
47	6	0	-3.537434	-3.456822	1.312124
48	6	0	-3.845140	-3.357432	-1.080309
49	6	0	-3.764978	-4.092617	0.096782
50	1	0	-3.477066	-4.037599	2.231911
51	1	0	-4.023794	-3.860973	-2.029644
52	1	0	-3.887127	-5.173998	0.067130
53	6	0	-3.126818	-1.370124	2.673814
54	1	0	-3.855789	-0.571654	2.869164
55	1	0	-3.168227	-2.072375	3.513216
56	1	0	-2.131388	-0.901444	2.679620
57	6	0	-3.760952	-1.165478	-2.328879
58	1	0	-4.462132	-0.323108	-2.255496
59	1	0	-2.776223	-0.740579	-2.574536
60	1	0	-4.072618	-1.787459	-3.174762
61	6	0	-2.041414	3.262580	-2.363478
62	1	0	-3.111674	3.479963	-2.242058
63	1	0	-1.699479	3.789487	-3.260689
64	1	0	-1.956335	2.182367	-2.552212
65	6	0	-0.867062	2.641473	2.509192
66	1	0	-1.928284	2.480814	2.742915
67	1	0	-0.392554	1.648346	2.481035
68	1	0	-0.418647	3.197319	3.339855
69	1	0	5.359895	-4.294302	0.910446
70	1	0	5.427984	-0.642798	-1.366569

Zero-point correction= 0.558103 (Hartree/Particle)
Thermal correction to Energy= 0.596691
Thermal correction to Enthalpy= 0.597635
Thermal correction to Gibbs Free Energy= 0.480673
Sum of electronic and zero-point Energies= -1761.434896
Sum of electronic and thermal Energies= -1761.396308
Sum of electronic and thermal Enthalpies= -1761.395364

Sum of electronic and thermal Free Energies= -1761.512326
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.81953393

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.699916	-0.138239	-0.065055
2	6	0	1.699632	-0.964444	-0.217406
3	6	0	5.547619	-2.372634	0.644608
4	6	0	5.857093	-2.113699	-0.723946
5	8	0	4.181491	-0.885256	-0.015036
6	6	0	4.953423	-1.192759	-1.101699
7	7	0	4.547878	-1.675530	1.103083
8	1	0	6.628820	-2.571396	-1.326413
9	79	0	-0.236638	-0.185630	-0.103389
10	6	0	-2.194664	0.413333	0.059712
11	7	0	-3.245383	-0.427731	0.182524
12	6	0	-4.105102	1.593135	0.228706
13	6	0	-4.432217	0.279573	0.288350
14	1	0	-4.709289	2.489955	0.272211
15	1	0	-5.385611	-0.221302	0.395642
16	7	0	-2.726603	1.653554	0.086555
17	6	0	-1.962504	2.866604	-0.005703
18	6	0	-1.782260	3.439798	-1.268342
19	6	0	-1.439305	3.412180	1.170595
20	6	0	-1.067745	4.635822	-1.331070
21	6	0	-0.727581	4.606466	1.059098
22	6	0	-0.553895	5.217484	-0.176946
23	1	0	-0.924194	5.115389	-2.299145
24	1	0	-0.312186	5.059892	1.958367
25	1	0	-0.009408	6.158495	-0.242288
26	6	0	-3.108832	-1.859278	0.194046
27	6	0	-2.883134	-2.493537	1.419243
28	6	0	-3.161729	-2.537806	-1.027794
29	6	0	-2.717053	-3.878304	1.399410
30	6	0	-2.987327	-3.921005	-0.998707
31	6	0	-2.771319	-4.585055	0.203528
32	1	0	-2.549611	-4.402339	2.340026
33	1	0	-3.029553	-4.478910	-1.933512
34	1	0	-2.649232	-5.667118	0.208483
35	6	0	-2.802920	-1.715423	2.697556
36	1	0	-3.688828	-1.085198	2.855416
37	1	0	-2.715468	-2.388038	3.557489
38	1	0	-1.928974	-1.046939	2.707151
39	6	0	-3.383982	-1.805747	-2.316734
40	1	0	-4.331272	-1.249003	-2.317504
41	1	0	-2.585370	-1.074322	-2.510173
42	1	0	-3.408829	-2.502779	-3.161175
43	6	0	-2.321981	2.782942	-2.502688
44	1	0	-3.411555	2.648424	-2.459756
45	1	0	-2.095202	3.378417	-3.393539
46	1	0	-1.885575	1.782909	-2.645984
47	6	0	-1.617531	2.727447	2.491392
48	1	0	-2.658498	2.422073	2.664733
49	1	0	-1.004289	1.815536	2.547877
50	1	0	-1.315688	3.381672	3.316278
51	6	0	2.985686	1.279097	0.062847
52	6	0	2.277909	2.182056	-0.744420
53	6	0	3.911669	1.763652	0.996377
54	6	0	2.485485	3.547048	-0.605143
55	1	0	1.567098	1.802151	-1.478713
56	6	0	4.115203	3.130170	1.124472
57	1	0	4.457182	1.068936	1.633029
58	6	0	3.401900	4.023294	0.328276
59	1	0	1.927043	4.239407	-1.231908
60	1	0	4.830884	3.501827	1.854773
61	1	0	3.566015	5.094155	0.432547
62	6	0	1.840215	-2.420442	-0.456845
63	8	0	2.650478	-2.918982	-1.208623
64	8	0	0.933838	-3.111995	0.234933
65	6	0	0.986456	-4.529158	0.063518
66	1	0	1.988070	-4.907968	0.290745
67	1	0	0.251402	-4.936398	0.759150

68	1	0	0.727012	-4.793583	-0.967226
69	1	0	6.038980	-3.060867	1.324707
70	1	0	4.706048	-0.665883	-2.014320

Zero-point correction= 0.560237 (Hartree/Particle)
Thermal correction to Energy= 0.597425
Thermal correction to Enthalpy= 0.598369
Thermal correction to Gibbs Free Energy= 0.487808
Sum of electronic and zero-point Energies= -1761.403976
Sum of electronic and thermal Energies= -1761.366788
Sum of electronic and thermal Enthalpies= -1761.365843
Sum of electronic and thermal Free Energies= -1761.476404
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.79114235

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.904982	0.061230	-0.135962
2	6	0	2.191851	-1.183144	-0.102193
3	6	0	2.559899	1.354968	-0.186968
4	6	0	3.826048	1.476291	-0.782557
5	6	0	1.932957	2.503357	0.317489
6	6	0	4.451330	2.711788	-0.853907
7	1	0	4.303099	0.594079	-1.206771
8	6	0	2.575238	3.732724	0.265817
9	1	0	0.937665	2.428228	0.759165
10	6	0	3.832441	3.840943	-0.320831
11	1	0	5.425957	2.797056	-1.330542
12	1	0	2.081050	4.612566	0.673944
13	1	0	4.327941	4.808455	-0.373979
14	79	0	-0.258564	0.004604	-0.068523
15	6	0	1.737520	-2.564044	-0.286154
16	8	0	2.709766	-3.418448	-0.589561
17	6	0	6.481314	-1.379967	0.386955
18	6	0	5.346917	-1.923745	-0.254882
19	6	0	5.942748	-0.582385	1.347525
20	1	0	7.524723	-1.562497	0.172489
21	8	0	0.565520	-2.858273	-0.204290
22	7	0	4.240890	-1.473650	0.289806
23	8	0	4.607545	-0.627204	1.300853
24	6	0	2.269893	-4.765752	-0.801901
25	1	0	1.573735	-4.809356	-1.645298
26	1	0	3.172475	-5.339274	-1.016488
27	1	0	1.772835	-5.147900	0.094894
28	6	0	-2.280641	0.285754	0.011212
29	7	0	-2.909484	1.481565	0.008145
30	6	0	-4.505981	-0.025843	0.082012
31	6	0	-4.284188	1.310553	0.050710
32	1	0	-5.419166	-0.605461	0.119139
33	1	0	-4.960564	2.155349	0.055900
34	7	0	-3.262529	-0.637980	0.057624
35	6	0	-3.048848	-2.059945	0.117440
36	6	0	-3.002643	-2.660137	1.379419
37	6	0	-2.904927	-2.765966	-1.079161
38	6	0	-2.823361	-4.041465	1.422881
39	6	0	-2.726648	-4.145968	-0.985963
40	6	0	-2.691135	-4.777428	0.251019
41	1	0	-2.789069	-4.540453	2.390630
42	1	0	-2.618905	-4.727121	-1.901195
43	1	0	-2.560073	-5.856724	0.303238
44	6	0	-2.227479	2.746770	-0.000384
45	6	0	-1.965081	3.351414	-1.233896
46	6	0	-1.844936	3.299160	1.226334
47	6	0	-1.294477	4.573974	-1.216573
48	6	0	-1.179935	4.525834	1.194732
49	6	0	-0.911008	5.157683	-0.014464
50	1	0	-1.077803	5.071909	-2.160740
51	1	0	-0.879217	4.988576	2.134468
52	1	0	-0.400061	6.119171	-0.020290
53	6	0	-2.381822	2.702893	-2.519019
54	1	0	-3.470815	2.568239	-2.576560
55	1	0	-2.075989	3.307625	-3.379234
56	1	0	-1.931818	1.705598	-2.631576

57	6	0	-2.107720	2.588097	2.519742
58	1	0	-3.139211	2.217395	2.590677
59	1	0	-1.448489	1.713751	2.633861
60	1	0	-1.928647	3.250247	3.373742
61	6	0	-3.123302	-1.844786	2.631481
62	1	0	-4.067571	-1.284173	2.674571
63	1	0	-3.076123	-2.483746	3.519725
64	1	0	-2.310940	-1.106661	2.706939
65	6	0	-2.914874	-2.067336	-2.404912
66	1	0	-3.752833	-1.363365	-2.500476
67	1	0	-1.991435	-1.487181	-2.553614
68	1	0	-2.987367	-2.788424	-3.226347
69	1	0	5.281940	-2.621141	-1.081760
70	1	0	6.361693	0.050216	2.119514

Zero-point correction= 0.557743 (Hartree/Particle)
Thermal correction to Energy= 0.596253
Thermal correction to Enthalpy= 0.597197
Thermal correction to Gibbs Free Energy= 0.481891
Sum of electronic and zero-point Energies= -1761.428575
Sum of electronic and thermal Energies= -1761.390065
Sum of electronic and thermal Enthalpies= -1761.389121
Sum of electronic and thermal Free Energies= -1761.504427
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.80847411

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.938084	-0.066551	-0.099622
2	6	0	2.464528	-1.248461	0.149923
3	6	0	2.654430	1.175095	-0.405862
4	6	0	3.762760	1.186947	-1.268939
5	6	0	2.208013	2.390912	0.136176
6	6	0	4.413963	2.377506	-1.560586
7	1	0	4.090037	0.262629	-1.742073
8	6	0	2.891507	3.570528	-0.126281
9	1	0	1.321570	2.410254	0.774498
10	6	0	3.992410	3.569323	-0.977304
11	1	0	5.258667	2.374246	-2.246754
12	1	0	2.544975	4.500539	0.320825
13	1	0	4.513349	4.498944	-1.198344
14	79	0	-0.165183	0.040164	-0.040903
15	6	0	2.069073	-2.632252	0.468013
16	8	0	0.761976	-2.806477	0.304412
17	6	0	5.934980	-2.109978	1.138387
18	6	0	5.860248	-2.424182	-0.255302
19	6	0	4.794758	-1.450895	1.393712
20	8	0	2.843333	-3.484586	0.840684
21	7	0	4.782183	-1.995132	-0.837439
22	8	0	4.102417	-1.315487	0.214822
23	1	0	6.727889	-2.358047	1.829828
24	6	0	0.276206	-4.114840	0.625588
25	1	0	0.723069	-4.856194	-0.044194
26	1	0	0.524691	-4.368281	1.661144
27	1	0	-0.805305	-4.063738	0.483101
28	6	0	-2.187858	0.431975	-0.010382
29	7	0	-3.258802	-0.380668	-0.148362
30	6	0	-4.089717	1.641152	0.099014
31	6	0	-4.439242	0.346111	-0.085105
32	1	0	-4.681486	2.541362	0.201720
33	1	0	-5.404136	-0.134327	-0.182695
34	7	0	-2.705392	1.672717	0.141381
35	6	0	-1.912796	2.854327	0.345810
36	6	0	-1.555049	3.616664	-0.770961
37	6	0	-1.529837	3.174896	1.652314
38	6	0	-0.789064	4.760084	-0.545559
39	6	0	-0.759890	4.325144	1.828992
40	6	0	-0.399645	5.113255	0.741504
41	1	0	-0.498972	5.377224	-1.395053
42	1	0	-0.455088	4.607218	2.836205
43	1	0	0.186391	6.017219	0.900161
44	6	0	-3.210447	-1.805468	-0.329501
45	6	0	-3.428347	-2.618554	0.787891

46	6	0	-2.995695	-2.308069	-1.616956
47	6	0	-3.459200	-3.998090	0.579688
48	6	0	-3.023964	-3.694128	-1.774708
49	6	0	-3.266172	-4.530214	-0.690849
50	1	0	-3.641688	-4.656709	1.428400
51	1	0	-2.870985	-4.115987	-2.767338
52	1	0	-3.303140	-5.608222	-0.837024
53	6	0	-3.621563	-2.029794	2.152885
54	1	0	-4.592473	-1.523946	2.250826
55	1	0	-3.581124	-2.808928	2.921723
56	1	0	-2.848148	-1.283183	2.383793
57	6	0	-2.750206	-1.397658	-2.781632
58	1	0	-3.484683	-0.581874	-2.829658
59	1	0	-1.756640	-0.929282	-2.722759
60	1	0	-2.799442	-1.950993	-3.725579
61	6	0	-1.963609	3.208378	-2.153437
62	1	0	-3.055043	3.140967	-2.260401
63	1	0	-1.599856	3.926696	-2.895685
64	1	0	-1.555762	2.220880	-2.414890
65	6	0	-1.909558	2.306315	2.813306
66	1	0	-2.975638	2.041805	2.802772
67	1	0	-1.346557	1.360277	2.804384
68	1	0	-1.697224	2.808949	3.763165
69	1	0	4.326125	-1.002318	2.260204
70	1	0	6.583785	-2.962995	-0.858653

Zero-point correction= 0.559629 (Hartree/Particle)
Thermal correction to Energy= 0.596851
Thermal correction to Enthalpy= 0.597795
Thermal correction to Gibbs Free Energy= 0.487726
Sum of electronic and zero-point Energies= -1761.400768
Sum of electronic and thermal Energies= -1761.363546
Sum of electronic and thermal Enthalpies= -1761.362602
Sum of electronic and thermal Free Energies= -1761.472671
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.78509297

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.365534	-1.407028	-0.234643
2	6	0	2.657063	-0.929384	-0.420506
3	79	0	-0.336466	-0.278563	-0.114071
4	6	0	1.195635	-2.871583	-0.120291
5	8	0	1.051644	-3.276828	1.136105
6	6	0	3.019927	0.493095	-0.621713
7	6	0	2.282599	1.296484	-1.497985
8	6	0	4.132102	1.031862	0.030422
9	6	0	2.658715	2.614904	-1.718950
10	1	0	1.433370	0.872504	-2.034962
11	6	0	4.495599	2.356865	-0.181807
12	1	0	4.697795	0.416283	0.730311
13	6	0	3.762708	3.148714	-1.060169
14	1	0	2.091207	3.224925	-2.420294
15	1	0	5.355520	2.771276	0.340710
16	1	0	4.053052	4.183666	-1.233831
17	8	0	1.148020	-3.571316	-1.105549
18	6	0	5.875524	-2.469078	-0.300598
19	6	0	5.453240	-2.602577	1.027681
20	6	0	4.797066	-1.998118	-1.016171
21	7	0	3.649210	-1.844971	-0.368303
22	8	0	4.283622	-2.206361	1.299790
23	1	0	6.835090	-2.756856	-0.707238
24	6	0	0.792351	-4.676516	1.300151
25	1	0	0.723380	-4.840012	2.376112
26	1	0	-0.147341	-4.945540	0.806881
27	1	0	1.606117	-5.269024	0.870645
28	6	0	-2.045113	0.860766	0.132774
29	7	0	-3.330087	0.447007	0.081166
30	6	0	-3.424683	2.593237	0.542826
31	6	0	-4.195654	1.498528	0.330526
32	1	0	-3.677128	3.619720	0.774782
33	1	0	-5.269138	1.360561	0.331889
34	7	0	-2.108437	2.180887	0.414689

35	6	0	-0.963410	3.031942	0.592292
36	6	0	-0.570670	3.842749	-0.477694
37	6	0	-0.305474	3.014643	1.826008
38	6	0	0.514725	4.691926	-0.271824
39	6	0	0.789996	3.865795	1.977123
40	6	0	1.188874	4.703471	0.943746
41	1	0	0.837392	5.345102	-1.082976
42	1	0	1.321787	3.877329	2.927788
43	1	0	2.037659	5.370381	1.085251
44	6	0	-3.731401	-0.910159	-0.176033
45	6	0	-3.893086	-1.766379	0.917526
46	6	0	-3.926974	-1.305763	-1.502418
47	6	0	-4.277658	-3.079252	0.647998
48	6	0	-4.311599	-2.627900	-1.723047
49	6	0	-4.485903	-3.505025	-0.659002
50	1	0	-4.417463	-3.770676	1.478226
51	1	0	-4.474701	-2.967786	-2.744964
52	1	0	-4.789838	-4.532287	-0.850733
53	6	0	-3.648914	-1.291303	2.318162
54	1	0	-4.286169	-0.435376	2.580779
55	1	0	-3.849710	-2.088631	3.041685
56	1	0	-2.607169	-0.966238	2.457563
57	6	0	-3.715058	-0.351710	-2.638994
58	1	0	-4.300314	0.570466	-2.519621
59	1	0	-2.659773	-0.051595	-2.720027
60	1	0	-4.003071	-0.809387	-3.591344
61	6	0	-1.267566	3.770805	-1.802788
62	1	0	-2.323500	4.067280	-1.739621
63	1	0	-0.784894	4.428553	-2.534397
64	1	0	-1.250529	2.746426	-2.205828
65	6	0	-0.744381	2.111369	2.939170
66	1	0	-1.837606	2.078207	3.042569
67	1	0	-0.407860	1.077134	2.769275
68	1	0	-0.324377	2.439739	3.896197
69	1	0	4.775655	-1.796772	-2.087856
70	1	0	6.037610	-3.069634	1.828344

Zero-point correction= 0.557673 (Hartree/Particle)
Thermal correction to Energy= 0.595785
Thermal correction to Enthalpy= 0.596730
Thermal correction to Gibbs Free Energy= 0.482825
Sum of electronic and zero-point Energies= -1761.435267
Sum of electronic and thermal Energies= -1761.397155
Sum of electronic and thermal Enthalpies= -1761.396211
Sum of electronic and thermal Free Energies= -1761.510115
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.82546217

TS6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.496448	-1.273896	-0.231363
2	6	0	2.670389	-0.681134	-0.704698
3	79	0	-0.310928	-0.331439	-0.054032
4	6	0	1.580230	-2.667191	0.242208
5	8	0	1.593272	-2.769125	1.563025
6	6	0	2.760714	0.713006	-1.200975
7	6	0	1.816706	1.205290	-2.107727
8	6	0	3.832826	1.522670	-0.817600
9	6	0	1.948348	2.488116	-2.625799
10	1	0	0.999410	0.564492	-2.442826
11	6	0	3.950187	2.811543	-1.324317
12	1	0	4.572211	1.137330	-0.117391
13	6	0	3.013573	3.293951	-2.233951
14	1	0	1.227700	2.850367	-3.357252
15	1	0	4.785304	3.437567	-1.015973
16	1	0	3.120363	4.295661	-2.647288
17	8	0	1.618219	-3.593874	-0.541047
18	6	0	5.169761	-3.154169	-0.018125
19	6	0	5.434407	-2.215408	0.988748
20	6	0	4.232248	-2.606972	-0.870848
21	7	0	3.821548	-1.370602	-0.651137
22	8	0	4.772805	-1.145168	0.988073
23	1	0	5.663534	-4.106056	-0.157279

24	6	0	1.648437	-4.107748	2.077489
25	1	0	1.669445	-4.005117	3.162643
26	1	0	0.766780	-4.671527	1.757813
27	1	0	2.550099	-4.614858	1.718152
28	6	0	-2.044932	0.741510	0.303987
29	7	0	-3.338649	0.394809	0.141176
30	6	0	-3.372986	2.447292	0.931410
31	6	0	-4.174091	1.433047	0.520463
32	1	0	-3.597861	3.436244	1.309126
33	1	0	-5.250845	1.344783	0.456305
34	7	0	-2.070113	2.001901	0.789993
35	6	0	-0.877633	2.750388	1.085244
36	6	0	-0.344876	3.559300	0.076677
37	6	0	-0.284316	2.591364	2.341135
38	6	0	0.843315	4.231069	0.357744
39	6	0	0.904339	3.282282	2.575922
40	6	0	1.464553	4.089620	1.593056
41	1	0	1.285536	4.867290	-0.407952
42	1	0	1.391098	3.181734	3.545320
43	1	0	2.393998	4.619526	1.793524
44	6	0	-3.778027	-0.870051	-0.383421
45	6	0	-4.115873	-1.880506	0.522210
46	6	0	-3.837816	-1.026026	-1.771595
47	6	0	-4.542470	-3.096794	-0.009102
48	6	0	-4.271905	-2.259503	-2.256437
49	6	0	-4.621790	-3.283483	-1.384431
50	1	0	-4.815877	-3.903913	0.669488
51	1	0	-4.335503	-2.412029	-3.333157
52	1	0	-4.961071	-4.238298	-1.781271
53	6	0	-4.013369	-1.663756	2.001979
54	1	0	-4.707290	-0.887969	2.354534
55	1	0	-4.245199	-2.584594	2.547715
56	1	0	-3.002871	-1.343186	2.295066
57	6	0	-3.432429	0.077841	-2.701996
58	1	0	-3.856600	1.047865	-2.408396
59	1	0	-2.338477	0.201157	-2.723408
60	1	0	-3.757950	-0.135801	-3.725832
61	6	0	-1.017757	3.678192	-1.257080
62	1	0	-2.053956	4.032765	-1.168718
63	1	0	-0.480841	4.381568	-1.903216
64	1	0	-1.056112	2.707256	-1.775037
65	6	0	-0.884031	1.695332	3.382737
66	1	0	-1.963086	1.861096	3.502872
67	1	0	-0.750873	0.634234	3.123468
68	1	0	-0.409079	1.857909	4.356314
69	1	0	3.823216	-3.100941	-1.753231
70	1	0	6.221137	-2.339333	1.744541

Zero-point correction= 0.557152 (Hartree/Particle)
Thermal correction to Energy= 0.595363
Thermal correction to Enthalpy= 0.596307
Thermal correction to Gibbs Free Energy= 0.481974
Sum of electronic and zero-point Energies= -1761.436347
Sum of electronic and thermal Energies= -1761.398136
Sum of electronic and thermal Enthalpies= -1761.397191
Sum of electronic and thermal Free Energies= -1761.511525
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.82172165

TS7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223979	-1.496722	1.036390
2	6	0	-2.296711	-1.746580	0.106051
3	79	0	0.273484	-0.220183	0.447927
4	6	0	-1.399484	-1.930946	2.437585
5	8	0	-1.046522	-3.159000	2.742858
6	6	0	-3.340190	-0.916528	-0.422881
7	6	0	-4.206441	-1.396083	-1.416380
8	6	0	-3.489505	0.378063	0.094202
9	6	0	-5.216951	-0.578544	-1.890426
10	1	0	-4.082279	-2.407147	-1.802403
11	6	0	-4.506166	1.188901	-0.387774
12	1	0	-2.813502	0.736538	0.873200

13	6	0	-5.365612	0.710882	-1.374440
14	1	0	-5.896562	-0.939893	-2.658630
15	1	0	-4.632244	2.192447	0.012382
16	1	0	-6.167209	1.347148	-1.744999
17	8	0	-1.830817	-1.079004	3.183877
18	6	0	-1.167826	-3.526841	-2.367419
19	6	0	-0.725049	-2.222526	-2.843619
20	6	0	-1.676522	-3.800354	-1.140721
21	7	0	-1.867573	-2.937195	-0.101620
22	8	0	-0.822804	-1.171311	-2.229319
23	1	0	-1.023345	-4.370931	-3.039055
24	1	0	-0.255945	-2.234702	-3.851554
25	1	0	-1.887179	-4.837908	-0.875658
26	6	0	-1.204041	-3.511188	4.128916
27	1	0	-0.613610	-2.836815	4.756220
28	1	0	-2.257942	-3.447186	4.415332
29	1	0	-0.841766	-4.535779	4.212126
30	6	0	1.620802	1.231721	-0.121462
31	7	0	1.342538	2.547727	-0.231279
32	6	0	3.446219	2.337378	-0.830558
33	6	0	2.455795	3.248163	-0.667775
34	1	0	4.473578	2.438173	-1.155629
35	1	0	2.427539	4.319149	-0.820335
36	7	0	2.912475	1.104913	-0.487870
37	6	0	3.609816	-0.150560	-0.558472
38	6	0	3.518553	-0.886116	-1.744577
39	6	0	4.331478	-0.574579	0.560955
40	6	0	4.200627	-2.101423	-1.793509
41	6	0	4.996456	-1.796429	0.465125
42	6	0	4.932848	-2.551017	-0.700563
43	1	0	4.157923	-2.696192	-2.705326
44	1	0	5.571171	-2.154447	1.318404
45	1	0	5.462627	-3.499915	-0.758753
46	6	0	0.047850	3.121418	0.019460
47	6	0	-0.205272	3.655983	1.287747
48	6	0	-0.893804	3.106644	-1.014471
49	6	0	-1.462656	4.217059	1.506231
50	6	0	-2.132915	3.693575	-0.752779
51	6	0	-2.413561	4.244824	0.491765
52	1	0	-1.689640	4.644035	2.482175
53	1	0	-2.880673	3.716943	-1.545601
54	1	0	-3.382476	4.707941	0.673803
55	6	0	0.830747	3.612382	2.369671
56	1	0	1.745312	4.151673	2.087182
57	1	0	0.450752	4.063412	3.292316
58	1	0	1.127664	2.578749	2.599658
59	6	0	-0.610384	2.457011	-2.335181
60	1	0	0.417614	2.635104	-2.678648
61	1	0	-0.745849	1.364799	-2.278511
62	1	0	-1.292612	2.832422	-3.106244
63	6	0	2.712414	-0.388872	-2.907082
64	1	0	3.022745	0.617335	-3.222269
65	1	0	2.825039	-1.054437	-3.770469
66	1	0	1.640298	-0.328161	-2.663223
67	6	0	4.377178	0.247315	1.813531
68	1	0	4.794014	1.248088	1.634790
69	1	0	3.372960	0.392285	2.237924
70	1	0	4.995139	-0.237928	2.576408

Zero-point correction= 0.556782 (Hartree/Particle)
Thermal correction to Energy= 0.595614
Thermal correction to Enthalpy= 0.596558
Thermal correction to Gibbs Free Energy= 0.481068
Sum of electronic and zero-point Energies= -1761.452129
Sum of electronic and thermal Energies= -1761.413297
Sum of electronic and thermal Enthalpies= -1761.412353
Sum of electronic and thermal Free Energies= -1761.527843
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83301344

TS8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.826743	2.018195	-0.102020

2	6	0	-2.296865	1.976782	0.091377
3	79	0	0.274915	0.311862	-0.046322
4	6	0	-0.274356	3.218880	-0.736941
5	8	0	0.410540	4.088164	-0.036509
6	6	0	-3.093484	1.050798	-0.713818
7	6	0	-2.654056	0.598593	-1.966066
8	6	0	-4.340869	0.642601	-0.220915
9	6	0	-3.462378	-0.242385	-2.719340
10	1	0	-1.703997	0.946851	-2.371509
11	6	0	-5.139469	-0.199658	-0.977659
12	1	0	-4.662667	0.996711	0.756173
13	6	0	-4.704262	-0.636887	-2.228056
14	1	0	-3.130859	-0.574350	-3.701302
15	1	0	-6.109442	-0.512806	-0.596554
16	1	0	-5.341240	-1.287111	-2.825764
17	8	0	-0.483433	3.225332	-1.935749
18	6	0	-1.064007	2.755763	2.622900
19	6	0	-0.984690	1.315056	2.918092
20	6	0	-2.028274	3.362242	1.865825
21	7	0	-2.846711	2.727971	0.988901
22	8	0	-1.702816	0.442344	2.470153
23	6	0	0.995462	5.165204	-0.799133
24	1	0	1.512029	5.788123	-0.069442
25	1	0	1.697971	4.760258	-1.533055
26	1	0	0.211626	5.731175	-1.310299
27	6	0	1.294904	-1.478692	0.067891
28	7	0	0.688847	-2.668617	0.268769
29	6	0	2.837932	-3.107582	0.159064
30	6	0	1.621208	-3.686081	0.329945
31	1	0	3.837195	-3.522866	0.136167
32	1	0	1.329219	-4.716301	0.487125
33	7	0	2.614523	-1.751194	-0.000511
34	6	0	3.638762	-0.761290	-0.201839
35	6	0	4.171466	-0.121874	0.921583
36	6	0	4.040884	-0.484824	-1.512153
37	6	0	5.167332	0.829204	0.700853
38	6	0	5.037644	0.475123	-1.683571
39	6	0	5.597122	1.122948	-0.588072
40	1	0	5.610303	1.339542	1.555305
41	1	0	5.377967	0.710160	-2.691274
42	1	0	6.380067	1.863325	-0.740638
43	6	0	-0.739228	-2.807679	0.393841
44	6	0	-1.484282	-3.006814	-0.773450
45	6	0	-1.307899	-2.680417	1.664288
46	6	0	-2.867570	-3.096327	-0.635798
47	6	0	-2.697277	-2.763871	1.748919
48	6	0	-3.467723	-2.972576	0.612451
49	1	0	-3.477876	-3.258419	-1.523764
50	1	0	-3.172402	-2.653649	2.722571
51	1	0	-4.551144	-3.037526	0.698582
52	6	0	-0.824552	-3.097877	-2.116548
53	1	0	-0.045682	-3.872276	-2.146661
54	1	0	-1.558176	-3.335165	-2.894843
55	1	0	-0.339682	-2.149382	-2.395090
56	6	0	-0.462524	-2.458959	2.880993
57	1	0	0.174735	-3.327975	3.098898
58	1	0	0.201855	-1.591260	2.760461
59	1	0	-1.090265	-2.271192	3.758226
60	6	0	3.676996	-0.429524	2.303148
61	1	0	3.647479	-1.508777	2.505814
62	1	0	4.317791	0.035602	3.059928
63	1	0	2.654601	-0.050642	2.455389
64	6	0	3.415999	-1.184659	-2.681242
65	1	0	3.532867	-2.275486	-2.620307
66	1	0	2.336150	-0.983717	-2.741339
67	1	0	3.868862	-0.854323	-3.621957
68	1	0	-0.449830	3.396358	3.255144
69	1	0	-0.189707	1.064886	3.659092
70	1	0	-2.228177	4.428800	2.003789

Zero-point correction= 0.557385 (Hartree/Particle)
Thermal correction to Energy= 0.595569
Thermal correction to Enthalpy= 0.596513
Thermal correction to Gibbs Free Energy= 0.484596
Sum of electronic and zero-point Energies= -1761.445460

Sum of electronic and thermal Energies= -1761.407276
Sum of electronic and thermal Enthalpies= -1761.406332
Sum of electronic and thermal Free Energies= -1761.518249
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83041226

TS9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.430539	-1.597374	1.096886
2	6	0	-1.228666	-2.438991	0.193360
3	79	0	0.075644	0.293811	0.524338
4	6	0	-0.221587	-2.122683	2.442310
5	8	0	0.882552	-2.723514	2.802597
6	6	0	-2.657656	-2.161433	-0.007954
7	6	0	-3.502075	-3.241747	-0.300218
8	6	0	-3.208430	-0.880815	0.140562
9	6	0	-4.863226	-3.043568	-0.468206
10	1	0	-3.088528	-4.246508	-0.369803
11	6	0	-4.571737	-0.688740	-0.033566
12	1	0	-2.574184	-0.022848	0.368458
13	6	0	-5.399999	-1.764599	-0.338186
14	1	0	-5.509990	-3.889676	-0.689721
15	1	0	-4.984450	0.312558	0.073791
16	1	0	-6.469674	-1.609455	-0.465101
17	8	0	-1.202482	-1.885686	3.122330
18	6	0	-0.837685	-3.456447	-2.727276
19	6	0	-0.813273	-2.034553	-3.016359
20	6	0	-0.734714	-4.029859	-1.496655
21	7	0	-0.537221	-3.395983	-0.310213
22	8	0	-0.786583	-1.118230	-2.203424
23	1	0	-0.869037	-4.124804	-3.585718
24	1	0	-0.662148	-5.119304	-1.432363
25	1	0	-0.802400	-1.798893	-4.104378
26	7	0	2.060710	-2.028312	0.166867
27	6	0	2.911899	-2.992560	0.421048
28	6	0	3.419703	-3.574511	-0.764330
29	1	0	3.126035	-3.244138	1.453074
30	6	0	2.787886	-2.871830	-1.739685
31	1	0	4.131979	-4.380814	-0.867893
32	1	0	2.808877	-2.906367	-2.822617
33	8	0	1.980440	-1.950415	-1.207184
34	6	0	0.915334	-3.145303	4.181527
35	1	0	0.094361	-3.839855	4.380715
36	1	0	1.878888	-3.637958	4.312132
37	1	0	0.831054	-2.275812	4.839612
38	6	0	0.602212	2.165090	-0.156090
39	7	0	1.838521	2.574744	-0.507777
40	6	0	0.513068	4.281783	-0.908409
41	6	0	1.805663	3.878318	-0.976301
42	1	0	0.033722	5.216064	-1.170146
43	1	0	2.702610	4.383157	-1.310683
44	7	0	-0.209649	3.212992	-0.402381
45	6	0	-1.634593	3.186169	-0.210395
46	6	0	-2.145122	3.608485	1.021902
47	6	0	-2.432923	2.720552	-1.260202
48	6	0	-3.528704	3.570196	1.187534
49	6	0	-3.813033	2.710061	-1.050649
50	6	0	-4.354722	3.132098	0.157975
51	1	0	-3.958244	3.896285	2.133840
52	1	0	-4.464725	2.364171	-1.852941
53	1	0	-5.434657	3.125227	0.298882
54	6	0	3.005519	1.736822	-0.439020
55	6	0	3.296100	0.918296	-1.534491
56	6	0	3.772714	1.764704	0.729691
57	6	0	4.431179	0.112890	-1.441471
58	6	0	4.890313	0.932996	0.780544
59	6	0	5.218418	0.117562	-0.296719
60	1	0	4.694001	-0.528585	-2.282868
61	1	0	5.510898	0.934789	1.675916
62	1	0	6.100375	-0.518548	-0.244431
63	6	0	2.407389	0.880838	-2.740744
64	1	0	2.217272	1.882956	-3.149086
65	1	0	2.862736	0.278791	-3.536220

66	1	0	1.428646	0.434108	-2.504422
67	6	0	3.397129	2.643272	1.884517
68	1	0	3.338973	3.701879	1.596481
69	1	0	2.413090	2.371122	2.293818
70	1	0	4.130130	2.559132	2.693956
71	6	0	-1.237887	4.064778	2.124172
72	1	0	-0.569055	4.874378	1.801837
73	1	0	-1.815954	4.429519	2.979817
74	1	0	-0.597126	3.244638	2.480125
75	6	0	-1.838889	2.216214	-2.540160
76	1	0	-1.017316	2.851607	-2.897524
77	1	0	-1.435775	1.197190	-2.420003
78	1	0	-2.598587	2.176957	-3.328877

Zero-point correction= 0.616987 (Hartree/Particle)
Thermal correction to Energy= 0.660415
Thermal correction to Enthalpy= 0.661359
Thermal correction to Gibbs Free Energy= 0.536940
Sum of electronic and zero-point Energies= -2007.280277
Sum of electronic and thermal Energies= -2007.236849
Sum of electronic and thermal Enthalpies= -2007.235905
Sum of electronic and thermal Free Energies= -2007.360324
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.78954867

TS10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.348047	-1.473226	0.484840
2	6	0	-2.430232	-1.268826	-0.428234
3	79	0	0.410242	-0.345993	0.209006
4	6	0	-1.719971	-1.634864	1.925060
5	8	0	-1.790583	-2.904996	2.302132
6	6	0	-3.754831	-0.723818	-0.440562
7	6	0	-4.779098	-1.350400	-1.162228
8	6	0	-3.984029	0.461810	0.269911
9	6	0	-6.046852	-0.794059	-1.155571
10	1	0	-4.569518	-2.271988	-1.705640
11	6	0	-5.256431	1.013450	0.262517
12	1	0	-3.162329	0.923049	0.820387
13	6	0	-6.280413	0.385687	-0.445286
14	1	0	-6.858039	-1.272580	-1.699263
15	1	0	-5.456994	1.928944	0.814689
16	1	0	-7.278738	0.819369	-0.442942
17	8	0	-1.893835	-0.673924	2.639661
18	6	0	-1.061063	-2.533033	-2.733251
19	6	0	-1.337609	-1.138495	-2.929165
20	6	0	-1.239093	-3.114365	-1.520974
21	7	0	-1.924208	-2.534775	-0.479598
22	8	0	-1.810148	-0.370624	-2.075327
23	1	0	-0.578565	-3.081160	-3.536286
24	6	0	-2.100528	-3.112734	3.685113
25	1	0	-1.339800	-2.644673	4.317784
26	1	0	-3.078865	-2.683723	3.922988
27	1	0	-2.109140	-4.193955	3.827392
28	6	0	1.898258	1.050418	-0.033663
29	7	0	1.621341	2.372702	-0.081486
30	6	0	3.795846	2.217278	-0.344190
31	6	0	2.778065	3.110122	-0.273140
32	1	0	4.860992	2.347299	-0.485074
33	1	0	2.761143	4.190373	-0.335274
34	7	0	3.233308	0.957755	-0.195127
35	6	0	3.962419	-0.280713	-0.219627
36	6	0	4.055841	-0.971468	-1.431199
37	6	0	4.532269	-0.735869	0.973125
38	6	0	4.777859	-2.164527	-1.432492
39	6	0	5.242680	-1.934723	0.924455
40	6	0	5.367678	-2.639710	-0.267008
41	1	0	4.878268	-2.722100	-2.363146
42	1	0	5.701630	-2.315069	1.836164
43	1	0	5.931392	-3.570387	-0.287206
44	6	0	0.285650	2.891723	0.049073
45	6	0	-0.208091	3.146566	1.331846
46	6	0	-0.476332	3.047503	-1.114715

47	6	0	-1.521765	3.608775	1.429801
48	6	0	-1.785822	3.500657	-0.967703
49	6	0	-2.300150	3.787258	0.292676
50	1	0	-1.931061	3.827510	2.415364
51	1	0	-2.404053	3.631503	-1.855055
52	1	0	-3.320036	4.156978	0.387846
53	6	0	0.614237	2.890008	2.558039
54	1	0	1.662021	3.193242	2.433871
55	1	0	0.205863	3.426311	3.421436
56	1	0	0.613965	1.818319	2.809296
57	6	0	0.088924	2.712467	-2.461589
58	1	0	0.971101	3.321107	-2.703992
59	1	0	0.405762	1.659347	-2.508866
60	1	0	-0.656001	2.876275	-3.248045
61	6	0	3.383881	-0.465435	-2.672523
62	1	0	3.558923	0.606767	-2.835999
63	1	0	3.741791	-1.003501	-3.557286
64	1	0	2.292288	-0.603901	-2.615839
65	6	0	4.368120	0.028486	2.251962
66	1	0	4.804261	1.035212	2.191231
67	1	0	3.306300	0.156512	2.509472
68	1	0	4.853447	-0.492909	3.083752
69	1	0	-1.054302	-0.693432	-3.898692
70	1	0	-0.845592	-4.104351	-1.294599

Zero-point correction= 0.558156 (Hartree/Particle)
Thermal correction to Energy= 0.596139
Thermal correction to Enthalpy= 0.597084
Thermal correction to Gibbs Free Energy= 0.484272
Sum of electronic and zero-point Energies= -1761.449771
Sum of electronic and thermal Energies= -1761.411787
Sum of electronic and thermal Enthalpies= -1761.410843
Sum of electronic and thermal Free Energies= -1761.523654
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83274912

TS11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.779605	-0.501985	-0.642696
2	6	0	-2.779125	0.488220	-0.309725
3	79	0	0.275604	-0.099847	-0.271213
4	6	0	-2.053822	-1.911897	-0.222199
5	8	0	-2.389781	-2.720398	-1.223396
6	6	0	-4.125970	0.261758	0.256196
7	6	0	-4.915611	-0.793575	-0.212668
8	6	0	-4.601875	1.083795	1.281869
9	6	0	-6.165202	-1.021858	0.347140
10	1	0	-4.562811	-1.413503	-1.034597
11	6	0	-5.848947	0.840118	1.842165
12	1	0	-3.995450	1.907255	1.650832
13	6	0	-6.633000	-0.210474	1.376755
14	1	0	-6.780464	-1.836678	-0.028535
15	1	0	-6.210093	1.478035	2.646004
16	1	0	-7.612018	-0.394953	1.814141
17	8	0	-1.894639	-2.254149	0.927425
18	6	0	-1.384496	2.036360	-2.192075
19	6	0	-1.497877	2.383271	-0.862989
20	6	0	-2.097477	0.930109	-2.633762
21	7	0	-2.576389	-0.037511	-1.829961
22	8	0	-2.321236	1.783284	-0.039963
23	1	0	-0.881183	2.714744	-2.874156
24	6	0	-2.596884	-4.084844	-0.846091
25	1	0	-2.843638	-4.613803	-1.767547
26	1	0	-1.689418	-4.496689	-0.392720
27	1	0	-3.420201	-4.155316	-0.126528
28	6	0	2.229861	0.243119	0.275034
29	7	0	2.806554	1.441949	0.513949
30	6	0	4.347536	-0.055190	0.974296
31	6	0	4.114792	1.279835	0.947297
32	1	0	5.223698	-0.627140	1.250415
33	1	0	4.742824	2.126599	1.192063
34	7	0	3.178693	-0.672388	0.558122
35	6	0	2.972161	-2.092194	0.444672

36	6	0	3.441020	-2.732088	-0.708516
37	6	0	2.287358	-2.752874	1.469153
38	6	0	3.219419	-4.103450	-0.813959
39	6	0	2.087748	-4.126052	1.317311
40	6	0	2.550279	-4.794154	0.190966
41	1	0	3.574671	-4.630913	-1.698368
42	1	0	1.562269	-4.670700	2.100899
43	1	0	2.389657	-5.866290	0.094359
44	6	0	2.119972	2.694455	0.366967
45	6	0	1.454850	3.218015	1.481648
46	6	0	2.130019	3.318647	-0.885221
47	6	0	0.787373	4.433550	1.318191
48	6	0	1.447709	4.531122	-1.003368
49	6	0	0.789227	5.087533	0.089589
50	1	0	0.272632	4.873381	2.171658
51	1	0	1.454255	5.051334	-1.961115
52	1	0	0.280303	6.044377	-0.014658
53	6	0	1.448143	2.490922	2.791952
54	1	0	2.464881	2.312338	3.167431
55	1	0	0.906934	3.061052	3.554307
56	1	0	0.966410	1.505834	2.701829
57	6	0	2.826383	2.697522	-2.057786
58	1	0	3.863498	2.422758	-1.823737
59	1	0	2.320856	1.774203	-2.378894
60	1	0	2.846938	3.384333	-2.910977
61	6	0	4.133719	-1.966433	-1.795459
62	1	0	5.101914	-1.562685	-1.468002
63	1	0	4.322674	-2.607241	-2.663256
64	1	0	3.529454	-1.111500	-2.133744
65	6	0	1.752991	-2.028958	2.668525
66	1	0	2.402203	-1.201046	2.983815
67	1	0	0.756359	-1.608731	2.461008
68	1	0	1.642471	-2.713634	3.516797
69	1	0	-1.048950	3.282766	-0.435808
70	1	0	-2.334139	0.811503	-3.693685

Zero-point correction= 0.559030 (Hartree/Particle)
Thermal correction to Energy= 0.596325
Thermal correction to Enthalpy= 0.597270
Thermal correction to Gibbs Free Energy= 0.486218
Sum of electronic and zero-point Energies= -1761.464428
Sum of electronic and thermal Energies= -1761.427133
Sum of electronic and thermal Enthalpies= -1761.426188
Sum of electronic and thermal Free Energies= -1761.537241
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.84777710

TS12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.759722	-0.416437	-0.801949
2	6	0	-2.353147	0.407235	0.267636
3	79	0	0.388570	0.013168	-0.477309
4	6	0	-1.632878	-1.896906	-0.519430
5	8	0	-1.680696	-2.610690	-1.646389
6	6	0	-2.308174	0.052736	1.723139
7	6	0	-3.068969	-0.967951	2.292441
8	6	0	-1.430511	0.784427	2.527923
9	6	0	-2.941898	-1.260956	3.641673
10	1	0	-3.752657	-1.550525	1.680742
11	6	0	-1.295171	0.478697	3.878097
12	1	0	-0.848235	1.596645	2.092810
13	6	0	-2.050280	-0.544896	4.437276
14	1	0	-3.541367	-2.058230	4.075793
15	1	0	-0.605896	1.052276	4.495550
16	1	0	-1.952696	-0.781406	5.495036
17	8	0	-1.404871	-2.394752	0.565359
18	6	0	-1.572699	2.168129	-2.124714
19	6	0	-1.592826	2.450891	-0.819866
20	6	0	-2.167416	0.966147	-2.691166
21	7	0	-2.266304	-0.171054	-2.120881
22	8	0	-2.268853	1.768101	0.163491
23	1	0	-1.082140	2.885937	-2.781228
24	6	0	-1.321733	-3.981496	-1.498367

25	1	0	-1.400361	-4.417007	-2.496088
26	1	0	-0.293949	-4.065104	-1.122112
27	1	0	-1.996214	-4.490326	-0.801754
28	6	0	2.360457	0.265637	0.002951
29	7	0	2.993028	1.432903	0.253040
30	6	0	4.453739	-0.143285	0.713549
31	6	0	4.288080	1.201991	0.693310
32	1	0	5.299903	-0.759126	0.988403
33	1	0	4.958037	2.013801	0.944528
34	7	0	3.257730	-0.700042	0.287577
35	6	0	2.981792	-2.106897	0.158797
36	6	0	3.475414	-2.763164	-0.975881
37	6	0	2.208699	-2.738627	1.138276
38	6	0	3.200183	-4.122643	-1.101762
39	6	0	1.956516	-4.101533	0.965642
40	6	0	2.452560	-4.787735	-0.134811
41	1	0	3.575494	-4.660866	-1.971320
42	1	0	1.354781	-4.620338	1.711126
43	1	0	2.251017	-5.851903	-0.244920
44	6	0	2.341771	2.708480	0.147863
45	6	0	1.800993	3.266593	1.312121
46	6	0	2.230043	3.303873	-1.112071
47	6	0	1.131108	4.484279	1.190385
48	6	0	1.555054	4.523662	-1.186032
49	6	0	1.014208	5.110314	-0.047021
50	1	0	0.706217	4.946700	2.080808
51	1	0	1.465887	5.019971	-2.152249
52	1	0	0.502147	6.068139	-0.122336
53	6	0	1.925598	2.573074	2.635442
54	1	0	2.963542	2.555960	2.995539
55	1	0	1.323336	3.080338	3.398126
56	1	0	1.592080	1.525277	2.577348
57	6	0	2.783379	2.645629	-2.339175
58	1	0	3.797997	2.257444	-2.179103
59	1	0	2.160274	1.790690	-2.644311
60	1	0	2.819107	3.348819	-3.178511
61	6	0	4.248527	-2.023210	-2.026160
62	1	0	5.229002	-1.685631	-1.662257
63	1	0	4.425385	-2.660269	-2.899296
64	1	0	3.708546	-1.127131	-2.366979
65	6	0	1.619471	-2.006312	2.306430
66	1	0	2.219235	-1.137813	2.609642
67	1	0	0.605089	-1.649495	2.062452
68	1	0	1.524907	-2.672515	3.171915
69	7	0	-4.186499	0.278255	-0.139186
70	6	0	-4.983425	1.174541	-0.675398
71	6	0	-6.003170	0.538325	-1.411049
72	6	0	-5.712233	-0.784259	-1.279551
73	1	0	-6.818248	0.994554	-1.954313
74	8	0	-4.623625	-0.954339	-0.523391
75	1	0	-6.172794	-1.694737	-1.640565
76	1	0	-4.790386	2.228504	-0.510662
77	1	0	-2.549638	1.034298	-3.715895
78	1	0	-1.135807	3.345679	-0.396182

Zero-point correction= 0.620666 (Hartree/Particle)
Thermal correction to Energy= 0.662115
Thermal correction to Enthalpy= 0.663059
Thermal correction to Gibbs Free Energy= 0.544333
Sum of electronic and zero-point Energies= -2007.307806
Sum of electronic and thermal Energies= -2007.266357
Sum of electronic and thermal Enthalpies= -2007.265413
Sum of electronic and thermal Free Energies= -2007.384140
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.82125156

TS13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.111872	-0.976290	-0.577164
2	6	0	-3.402382	-0.466513	-0.321125
3	79	0	0.754666	0.062473	-0.504304
4	6	0	-1.715193	-2.329718	-0.235309
5	8	0	-0.475160	-2.616119	-0.687972

6	8	0	-2.367405	-3.144751	0.403225
7	6	0	-2.819792	0.646365	-3.000335
8	6	0	-1.578778	0.558497	-2.310482
9	6	0	-4.060350	0.133026	-2.719271
10	1	0	-2.787327	1.276872	-3.886747
11	8	0	-4.459495	-0.606683	-1.731026
12	7	0	-1.204500	-0.168185	-1.283685
13	6	0	0.047284	-3.873836	-0.284025
14	1	0	-0.578766	-4.692573	-0.654570
15	1	0	1.050541	-3.929305	-0.714747
16	1	0	0.102603	-3.939000	0.809977
17	6	0	2.581785	0.435490	0.283291
18	7	0	3.579776	-0.422779	0.588719
19	6	0	4.326172	1.567555	1.154368
20	6	0	4.663589	0.256831	1.126013
21	1	0	4.864046	2.445179	1.488570
22	1	0	5.561693	-0.265516	1.429072
23	7	0	3.044838	1.657312	0.634473
24	6	0	2.317650	2.884363	0.455090
25	6	0	1.468427	3.313705	1.479212
26	6	0	2.496060	3.584167	-0.742191
27	6	0	0.786243	4.513931	1.280620
28	6	0	1.787752	4.775120	-0.898802
29	6	0	0.943591	5.237141	0.103909
30	1	0	0.131704	4.887389	2.068381
31	1	0	1.907188	5.344935	-1.819490
32	1	0	0.405287	6.173190	-0.031657
33	6	0	3.565508	-1.844078	0.370739
34	6	0	3.992182	-2.327995	-0.869995
35	6	0	3.175460	-2.672505	1.427564
36	6	0	4.046003	-3.713028	-1.031131
37	6	0	3.253738	-4.049770	1.223672
38	6	0	3.691541	-4.565161	0.008786
39	1	0	4.382586	-4.121555	-1.983206
40	1	0	2.966281	-4.721602	2.031999
41	1	0	3.755180	-5.642837	-0.130259
42	6	0	4.365823	-1.396817	-1.983400
43	1	0	5.059805	-0.611574	-1.653089
44	1	0	4.841098	-1.941491	-2.806200
45	1	0	3.478587	-0.889150	-2.390095
46	6	0	2.671908	-2.099145	2.717528
47	1	0	3.402514	-1.426897	3.188215
48	1	0	1.754940	-1.511306	2.559183
49	1	0	2.440770	-2.894253	3.434671
50	6	0	1.287176	2.506144	2.729037
51	1	0	2.243821	2.284276	3.221777
52	1	0	0.655903	3.037331	3.450389
53	1	0	0.810516	1.537227	2.513682
54	6	0	3.400539	3.062504	-1.817406
55	1	0	4.430724	2.925512	-1.460342
56	1	0	3.060410	2.083863	-2.187330
57	1	0	3.432505	3.749847	-2.669437
58	1	0	-0.787096	1.191393	-2.719604
59	1	0	-4.871073	0.421574	-3.400294
60	7	0	-4.248076	-1.372077	0.471559
61	6	0	-5.109079	-2.320091	0.170884
62	6	0	-5.483780	-2.968533	1.354885
63	1	0	-5.393819	-2.470643	-0.861937
64	6	0	-4.761702	-2.337948	2.322575
65	1	0	-6.177390	-3.789274	1.465147
66	1	0	-4.687058	-2.450202	3.396167
67	6	0	-3.598571	0.951075	0.135997
68	6	0	-4.829078	1.600088	-0.002215
69	6	0	-2.567953	1.589121	0.831554
70	6	0	-5.013824	2.873818	0.520969
71	1	0	-5.641903	1.103679	-0.528507
72	6	0	-2.752367	2.866176	1.345014
73	1	0	-1.617506	1.075643	0.975863
74	6	0	-3.974188	3.513466	1.189037
75	1	0	-5.975152	3.369913	0.403008
76	1	0	-1.935161	3.352842	1.875599
77	1	0	-4.119843	4.512936	1.594531
78	8	0	-4.013770	-1.361770	1.806578

Zero-point correction= 0.621681 (Hartree/Particle)

Thermal correction to Energy= 0.663048
Thermal correction to Enthalpy= 0.663992
Thermal correction to Gibbs Free Energy= 0.544138
Sum of electronic and zero-point Energies= -2007.307899
Sum of electronic and thermal Energies= -2007.266532
Sum of electronic and thermal Enthalpies= -2007.265588
Sum of electronic and thermal Free Energies= -2007.385442
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.82479790

TS14b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.133018	0.213608	0.186027
2	6	0	-3.470950	0.006058	-0.187713
3	79	0	0.820240	-0.273491	0.253799
4	6	0	-1.600385	1.626568	0.095213
5	8	0	-1.430925	2.137060	1.310882
6	8	0	-1.364440	2.187953	-0.947741
7	6	0	-2.481787	-2.283991	1.989560
8	6	0	-1.539673	-1.937663	1.077711
9	6	0	-3.395316	-1.412572	2.712358
10	1	0	-2.504878	-3.334095	2.277010
11	8	0	-3.513298	-0.203792	2.573827
12	7	0	-1.236047	-0.686466	0.570051
13	6	0	-0.847191	3.443225	1.356770
14	1	0	-1.370937	4.121160	0.673516
15	1	0	-0.944017	3.775539	2.391221
16	1	0	0.208888	3.386504	1.067667
17	6	0	2.767220	0.042002	-0.195397
18	7	0	3.398354	1.199823	-0.486019
19	6	0	4.904026	-0.382036	-0.758570
20	6	0	4.718043	0.957035	-0.837479
21	1	0	5.770409	-1.003224	-0.944791
22	1	0	5.385805	1.763347	-1.110931
23	7	0	3.693897	-0.926738	-0.361505
24	6	0	3.428451	-2.329790	-0.189506
25	6	0	2.997234	-3.056868	-1.303901
26	6	0	3.593549	-2.887988	1.081626
27	6	0	2.726059	-4.411369	-1.115303
28	6	0	3.310520	-4.246498	1.221720
29	6	0	2.881459	-4.999877	0.134993
30	1	0	2.393006	-5.007858	-1.963820
31	1	0	3.433466	-4.714300	2.197764
32	1	0	2.670340	-6.059877	0.262817
33	6	0	2.805409	2.509684	-0.448553
34	6	0	3.104056	3.327323	0.649557
35	6	0	1.996274	2.917295	-1.513739
36	6	0	2.584272	4.620664	0.645590
37	6	0	1.487275	4.216906	-1.465689
38	6	0	1.789735	5.063950	-0.407858
39	1	0	2.809428	5.283992	1.480078
40	1	0	0.851647	4.560798	-2.280642
41	1	0	1.398318	6.079818	-0.398976
42	6	0	3.940364	2.825558	1.788391
43	1	0	4.989430	2.674059	1.498753
44	1	0	3.931236	3.537198	2.620836
45	1	0	3.571222	1.860158	2.164776
46	6	0	1.659223	2.008731	-2.656307
47	1	0	2.470615	1.307182	-2.891147
48	1	0	0.760797	1.416457	-2.424831
49	1	0	1.437873	2.588119	-3.559627
50	6	0	2.820828	-2.399413	-2.639590
51	1	0	3.748528	-1.928971	-2.993910
52	1	0	2.508674	-3.127764	-3.395587
53	1	0	2.057987	-1.607118	-2.602135
54	6	0	4.038744	-2.055836	2.246144
55	1	0	4.965452	-1.506483	2.030854
56	1	0	3.280511	-1.306932	2.518828
57	1	0	4.218163	-2.681326	3.127036
58	1	0	-0.846038	-2.715437	0.745996
59	1	0	-4.014086	-1.943435	3.469671
60	7	0	-4.247038	1.105153	-0.131702
61	6	0	-4.494275	2.050080	0.760730

62	6	0	-4.972027	3.234114	0.214802
63	1	0	-4.342719	1.776457	1.804743
64	6	0	-5.062678	3.008081	-1.148467
65	1	0	-5.303745	4.108209	0.756579
66	1	0	-5.504726	3.662006	-1.901728
67	6	0	-4.077538	-1.269307	-0.593710
68	6	0	-5.338575	-1.634938	-0.113802
69	6	0	-3.402801	-2.130272	-1.465148
70	6	0	-5.910531	-2.844176	-0.491459
71	1	0	-5.866446	-0.967574	0.567975
72	6	0	-3.973411	-3.339978	-1.836858
73	1	0	-2.429081	-1.838615	-1.860510
74	6	0	-5.227568	-3.700877	-1.349398
75	1	0	-6.892514	-3.120092	-0.111891
76	1	0	-3.444432	-4.000257	-2.521637
77	1	0	-5.675027	-4.648128	-1.643899
78	8	0	-4.633387	1.864940	-1.548519

Zero-point correction= 0.618906 (Hartree/Particle)
Thermal correction to Energy= 0.661616
Thermal correction to Enthalpy= 0.662560
Thermal correction to Gibbs Free Energy= 0.539370
Sum of electronic and zero-point Energies= -2007.327271
Sum of electronic and thermal Energies= -2007.284561
Sum of electronic and thermal Enthalpies= -2007.283617
Sum of electronic and thermal Free Energies= -2007.406808
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.84359900

TS15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.896571	-1.093625	-0.273627
2	6	0	-3.857713	0.185800	0.477207
3	79	0	1.639296	-0.573747	-0.487265
4	6	0	-4.771468	-2.251843	0.098140
5	8	0	-5.443534	-2.711728	-0.950380
6	6	0	-4.900145	0.606107	1.412196
7	6	0	-6.227706	0.203701	1.232147
8	6	0	-4.576222	1.465101	2.467960
9	6	0	-7.215003	0.646257	2.101667
10	1	0	-6.503704	-0.424994	0.384516
11	6	0	-5.562362	1.895058	3.342123
12	1	0	-3.541321	1.779013	2.593458
13	6	0	-6.881981	1.484830	3.161067
14	1	0	-8.247566	0.339747	1.950234
15	1	0	-5.304931	2.552743	4.169677
16	1	0	-7.655065	1.824504	3.847425
17	8	0	-4.800441	-2.684787	1.219857
18	6	0	-1.498766	0.968052	-1.880739
19	6	0	-2.510922	1.369955	-2.808279
20	6	0	-1.868529	0.363864	-0.656400
21	7	0	-2.799819	0.873428	0.238639
22	8	0	-3.687563	1.035012	-2.697402
23	1	0	-1.035630	-0.096106	-0.101514
24	1	0	-2.163008	1.944646	-3.697128
25	7	0	-2.948278	-1.157438	-1.136199
26	6	0	-2.816576	-1.836371	-2.300930
27	6	0	-1.654509	-1.848116	-3.011752
28	6	0	-0.359996	-1.470721	-2.524490
29	1	0	-1.715305	-2.117315	-4.065230
30	8	0	0.043453	-1.697588	-1.356662
31	1	0	0.346120	-1.073602	-3.273771
32	1	0	-3.749028	-2.160283	-2.762693
33	1	0	-0.445515	1.181971	-2.065956
34	6	0	-6.308462	-3.828373	-0.677938
35	1	0	-6.808937	-4.049806	-1.620582
36	1	0	-5.719401	-4.684327	-0.335725
37	1	0	-7.034066	-3.555522	0.094724
38	6	0	2.973097	0.632076	0.400128
39	7	0	2.848977	1.972745	0.508681
40	6	0	4.726343	1.456380	1.530369
41	6	0	3.925062	2.499648	1.203445
42	1	0	5.663717	1.406604	2.069002

43	1	0	4.008780	3.561522	1.394523
44	7	0	4.123429	0.314995	1.026745
45	6	0	4.645712	-1.020470	1.153932
46	6	0	5.478749	-1.504103	0.140621
47	6	0	4.288887	-1.762200	2.284187
48	6	0	5.975605	-2.798436	0.290212
49	6	0	4.808500	-3.051757	2.388379
50	6	0	5.644065	-3.563594	1.402221
51	1	0	6.631387	-3.205347	-0.478449
52	1	0	4.552236	-3.656883	3.256988
53	1	0	6.043351	-4.570892	1.502596
54	6	0	1.758383	2.732695	-0.044986
55	6	0	0.579821	2.852699	0.699253
56	6	0	1.931211	3.297732	-1.313604
57	6	0	-0.464897	3.578604	0.127300
58	6	0	0.859534	4.017139	-1.842923
59	6	0	-0.325715	4.155921	-1.129560
60	1	0	-1.402544	3.675289	0.673317
61	1	0	0.963047	4.472308	-2.827281
62	1	0	-1.153767	4.716259	-1.559861
63	6	0	0.429388	2.200313	2.040648
64	1	0	1.295894	2.379574	2.691657
65	1	0	-0.462726	2.572398	2.556021
66	1	0	0.323726	1.107661	1.947326
67	6	0	3.213366	3.131325	-2.072557
68	1	0	4.052127	3.642393	-1.579564
69	1	0	3.498123	2.073074	-2.166600
70	1	0	3.125409	3.546424	-3.082169
71	6	0	5.808566	-0.673516	-1.063019
72	1	0	6.181078	0.323754	-0.791414
73	1	0	6.575122	-1.160721	-1.674878
74	1	0	4.924596	-0.521552	-1.700385
75	6	0	3.381169	-1.194183	3.333356
76	1	0	3.795694	-0.283338	3.787572
77	1	0	2.399158	-0.923911	2.917672
78	1	0	3.213629	-1.918335	4.137494

Zero-point correction= 0.617365 (Hartree/Particle)
Thermal correction to Energy= 0.660677
Thermal correction to Enthalpy= 0.661621
Thermal correction to Gibbs Free Energy= 0.535089
Sum of electronic and zero-point Energies= -2007.325393
Sum of electronic and thermal Energies= -2007.282082
Sum of electronic and thermal Enthalpies= -2007.281137
Sum of electronic and thermal Free Energies= -2007.407670
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.84711684

TS16b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.131258	-1.067593	0.035620
2	6	0	-3.707369	0.196449	0.579564
3	79	0	1.554363	-0.744411	-0.308580
4	6	0	-5.373492	-1.828443	0.331160
5	8	0	-5.209352	-3.139097	0.140181
6	6	0	-4.392123	1.113022	1.500610
7	6	0	-5.736689	1.465291	1.352536
8	6	0	-3.628066	1.719103	2.506509
9	6	0	-6.306502	2.400227	2.207950
10	1	0	-6.332720	1.014450	0.565128
11	6	0	-4.205625	2.642820	3.365325
12	1	0	-2.580464	1.441329	2.615495
13	6	0	-5.547521	2.985157	3.216307
14	1	0	-7.351878	2.674229	2.082526
15	1	0	-3.609942	3.095805	4.155475
16	1	0	-6.001709	3.711158	3.887999
17	8	0	-6.390485	-1.311186	0.716129
18	6	0	-1.292802	-0.387413	-1.907868
19	6	0	-2.141131	0.111512	-3.051612
20	6	0	-2.060986	-0.573488	-0.611089
21	7	0	-2.475232	0.463763	0.166287
22	8	0	-3.305009	0.401715	-2.948100
23	1	0	-1.097521	-1.304880	-0.160504

24	1	0	-1.593423	0.211285	-4.019031
25	7	0	-3.125994	-1.508405	-0.731418
26	6	0	-2.963942	-2.633606	-1.568120
27	6	0	-1.806637	-2.781275	-2.224964
28	6	0	-0.669153	-1.797952	-2.040874
29	1	0	-1.673088	-3.655554	-2.856604
30	8	0	-0.067182	-2.048952	-0.786898
31	1	0	0.068031	-1.856835	-2.852152
32	1	0	-3.802561	-3.316433	-1.613602
33	1	0	-0.487191	0.348485	-1.744108
34	6	0	-6.362846	-3.941529	0.440233
35	1	0	-6.061520	-4.971844	0.249556
36	1	0	-6.648146	-3.807506	1.487688
37	1	0	-7.200357	-3.652529	-0.201750
38	6	0	2.872140	0.713337	0.112676
39	7	0	2.657994	2.008245	-0.217133
40	6	0	4.577251	1.971591	0.852373
41	6	0	3.702567	2.799856	0.230796
42	1	0	5.521876	2.158624	1.346313
43	1	0	3.716139	3.869005	0.064335
44	7	0	4.048655	0.692591	0.768196
45	6	0	4.661974	-0.491627	1.309349
46	6	0	5.511840	-1.232934	0.483576
47	6	0	4.370935	-0.837938	2.632284
48	6	0	6.099556	-2.371221	1.034375
49	6	0	4.980501	-1.985067	3.138404
50	6	0	5.837282	-2.742447	2.347879
51	1	0	6.771042	-2.969799	0.420130
52	1	0	4.777499	-2.282750	4.166313
53	1	0	6.307002	-3.632898	2.760998
54	6	0	1.502331	2.459575	-0.947437
55	6	0	0.313944	2.691908	-0.246451
56	6	0	1.615803	2.592830	-2.337327
57	6	0	-0.806353	3.068883	-0.990986
58	6	0	0.473114	2.978656	-3.037832
59	6	0	-0.726673	3.213693	-2.371097
60	1	0	-1.750407	3.233407	-0.472534
61	1	0	0.531319	3.098572	-4.119360
62	1	0	-1.609785	3.512449	-2.933877
63	6	0	0.222667	2.502511	1.237084
64	1	0	1.114433	2.870876	1.761409
65	1	0	-0.653295	3.023905	1.638723
66	1	0	0.112036	1.436293	1.491802
67	6	0	2.910663	2.318246	-3.041089
68	1	0	3.682525	3.056269	-2.782125
69	1	0	3.315968	1.330184	-2.777795
70	1	0	2.779279	2.350863	-4.127907
71	6	0	5.764250	-0.832127	-0.938673
72	1	0	6.060821	0.222019	-1.027993
73	1	0	6.559864	-1.441521	-1.380348
74	1	0	4.864096	-0.965175	-1.557316
75	6	0	3.436260	-0.012200	3.464123
76	1	0	3.794004	1.020034	3.584333
77	1	0	2.436109	0.048565	3.009677
78	1	0	3.322098	-0.441671	4.465008

Zero-point correction= 0.619161 (Hartree/Particle)
Thermal correction to Energy= 0.660464
Thermal correction to Enthalpy= 0.661408
Thermal correction to Gibbs Free Energy= 0.541023
Sum of electronic and zero-point Energies= -2007.367481
Sum of electronic and thermal Energies= -2007.326178
Sum of electronic and thermal Enthalpies= -2007.325234
Sum of electronic and thermal Free Energies= -2007.445620

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.88493066

TS17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.789282	1.254201	0.088908
2	6	0	-2.562476	0.015076	0.706591
3	6	0	-3.951841	1.759800	-0.594335
4	8	0	-3.748116	2.987470	-1.162183

5	6	0	-3.383331	-1.202119	0.836915
6	6	0	-4.413873	-1.567309	-0.035535
7	6	0	-3.046732	-2.082217	1.877071
8	6	0	-5.095640	-2.766185	0.141011
9	1	0	-4.688983	-0.902330	-0.847153
10	6	0	-3.736030	-3.272608	2.054582
11	1	0	-2.223103	-1.806807	2.532421
12	6	0	-4.767223	-3.621821	1.186887
13	1	0	-5.893466	-3.032444	-0.552181
14	1	0	-3.461604	-3.935571	2.874676
15	1	0	-5.309019	-4.557785	1.323007
16	8	0	-5.034607	1.210372	-0.697196
17	6	0	0.567803	1.572458	1.376626
18	6	0	1.097246	1.262447	2.688432
19	6	0	-0.754910	1.147372	1.024025
20	7	0	-1.328098	-0.026333	1.264253
21	8	0	0.642584	0.521423	3.543216
22	1	0	1.216073	2.161536	-1.183489
23	1	0	2.065205	1.808045	2.877501
24	7	0	-1.595238	1.974383	0.310603
25	6	0	-1.242655	3.305069	0.074428
26	6	0	0.007160	3.730568	0.299328
27	6	0	1.107613	2.781531	0.658975
28	1	0	0.245181	4.776138	0.112626
29	8	0	1.863559	2.488967	-0.537196
30	1	0	1.849177	3.274849	1.306487
31	1	0	-2.042883	3.944671	-0.273977
32	1	0	1.376752	0.270948	0.589760
33	6	0	-4.869893	3.508305	-1.847786
34	1	0	-4.554902	4.475586	-2.249174
35	1	0	-5.177783	2.843436	-2.663354
36	1	0	-5.724123	3.638183	-1.172481
37	7	0	1.880801	-0.522174	-0.019092
38	16	0	1.293473	-0.694940	-1.563990
39	8	0	0.244430	0.296700	-1.726445
40	8	0	2.338504	-0.860487	-2.550717
41	16	0	3.407652	-0.952550	0.488584
42	8	0	3.370425	-0.997706	1.932221
43	8	0	3.925605	-2.036828	-0.316165
44	6	0	0.441245	-2.332932	-1.450878
45	6	0	4.428919	0.542010	0.077691
46	9	0	5.698865	0.211191	0.292019
47	9	0	4.276773	0.888719	-1.181374
48	9	0	4.103529	1.539016	0.874016
49	9	0	1.320290	-3.261322	-1.120911
50	9	0	-0.053352	-2.600884	-2.652572
51	9	0	-0.527486	-2.294596	-0.569003

Zero-point correction= 0.332608 (Hartree/Particle)
Thermal correction to Energy= 0.366179
Thermal correction to Enthalpy= 0.367123
Thermal correction to Gibbs Free Energy= 0.265883
Sum of electronic and zero-point Energies= -2854.330434
Sum of electronic and thermal Energies= -2854.296863
Sum of electronic and thermal Enthalpies= -2854.295919
Sum of electronic and thermal Free Energies= -2854.397159
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -2855.32797841

TS18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.051436	-0.638337	-1.084828
2	6	0	-3.161113	0.011728	-0.522112
3	6	0	-1.603402	-2.001158	-0.952927
4	8	0	-0.250790	-2.113198	-1.146953
5	6	0	-4.400864	-0.522516	0.062039
6	6	0	-5.123933	0.309685	0.928953
7	6	0	-4.925301	-1.781804	-0.247236
8	6	0	-6.319616	-0.115096	1.488886
9	1	0	-4.722979	1.299384	1.136419
10	6	0	-6.126244	-2.201985	0.313385
11	1	0	-4.374834	-2.435006	-0.916521
12	6	0	-6.826962	-1.376281	1.185743

13	1	0	-6.862310	0.544955	2.165362
14	1	0	-6.517875	-3.187307	0.061119
15	1	0	-7.766760	-1.711304	1.624963
16	8	0	-2.286810	-2.977118	-0.697396
17	6	0	-1.140036	2.830046	-1.287935
18	6	0	-1.744485	4.120725	-1.153975
19	6	0	-1.804794	1.603407	-1.057840
20	7	0	-2.998072	1.354839	-0.514443
21	8	0	-2.883862	4.419024	-0.824740
22	1	0	-1.010335	4.940557	-1.411841
23	7	0	-1.189702	0.419593	-1.445137
24	6	0	-0.075275	0.427949	-2.260102
25	6	0	0.635816	1.555339	-2.429058
26	6	0	0.288974	2.757023	-1.634945
27	1	0	1.504173	1.556066	-3.083616
28	8	0	1.141711	2.699346	-0.353610
29	1	0	0.637594	3.686930	-2.102440
30	1	0	0.159502	-0.511323	-2.747089
31	7	0	2.130135	0.439705	0.289078
32	16	0	1.255245	-0.311640	1.480647
33	8	0	-0.108750	0.136564	1.316962
34	8	0	1.635190	-1.700019	1.624247
35	16	0	3.679178	0.113648	-0.184644
36	8	0	4.068603	1.213576	-1.041494
37	8	0	4.508682	-0.353803	0.906174
38	6	0	1.825378	0.557063	3.013248
39	6	0	3.509470	-1.345899	-1.312611
40	9	0	4.684678	-1.507051	-1.908043
41	9	0	3.216684	-2.435689	-0.632108
42	9	0	2.585361	-1.130283	-2.229697
43	9	0	3.071309	0.252360	3.312108
44	9	0	1.032057	0.190801	4.006804
45	9	0	1.721628	1.865393	2.827145
46	1	0	1.677204	1.430809	-0.079711
47	1	0	0.500396	2.897380	0.353759
48	6	0	0.292972	-3.414346	-1.009414
49	1	0	1.144031	-3.473154	-1.694780
50	1	0	0.647345	-3.562129	0.018459
51	1	0	-0.454607	-4.174952	-1.253648

Zero-point correction= 0.331914 (Hartree/Particle)
Thermal correction to Energy= 0.365292
Thermal correction to Enthalpy= 0.366237
Thermal correction to Gibbs Free Energy= 0.266638
Sum of electronic and zero-point Energies= -2854.335987
Sum of electronic and thermal Energies= -2854.302609
Sum of electronic and thermal Enthalpies= -2854.301665
Sum of electronic and thermal Free Energies= -2854.401263
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -2855.33581206

TS19b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.404497	-0.470924	-0.485012
2	7	0	-3.773679	-0.078984	-0.341064
3	16	0	-4.208287	1.243663	0.518829
4	8	0	-5.435083	1.093230	1.274790
5	8	0	-2.997139	1.749276	1.150270
6	16	0	-4.792929	-1.242932	-0.880646
7	8	0	-6.164804	-0.810225	-1.039785
8	8	0	-4.071794	-1.938128	-1.931646
9	6	0	-4.788900	-2.419375	0.540891
10	6	0	-4.560737	2.462836	-0.819220
11	9	0	-4.902404	3.611434	-0.258744
12	9	0	-5.540404	2.034134	-1.589923
13	9	0	-3.469730	2.641492	-1.551886
14	9	0	-5.568857	-3.445887	0.249821
15	9	0	-3.552121	-2.857757	0.755055
16	9	0	-5.227637	-1.826976	1.638190
17	6	0	-0.519544	0.187163	0.368621
18	6	0	-0.282965	1.404582	-0.355734
19	79	0	1.653886	-0.250056	0.225498
20	6	0	-0.895110	0.116100	1.809653

21	8	0	-1.816969	-0.840924	1.990815
22	6	0	0.117252	2.737218	0.098519
23	6	0	0.874242	2.965573	1.256361
24	6	0	-0.266494	3.831932	-0.691857
25	6	0	1.228415	4.258484	1.614376
26	1	0	1.172744	2.127062	1.880532
27	6	0	0.082193	5.122893	-0.321686
28	1	0	-0.858895	3.649590	-1.584989
29	6	0	0.831170	5.339498	0.831913
30	1	0	1.821342	4.421594	2.512901
31	1	0	-0.238981	5.964686	-0.932684
32	1	0	1.104239	6.353129	1.123137
33	8	0	-0.434973	0.782240	2.707988
34	6	0	-1.144169	-0.714393	-0.656474
35	6	0	-0.956236	-2.191117	-0.654699
36	6	0	-0.985550	0.025085	-1.873350
37	7	0	-0.536035	1.248675	-1.704966
38	8	0	-0.868176	-2.858949	-1.660702
39	6	0	-2.398718	-0.888725	3.291432
40	1	0	-3.126118	-1.701897	3.256810
41	1	0	-1.634988	-1.077379	4.053400
42	1	0	-2.899098	0.063043	3.504376
43	6	0	3.582729	-0.743853	-0.210222
44	7	0	4.569312	0.119249	-0.533037
45	6	0	5.374006	-1.887697	-0.938881
46	6	0	5.684464	-0.568487	-0.985556
47	1	0	5.941038	-2.771594	-1.199701
48	1	0	6.581034	-0.049702	-1.298064
49	7	0	4.076670	-1.974137	-0.459596
50	6	0	3.312249	-3.179292	-0.271524
51	6	0	2.415276	-3.562895	-1.273408
52	6	0	3.456667	-3.865723	0.938890
53	6	0	1.638715	-4.698010	-1.034389
54	6	0	2.669373	-4.999317	1.127993
55	6	0	1.766743	-5.408370	0.151864
56	1	0	0.905634	-4.998209	-1.780695
57	1	0	2.758728	-5.555977	2.060433
58	1	0	1.149642	-6.288745	0.321693
59	6	0	4.437703	1.549146	-0.438773
60	6	0	4.960971	2.177429	0.698883
61	6	0	3.760352	2.237158	-1.450170
62	6	0	4.815223	3.558120	0.795860
63	6	0	3.636370	3.621238	-1.306512
64	6	0	4.156536	4.274085	-0.199051
65	1	0	5.210596	4.072162	1.671577
66	1	0	3.101530	4.182186	-2.072728
67	1	0	4.037462	5.351916	-0.102471
68	6	0	5.617249	1.383919	1.788317
69	1	0	6.499314	0.833036	1.433623
70	1	0	5.940227	2.038041	2.605470
71	1	0	4.925001	0.639663	2.209089
72	6	0	3.141684	1.550277	-2.630853
73	1	0	3.580832	0.564800	-2.831007
74	1	0	2.059692	1.406627	-2.473803
75	1	0	3.251785	2.161973	-3.534507
76	6	0	2.250256	-2.768556	-2.533781
77	1	0	3.213939	-2.451329	-2.955843
78	1	0	1.712864	-3.349292	-3.290625
79	1	0	1.655964	-1.858251	-2.353284
80	6	0	4.391565	-3.374906	2.002867
81	1	0	5.428142	-3.298622	1.646454
82	1	0	4.101563	-2.374332	2.356385
83	1	0	4.384921	-4.047572	2.867458
84	1	0	-1.244475	-0.359799	-2.859115
85	1	0	-0.878557	-2.649039	0.358290

Zero-point correction= 0.614179 (Hartree/Particle)
Thermal correction to Energy= 0.666429
Thermal correction to Enthalpy= 0.667374
Thermal correction to Gibbs Free Energy= 0.525917
Sum of electronic and zero-point Energies= -3588.384494
Sum of electronic and thermal Energies= -3588.332243
Sum of electronic and thermal Enthalpies= -3588.331299
Sum of electronic and thermal Free Energies= -3588.472755
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3590.14839920

TS20b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.509850	2.237169	0.297262
2	6	0	1.745604	3.453159	-3.001823
3	6	0	1.285341	2.792294	-1.774470
4	6	0	1.103631	1.440463	-1.716361
5	6	0	0.898560	3.313915	-0.479730
6	8	0	2.030332	2.836660	-4.010183
7	7	0	0.662209	1.056358	-0.458689
8	79	0	-1.141053	-0.136449	-0.409000
9	1	0	1.606974	0.174670	-0.061125
10	7	0	2.542369	-0.590098	0.213057
11	16	0	2.032563	-2.137218	0.486911
12	8	0	2.014431	-2.508985	1.887711
13	8	0	0.849071	-2.279276	-0.346522
14	16	0	3.823423	0.167341	0.959758
15	8	0	3.384993	1.503428	1.307824
16	8	0	4.517148	-0.701084	1.885919
17	6	0	4.941613	0.395243	-0.492059
18	6	0	3.301378	-3.209285	-0.327046
19	9	0	3.445406	-2.843658	-1.586550
20	9	0	2.843088	-4.450577	-0.275370
21	9	0	4.456565	-3.138226	0.299050
22	9	0	6.014522	1.041527	-0.072613
23	9	0	4.329561	1.100232	-1.423444
24	9	0	5.295565	-0.779986	-0.983037
25	6	0	-2.896245	-1.133816	-0.275674
26	7	0	-3.121670	-2.457574	-0.122082
27	6	0	-5.111035	-1.517600	-0.098511
28	6	0	-4.479927	-2.712118	-0.010123
29	1	0	-6.157829	-1.246693	-0.057981
30	1	0	-4.852478	-3.719241	0.122799
31	7	0	-4.122167	-0.561185	-0.262061
32	6	0	-4.349022	0.855337	-0.339011
33	6	0	-4.536197	1.433285	-1.597569
34	6	0	-4.343624	1.585281	0.853003
35	6	0	-4.737641	2.811839	-1.643203
36	6	0	-4.550034	2.961392	0.758723
37	6	0	-4.744163	3.568058	-0.476394
38	1	0	-4.884356	3.293428	-2.609424
39	1	0	-4.550174	3.559175	1.669900
40	1	0	-4.900323	4.643939	-0.531128
41	6	0	-2.113143	-3.482536	-0.062031
42	6	0	-1.463536	-3.714586	1.152130
43	6	0	-1.844039	-4.203284	-1.229101
44	6	0	-0.530398	-4.750785	1.188044
45	6	0	-0.904095	-5.228143	-1.146776
46	6	0	-0.259684	-5.504547	0.053560
47	1	0	0.001130	-4.948015	2.118381
48	1	0	-0.673549	-5.807857	-2.040113
49	1	0	0.474235	-6.307232	0.101157
50	6	0	-1.706578	-2.852088	2.352264
51	1	0	-2.771105	-2.621874	2.498887
52	1	0	-1.329033	-3.332852	3.261565
53	1	0	-1.179359	-1.889630	2.250261
54	6	0	-2.522693	-3.863664	-2.522005
55	1	0	-3.611886	-4.004062	-2.473440
56	1	0	-2.348864	-2.812688	-2.796992
57	1	0	-2.142919	-4.489428	-3.337094
58	6	0	-4.492454	0.604270	-2.845308
59	1	0	-4.725173	1.212122	-3.726454
60	1	0	-3.495385	0.164925	-2.996296
61	1	0	-5.206171	-0.230646	-2.813061
62	6	0	-4.088147	0.916627	2.168641
63	1	0	-4.702948	0.015539	2.301716
64	1	0	-3.034053	0.608825	2.257473
65	1	0	-4.296320	1.597571	3.001364
66	1	0	1.305856	0.696851	-2.481385
67	1	0	1.812352	4.559162	-2.970059
68	6	0	-0.017654	2.122024	1.665731
69	6	0	-0.955789	3.036058	2.160812
70	6	0	0.342917	1.033828	2.475788

71	6	0	-1.495404	2.877427	3.432022
72	1	0	-1.246347	3.880776	1.544435
73	6	0	-0.204824	0.873605	3.742318
74	1	0	1.080484	0.313527	2.127183
75	6	0	-1.124922	1.798495	4.228814
76	1	0	-2.215987	3.606981	3.801154
77	1	0	0.105767	0.027677	4.353779
78	1	0	-1.548158	1.679256	5.225197
79	6	0	1.037134	4.702306	-0.019066
80	8	0	0.497840	5.210228	0.939910
81	8	0	1.888142	5.393219	-0.808440
82	6	0	2.103936	6.742485	-0.416675
83	1	0	2.534100	6.787511	0.589679
84	1	0	2.800205	7.158720	-1.147751
85	1	0	1.163236	7.304584	-0.419025

Zero-point correction= 0.615590 (Hartree/Particle)
Thermal correction to Energy= 0.668132
Thermal correction to Enthalpy= 0.669076
Thermal correction to Gibbs Free Energy= 0.524970
Sum of electronic and zero-point Energies= -3588.410735
Sum of electronic and thermal Energies= -3588.358194
Sum of electronic and thermal Enthalpies= -3588.357250
Sum of electronic and thermal Free Energies= -3588.501355
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3590.17149602

TS21b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.323555	-0.922619	0.766185
2	6	0	-2.220402	0.004003	0.013522
3	79	0	0.631723	-0.250320	0.184726
4	6	0	-1.556595	-0.909086	2.274091
5	8	0	-2.841314	-1.181543	2.542484
6	6	0	-2.446445	1.339861	0.660784
7	6	0	-1.569823	1.929942	1.581098
8	6	0	-3.616973	2.032486	0.321277
9	6	0	-1.868088	3.161469	2.154675
10	1	0	-0.630531	1.450633	1.850052
11	6	0	-3.915710	3.257322	0.899813
12	1	0	-4.285059	1.595044	-0.417696
13	6	0	-3.042858	3.826465	1.823958
14	1	0	-1.167253	3.602856	2.862029
15	1	0	-4.836666	3.770445	0.629062
16	1	0	-3.277585	4.786282	2.280727
17	8	0	-0.715383	-0.716632	3.114449
18	6	0	-2.288489	-2.608755	-1.710585
19	6	0	-1.575793	-2.996277	-0.581950
20	6	0	-2.904501	-1.260051	-1.962961
21	7	0	-2.794799	-0.135501	-1.125455
22	8	0	-1.394081	-2.367716	0.514783
23	6	0	4.510548	1.065790	-1.047307
24	6	0	3.742710	2.117921	-1.422387
25	1	0	5.574838	0.885661	-1.124614
26	1	0	3.990230	3.056265	-1.901223
27	7	0	3.657242	0.133004	-0.476941
28	7	0	2.440273	1.800659	-1.072762
29	6	0	2.386021	0.582004	-0.489290
30	1	0	-2.682141	-0.958879	-2.994408
31	1	0	-1.154722	-4.006275	-0.546792
32	6	0	-4.070952	-3.580360	-1.512208
33	6	0	-4.606012	-3.009798	-0.302290
34	6	0	-4.850814	-1.733776	-0.659687
35	8	0	-4.496063	-2.844992	-2.553771
36	1	0	-4.691993	-3.482002	0.667793
37	1	0	-5.163794	-0.882540	-0.066348
38	7	0	-4.494887	-1.524815	-2.015204
39	1	0	-3.911674	-4.635485	-1.727888
40	1	0	-2.013828	-3.176151	-2.602315
41	6	0	-3.184614	-1.149583	3.931656
42	1	0	-4.249004	-1.384036	3.984601
43	1	0	-2.596765	-1.885455	4.489212
44	1	0	-2.989908	-0.151532	4.339238

45	6	0	1.290081	2.649814	-1.236500
46	6	0	1.065209	3.637725	-0.271549
47	6	0	0.428310	2.420468	-2.313834
48	6	0	-0.066440	4.436794	-0.423612
49	6	0	-0.696957	3.238285	-2.418401
50	6	0	-0.939897	4.239665	-1.486459
51	1	0	-0.268156	5.214321	0.312581
52	1	0	-1.388075	3.081502	-3.245905
53	1	0	-1.824323	4.866714	-1.582861
54	6	0	4.064635	-1.127952	0.079971
55	6	0	4.264138	-1.210358	1.461178
56	6	0	4.231118	-2.210702	-0.789371
57	6	0	4.667339	-2.443573	1.974033
58	6	0	4.632831	-3.423081	-0.231266
59	6	0	4.852029	-3.537123	1.137230
60	1	0	4.837852	-2.539237	3.045686
61	1	0	4.776447	-4.284503	-0.882675
62	1	0	5.171551	-4.489606	1.555780
63	6	0	4.029989	-0.034615	2.361166
64	1	0	2.954898	0.115514	2.544785
65	1	0	4.508720	-0.187636	3.334536
66	1	0	4.419313	0.900351	1.935371
67	6	0	1.981439	3.801616	0.903503
68	1	0	2.099506	2.857085	1.456545
69	1	0	2.989679	4.122897	0.607371
70	1	0	1.589222	4.551331	1.599744
71	6	0	0.674059	1.319077	-3.300917
72	1	0	1.733998	1.229393	-3.573827
73	1	0	0.366948	0.344049	-2.888488
74	1	0	0.100703	1.485046	-4.219919
75	6	0	3.976081	-2.070740	-2.260172
76	1	0	2.973973	-1.662671	-2.459670
77	1	0	4.694864	-1.393266	-2.741976
78	1	0	4.052826	-3.040778	-2.763239

Zero-point correction= 0.621920 (Hartree/Particle)
Thermal correction to Energy= 0.662367
Thermal correction to Enthalpy= 0.663312
Thermal correction to Gibbs Free Energy= 0.546778
Sum of electronic and zero-point Energies= -2007.239955
Sum of electronic and thermal Energies= -2007.199507
Sum of electronic and thermal Enthalpies= -2007.198563
Sum of electronic and thermal Free Energies= -2007.315097
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.75900141

TS22b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.149516	-1.738428	0.904201
2	6	0	-3.024664	-1.883042	-0.234235
3	79	0	0.529316	-0.516744	0.198551
4	6	0	-2.428267	-0.665778	1.887529
5	8	0	-1.446031	-0.527269	2.785922
6	6	0	-3.627211	-0.949662	-1.134185
7	6	0	-4.577137	-1.418471	-2.061770
8	6	0	-3.239813	0.403656	-1.144448
9	6	0	-5.127065	-0.549472	-2.987219
10	1	0	-4.877675	-2.463429	-2.034982
11	6	0	-3.796094	1.260648	-2.076383
12	1	0	-2.507125	0.779410	-0.429167
13	6	0	-4.736339	0.788836	-2.993131
14	1	0	-5.864902	-0.908041	-3.700780
15	1	0	-3.498776	2.306820	-2.086151
16	1	0	-5.172532	1.473744	-3.717939
17	8	0	-3.478455	-0.062577	1.923454
18	6	0	-1.483176	-4.314166	0.822231
19	6	0	-0.493150	-3.376043	0.518385
20	6	0	-2.745541	-3.747316	0.810877
21	1	0	-1.247339	-5.266873	1.288056
22	8	0	-3.151576	-3.162657	-0.460445
23	7	0	-0.800503	-2.088306	0.637607
24	6	0	-1.748628	0.355071	3.867070
25	1	0	-2.636468	0.006119	4.404589

26	1	0	-0.874284	0.339247	4.520570
27	1	0	-1.939448	1.367032	3.491973
28	6	0	1.777657	1.019527	-0.212562
29	7	0	1.469898	2.334898	-0.183771
30	6	0	3.602215	2.237403	-0.709097
31	6	0	2.584931	3.103065	-0.484817
32	1	0	4.640634	2.395716	-0.969693
33	1	0	2.539222	4.184111	-0.503689
34	7	0	3.086197	0.962462	-0.537950
35	6	0	3.843409	-0.255491	-0.653682
36	6	0	3.929413	-0.867128	-1.907983
37	6	0	4.450542	-0.764328	0.498637
38	6	0	4.670905	-2.045092	-1.992343
39	6	0	5.182511	-1.943633	0.365040
40	6	0	5.292037	-2.576716	-0.867817
41	1	0	4.761512	-2.545367	-2.955725
42	1	0	5.673113	-2.364182	1.241994
43	1	0	5.871506	-3.493866	-0.954107
44	6	0	0.177286	2.863157	0.154647
45	6	0	-0.169696	2.958833	1.506730
46	6	0	-0.662909	3.275073	-0.885763
47	6	0	-1.420899	3.499702	1.808383
48	6	0	-1.893872	3.828445	-0.532467
49	6	0	-2.273606	3.933956	0.800933
50	1	0	-1.713746	3.608331	2.852588
51	1	0	-2.553344	4.198023	-1.318073
52	1	0	-3.237246	4.368681	1.057924
53	6	0	0.754344	2.487673	2.589114
54	1	0	1.800530	2.757581	2.391508
55	1	0	0.472138	2.915948	3.557775
56	1	0	0.719804	1.390368	2.686392
57	6	0	-0.263017	3.105470	-2.320326
58	1	0	0.638180	3.679746	-2.574206
59	1	0	-0.043615	2.051694	-2.550311
60	1	0	-1.063062	3.436416	-2.991890
61	6	0	3.245030	-0.282985	-3.106852
62	1	0	3.598880	0.733537	-3.328285
63	1	0	3.424191	-0.896778	-3.995945
64	1	0	2.157110	-0.216543	-2.958912
65	6	0	4.304939	-0.078157	1.823539
66	1	0	4.586676	0.982852	1.774271
67	1	0	3.265572	-0.115622	2.182952
68	1	0	4.934741	-0.555428	2.581804
69	1	0	-3.627630	-4.135787	1.317088
70	1	0	0.549098	-3.621703	0.318776

Zero-point correction= 0.560904 (Hartree/Particle)
Thermal correction to Energy= 0.597520
Thermal correction to Enthalpy= 0.598464
Thermal correction to Gibbs Free Energy= 0.490474
Sum of electronic and zero-point Energies= -1761.473838
Sum of electronic and thermal Energies= -1761.437222
Sum of electronic and thermal Enthalpies= -1761.436278
Sum of electronic and thermal Free Energies= -1761.544268
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.85812975

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.714899	-0.976848	-0.232815
2	6	0	2.850018	-0.269546	-0.078952
3	79	0	-0.200323	-0.184767	-0.127314
4	6	0	1.809684	-2.442975	-0.484024
5	8	0	0.746392	-3.086924	0.007756
6	6	0	3.048067	1.184146	0.043359
7	6	0	2.255443	2.074809	-0.691105
8	6	0	4.035912	1.698706	0.893237
9	6	0	2.433605	3.444969	-0.558143
10	1	0	1.506468	1.684067	-1.380193
11	6	0	4.207723	3.070221	1.027614
12	1	0	4.656639	1.020135	1.480043
13	6	0	3.404351	3.947124	0.304129
14	1	0	1.808230	4.123081	-1.135801
15	1	0	4.967568	3.455747	1.704533

16	1	0	3.541733	5.022061	0.405616
17	8	0	2.706085	-3.004379	-1.085157
18	6	0	6.008634	-2.056356	-0.483902
19	6	0	5.455962	-2.529581	0.669512
20	6	0	5.107655	-1.073612	-0.912915
21	7	0	4.117474	-0.991869	-0.048690
22	8	0	4.321202	-1.889558	0.957388
23	1	0	6.920281	-2.375638	-0.968114
24	6	0	0.731191	-4.497762	-0.201889
25	1	0	-0.170936	-4.859157	0.295255
26	1	0	0.695777	-4.722165	-1.273366
27	1	0	1.625278	-4.961951	0.228103
28	6	0	-2.158338	0.448063	0.037229
29	7	0	-3.225415	-0.374249	0.163283
30	6	0	-4.054790	1.658629	0.204446
31	6	0	-4.401664	0.351371	0.269158
32	1	0	-4.644467	2.565107	0.246958
33	1	0	-5.361963	-0.135653	0.379159
34	7	0	-2.675519	1.696661	0.059770
35	6	0	-1.907080	2.908567	-0.001480
36	6	0	-1.754664	3.535622	-1.242391
37	6	0	-1.375172	3.417024	1.187706
38	6	0	-1.059987	4.744662	-1.268049
39	6	0	-0.683264	4.626229	1.113015
40	6	0	-0.538420	5.289369	-0.099364
41	1	0	-0.937854	5.263588	-2.218534
42	1	0	-0.261326	5.049816	2.023777
43	1	0	-0.009425	6.240639	-0.135277
44	6	0	-3.136049	-1.808510	0.208112
45	6	0	-2.974845	-2.421700	1.454358
46	6	0	-3.207603	-2.517732	-0.994723
47	6	0	-2.905074	-3.814647	1.477415
48	6	0	-3.129089	-3.908362	-0.923955
49	6	0	-2.988226	-4.550915	0.300935
50	1	0	-2.790647	-4.321056	2.435330
51	1	0	-3.191131	-4.488720	-1.843934
52	1	0	-2.947028	-5.638476	0.339638
53	6	0	-2.860988	-1.612801	2.710540
54	1	0	-3.706241	-0.922664	2.839475
55	1	0	-2.824911	-2.262937	3.591360
56	1	0	-1.946697	-1.000662	2.708008
57	6	0	-3.350594	-1.810773	-2.308156
58	1	0	-4.205298	-1.120674	-2.315328
59	1	0	-2.456801	-1.213301	-2.540066
60	1	0	-3.492770	-2.528569	-3.123149
61	6	0	-2.310716	2.925785	-2.493363
62	1	0	-3.404553	2.828633	-2.457058
63	1	0	-2.061231	3.534512	-3.369120
64	1	0	-1.908299	1.915595	-2.658399
65	6	0	-1.516223	2.678856	2.484067
66	1	0	-2.532950	2.292109	2.638202
67	1	0	-0.837858	1.812708	2.516464
68	1	0	-1.267099	3.325619	3.332394
69	1	0	5.750776	-3.286675	1.384617
70	1	0	5.104883	-0.437660	-1.790827

Zero-point correction= 0.562540 (Hartree/Particle)
Thermal correction to Energy= 0.599903
Thermal correction to Enthalpy= 0.600847
Thermal correction to Gibbs Free Energy= 0.489155
Sum of electronic and zero-point Energies= -1761.458176
Sum of electronic and thermal Energies= -1761.420813
Sum of electronic and thermal Enthalpies= -1761.419869
Sum of electronic and thermal Free Energies= -1761.531561
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.85056194

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333791	-1.452518	-0.150099
2	6	0	2.600579	-0.968335	-0.643672
3	79	0	-0.370164	-0.367258	0.002546
4	6	0	1.323612	-2.865045	0.254890

5	8	0	1.523396	-3.121518	1.524034
6	6	0	2.734875	0.391283	-1.209053
7	6	0	1.876687	0.828461	-2.224936
8	6	0	3.753404	1.234153	-0.750977
9	6	0	2.058788	2.081810	-2.795761
10	1	0	1.088990	0.168467	-2.592071
11	6	0	3.914493	2.496952	-1.307453
12	1	0	4.398347	0.900791	0.062027
13	6	0	3.074942	2.916800	-2.336024
14	1	0	1.411597	2.404932	-3.609229
15	1	0	4.699558	3.154345	-0.939256
16	1	0	3.214571	3.899139	-2.784450
17	8	0	1.071083	-3.644376	-0.640093
18	6	0	5.987879	-1.756261	-0.310924
19	6	0	5.863848	-1.922565	1.130070
20	6	0	4.841466	-1.623005	-1.016979
21	7	0	3.600185	-1.791001	-0.478818
22	8	0	4.811558	-1.736839	1.716923
23	1	0	6.955916	-1.749081	-0.802730
24	6	0	1.493355	-4.512471	1.890267
25	1	0	1.666542	-4.534193	2.965864
26	1	0	0.519720	-4.945452	1.641766
27	1	0	2.283134	-5.052420	1.360132
28	6	0	-2.042240	0.822408	0.288724
29	7	0	-3.344923	0.520338	0.108674
30	6	0	-3.312992	2.603271	0.812754
31	6	0	-4.145382	1.605103	0.423850
32	1	0	-3.505819	3.615203	1.144719
33	1	0	-5.223089	1.557401	0.336534
34	7	0	-2.026342	2.101877	0.721101
35	6	0	-0.817842	2.824716	1.015887
36	6	0	-0.220108	3.551812	-0.018668
37	6	0	-0.287405	2.739392	2.306674
38	6	0	0.966241	4.221601	0.275169
39	6	0	0.902386	3.424784	2.552540
40	6	0	1.523151	4.156527	1.547225
41	1	0	1.454894	4.800248	-0.508233
42	1	0	1.340954	3.381082	3.548659
43	1	0	2.449474	4.687390	1.759396
44	6	0	-3.821111	-0.745600	-0.382334
45	6	0	-4.221598	-1.708749	0.549055
46	6	0	-3.850141	-0.949279	-1.765556
47	6	0	-4.679473	-2.926857	0.048971
48	6	0	-4.317673	-2.182656	-2.218270
49	6	0	-4.728684	-3.160579	-1.320542
50	1	0	-5.001100	-3.698240	0.747584
51	1	0	-4.358166	-2.372137	-3.290172
52	1	0	-5.092410	-4.116313	-1.692588
53	6	0	-4.151890	-1.442724	2.022653
54	1	0	-4.820246	-0.625095	2.326578
55	1	0	-4.440016	-2.332004	2.593164
56	1	0	-3.137004	-1.156868	2.335603
57	6	0	-3.378467	0.103608	-2.723624
58	1	0	-3.762150	1.101466	-2.470193
59	1	0	-2.279632	0.175865	-2.729779
60	1	0	-3.696139	-0.129200	-3.745731
61	6	0	-0.825026	3.591642	-1.389230
62	1	0	-1.861898	3.954953	-1.374767
63	1	0	-0.250890	4.250894	-2.050032
64	1	0	-0.844581	2.590962	-1.848221
65	6	0	-0.957271	1.929788	3.375748
66	1	0	-2.023165	2.175411	3.475638
67	1	0	-0.896567	0.852229	3.162447
68	1	0	-0.482536	2.099502	4.347969
69	1	0	6.767881	-2.261389	1.677526
70	1	0	4.862845	-1.425970	-2.095164

Zero-point correction= 0.556994 (Hartree/Particle)
Thermal correction to Energy= 0.596438
Thermal correction to Enthalpy= 0.597382
Thermal correction to Gibbs Free Energy= 0.479000
Sum of electronic and zero-point Energies= -1761.444252
Sum of electronic and thermal Energies= -1761.404808
Sum of electronic and thermal Enthalpies= -1761.403864
Sum of electronic and thermal Free Energies= -1761.522246

M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83417431

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.435045	-1.335014	-0.409364
2	6	0	2.650714	-0.755256	-0.922577
3	79	0	-0.311710	-0.342141	-0.120699
4	6	0	1.487968	-2.731025	0.043031
5	8	0	1.590742	-2.896806	1.344384
6	6	0	2.683439	0.654059	-1.375187
7	6	0	1.695692	1.168626	-2.222376
8	6	0	3.768671	1.455789	-1.007643
9	6	0	1.804286	2.465271	-2.709421
10	1	0	0.866848	0.536526	-2.545972
11	6	0	3.859061	2.759143	-1.478110
12	1	0	4.530452	1.042946	-0.348494
13	6	0	2.883106	3.262305	-2.335200
14	1	0	1.053565	2.847818	-3.398846
15	1	0	4.701071	3.382186	-1.183203
16	1	0	2.967682	4.277540	-2.720076
17	8	0	1.388994	-3.594264	-0.805201
18	6	0	4.925215	-3.155202	0.252335
19	6	0	5.234630	-2.200013	1.286947
20	6	0	4.159746	-2.676463	-0.766991
21	7	0	3.786073	-1.393367	-0.884534
22	8	0	4.758203	-1.070883	1.286931
23	1	0	5.324638	-4.163760	0.240694
24	6	0	1.642441	-4.261809	1.795488
25	1	0	1.711542	-4.207951	2.881806
26	1	0	0.738448	-4.795082	1.487277
27	1	0	2.523922	-4.756572	1.373959
28	6	0	-1.978169	0.781600	0.376748
29	7	0	-3.289127	0.483175	0.269989
30	6	0	-3.208270	2.501081	1.141338
31	6	0	-4.065725	1.531589	0.733697
32	1	0	-3.378186	3.479760	1.570985
33	1	0	-5.146851	1.482433	0.723434
34	7	0	-1.931597	2.020189	0.912066
35	6	0	-0.700038	2.713701	1.182456
36	6	0	-0.203374	3.576732	0.200390
37	6	0	-0.042747	2.455961	2.389344
38	6	0	1.013270	4.204462	0.460546
39	6	0	1.173666	3.104228	2.602599
40	6	0	1.697043	3.967228	1.647286
41	1	0	1.427014	4.884507	-0.283072
42	1	0	1.711444	2.926307	3.532962
43	1	0	2.648099	4.463700	1.830939
44	6	0	-3.795714	-0.747242	-0.276882
45	6	0	-4.119650	-1.779513	0.609205
46	6	0	-3.927967	-0.849978	-1.665150
47	6	0	-4.608344	-2.962867	0.057337
48	6	0	-4.422739	-2.052037	-2.170314
49	6	0	-4.760456	-3.096663	-1.318097
50	1	0	-4.872887	-3.786089	0.719842
51	1	0	-4.543999	-2.163394	-3.247074
52	1	0	-5.147566	-4.026215	-1.730721
53	6	0	-3.940811	-1.618854	2.088963
54	1	0	-4.612326	-0.854518	2.504464
55	1	0	-4.150952	-2.558321	2.611128
56	1	0	-2.915401	-1.313000	2.343563
57	6	0	-3.537469	0.275667	-2.575925
58	1	0	-3.918863	1.245528	-2.228200
59	1	0	-2.442899	0.370903	-2.650458
60	1	0	-3.919693	0.107963	-3.588603
61	6	0	-0.946961	3.805600	-1.080411
62	1	0	-1.937328	4.250233	-0.909638
63	1	0	-0.390265	4.483160	-1.737401
64	1	0	-1.110086	2.864187	-1.627320
65	6	0	-0.608136	1.506345	3.402670
66	1	0	-1.672295	1.693972	3.600090
67	1	0	-0.524733	0.461772	3.065854
68	1	0	-0.071238	1.587620	4.353877

69	1	0	3.873465	-3.312476	-1.610336
70	1	0	5.957024	-2.501632	2.071797

Zero-point correction= 0.557096 (Hartree/Particle)
Thermal correction to Energy= 0.596126
Thermal correction to Enthalpy= 0.597070
Thermal correction to Gibbs Free Energy= 0.481081
Sum of electronic and zero-point Energies= -1761.439502
Sum of electronic and thermal Energies= -1761.400473
Sum of electronic and thermal Enthalpies= -1761.399529
Sum of electronic and thermal Free Energies= -1761.515517
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.82743171

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.761613	2.050668	-0.211609
2	6	0	-2.188404	1.904190	0.053661
3	79	0	0.395980	0.386925	-0.050261
4	6	0	-0.280972	3.339763	-0.720118
5	8	0	0.087893	4.265918	0.125975
6	6	0	-3.096205	1.052190	-0.692294
7	6	0	-4.347106	0.681235	-0.181921
8	6	0	-2.713745	0.648585	-1.979244
9	6	0	-5.198578	-0.095422	-0.951595
10	1	0	-4.645522	0.999340	0.815199
11	6	0	-3.573646	-0.124611	-2.745739
12	1	0	-1.753113	0.971091	-2.384101
13	6	0	-4.813848	-0.495269	-2.231264
14	1	0	-6.170300	-0.386647	-0.558827
15	1	0	-3.283220	-0.427305	-3.749920
16	1	0	-5.492136	-1.095728	-2.835188
17	8	0	-0.248535	3.373137	-1.934568
18	6	0	-3.146171	1.549325	3.175205
19	6	0	-2.383505	0.311937	3.100883
20	6	0	-3.094567	2.534101	2.243418
21	7	0	-2.310464	2.578523	1.132957
22	8	0	-1.668415	-0.017173	2.168096
23	1	0	-3.748239	1.724716	4.063983
24	1	0	-2.485518	-0.353935	3.987185
25	1	0	-3.625310	3.471710	2.428942
26	6	0	0.589002	5.479609	-0.468404
27	1	0	1.467508	5.258566	-1.081504
28	1	0	-0.185994	5.941082	-1.087018
29	1	0	0.851937	6.124764	0.369416
30	6	0	1.459657	-1.381496	-0.021133
31	7	0	0.902018	-2.612228	-0.020730
32	6	0	3.073101	-2.946327	-0.047024
33	6	0	1.879325	-3.591111	-0.035934
34	1	0	4.091311	-3.313110	-0.056208
35	1	0	1.628262	-4.643856	-0.035243
36	7	0	2.792490	-1.590960	-0.038880
37	6	0	3.778647	-0.544170	-0.012100
38	6	0	4.167242	-0.037270	1.231701
39	6	0	4.291273	-0.085280	-1.229178
40	6	0	5.129177	0.972602	1.234997
41	6	0	5.248511	0.927025	-1.175774
42	6	0	5.664824	1.448488	0.043997
43	1	0	5.459848	1.384886	2.187567
44	1	0	5.670962	1.305292	-2.105844
45	1	0	6.418080	2.233689	0.066492
46	6	0	-0.517508	-2.846078	0.025418
47	6	0	-1.229234	-2.870617	-1.178343
48	6	0	-1.114029	-3.007358	1.278995
49	6	0	-2.605491	-3.077935	-1.099555
50	6	0	-2.493221	-3.208370	1.306888
51	6	0	-3.231479	-3.243329	0.130704
52	1	0	-3.188214	-3.112340	-2.019804
53	1	0	-2.987888	-3.335005	2.269710
54	1	0	-4.307488	-3.405377	0.170937
55	6	0	-0.547981	-2.655622	-2.496253
56	1	0	0.346130	-3.283136	-2.611807
57	1	0	-1.225760	-2.882626	-3.326937

58	1	0	-0.218713	-1.610998	-2.611833
59	6	0	-0.309741	-2.928009	2.539655
60	1	0	0.528810	-3.637727	2.547855
61	1	0	0.107125	-1.919141	2.669958
62	1	0	-0.935771	-3.143037	3.413111
63	6	0	3.559492	-0.541489	2.506308
64	1	0	3.529675	-1.638947	2.548951
65	1	0	4.124881	-0.187023	3.374891
66	1	0	2.522826	-0.190538	2.621516
67	6	0	3.821264	-0.653600	-2.534118
68	1	0	4.040799	-1.726969	-2.619196
69	1	0	2.733950	-0.540143	-2.655813
70	1	0	4.305973	-0.149180	-3.376653

Zero-point correction= 0.557478 (Hartree/Particle)
Thermal correction to Energy= 0.596864
Thermal correction to Enthalpy= 0.597808
Thermal correction to Gibbs Free Energy= 0.481402
Sum of electronic and zero-point Energies= -1761.451602
Sum of electronic and thermal Energies= -1761.412216
Sum of electronic and thermal Enthalpies= -1761.411272
Sum of electronic and thermal Free Energies= -1761.527678
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83440866

INT6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.935102	1.885717	-0.373734
2	6	0	-2.264782	1.754287	0.214322
3	79	0	0.305206	0.315954	-0.116731
4	6	0	-0.659283	3.070332	-1.191219
5	8	0	-0.405621	4.197315	-0.568963
6	6	0	-3.300962	0.894571	-0.342056
7	6	0	-3.134456	0.356226	-1.623824
8	6	0	-4.468976	0.640892	0.385447
9	6	0	-4.137548	-0.427501	-2.176926
10	1	0	-2.229703	0.571771	-2.194894
11	6	0	-5.462680	-0.148641	-0.170764
12	1	0	-4.580744	1.069587	1.379872
13	6	0	-5.299152	-0.678681	-1.451415
14	1	0	-4.015594	-0.837797	-3.177658
15	1	0	-6.373582	-0.348487	0.389435
16	1	0	-6.087569	-1.290135	-1.887063
17	8	0	-0.708101	2.863976	-2.385360
18	6	0	-0.727388	2.990347	3.039069
19	6	0	-0.159892	1.682842	3.277193
20	6	0	-1.663573	3.260187	2.092768
21	7	0	-2.354421	2.383754	1.322468
22	8	0	-0.388146	0.679627	2.608629
23	6	0	-0.126196	5.328195	-1.423185
24	1	0	0.092392	6.154306	-0.747185
25	1	0	0.735025	5.107419	-2.059855
26	1	0	-0.998943	5.550350	-2.043445
27	6	0	1.366607	-1.451988	-0.060007
28	7	0	0.805396	-2.674602	0.051851
29	6	0	2.971791	-3.022077	-0.074117
30	6	0	1.778115	-3.657683	0.044648
31	1	0	3.986765	-3.395722	-0.113422
32	1	0	1.525545	-4.706516	0.131008
33	7	0	2.695311	-1.667696	-0.140405
34	6	0	3.674560	-0.617686	-0.224826
35	6	0	4.077352	0.001120	0.963251
36	6	0	4.157574	-0.259590	-1.486797
37	6	0	5.026174	1.017961	0.859968
38	6	0	5.104096	0.763122	-1.539507
39	6	0	5.535939	1.392839	-0.377906
40	1	0	5.369428	1.515251	1.766408
41	1	0	5.503906	1.064326	-2.506955
42	1	0	6.279761	2.185039	-0.437959
43	6	0	-0.609103	-2.889856	0.216210
44	6	0	-1.398222	-3.036502	-0.929690
45	6	0	-1.122461	-2.910710	1.517390
46	6	0	-2.765484	-3.228730	-0.740503

47	6	0	-2.498118	-3.100204	1.653812
48	6	0	-3.310082	-3.259528	0.538160
49	1	0	-3.406989	-3.356415	-1.612002
50	1	0	-2.929187	-3.126198	2.653848
51	1	0	-4.380424	-3.413004	0.665477
52	6	0	-0.804711	-2.965866	-2.304423
53	1	0	0.014264	-3.685099	-2.442360
54	1	0	-1.563363	-3.176444	-3.066655
55	1	0	-0.388905	-1.968409	-2.514450
56	6	0	-0.245191	-2.703656	2.714246
57	1	0	0.700679	-3.256865	2.641992
58	1	0	-0.001389	-1.637371	2.835598
59	1	0	-0.754492	-3.030563	3.627537
60	6	0	3.504169	-0.404282	2.288575
61	1	0	3.580531	-1.487650	2.456578
62	1	0	4.029728	0.097079	3.108571
63	1	0	2.436214	-0.147117	2.367216
64	6	0	3.667031	-0.939960	-2.729114
65	1	0	3.928767	-2.007060	-2.745830
66	1	0	2.572458	-0.878778	-2.818213
67	1	0	4.101516	-0.480347	-3.623101
68	1	0	-0.394797	3.813992	3.666192
69	1	0	0.537986	1.623204	4.140289
70	1	0	-2.029913	4.286757	2.000680

Zero-point correction= 0.557437 (Hartree/Particle)
Thermal correction to Energy= 0.596738
Thermal correction to Enthalpy= 0.597682
Thermal correction to Gibbs Free Energy= 0.481921
Sum of electronic and zero-point Energies= -1761.450593
Sum of electronic and thermal Energies= -1761.411293
Sum of electronic and thermal Enthalpies= -1761.410348
Sum of electronic and thermal Free Energies= -1761.526109
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.83284413

INT6d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683289	-1.831559	0.854400
2	6	0	-1.649831	-2.133297	-0.247381
3	79	0	0.245265	0.097178	0.357450
4	6	0	-1.218451	-1.623477	2.238778
5	8	0	-0.351392	-2.042345	3.182064
6	6	0	-2.950912	-1.424941	-0.338793
7	6	0	-4.087522	-2.209332	-0.565216
8	6	0	-3.096088	-0.038184	-0.238473
9	6	0	-5.341342	-1.626932	-0.688528
10	1	0	-3.987691	-3.292944	-0.622381
11	6	0	-4.348005	0.543876	-0.379490
12	1	0	-2.227112	0.599496	-0.062893
13	6	0	-5.472753	-0.245459	-0.601444
14	1	0	-6.215629	-2.253536	-0.851919
15	1	0	-4.442578	1.625814	-0.306384
16	1	0	-6.452814	0.217085	-0.702638
17	8	0	-2.281699	-1.113858	2.486994
18	6	0	-1.800423	-2.506849	-3.391939
19	6	0	-1.178280	-1.202147	-3.449285
20	6	0	-1.852808	-3.306758	-2.294241
21	7	0	-1.303483	-3.052789	-1.074524
22	8	0	-0.608310	-0.615825	-2.534017
23	1	0	-2.212051	-2.894306	-4.321752
24	1	0	-2.271853	-4.311650	-2.407354
25	1	0	-1.225358	-0.724426	-4.453919
26	7	0	0.384502	-2.815451	0.827214
27	6	0	0.452446	-4.070054	1.226579
28	6	0	1.636620	-4.645983	0.753126
29	1	0	-0.343629	-4.481925	1.835327
30	6	0	2.219443	-3.646592	0.028196
31	1	0	1.998602	-5.650583	0.918850
32	1	0	3.139926	-3.558379	-0.536778
33	8	0	1.480909	-2.541670	0.058302
34	6	0	-0.761402	-1.767879	4.525032
35	1	0	-1.720565	-2.248694	4.740760

36	1	0	0.025566	-2.170400	5.164686
37	1	0	-0.864777	-0.688473	4.675351
38	6	0	1.267948	1.810350	-0.095272
39	7	0	2.578525	1.885024	-0.415377
40	6	0	1.832140	3.950182	-0.501690
41	6	0	2.945830	3.197952	-0.671404
42	1	0	1.657668	5.013644	-0.600280
43	1	0	3.958380	3.459765	-0.949697
44	7	0	0.813723	3.078415	-0.146717
45	6	0	-0.561238	3.447820	0.052129
46	6	0	-0.975943	3.802698	1.339067
47	6	0	-1.414428	3.411318	-1.055728
48	6	0	-2.314870	4.153810	1.503449
49	6	0	-2.741725	3.787506	-0.845250
50	6	0	-3.186110	4.155684	0.419757
51	1	0	-2.670777	4.435640	2.493471
52	1	0	-3.430402	3.785058	-1.690005
53	1	0	-4.225216	4.447125	0.564158
54	6	0	3.435640	0.740459	-0.555802
55	6	0	3.473532	0.101274	-1.799722
56	6	0	4.174767	0.316669	0.553640
57	6	0	4.320621	-1.002288	-1.923346
58	6	0	4.999064	-0.796171	0.386387
59	6	0	5.080268	-1.441897	-0.844029
60	1	0	4.392795	-1.505132	-2.887597
61	1	0	5.599376	-1.140043	1.228134
62	1	0	5.758593	-2.285828	-0.966979
63	6	0	2.618664	0.562088	-2.939922
64	1	0	2.669307	1.650122	-3.082564
65	1	0	2.931355	0.086419	-3.876096
66	1	0	1.559603	0.307631	-2.771168
67	6	0	4.069829	1.022626	1.870987
68	1	0	4.311007	2.090825	1.785796
69	1	0	3.049766	0.958689	2.277661
70	1	0	4.753907	0.584601	2.605742
71	6	0	-0.022188	3.788516	2.494777
72	1	0	0.839733	4.448824	2.326441
73	1	0	-0.519038	4.116442	3.414050
74	1	0	0.378632	2.779333	2.671040
75	6	0	-0.934661	2.946426	-2.397109
76	1	0	0.024293	3.403815	-2.677932
77	1	0	-0.786366	1.853982	-2.409719
78	1	0	-1.664781	3.191418	-3.176340

Zero-point correction= 0.622131 (Hartree/Particle)
Thermal correction to Energy= 0.664408
Thermal correction to Enthalpy= 0.665352
Thermal correction to Gibbs Free Energy= 0.545052
Sum of electronic and zero-point Energies= -2007.337245
Sum of electronic and thermal Energies= -2007.294969
Sum of electronic and thermal Enthalpies= -2007.294025
Sum of electronic and thermal Free Energies= -2007.414324
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.85726827

INT7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.213339	-1.592835	0.997713
2	6	0	-2.220175	-1.626052	-0.012017
3	79	0	0.299737	-0.226367	0.482911
4	6	0	-1.607818	-1.772344	2.425608
5	8	0	-1.547377	-3.041419	2.817629
6	6	0	-3.300756	-0.950456	-0.615991
7	6	0	-4.058729	-1.547155	-1.639314
8	6	0	-3.605654	0.337308	-0.139472
9	6	0	-5.129223	-0.856760	-2.173565
10	1	0	-3.800920	-2.546289	-1.988411
11	6	0	-4.674137	1.022479	-0.693428
12	1	0	-2.997135	0.775234	0.654017
13	6	0	-5.431790	0.424023	-1.700200
14	1	0	-5.733807	-1.303725	-2.958838
15	1	0	-4.924962	2.018943	-0.336892
16	1	0	-6.276689	0.962566	-2.125661

17	8	0	-1.919185	-0.831046	3.115299
18	6	0	-0.434049	-3.475911	-2.020977
19	6	0	-0.603874	-2.279894	-2.850864
20	6	0	-0.823257	-3.632904	-0.740800
21	7	0	-1.568348	-2.755993	0.031078
22	8	0	-1.088539	-1.228074	-2.474301
23	1	0	0.128009	-4.297292	-2.462519
24	1	0	-0.212602	-2.377606	-3.886491
25	1	0	-0.533028	-4.522389	-0.183996
26	6	0	-1.894252	-3.268532	4.189560
27	1	0	-1.229639	-2.698274	4.845919
28	1	0	-2.929005	-2.963736	4.374620
29	1	0	-1.773245	-4.339995	4.353094
30	6	0	1.621932	1.238632	-0.094981
31	7	0	1.315967	2.547201	-0.225783
32	6	0	3.424367	2.374035	-0.821236
33	6	0	2.414255	3.265546	-0.672206
34	1	0	4.450030	2.493799	-1.145250
35	1	0	2.364064	4.333450	-0.840003
36	7	0	2.916815	1.135061	-0.460300
37	6	0	3.634526	-0.109398	-0.508258
38	6	0	3.545403	-0.874451	-1.675691
39	6	0	4.361940	-0.503581	0.617995
40	6	0	4.234275	-2.086381	-1.699356
41	6	0	5.037126	-1.721987	0.547409
42	6	0	4.974922	-2.504712	-0.599384
43	1	0	4.191978	-2.702487	-2.597180
44	1	0	5.616893	-2.055842	1.407033
45	1	0	5.511748	-3.450712	-0.637100
46	6	0	0.004251	3.086412	0.013599
47	6	0	-0.283189	3.589640	1.287544
48	6	0	-0.925810	3.056956	-1.030436
49	6	0	-1.562219	4.101588	1.500756
50	6	0	-2.188806	3.593810	-0.773583
51	6	0	-2.503529	4.111820	0.476922
52	1	0	-1.814979	4.502031	2.481538
53	1	0	-2.927614	3.604161	-1.575368
54	1	0	-3.490758	4.535332	0.656647
55	6	0	0.737679	3.556616	2.383997
56	1	0	1.666967	4.068807	2.099895
57	1	0	0.353805	4.038205	3.289405
58	1	0	1.008434	2.523200	2.645745
59	6	0	-0.612573	2.436237	-2.358429
60	1	0	0.429228	2.597931	-2.665255
61	1	0	-0.777838	1.347033	-2.333833
62	1	0	-1.261416	2.845428	-3.141259
63	6	0	2.733745	-0.409490	-2.847408
64	1	0	3.067617	0.570639	-3.216262
65	1	0	2.810067	-1.117995	-3.680280
66	1	0	1.669530	-0.300569	-2.587683
67	6	0	4.399543	0.343352	1.853850
68	1	0	4.803922	1.345333	1.654854
69	1	0	3.393633	0.484051	2.275729
70	1	0	5.023536	-0.119429	2.625693

Zero-point correction= 0.558458 (Hartree/Particle)
Thermal correction to Energy= 0.597492
Thermal correction to Enthalpy= 0.598436
Thermal correction to Gibbs Free Energy= 0.482710
Sum of electronic and zero-point Energies= -1761.458668
Sum of electronic and thermal Energies= -1761.419634
Sum of electronic and thermal Enthalpies= -1761.418689
Sum of electronic and thermal Free Energies= -1761.534415
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.84347487

INT8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.657094	2.331455	0.415405
2	6	0	-1.939518	1.717328	0.553719
3	79	0	0.201757	0.283324	0.070575
4	6	0	-0.173680	3.130964	-0.744765
5	8	0	0.791380	3.970475	-0.338800

6	6	0	-2.913215	1.243463	-0.410636
7	6	0	-2.604690	0.975084	-1.758794
8	6	0	-4.229685	1.026465	0.044050
9	6	0	-3.588958	0.523966	-2.621313
10	1	0	-1.594095	1.129384	-2.125264
11	6	0	-5.212888	0.597924	-0.832760
12	1	0	-4.463600	1.211048	1.088904
13	6	0	-4.895266	0.345810	-2.165123
14	1	0	-3.339949	0.318044	-3.660139
15	1	0	-6.230784	0.456183	-0.475790
16	1	0	-5.667653	0.004862	-2.852491
17	8	0	-0.558845	3.054756	-1.887284
18	6	0	-0.261357	2.740836	1.829720
19	6	0	1.104753	2.221184	2.264401
20	6	0	-1.379756	2.160218	2.614557
21	7	0	-2.298067	1.594058	1.912895
22	8	0	1.258021	1.476454	3.199931
23	6	0	1.355904	4.792034	-1.368333
24	1	0	2.106591	5.410241	-0.874472
25	1	0	1.815049	4.167742	-2.141249
26	1	0	0.580690	5.415264	-1.823900
27	6	0	0.963031	-1.599376	-0.094067
28	7	0	0.206115	-2.704864	0.058395
29	6	0	2.255460	-3.416972	-0.294325
30	6	0	0.987577	-3.841474	-0.061879
31	1	0	3.180569	-3.958148	-0.444538
32	1	0	0.566606	-4.833779	0.033630
33	7	0	2.218241	-2.031063	-0.310518
34	6	0	3.351631	-1.158887	-0.475584
35	6	0	4.007829	-0.705354	0.673140
36	6	0	3.722760	-0.795649	-1.774711
37	6	0	5.096384	0.148168	0.486109
38	6	0	4.815323	0.059130	-1.909805
39	6	0	5.495699	0.525496	-0.790041
40	1	0	5.637493	0.511292	1.359192
41	1	0	5.134548	0.356307	-2.907962
42	1	0	6.351822	1.185763	-0.914879
43	6	0	-1.203899	-2.640242	0.343804
44	6	0	-2.100764	-2.729013	-0.726985
45	6	0	-1.600625	-2.415134	1.666803
46	6	0	-3.457582	-2.602677	-0.434669
47	6	0	-2.969260	-2.287514	1.907868
48	6	0	-3.887137	-2.382910	0.869505
49	1	0	-4.181536	-2.669874	-1.246161
50	1	0	-3.311291	-2.115049	2.927573
51	1	0	-4.951308	-2.285397	1.078013
52	6	0	-1.621396	-2.930426	-2.132757
53	1	0	-1.122721	-3.900415	-2.265981
54	1	0	-2.459343	-2.890857	-2.837384
55	1	0	-0.897659	-2.156545	-2.429331
56	6	0	-0.606922	-2.280747	2.782135
57	1	0	0.234135	-2.979440	2.681637
58	1	0	-0.176786	-1.267040	2.821299
59	1	0	-1.083935	-2.465857	3.750825
60	6	0	3.557696	-1.093096	2.049742
61	1	0	3.217549	-2.135770	2.101888
62	1	0	4.371967	-0.970055	2.772308
63	1	0	2.725180	-0.460971	2.394963
64	6	0	2.965672	-1.292396	-2.969344
65	1	0	2.929049	-2.389556	-3.010586
66	1	0	1.924102	-0.938605	-2.961767
67	1	0	3.427965	-0.940936	-3.897753
68	1	0	-0.248885	3.841602	1.921408
69	1	0	1.951543	2.570991	1.632891
70	1	0	-1.428761	2.170642	3.703133

Zero-point correction= 0.561311 (Hartree/Particle)
Thermal correction to Energy= 0.598930
Thermal correction to Enthalpy= 0.599874
Thermal correction to Gibbs Free Energy= 0.489727
Sum of electronic and zero-point Energies= -1761.533478
Sum of electronic and thermal Energies= -1761.495858
Sum of electronic and thermal Enthalpies= -1761.494914
Sum of electronic and thermal Free Energies= -1761.605061
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.92410058

INT9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.725855	-0.505782	-0.552276
2	6	0	-2.745456	0.320118	0.160470
3	79	0	0.316888	-0.184390	-0.210542
4	6	0	-2.156271	-1.891741	-0.900829
5	8	0	-2.717959	-1.988183	-2.103889
6	6	0	-4.084901	-0.163039	0.566198
7	6	0	-5.232824	0.313535	-0.067947
8	6	0	-4.182599	-1.080083	1.615411
9	6	0	-6.482453	-0.127118	0.350634
10	1	0	-5.144443	1.019363	-0.893894
11	6	0	-5.434118	-1.512712	2.031929
12	1	0	-3.275688	-1.457199	2.087240
13	6	0	-6.581211	-1.036102	1.400607
14	1	0	-7.380719	0.238035	-0.142677
15	1	0	-5.517236	-2.230120	2.845306
16	1	0	-7.560423	-1.380507	1.727461
17	8	0	-1.970514	-2.810015	-0.138059
18	6	0	-2.341690	2.901410	-0.754473
19	6	0	-2.261231	2.578972	0.581564
20	6	0	-2.203884	1.818907	-1.637381
21	7	0	-2.498688	0.606934	-1.214387
22	8	0	-2.273104	1.360286	1.064365
23	1	0	-2.260502	3.933429	-1.073296
24	6	0	-3.117635	-3.311561	-2.474456
25	1	0	-2.251322	-3.980610	-2.484359
26	1	0	-3.858002	-3.696052	-1.765837
27	1	0	-3.548944	-3.222657	-3.472400
28	6	0	2.285528	0.270311	0.183185
29	7	0	3.329185	-0.553499	0.410099
30	6	0	4.145648	1.481492	0.582177
31	6	0	4.484014	0.171896	0.657914
32	1	0	4.726822	2.386125	0.705373
33	1	0	5.427094	-0.318739	0.861298
34	7	0	2.789694	1.521030	0.291027
35	6	0	2.016344	2.719766	0.126015
36	6	0	1.398899	3.271392	1.253781
37	6	0	1.925867	3.283378	-1.151470
38	6	0	0.683997	4.457480	1.077224
39	6	0	1.194537	4.464910	-1.281530
40	6	0	0.588780	5.052770	-0.176424
41	1	0	0.220490	4.928220	1.944875
42	1	0	1.120936	4.935019	-2.261820
43	1	0	0.048135	5.991227	-0.291038
44	6	0	3.240177	-1.989971	0.389894
45	6	0	3.464491	-2.647909	-0.822951
46	6	0	2.913747	-2.650125	1.578347
47	6	0	3.363575	-4.038341	-0.821747
48	6	0	2.821555	-4.040339	1.530016
49	6	0	3.045533	-4.727403	0.342739
50	1	0	3.536116	-4.581237	-1.750258
51	1	0	2.567656	-4.585345	2.438251
52	1	0	2.969947	-5.812750	0.324604
53	6	0	3.780629	-1.887614	-2.075580
54	1	0	4.654782	-1.232739	-1.955500
55	1	0	3.990661	-2.572925	-2.903692
56	1	0	2.939855	-1.245994	-2.379415
57	6	0	2.658423	-1.892719	2.846449
58	1	0	3.524048	-1.285638	3.146817
59	1	0	1.804957	-1.205903	2.742882
60	1	0	2.433442	-2.578890	3.669809
61	6	0	1.490952	2.606102	2.593338
62	1	0	2.531075	2.407973	2.885450
63	1	0	1.038342	3.228447	3.372979
64	1	0	0.973806	1.634429	2.593349
65	6	0	2.586262	2.638565	-2.331965
66	1	0	3.671930	2.541871	-2.194598
67	1	0	2.198670	1.623677	-2.504861
68	1	0	2.418533	3.223426	-3.242659
69	1	0	-2.104943	3.332175	1.353932
70	1	0	-1.810930	1.922095	-2.650168

Zero-point correction= 0.562527 (Hartree/Particle)
Thermal correction to Energy= 0.599341
Thermal correction to Enthalpy= 0.600285
Thermal correction to Gibbs Free Energy= 0.491374
Sum of electronic and zero-point Energies= -1761.466920
Sum of electronic and thermal Energies= -1761.430106
Sum of electronic and thermal Enthalpies= -1761.429162
Sum of electronic and thermal Free Energies= -1761.538073
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.85656729

INT10b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.089479	2.156949	-1.535471
2	6	0	0.939687	2.375074	-0.601705
3	79	0	0.054584	0.034447	-0.479650
4	6	0	-1.549577	2.201064	-1.134806
5	8	0	-2.318103	1.931390	-2.182886
6	6	0	0.888116	2.929570	0.754878
7	6	0	0.044425	3.990740	1.100408
8	6	0	1.780575	2.414599	1.708140
9	6	0	0.077632	4.507955	2.386750
10	1	0	-0.627904	4.416323	0.361213
11	6	0	1.789520	2.917810	2.999592
12	1	0	2.459335	1.608025	1.426432
13	6	0	0.936975	3.966256	3.339636
14	1	0	-0.568705	5.342928	2.647281
15	1	0	2.471986	2.504078	3.739576
16	1	0	0.951059	4.371254	4.349587
17	8	0	-1.966605	2.367226	-0.008730
18	6	0	2.100049	0.839090	-2.953321
19	6	0	2.599542	1.115389	-1.747354
20	6	0	1.079969	1.699985	-3.544948
21	7	0	0.135021	2.276502	-2.912138
22	8	0	2.235247	2.224424	-1.009719
23	1	0	2.509868	0.002087	-3.515694
24	6	0	-3.713075	1.802944	-1.896028
25	1	0	-4.193764	1.626432	-2.859066
26	1	0	-3.883337	0.958458	-1.214880
27	1	0	-4.095033	2.719419	-1.435866
28	6	0	-0.167266	-1.769933	0.439335
29	7	0	0.842733	-2.592363	0.790361
30	6	0	-0.987421	-3.510737	1.588191
31	6	0	0.355933	-3.676209	1.503384
32	1	0	-1.757751	-4.110244	2.055148
33	1	0	1.011887	-4.451222	1.878036
34	7	0	-1.290751	-2.330617	0.927008
35	6	0	-2.610790	-1.768059	0.794723
36	6	0	-3.470493	-2.332723	-0.155896
37	6	0	-2.970384	-0.694883	1.617789
38	6	0	-4.756685	-1.804256	-0.249661
39	6	0	-4.268200	-0.198559	1.483296
40	6	0	-5.155160	-0.752416	0.569229
41	1	0	-5.450660	-2.228057	-0.974513
42	1	0	-4.578365	0.634502	2.112712
43	1	0	-6.166273	-0.357404	0.488673
44	6	0	2.220542	-2.305516	0.493327
45	6	0	2.957838	-1.577186	1.434388
46	6	0	2.737780	-2.722445	-0.737036
47	6	0	4.277568	-1.263185	1.107399
48	6	0	4.063794	-2.388930	-1.018425
49	6	0	4.826646	-1.668365	-0.105518
50	1	0	4.881100	-0.703918	1.821630
51	1	0	4.500392	-2.711543	-1.963154
52	1	0	5.862247	-1.426308	-0.337453
53	6	0	2.353459	-1.144644	2.736549
54	1	0	2.023057	-1.999560	3.342195
55	1	0	3.080400	-0.581694	3.333085
56	1	0	1.473377	-0.500306	2.585914
57	6	0	1.896394	-3.474435	-1.722658
58	1	0	1.411693	-4.349423	-1.269205
59	1	0	1.093420	-2.841261	-2.129233

60	1	0	2.501714	-3.826827	-2.564686
61	6	0	-3.027538	-3.455973	-1.044583
62	1	0	-2.903600	-4.398719	-0.493744
63	1	0	-3.763884	-3.636465	-1.834827
64	1	0	-2.063766	-3.238079	-1.527115
65	6	0	-2.015665	-0.069157	2.589612
66	1	0	-1.332823	-0.800979	3.041737
67	1	0	-1.402640	0.700789	2.092333
68	1	0	-2.560862	0.429393	3.398710
69	1	0	3.395658	0.548245	-1.260717
70	1	0	1.128466	1.880916	-4.622965

Zero-point correction= 0.562386 (Hartree/Particle)
Thermal correction to Energy= 0.599387
Thermal correction to Enthalpy= 0.600331
Thermal correction to Gibbs Free Energy= 0.492594
Sum of electronic and zero-point Energies= -1761.495810
Sum of electronic and thermal Energies= -1761.458808
Sum of electronic and thermal Enthalpies= -1761.457864
Sum of electronic and thermal Free Energies= -1761.565601
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.88186930

1NT11b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.125824	-1.282656	0.643036
2	6	0	-3.123119	-1.652367	-0.204484
3	79	0	0.708404	-0.492345	0.183354
4	6	0	-2.301877	-0.217438	1.665531
5	8	0	-1.246417	-0.179502	2.501712
6	6	0	-4.300529	-0.894843	-0.608516
7	6	0	-5.515001	-1.558626	-0.823927
8	6	0	-4.206106	0.476249	-0.878511
9	6	0	-6.627874	-0.852798	-1.256894
10	1	0	-5.586737	-2.628704	-0.636957
11	6	0	-5.314966	1.173127	-1.328456
12	1	0	-3.250945	0.983460	-0.748870
13	6	0	-6.529478	0.513019	-1.508809
14	1	0	-7.574138	-1.368648	-1.404217
15	1	0	-5.233921	2.237092	-1.546070
16	1	0	-7.401083	1.064272	-1.856342
17	8	0	-3.275817	0.481961	1.803383
18	6	0	-1.716361	-4.159910	0.650024
19	6	0	-0.660450	-3.173251	0.674913
20	6	0	-2.795985	-3.980559	-0.119451
21	1	0	-1.563288	-5.121764	1.132131
22	8	0	-3.041374	-2.865064	-0.864889
23	7	0	-0.834039	-1.899822	0.606132
24	6	0	-1.390566	0.733186	3.589135
25	1	0	-2.236078	0.442249	4.220887
26	1	0	-0.455275	0.680153	4.149692
27	1	0	-1.566158	1.746660	3.212294
28	6	0	2.033116	0.948850	-0.316353
29	7	0	1.702424	2.247558	-0.485409
30	6	0	3.858643	2.122140	-0.891353
31	6	0	2.817732	2.988881	-0.841116
32	1	0	4.906076	2.265766	-1.122724
33	1	0	2.757723	4.054557	-1.019723
34	7	0	3.355495	0.871983	-0.564773
35	6	0	4.124597	-0.341358	-0.489398
36	6	0	4.306802	-1.081270	-1.661726
37	6	0	4.632587	-0.725142	0.755349
38	6	0	5.046534	-2.258999	-1.562269
39	6	0	5.366992	-1.909659	0.805114
40	6	0	5.572349	-2.667808	-0.341841
41	1	0	5.210776	-2.857221	-2.457592
42	1	0	5.782348	-2.235086	1.758144
43	1	0	6.152284	-3.586963	-0.285236
44	6	0	0.366872	2.749927	-0.301511
45	6	0	-0.007069	3.178713	0.976813
46	6	0	-0.500676	2.746152	-1.398575
47	6	0	-1.316301	3.630210	1.140918
48	6	0	-1.801808	3.203215	-1.183759

49	6	0	-2.206852	3.637816	0.073042
50	1	0	-1.638258	3.982768	2.120606
51	1	0	-2.501694	3.214359	-2.020045
52	1	0	-3.227369	3.984812	0.224631
53	6	0	0.955404	3.133811	2.124959
54	1	0	1.876973	3.694654	1.917607
55	1	0	0.505586	3.560709	3.028457
56	1	0	1.256562	2.100026	2.355277
57	6	0	-0.057665	2.253465	-2.742685
58	1	0	0.844888	2.770622	-3.095625
59	1	0	0.179029	1.179084	-2.720561
60	1	0	-0.842228	2.404278	-3.491768
61	6	0	3.724376	-0.628884	-2.966598
62	1	0	4.169672	0.315180	-3.310491
63	1	0	3.893356	-1.376812	-3.748533
64	1	0	2.639939	-0.460339	-2.890983
65	6	0	4.380380	0.091667	1.986726
66	1	0	4.588251	1.158600	1.826999
67	1	0	3.330586	0.017418	2.308462
68	1	0	5.005734	-0.251566	2.817803
69	1	0	-3.546271	-4.755974	-0.276417
70	1	0	0.374138	-3.524775	0.704894

Zero-point correction= 0.563991 (Hartree/Particle)
Thermal correction to Energy= 0.600564
Thermal correction to Enthalpy= 0.601508
Thermal correction to Gibbs Free Energy= 0.493750
Sum of electronic and zero-point Energies= -1761.509657
Sum of electronic and thermal Energies= -1761.473084
Sum of electronic and thermal Enthalpies= -1761.472140
Sum of electronic and thermal Free Energies= -1761.579899
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.89988870

INT12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.682901	-0.541338	-0.833073
2	6	0	-2.559188	0.239882	0.144889
3	79	0	0.391346	0.012828	-0.446602
4	6	0	-1.512957	-2.003261	-0.488954
5	8	0	-1.211764	-2.718257	-1.581566
6	6	0	-2.552921	-0.126660	1.617425
7	6	0	-3.485445	-0.979824	2.201503
8	6	0	-1.557695	0.443677	2.413168
9	6	0	-3.411267	-1.277089	3.556097
10	1	0	-4.263298	-1.453569	1.607926
11	6	0	-1.478626	0.135504	3.765963
12	1	0	-0.848954	1.144400	1.972554
13	6	0	-2.404365	-0.727710	4.341710
14	1	0	-4.143037	-1.950750	3.997044
15	1	0	-0.695590	0.582695	4.376375
16	1	0	-2.346732	-0.965708	5.401910
17	8	0	-1.523680	-2.485755	0.625722
18	6	0	-1.711270	2.035316	-2.185098
19	6	0	-1.809083	2.340692	-0.884212
20	6	0	-2.079862	0.762215	-2.776648
21	7	0	-2.079292	-0.382610	-2.205476
22	8	0	-2.402953	1.633864	0.121292
23	1	0	-1.306679	2.812215	-2.833332
24	6	0	-0.745700	-4.035895	-1.317889
25	1	0	-0.558591	-4.485951	-2.294884
26	1	0	0.181749	-3.996972	-0.730894
27	1	0	-1.491308	-4.616436	-0.764377
28	6	0	2.344019	0.419332	0.035270
29	7	0	2.881008	1.629948	0.307217
30	6	0	4.480326	0.176425	0.702869
31	6	0	4.198008	1.501639	0.723455
32	1	0	5.380576	-0.372372	0.946907
33	1	0	4.798161	2.362515	0.987800
34	7	0	3.329202	-0.470228	0.277297
35	6	0	3.180867	-1.895799	0.149040
36	6	0	3.654357	-2.502738	-1.019946
37	6	0	2.563913	-2.602508	1.186443

38	6	0	3.533321	-3.887749	-1.117892
39	6	0	2.471000	-3.988647	1.045845
40	6	0	2.958273	-4.625525	-0.088642
41	1	0	3.897777	-4.388032	-2.014327
42	1	0	2.003373	-4.566539	1.842210
43	1	0	2.882265	-5.707882	-0.176405
44	6	0	2.127719	2.850945	0.247829
45	6	0	1.513482	3.302215	1.421767
46	6	0	2.007559	3.505296	-0.981574
47	6	0	0.754139	4.469737	1.342113
48	6	0	1.244347	4.673318	-1.013129
49	6	0	0.626551	5.152994	0.136792
50	1	0	0.269613	4.848043	2.241637
51	1	0	1.145366	5.213240	-1.954602
52	1	0	0.044915	6.072502	0.095964
53	6	0	1.664014	2.555164	2.712704
54	1	0	2.683766	2.635890	3.114653
55	1	0	0.978850	2.949116	3.472318
56	1	0	1.457635	1.480861	2.588565
57	6	0	2.654424	2.963404	-2.219292
58	1	0	3.712793	2.719505	-2.056916
59	1	0	2.162796	2.037500	-2.553094
60	1	0	2.597281	3.687571	-3.039250
61	6	0	4.244203	-1.690729	-2.133252
62	1	0	5.162892	-1.169817	-1.830050
63	1	0	4.494097	-2.327479	-2.988639
64	1	0	3.540277	-0.920699	-2.483186
65	6	0	1.979200	-1.916579	2.384188
66	1	0	2.574596	-1.050600	2.705046
67	1	0	0.959633	-1.558424	2.164433
68	1	0	1.904022	-2.609592	3.229643
69	7	0	-4.027416	0.083805	-0.387737
70	6	0	-4.902971	0.960633	-0.831990
71	6	0	-5.927256	0.276054	-1.506687
72	6	0	-5.556555	-1.032711	-1.428461
73	1	0	-6.801553	0.697430	-1.981943
74	8	0	-4.407934	-1.161914	-0.759958
75	1	0	-5.987949	-1.961678	-1.778700
76	1	0	-4.752385	2.017295	-0.647820
77	1	0	-2.348924	0.774791	-3.839086
78	1	0	-1.487601	3.305537	-0.492922

Zero-point correction= 0.623740 (Hartree/Particle)
Thermal correction to Energy= 0.664663
Thermal correction to Enthalpy= 0.665607
Thermal correction to Gibbs Free Energy= 0.550085
Sum of electronic and zero-point Energies= -2007.308501
Sum of electronic and thermal Energies= -2007.267578
Sum of electronic and thermal Enthalpies= -2007.266634
Sum of electronic and thermal Free Energies= -2007.382156
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.83321336

INT13b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.015255	-0.944138	0.266834
2	6	0	3.215843	-0.506331	-0.225602
3	79	0	-0.782535	0.110314	0.437455
4	6	0	1.470126	-2.275821	-0.184029
5	8	0	0.446337	-2.657798	0.572920
6	8	0	1.885295	-2.906856	-1.132834
7	6	0	2.777350	0.452590	2.915273
8	6	0	1.662381	0.552182	2.119901
9	6	0	3.771637	-0.578648	2.965266
10	1	0	2.864178	1.217125	3.685968
11	8	0	3.830512	-1.597632	2.274855
12	7	0	1.210504	-0.189999	1.077770
13	6	0	-0.258444	-3.817021	0.131810
14	1	0	0.353171	-4.713444	0.277345
15	1	0	-1.164302	-3.859616	0.740713
16	1	0	-0.514342	-3.724082	-0.930167
17	6	0	-2.642871	0.563479	-0.223425
18	7	0	-3.722075	-0.228550	-0.400600

19	6	0	-4.362664	1.785948	-1.012948
20	6	0	-4.792526	0.507961	-0.888077
21	1	0	-4.860239	2.685113	-1.352250
22	1	0	-5.749001	0.044133	-1.091709
23	7	0	-3.040313	1.799963	-0.599594
24	6	0	-2.175018	2.948353	-0.597565
25	6	0	-1.363598	3.164713	-1.716319
26	6	0	-2.163800	3.769882	0.533931
27	6	0	-0.511846	4.268676	-1.682733
28	6	0	-1.295973	4.861378	0.522107
29	6	0	-0.480051	5.109186	-0.575650
30	1	0	0.127642	4.470001	-2.541905
31	1	0	-1.266957	5.522473	1.387338
32	1	0	0.184935	5.971149	-0.570033
33	6	0	-3.765943	-1.646367	-0.165344
34	6	0	-4.127586	-2.102000	1.106364
35	6	0	-3.483310	-2.498869	-1.237745
36	6	0	-4.223569	-3.482561	1.286343
37	6	0	-3.604063	-3.870252	-1.014155
38	6	0	-3.976100	-4.357173	0.234223
39	1	0	-4.511800	-3.868571	2.263290
40	1	0	-3.403137	-4.559587	-1.833900
41	1	0	-4.074344	-5.430104	0.389026
42	6	0	-4.400078	-1.146976	2.228284
43	1	0	-5.164683	-0.404532	1.961103
44	1	0	-4.748854	-1.680722	3.118635
45	1	0	-3.495337	-0.588057	2.507590
46	6	0	-3.038587	-1.959384	-2.563865
47	1	0	-3.755280	-1.241746	-2.986408
48	1	0	-2.076453	-1.431094	-2.475438
49	1	0	-2.909535	-2.767914	-3.291613
50	6	0	-1.386001	2.236101	-2.892732
51	1	0	-2.408363	2.008894	-3.224009
52	1	0	-0.847102	2.670933	-3.741540
53	1	0	-0.908073	1.273421	-2.653297
54	6	0	-3.033811	3.475150	1.717853
55	1	0	-4.100327	3.464043	1.454633
56	1	0	-2.802661	2.491004	2.151622
57	1	0	-2.893890	4.227180	2.501631
58	1	0	0.966157	1.350244	2.394525
59	1	0	4.547590	-0.411405	3.745662
60	7	0	4.074295	-1.487796	-0.786895
61	6	0	4.693044	-2.542201	-0.285621
62	6	0	5.297225	-3.248643	-1.333082
63	1	0	4.661248	-2.683894	0.793898
64	6	0	4.993309	-2.524495	-2.448928
65	1	0	5.884697	-4.152852	-1.266429
66	1	0	5.245013	-2.632800	-3.496473
67	6	0	3.763256	0.852722	-0.179923
68	6	0	5.110665	1.066985	0.131321
69	6	0	2.945210	1.955995	-0.460570
70	6	0	5.630637	2.355305	0.167352
71	1	0	5.751236	0.216845	0.369448
72	6	0	3.468318	3.239379	-0.422803
73	1	0	1.894169	1.802077	-0.712449
74	6	0	4.810983	3.444011	-0.108035
75	1	0	6.678827	2.508872	0.416150
76	1	0	2.827669	4.089842	-0.649697
77	1	0	5.217201	4.453121	-0.079275
78	8	0	4.260100	-1.455326	-2.152689

Zero-point correction= 0.623503 (Hartree/Particle)
Thermal correction to Energy= 0.665276
Thermal correction to Enthalpy= 0.666221
Thermal correction to Gibbs Free Energy= 0.546593
Sum of electronic and zero-point Energies= -2007.333776
Sum of electronic and thermal Energies= -2007.292002
Sum of electronic and thermal Enthalpies= -2007.291058
Sum of electronic and thermal Free Energies= -2007.410686
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.85636320

INT14b

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

1	6	0	-2.458091	-0.125455	0.196046
2	6	0	-3.849533	-0.697451	0.205589
3	79	0	0.629693	-0.137840	-0.122681
4	6	0	-2.261942	1.329477	0.542904
5	8	0	-1.286510	1.491714	1.424176
6	8	0	-2.892398	2.192988	-0.007582
7	6	0	-1.012913	-3.248545	-0.268072
8	6	0	-1.652214	-2.134056	-0.659117
9	6	0	-0.017872	-3.326165	0.809590
10	1	0	-1.248503	-4.171144	-0.795535
11	8	0	0.272850	-2.404266	1.549401
12	7	0	-1.439161	-0.836959	-0.136651
13	6	0	-1.056333	2.852986	1.812383
14	1	0	-1.982015	3.272352	2.220084
15	1	0	-0.273872	2.813090	2.572567
16	1	0	-0.724669	3.439722	0.948140
17	6	0	2.574051	0.372208	-0.295978
18	7	0	3.148932	1.592388	-0.341612
19	6	0	4.800884	0.150683	-0.526026
20	6	0	4.523587	1.475739	-0.484469
21	1	0	5.733375	-0.389733	-0.623708
22	1	0	5.159727	2.349288	-0.543185
23	7	0	3.589660	-0.511508	-0.407470
24	6	0	3.435275	-1.941926	-0.377675
25	6	0	3.257945	-2.611282	-1.594380
26	6	0	3.474195	-2.588776	0.861020
27	6	0	3.124953	-3.998465	-1.547122
28	6	0	3.355279	-3.979697	0.856478
29	6	0	3.184483	-4.676948	-0.333529
30	1	0	2.992865	-4.549650	-2.477472
31	1	0	3.396375	-4.514662	1.804979
32	1	0	3.102059	-5.762500	-0.317392
33	6	0	2.454438	2.848434	-0.249551
34	6	0	2.406658	3.483047	0.996007
35	6	0	1.898987	3.389856	-1.413278
36	6	0	1.786208	4.730809	1.053993
37	6	0	1.276336	4.633691	-1.303368
38	6	0	1.229361	5.302169	-0.085020
39	1	0	1.740731	5.255392	2.008184
40	1	0	0.837443	5.085506	-2.191972
41	1	0	0.752961	6.278686	-0.022873
42	6	0	2.980062	2.835821	2.220634
43	1	0	4.067516	2.695953	2.147662
44	1	0	2.786663	3.444441	3.110900
45	1	0	2.543403	1.839877	2.390086
46	6	0	1.968838	2.664014	-2.722921
47	1	0	2.983789	2.304541	-2.942126
48	1	0	1.311397	1.781832	-2.727725
49	1	0	1.657156	3.314560	-3.546987
50	6	0	3.215194	-1.862891	-2.892488
51	1	0	4.149535	-1.315879	-3.080615
52	1	0	3.057519	-2.546799	-3.733211
53	1	0	2.404695	-1.119280	-2.905825
54	6	0	3.584553	-1.828131	2.146243
55	1	0	4.279716	-0.981041	2.079220
56	1	0	2.599119	-1.431906	2.434059
57	1	0	3.924193	-2.480581	2.958047
58	1	0	-2.389738	-2.182944	-1.464393
59	1	0	0.488473	-4.310129	0.909197
60	7	0	-4.171122	-1.542199	1.108987
61	6	0	-3.454509	-1.932915	2.206332
62	6	0	-3.150000	-1.204231	3.307313
63	1	0	-3.256730	-3.009289	2.223043
64	6	0	-3.476933	0.203192	3.483245
65	1	0	-2.734370	-1.732613	4.162864
66	1	0	-3.448521	0.559312	4.536519
67	6	0	-4.765070	-0.352196	-0.883225
68	6	0	-6.099760	-0.775764	-0.813007
69	6	0	-4.318610	0.344643	-2.012937
70	6	0	-6.970163	-0.497986	-1.853060
71	1	0	-6.433495	-1.317725	0.069281
72	6	0	-5.193412	0.611747	-3.057337
73	1	0	-3.290163	0.698731	-2.073713
74	6	0	-6.517966	0.193840	-2.977089

75	1	0	-8.007788	-0.818747	-1.791248
76	1	0	-4.842693	1.154803	-3.932052
77	1	0	-7.205052	0.410399	-3.792818
78	8	0	-3.772797	0.979137	2.587538

Zero-point correction= 0.618106 (Hartree/Particle)
Thermal correction to Energy= 0.662397
Thermal correction to Enthalpy= 0.663342
Thermal correction to Gibbs Free Energy= 0.535782
Sum of electronic and zero-point Energies= -2007.372516
Sum of electronic and thermal Energies= -2007.328225
Sum of electronic and thermal Enthalpies= -2007.327280
Sum of electronic and thermal Free Energies= -2007.454840
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.89069901

INT15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.933197	-1.466999	-0.103421
2	6	0	3.563554	-0.170976	0.339416
3	79	0	-1.215042	-0.463373	0.207428
4	6	0	2.128611	-1.400230	-1.381435
5	8	0	2.000851	-2.579697	-1.963113
6	6	0	4.803229	0.238295	-0.324502
7	6	0	5.405553	-0.580155	-1.286037
8	6	0	5.386819	1.470586	-0.005148
9	6	0	6.571378	-0.171863	-1.921843
10	1	0	4.975021	-1.551175	-1.536307
11	6	0	6.550707	1.873545	-0.638305
12	1	0	4.911537	2.089325	0.753777
13	6	0	7.143565	1.054215	-1.599575
14	1	0	7.036775	-0.814687	-2.665797
15	1	0	7.004861	2.828814	-0.383249
16	1	0	8.058190	1.372983	-2.095610
17	8	0	1.658891	-0.354198	-1.760596
18	6	0	1.571244	-0.344555	3.002749
19	6	0	2.550173	-1.207641	3.654336
20	6	0	1.817941	0.374851	1.882641
21	7	0	3.002786	0.541667	1.228231
22	8	0	3.669859	-1.434496	3.235988
23	1	0	1.029662	1.030263	1.488560
24	1	0	2.194734	-1.673929	4.603458
25	7	0	2.995555	-2.486449	0.626081
26	6	0	2.503973	-3.689133	0.857455
27	6	0	1.212070	-3.991660	1.247356
28	6	0	0.116223	-3.121135	1.087824
29	1	0	1.031565	-4.967261	1.689892
30	8	0	0.168993	-2.057481	0.417948
31	1	0	-0.842481	-3.421337	1.542015
32	1	0	3.262938	-4.474965	0.884881
33	1	0	0.588121	-0.240432	3.462862
34	6	0	1.139572	-2.596483	-3.108445
35	1	0	1.142350	-3.625309	-3.468624
36	1	0	0.128031	-2.288846	-2.816273
37	1	0	1.518281	-1.913256	-3.874842
38	6	0	-2.396803	1.122880	-0.129328
39	7	0	-1.985249	2.404770	-0.232151
40	6	0	-4.152188	2.439525	-0.602892
41	6	0	-3.056114	3.232617	-0.526671
42	1	0	-5.190817	2.661119	-0.811294
43	1	0	-2.926783	4.299215	-0.655536
44	7	0	-3.726474	1.143812	-0.355550
45	6	0	-4.573217	-0.019583	-0.377914
46	6	0	-5.252656	-0.369467	0.793197
47	6	0	-4.671986	-0.738726	-1.573489
48	6	0	-6.072666	-1.496220	0.741222
49	6	0	-5.504691	-1.857197	-1.576685
50	6	0	-6.198956	-2.230871	-0.432020
51	1	0	-6.619627	-1.793543	1.635070
52	1	0	-5.609368	-2.435388	-2.493975
53	1	0	-6.847784	-3.104280	-0.454554
54	6	0	-0.613389	2.822883	-0.110106
55	6	0	0.232356	2.638329	-1.209570

56	6	0	-0.189353	3.362800	1.109824
57	6	0	1.569377	3.007160	-1.052111
58	6	0	1.148049	3.744209	1.208318
59	6	0	2.019130	3.562165	0.139318
60	1	0	2.260612	2.851387	-1.880015
61	1	0	1.510063	4.167305	2.144544
62	1	0	3.063517	3.852940	0.238602
63	6	0	-0.262788	2.045220	-2.493311
64	1	0	-1.239049	2.451091	-2.792067
65	1	0	0.449484	2.234068	-3.303780
66	1	0	-0.366423	0.953559	-2.406533
67	6	0	-1.119254	3.472379	2.280411
68	1	0	-1.990603	4.106880	2.069159
69	1	0	-1.509379	2.485143	2.574001
70	1	0	-0.604117	3.898033	3.148001
71	6	0	-5.099113	0.427546	2.053211
72	1	0	-5.459141	1.459062	1.936165
73	1	0	-5.665943	-0.027743	2.872189
74	1	0	-4.047362	0.489915	2.368663
75	6	0	-3.900989	-0.338065	-2.795029
76	1	0	-4.008251	0.731089	-3.023965
77	1	0	-2.823756	-0.529044	-2.670164
78	1	0	-4.236999	-0.903653	-3.670827

Zero-point correction= 0.621145 (Hartree/Particle)
Thermal correction to Energy= 0.664015
Thermal correction to Enthalpy= 0.664959
Thermal correction to Gibbs Free Energy= 0.544140
Sum of electronic and zero-point Energies= -2007.365216
Sum of electronic and thermal Energies= -2007.322346
Sum of electronic and thermal Enthalpies= -2007.321402
Sum of electronic and thermal Free Energies= -2007.442220
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.88618403

INT16b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.181666	-1.204014	0.200369
2	6	0	-3.908507	0.177901	0.638662
3	79	0	1.740282	-0.735320	-0.330315
4	6	0	-5.397848	-2.023634	0.490469
5	8	0	-5.706316	-2.835600	-0.511105
6	6	0	-4.845650	1.101881	1.273796
7	6	0	-6.213052	1.087815	0.980877
8	6	0	-4.334409	2.074643	2.141259
9	6	0	-7.056289	2.030082	1.553236
10	1	0	-6.622127	0.366509	0.275966
11	6	0	-5.182551	3.005408	2.721313
12	1	0	-3.268509	2.077052	2.362316
13	6	0	-6.544330	2.983438	2.428241
14	1	0	-8.117001	2.021818	1.313047
15	1	0	-4.783513	3.749506	3.407360
16	1	0	-7.209940	3.714661	2.882413
17	8	0	-5.975956	-1.922176	1.540485
18	6	0	-1.312251	-0.450236	-1.542802
19	6	0	-2.201894	-0.014621	-2.672537
20	6	0	-2.047253	-0.614415	-0.225624
21	7	0	-2.681331	0.494741	0.360978
22	8	0	-3.399982	0.107465	-2.588597
23	1	0	-1.295897	-1.049371	0.467754
24	1	0	-1.662637	0.180552	-3.629522
25	7	0	-3.095073	-1.653777	-0.368400
26	6	0	-2.788705	-2.851176	-1.035934
27	6	0	-1.649771	-2.921137	-1.741870
28	6	0	-0.609619	-1.819703	-1.794860
29	1	0	-1.415807	-3.862041	-2.235109
30	8	0	0.286785	-2.140454	-0.810346
31	1	0	-0.160763	-1.781608	-2.808730
32	1	0	-3.526719	-3.640999	-0.960947
33	1	0	-0.522568	0.310635	-1.416719
34	6	0	-6.871907	-3.655874	-0.299448
35	1	0	-7.034402	-4.179080	-1.241552
36	1	0	-6.687830	-4.361530	0.515933

37	1	0	-7.730275	-3.026519	-0.048319
38	6	0	2.999859	0.764946	0.136145
39	7	0	2.734263	2.067631	-0.124713
40	6	0	4.689245	2.052612	0.877453
41	6	0	3.767219	2.876305	0.324006
42	1	0	5.644123	2.249289	1.347425
43	1	0	3.739177	3.951418	0.204993
44	7	0	4.200014	0.760453	0.751823
45	6	0	4.878082	-0.423668	1.206580
46	6	0	5.709417	-1.096054	0.306082
47	6	0	4.665971	-0.843752	2.523242
48	6	0	6.362045	-2.237071	0.771035
49	6	0	5.337634	-1.991074	2.942437
50	6	0	6.178476	-2.679765	2.075625
51	1	0	7.019861	-2.782213	0.095292
52	1	0	5.194270	-2.344976	3.962609
53	1	0	6.696888	-3.572151	2.420827
54	6	0	1.547320	2.513582	-0.801534
55	6	0	0.374172	2.689627	-0.059124
56	6	0	1.615355	2.709727	-2.186128
57	6	0	-0.772926	3.081612	-0.752911
58	6	0	0.445375	3.100350	-2.837223
59	6	0	-0.737390	3.285533	-2.127443
60	1	0	-1.703159	3.213972	-0.200935
61	1	0	0.469793	3.263929	-3.914163
62	1	0	-1.641101	3.591589	-2.652200
63	6	0	0.328224	2.427614	1.415203
64	1	0	1.223500	2.795608	1.933510
65	1	0	-0.548387	2.905706	1.866252
66	1	0	0.259591	1.348140	1.623430
67	6	0	2.894492	2.494086	-2.936122
68	1	0	3.655045	3.240943	-2.669248
69	1	0	3.329012	1.507412	-2.719518
70	1	0	2.731005	2.563423	-4.016794
71	6	0	5.871911	-0.622976	-1.106578
72	1	0	6.113479	0.447460	-1.161854
73	1	0	6.671252	-1.173996	-1.613585
74	1	0	4.947207	-0.773073	-1.683331
75	6	0	3.745104	-0.096157	3.439562
76	1	0	4.076462	0.938707	3.604533
77	1	0	2.724833	-0.043563	3.031775
78	1	0	3.688232	-0.585183	4.417933

Zero-point correction= 0.624847 (Hartree/Particle)
Thermal correction to Energy= 0.665931
Thermal correction to Enthalpy= 0.666875
Thermal correction to Gibbs Free Energy= 0.547652
Sum of electronic and zero-point Energies= -2007.376520
Sum of electronic and thermal Energies= -2007.335435
Sum of electronic and thermal Enthalpies= -2007.334491
Sum of electronic and thermal Free Energies= -2007.453715
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.90276651

INT17b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.140823	0.777037	0.106784
2	6	0	-0.867503	-0.406583	-0.027625
3	6	0	-0.600440	2.161821	0.089467
4	8	0	0.408897	3.041181	-0.113687
5	6	0	-2.307854	-0.682618	-0.079134
6	6	0	-3.259911	0.060379	0.625933
7	6	0	-2.732026	-1.794550	-0.819693
8	6	0	-4.602877	-0.290483	0.571813
9	1	0	-2.944941	0.914799	1.215459
10	6	0	-4.074964	-2.135083	-0.879065
11	1	0	-1.985918	-2.388394	-1.343151
12	6	0	-5.016828	-1.382201	-0.183391
13	1	0	-5.331297	0.294861	1.130264
14	1	0	-4.387666	-2.996247	-1.467417
15	1	0	-6.071239	-1.650863	-0.225021
16	8	0	-1.748779	2.522959	0.215250
17	6	0	2.476304	-1.722619	-0.041417

18	6	0	2.829606	-2.101748	1.390062
19	6	0	1.197063	-0.973791	-0.090290
20	7	0	-0.008544	-1.470759	-0.159247
21	8	0	2.274583	-1.689390	2.372631
22	1	0	2.984617	-0.355958	-2.361280
23	1	0	3.703362	-2.795730	1.457004
24	7	0	1.205112	0.381107	0.061672
25	6	0	2.411430	1.095832	0.176777
26	6	0	3.578010	0.509818	-0.108913
27	6	0	3.645376	-0.900993	-0.621698
28	1	0	4.492594	1.092346	-0.041902
29	8	0	3.679486	-0.945490	-2.032239
30	1	0	4.586174	-1.374065	-0.304098
31	1	0	2.312032	2.125319	0.494156
32	1	0	2.390330	-2.651033	-0.624601
33	6	0	0.003200	4.406390	-0.155671
34	1	0	0.912594	4.982009	-0.339393
35	1	0	-0.721726	4.568757	-0.959719
36	1	0	-0.454982	4.704032	0.793450

Zero-point correction= 0.278382 (Hartree/Particle)
Thermal correction to Energy= 0.297539
Thermal correction to Enthalpy= 0.298483
Thermal correction to Gibbs Free Energy= 0.229681
Sum of electronic and zero-point Energies= -1027.575669
Sum of electronic and thermal Energies= -1027.556512
Sum of electronic and thermal Enthalpies= -1027.555568
Sum of electronic and thermal Free Energies= -1027.624370
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -1028.14147065

INT18b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.929784	-0.980539	-0.104392
2	6	0	2.496881	0.143682	0.607541
3	6	0	4.233782	-1.270923	-0.671299
4	8	0	4.357868	-2.557986	-1.094560
5	6	0	3.113362	1.450657	0.874524
6	6	0	4.039405	2.064260	0.024782
7	6	0	2.678417	2.150742	2.008847
8	6	0	4.536229	3.327774	0.320635
9	1	0	4.373117	1.545930	-0.867646
10	6	0	3.182239	3.408531	2.304239
11	1	0	1.925272	1.688699	2.642889
12	6	0	4.118334	4.002518	1.462070
13	1	0	5.253905	3.790347	-0.356038
14	1	0	2.835027	3.932398	3.193897
15	1	0	4.512416	4.992562	1.689872
16	8	0	5.163115	-0.495220	-0.763210
17	6	0	-0.377938	-1.966471	1.031112
18	6	0	-0.311876	-2.697919	2.351069
19	6	0	0.902034	-1.277622	0.731017
20	7	0	1.257315	-0.083561	1.131921
21	8	0	0.686770	-2.923835	2.987125
22	1	0	-1.043586	-1.711138	-1.480280
23	1	0	-1.314005	-3.061851	2.691062
24	7	0	1.866892	-1.892983	-0.004912
25	6	0	1.647831	-3.157678	-0.583464
26	6	0	0.436242	-3.714731	-0.565822
27	6	0	-0.784061	-3.002895	-0.048884
28	1	0	0.297408	-4.674388	-1.058374
29	8	0	-1.527124	-2.480935	-1.111972
30	1	0	-1.455089	-3.732322	0.434479
31	1	0	2.518879	-3.614640	-1.032415
32	1	0	-1.179996	-1.209801	1.094419
33	6	0	5.630534	-2.879902	-1.630215
34	1	0	5.577973	-3.933273	-1.916511
35	1	0	5.858200	-2.259510	-2.504410
36	1	0	6.418061	-2.727188	-0.883826
37	7	0	-2.081032	0.559532	0.101878
38	16	0	-1.582158	0.909852	-1.375642
39	8	0	-0.444076	0.028926	-1.686868
40	8	0	-2.594344	1.109643	-2.401643

41	16	0	-3.580862	0.796679	0.638230
42	8	0	-3.538272	0.813469	2.092833
43	8	0	-4.370313	1.787738	-0.076482
44	6	0	-0.801002	2.565676	-1.158767
45	6	0	-4.386961	-0.823861	0.259130
46	9	0	-5.658583	-0.772718	0.650669
47	9	0	-4.352314	-1.097737	-1.032781
48	9	0	-3.787297	-1.805345	0.930642
49	9	0	-1.711654	3.426820	-0.726654
50	9	0	-0.337481	2.983007	-2.333613
51	9	0	0.198452	2.520035	-0.297735

Zero-point correction= 0.337497 (Hartree/Particle)
Thermal correction to Energy= 0.371356
Thermal correction to Enthalpy= 0.372300
Thermal correction to Gibbs Free Energy= 0.269657
Sum of electronic and zero-point Energies= -2854.366029
Sum of electronic and thermal Energies= -2854.332171
Sum of electronic and thermal Enthalpies= -2854.331227
Sum of electronic and thermal Free Energies= -2854.433870
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -2855.37214490

INT19b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.884932	-0.288975	-1.160277
2	6	0	-3.009370	0.228191	-0.496236
3	6	0	-1.241648	-1.573918	-1.184909
4	8	0	-2.047262	-2.599646	-0.807769
5	6	0	-4.242355	-0.439755	-0.059563
6	6	0	-4.973710	0.128073	0.991190
7	6	0	-4.761137	-1.568388	-0.701578
8	6	0	-6.171385	-0.436312	1.407422
9	1	0	-4.580470	1.029382	1.456876
10	6	0	-5.961849	-2.130262	-0.285958
11	1	0	-4.216444	-1.999849	-1.537063
12	6	0	-6.670112	-1.571354	0.773606
13	1	0	-6.723271	0.017307	2.230366
14	1	0	-6.352495	-3.007505	-0.801600
15	1	0	-7.612109	-2.013077	1.098498
16	8	0	-0.068060	-1.768220	-1.478207
17	6	0	-1.042265	3.173533	-0.765549
18	6	0	-1.645050	4.420830	-0.412134
19	6	0	-1.701934	1.925271	-0.764779
20	7	0	-2.892429	1.553731	-0.268746
21	8	0	-2.790962	4.665228	-0.057036
22	1	0	-0.902297	5.268112	-0.502823
23	7	0	-1.071855	0.843362	-1.357171
24	6	0	0.043603	0.991650	-2.158360
25	6	0	0.746858	2.134851	-2.119507
26	6	0	0.404633	3.150068	-1.087422
27	1	0	1.615441	2.262102	-2.762011
28	8	0	1.216974	2.799983	0.128593
29	1	0	0.752231	4.155075	-1.367461
30	1	0	0.278591	0.141019	-2.787767
31	7	0	2.125863	0.284081	0.331833
32	16	0	1.232880	-0.620539	1.410497
33	8	0	-0.119175	-0.117420	1.351068
34	8	0	1.579618	-2.020134	1.336127
35	16	0	3.645722	-0.041479	-0.259791
36	8	0	4.115655	1.199049	-0.836922
37	8	0	4.425623	-0.813495	0.682841
38	6	0	1.879893	-0.004848	3.030940
39	6	0	3.323664	-1.184432	-1.680548
40	9	0	4.514838	-1.497685	-2.182619
41	9	0	2.719205	-2.272643	-1.273912
42	9	0	2.614397	-0.572597	-2.606925
43	9	0	3.151319	-0.312543	3.191469
44	9	0	1.164495	-0.566580	3.992912
45	9	0	1.734278	1.310016	3.083995
46	1	0	1.745987	1.276603	0.138353
47	1	0	0.598063	2.925899	0.869150
48	6	0	-1.379673	-3.837957	-0.652629

49	1	0	-2.135447	-4.541161	-0.291532
50	1	0	-0.960861	-4.188228	-1.604197
51	1	0	-0.561051	-3.753679	0.072381

Zero-point correction= 0.335959 (Hartree/Particle)
Thermal correction to Energy= 0.369589
Thermal correction to Enthalpy= 0.370533
Thermal correction to Gibbs Free Energy= 0.271051
Sum of electronic and zero-point Energies= -2854.332733
Sum of electronic and thermal Energies= -2854.299103
Sum of electronic and thermal Enthalpies= -2854.298159
Sum of electronic and thermal Free Energies= -2854.397641
M06/6-311++G(d,p)/SMD//M06/6-31G(d) energy in DCE solvent = -2855.33817471

INT20b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.757344	2.176213	0.215384
2	6	0	-2.048383	1.609222	0.628575
3	79	0	0.272403	0.267258	-0.062314
4	6	0	-0.590736	2.978505	-1.019745
5	8	0	0.398654	3.889794	-0.881715
6	6	0	-3.147889	1.083337	-0.195381
7	6	0	-2.967389	0.582343	-1.490641
8	6	0	-4.429846	1.026575	0.368527
9	6	0	-4.038736	0.059598	-2.203932
10	1	0	-1.978157	0.608991	-1.943544
11	6	0	-5.500951	0.507817	-0.347239
12	1	0	-4.562358	1.400755	1.381775
13	6	0	-5.311125	0.023780	-1.639292
14	1	0	-3.875735	-0.324050	-3.210977
15	1	0	-6.492245	0.486726	0.104519
16	1	0	-6.151246	-0.379193	-2.203977
17	8	0	-1.226888	2.873448	-2.045498
18	6	0	-0.125009	2.515638	1.506882
19	6	0	1.229983	2.972005	1.782069
20	6	0	-1.022297	2.108814	2.471148
21	7	0	-2.159484	1.566529	1.957186
22	8	0	1.669937	3.163442	2.903376
23	6	0	0.636195	4.690606	-2.029858
24	1	0	1.445828	5.371410	-1.757502
25	1	0	0.929989	4.070942	-2.885125
26	1	0	-0.261579	5.256019	-2.302948
27	6	0	1.087510	-1.602224	-0.015021
28	7	0	0.369055	-2.715445	0.252724
29	6	0	2.465711	-3.372090	0.168407
30	6	0	1.200891	-3.817326	0.369898
31	1	0	3.419279	-3.883529	0.170762
32	1	0	0.810231	-4.802584	0.587506
33	7	0	2.373932	-2.007362	-0.066576
34	6	0	3.473461	-1.108926	-0.285112
35	6	0	3.943138	-0.355132	0.795278
36	6	0	3.983719	-0.993562	-1.581882
37	6	0	4.987212	0.536272	0.544989
38	6	0	5.029968	-0.095281	-1.783110
39	6	0	5.526792	0.662842	-0.728782
40	1	0	5.370428	1.140869	1.366261
41	1	0	5.447332	0.015805	-2.783484
42	1	0	6.340352	1.364693	-0.903636
43	6	0	-1.057573	-2.683800	0.448736
44	6	0	-1.882981	-2.936396	-0.651522
45	6	0	-1.547463	-2.301757	1.702149
46	6	0	-3.258732	-2.833399	-0.458764
47	6	0	-2.930849	-2.196330	1.843021
48	6	0	-3.777995	-2.463466	0.776100
49	1	0	-3.926544	-3.008861	-1.301570
50	1	0	-3.337816	-1.868473	2.798918
51	1	0	-4.854203	-2.355957	0.898018
52	6	0	-1.307395	-3.233202	-2.002931
53	1	0	-0.634896	-4.102314	-1.994652
54	1	0	-2.104279	-3.430770	-2.728863
55	1	0	-0.721607	-2.378949	-2.375876
56	6	0	-0.634334	-1.949641	2.837269

57	1	0	0.247146	-2.602891	2.888503
58	1	0	-0.270224	-0.914580	2.737179
59	1	0	-1.163278	-2.013040	3.794814
60	6	0	3.334252	-0.464625	2.160274
61	1	0	3.113105	-1.505060	2.434739
62	1	0	4.001604	-0.043048	2.919823
63	1	0	2.386862	0.093928	2.217986
64	6	0	3.397217	-1.780159	-2.715001
65	1	0	3.488280	-2.864348	-2.561111
66	1	0	2.324933	-1.565020	-2.833388
67	1	0	3.895012	-1.534358	-3.659448
68	1	0	1.880570	3.107289	0.886968
69	1	0	-0.858887	2.149204	3.545534

Zero-point correction= 0.548408 (Hartree/Particle)
Thermal correction to Energy= 0.586153
Thermal correction to Enthalpy= 0.587097
Thermal correction to Gibbs Free Energy= 0.475339
Sum of electronic and zero-point Energies= -1761.156979
Sum of electronic and thermal Energies= -1761.119235
Sum of electronic and thermal Enthalpies= -1761.118290
Sum of electronic and thermal Free Energies= -1761.230049
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.50407890

INT21b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.605454	-0.391827	0.243926
2	6	0	4.057470	-3.351003	-1.458428
3	6	0	3.327543	-2.264408	-0.818055
4	6	0	1.945053	-2.214561	-0.815555
5	6	0	3.762468	-1.075769	-0.134983
6	8	0	3.511042	-4.300548	-1.995526
7	7	0	1.507461	-1.102671	-0.175500
8	79	0	-0.436358	-0.390934	-0.171444
9	6	0	-2.314847	0.370909	-0.235888
10	7	0	-2.639256	1.634952	-0.594904
11	6	0	-4.550019	0.658734	-0.123178
12	6	0	-4.009418	1.831672	-0.531040
13	1	0	-5.573436	0.359985	0.061976
14	1	0	-4.456637	2.784721	-0.781304
15	7	0	-3.494644	-0.224687	0.052124
16	6	0	-3.623451	-1.577322	0.516223
17	6	0	-3.462494	-1.826684	1.882241
18	6	0	-3.884706	-2.579750	-0.422113
19	6	0	-3.595723	-3.146806	2.311585
20	6	0	-4.008307	-3.884841	0.051980
21	6	0	-3.867590	-4.165201	1.406149
22	1	0	-3.475641	-3.372810	3.370635
23	1	0	-4.208424	-4.688226	-0.656167
24	1	0	-3.964643	-5.190407	1.758723
25	6	0	-1.662513	2.629179	-0.946932
26	6	0	-1.239658	2.708202	-2.276398
27	6	0	-1.147445	3.432327	0.074723
28	6	0	-0.255354	3.648750	-2.577569
29	6	0	-0.164194	4.356798	-0.272499
30	6	0	0.280002	4.460865	-1.584932
31	1	0	0.099576	3.731582	-3.604354
32	1	0	0.268883	4.984487	0.505496
33	1	0	1.056303	5.181327	-1.836701
34	6	0	-1.795576	1.793359	-3.325264
35	1	0	-2.894332	1.784207	-3.328513
36	1	0	-1.457284	2.092880	-4.323354
37	1	0	-1.467093	0.756484	-3.159921
38	6	0	-1.619001	3.279115	1.488284
39	1	0	-2.708991	3.391302	1.576385
40	1	0	-1.358464	2.285418	1.881893
41	1	0	-1.145805	4.022023	2.140002
42	6	0	-3.122035	-0.725399	2.840285
43	1	0	-3.241359	-1.058558	3.877274
44	1	0	-2.077199	-0.402211	2.711731
45	1	0	-3.750093	0.164280	2.693533
46	6	0	-3.996287	-2.261220	-1.882275

47	1	0	-4.801604	-1.542969	-2.090017
48	1	0	-3.065788	-1.815344	-2.263154
49	1	0	-4.196306	-3.166799	-2.465241
50	1	0	1.257849	-2.924727	-1.263161
51	1	0	5.164294	-3.271299	-1.441361
52	6	0	5.116662	-0.658735	0.212530
53	8	0	5.439692	0.388915	0.735768
54	8	0	6.038456	-1.598851	-0.114115
55	6	0	7.377082	-1.251189	0.196663
56	1	0	7.498267	-1.082524	1.272924
57	1	0	7.990443	-2.095845	-0.126295
58	1	0	7.678710	-0.338247	-0.330213
59	6	0	2.410164	0.850460	1.007380
60	6	0	1.548835	0.856433	2.113495
61	6	0	3.032540	2.048009	0.640750
62	6	0	1.319090	2.024291	2.833739
63	1	0	1.084265	-0.079547	2.426648
64	6	0	2.800075	3.214704	1.357966
65	1	0	3.713101	2.049499	-0.207026
66	6	0	1.943682	3.209317	2.456696
67	1	0	0.661544	2.003443	3.703323
68	1	0	3.295514	4.137647	1.057700
69	1	0	1.773176	4.124294	3.024510

Zero-point correction= 0.548423 (Hartree/Particle)
Thermal correction to Energy= 0.586645
Thermal correction to Enthalpy= 0.587589
Thermal correction to Gibbs Free Energy= 0.471644
Sum of electronic and zero-point Energies= -1761.173912
Sum of electronic and thermal Energies= -1761.135691
Sum of electronic and thermal Enthalpies= -1761.134746
Sum of electronic and thermal Free Energies= -1761.250691
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.52423442

INT22b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.809353	2.241623	-0.981536
2	6	0	-2.258223	-0.618455	-3.318624
3	6	0	-1.860333	0.407036	-2.331574
4	6	0	-0.514416	0.783064	-2.127331
5	6	0	-2.676530	1.343536	-1.625241
6	8	0	-1.642157	-1.643927	-3.508817
7	7	0	-0.542622	1.914482	-1.345216
8	79	0	-0.603933	-0.963111	-0.622625
9	1	0	0.285227	2.483998	-1.112265
10	7	0	2.561995	1.402102	-0.773407
11	16	0	2.656337	0.006333	0.010149
12	8	0	1.974598	-0.025292	1.304259
13	8	0	2.369012	-1.050895	-0.954867
14	16	0	2.652100	2.852394	-0.081737
15	8	0	1.592463	3.683488	-0.670066
16	8	0	2.856926	2.897355	1.357568
17	6	0	4.194025	3.518235	-0.837757
18	6	0	4.444932	-0.220744	0.420087
19	9	0	5.180397	-0.083975	-0.669181
20	9	0	4.620145	-1.443366	0.910633
21	9	0	4.826485	0.663058	1.324649
22	9	0	4.383196	4.747943	-0.387189
23	9	0	4.087331	3.544125	-2.153923
24	9	0	5.224801	2.761064	-0.495233
25	6	0	-0.763996	-2.256170	0.947863
26	7	0	-0.120098	-3.407528	1.227832
27	6	0	-1.611116	-3.155942	2.828518
28	6	0	-0.632038	-3.979033	2.382675
29	1	0	-2.266155	-3.211028	3.687821
30	1	0	-0.245958	-4.913474	2.767353
31	7	0	-1.677084	-2.101941	1.931742
32	6	0	-2.592658	-0.995812	1.993571
33	6	0	-3.807224	-1.105088	1.308587
34	6	0	-2.200804	0.153703	2.688281
35	6	0	-4.666990	-0.009273	1.357399
36	6	0	-3.092687	1.227079	2.700125

37	6	0	-4.312266	1.148038	2.040038
38	1	0	-5.626372	-0.065624	0.843331
39	1	0	-2.809809	2.145321	3.214364
40	1	0	-4.985247	2.003734	2.038550
41	6	0	0.970609	-3.941099	0.457607
42	6	0	2.256319	-3.848863	1.002896
43	6	0	0.701438	-4.506227	-0.791946
44	6	0	3.308272	-4.357749	0.244494
45	6	0	1.789659	-4.993966	-1.516084
46	6	0	3.078394	-4.919237	-1.005352
47	1	0	4.322124	-4.289096	0.636619
48	1	0	1.612432	-5.437226	-2.495696
49	1	0	3.914212	-5.302433	-1.588168
50	6	0	2.495052	-3.200387	2.333619
51	1	0	2.052565	-3.771350	3.161986
52	1	0	3.567979	-3.109633	2.532189
53	1	0	2.066471	-2.187349	2.361816
54	6	0	-0.685489	-4.583144	-1.357683
55	1	0	-1.444740	-4.744584	-0.580169
56	1	0	-0.954080	-3.656729	-1.889014
57	1	0	-0.760396	-5.403686	-2.081042
58	6	0	-4.144815	-2.323155	0.503095
59	1	0	-5.206806	-2.328603	0.230428
60	1	0	-3.561945	-2.347099	-0.432137
61	1	0	-3.927276	-3.256776	1.039461
62	6	0	-0.860924	0.244126	3.352938
63	1	0	-0.691868	-0.583270	4.056442
64	1	0	-0.038744	0.208860	2.621365
65	1	0	-0.768432	1.183488	3.910023
66	1	0	0.368585	0.531741	-2.710408
67	1	0	-3.152306	-0.363626	-3.924315
68	6	0	-1.983424	3.234938	0.082325
69	6	0	-3.058683	4.128201	0.133366
70	6	0	-1.013071	3.271792	1.095730
71	6	0	-3.150551	5.041069	1.177515
72	1	0	-3.819765	4.093558	-0.640238
73	6	0	-1.103402	4.194319	2.127766
74	1	0	-0.190577	2.556160	1.093487
75	6	0	-2.175410	5.081540	2.171321
76	1	0	-3.987471	5.736675	1.207237
77	1	0	-0.330599	4.213877	2.894374
78	1	0	-2.250694	5.807929	2.979054
79	6	0	-4.133861	1.278328	-1.524159
80	8	0	-4.880392	2.168480	-1.181112
81	8	0	-4.588665	0.066677	-1.928076
82	6	0	-6.001892	-0.038703	-2.043646
83	1	0	-6.390623	0.707346	-2.745834
84	1	0	-6.198370	-1.048949	-2.409411
85	1	0	-6.487706	0.115950	-1.073268

Zero-point correction= 0.621655 (Hartree/Particle)
Thermal correction to Energy= 0.673594
Thermal correction to Enthalpy= 0.674538
Thermal correction to Gibbs Free Energy= 0.534384
Sum of electronic and zero-point Energies= -3588.439563
Sum of electronic and thermal Energies= -3588.387624
Sum of electronic and thermal Enthalpies= -3588.386680
Sum of electronic and thermal Free Energies= -3588.526834
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -3590.20155134

INT23b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.164932	2.203669	-0.476344
2	6	0	0.909252	3.006040	0.241470
3	79	0	-0.155289	0.069744	-0.284361
4	6	0	-1.526380	2.453248	0.096175
5	8	0	-2.487873	2.380353	-0.828623
6	6	0	2.217569	2.484292	0.583290
7	6	0	2.965845	3.129785	1.585875
8	6	0	2.785712	1.403807	-0.113753
9	6	0	4.235172	2.680415	1.905420
10	1	0	2.513707	3.959613	2.124595

11	6	0	4.072111	0.985012	0.186488
12	1	0	2.240107	0.923421	-0.926195
13	6	0	4.790224	1.609748	1.204330
14	1	0	4.796945	3.164389	2.701105
15	1	0	4.511429	0.162783	-0.374140
16	1	0	5.793319	1.265025	1.449523
17	8	0	-1.716966	2.598797	1.284248
18	6	0	-0.600809	4.947146	-1.437028
19	6	0	-0.379879	3.842418	-2.230498
20	6	0	-0.204535	5.053807	-0.092328
21	7	0	0.658945	4.254472	0.493555
22	8	0	-0.040354	2.631390	-1.864011
23	1	0	-1.038523	5.817859	-1.919024
24	1	0	-0.484895	3.911506	-3.313773
25	1	0	-0.524100	5.921557	0.487415
26	6	0	-3.819814	2.373780	-0.310040
27	1	0	-3.949274	1.528037	0.375147
28	1	0	-4.029852	3.306706	0.223417
29	1	0	-4.475848	2.269588	-1.175734
30	6	0	-0.334762	-1.952910	0.042881
31	7	0	0.607163	-2.920567	0.033043
32	6	0	-1.262793	-3.932162	0.592832
33	6	0	0.054930	-4.148232	0.369652
34	1	0	-2.065852	-4.598495	0.879587
35	1	0	0.658307	-5.045705	0.413267
36	7	0	-1.483001	-2.579478	0.385745
37	6	0	-2.759223	-1.935431	0.549927
38	6	0	-3.662752	-1.981311	-0.518085
39	6	0	-3.045205	-1.320360	1.773502
40	6	0	-4.917241	-1.405851	-0.321687
41	6	0	-4.316774	-0.764785	1.926363
42	6	0	-5.246492	-0.816391	0.894281
43	1	0	-5.644635	-1.434992	-1.132152
44	1	0	-4.573647	-0.291006	2.873146
45	1	0	-6.237178	-0.387814	1.036952
46	6	0	2.003991	-2.728493	-0.246873
47	6	0	2.864172	-2.486970	0.829318
48	6	0	2.441566	-2.848484	-1.569625
49	6	0	4.229315	-2.412584	0.552604
50	6	0	3.813880	-2.744900	-1.801176
51	6	0	4.700941	-2.549722	-0.748198
52	1	0	4.925962	-2.242176	1.373488
53	1	0	4.186571	-2.842939	-2.820025
54	1	0	5.770739	-2.501529	-0.944943
55	6	0	2.335860	-2.285049	2.216433
56	1	0	1.655579	-3.090163	2.525772
57	1	0	3.153086	-2.235925	2.943993
58	1	0	1.768901	-1.343427	2.285468
59	6	0	1.476363	-3.086111	-2.691016
60	1	0	0.885294	-3.999590	-2.537211
61	1	0	0.761048	-2.257183	-2.791721
62	1	0	2.004441	-3.189344	-3.644943
63	6	0	-3.294229	-2.623941	-1.820808
64	1	0	-3.133007	-3.705955	-1.715985
65	1	0	-4.085702	-2.480489	-2.564129
66	1	0	-2.365671	-2.201272	-2.231193
67	6	0	-2.028057	-1.228870	2.870045
68	1	0	-1.436444	-2.148496	2.973042
69	1	0	-1.321354	-0.406771	2.677310
70	1	0	-2.509959	-1.025950	3.832630

Zero-point correction= 0.563621 (Hartree/Particle)
Thermal correction to Energy= 0.600174
Thermal correction to Enthalpy= 0.601118
Thermal correction to Gibbs Free Energy= 0.494344
Sum of electronic and zero-point Energies= -1761.490955
Sum of electronic and thermal Energies= -1761.454402
Sum of electronic and thermal Enthalpies= -1761.453458
Sum of electronic and thermal Free Energies= -1761.560233
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.87718798

INT24b

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

1	6	0	-1.177671	-0.578622	-1.492146
2	6	0	-2.312719	-0.247183	-0.529847
3	79	0	0.609504	-0.193048	-0.377583
4	6	0	-1.154614	-2.012676	-1.997721
5	8	0	-2.162923	-2.278218	-2.820126
6	6	0	-3.098623	-1.330171	0.113988
7	6	0	-2.509456	-2.524142	0.547587
8	6	0	-4.444014	-1.088075	0.416641
9	6	0	-3.261006	-3.462249	1.249139
10	1	0	-1.452421	-2.718001	0.377391
11	6	0	-5.192242	-2.031467	1.104159
12	1	0	-4.890148	-0.146039	0.105814
13	6	0	-4.602955	-3.223187	1.522765
14	1	0	-2.787577	-4.381861	1.588983
15	1	0	-6.241366	-1.836654	1.318167
16	1	0	-5.190265	-3.961458	2.065269
17	8	0	-0.316241	-2.816629	-1.657924
18	6	0	-1.115180	2.360212	-1.809934
19	6	0	-1.510674	1.430450	-2.849110
20	6	0	-1.809634	2.079836	-0.416959
21	7	0	-2.638858	0.953025	-0.208855
22	8	0	-1.474972	0.181301	-2.742860
23	6	0	3.873547	0.273284	2.369845
24	6	0	2.798748	0.479621	3.170224
25	1	0	4.935453	0.262051	2.578017
26	1	0	2.719616	0.690742	4.228630
27	7	0	3.383264	0.041236	1.093196
28	7	0	1.680119	0.366861	2.363599
29	6	0	2.037097	0.098971	1.085329
30	1	0	-1.022356	2.060438	0.352106
31	1	0	-1.824551	1.764509	-3.844988
32	6	0	-1.560799	3.826581	-2.038004
33	6	0	-3.036209	3.754116	-2.385629
34	6	0	-3.597667	3.410826	-1.223805
35	8	0	-1.603460	4.280504	-0.693106
36	1	0	-3.501274	3.919779	-3.350833
37	1	0	-4.616951	3.152988	-0.961852
38	7	0	-2.573239	3.350306	-0.201188
39	1	0	-0.903323	4.458880	-2.638402
40	1	0	-0.023908	2.229993	-1.660353
41	6	0	-2.243040	-3.634923	-3.271884
42	1	0	-3.107359	-3.675398	-3.935596
43	1	0	-1.328884	-3.914476	-3.804461
44	1	0	-2.381315	-4.302185	-2.414376
45	6	0	0.304205	0.502645	2.765901
46	6	0	-0.416681	-0.662773	3.054622
47	6	0	-0.270147	1.779332	2.760090
48	6	0	-1.777138	-0.523686	3.329280
49	6	0	-1.633732	1.868621	3.044821
50	6	0	-2.380520	0.728618	3.316683
51	1	0	-2.369670	-1.414345	3.539115
52	1	0	-2.113950	2.846503	3.023746
53	1	0	-3.447148	0.815318	3.514680
54	6	0	4.188774	-0.247854	-0.062593
55	6	0	4.355413	-1.583403	-0.441490
56	6	0	4.759447	0.826806	-0.752862
57	6	0	5.152539	-1.832699	-1.559398
58	6	0	5.545458	0.528347	-1.864337
59	6	0	5.743506	-0.789549	-2.261001
60	1	0	5.308716	-2.863319	-1.875830
61	1	0	6.008262	1.343357	-2.419615
62	1	0	6.365506	-1.006251	-3.127322
63	6	0	3.686894	-2.703413	0.297312
64	1	0	2.631019	-2.800171	0.000404
65	1	0	4.175119	-3.659374	0.078139
66	1	0	3.705133	-2.555736	1.385783
67	6	0	0.241980	-2.009293	3.046915
68	1	0	0.652780	-2.258380	2.056408
69	1	0	1.080356	-2.059246	3.755817
70	1	0	-0.474172	-2.792826	3.318385
71	6	0	0.531474	3.004987	2.435038
72	1	0	1.161147	3.315945	3.280815
73	1	0	1.206234	2.844130	1.581214
74	1	0	-0.128782	3.845226	2.188354
75	6	0	4.523786	2.242545	-0.320043

76	1	0	3.449899	2.463522	-0.228387
77	1	0	4.975618	2.457918	0.658220
78	1	0	4.952640	2.946962	-1.040932

Zero-point correction= 0.625069 (Hartree/Particle)
Thermal correction to Energy= 0.664650
Thermal correction to Enthalpy= 0.665595
Thermal correction to Gibbs Free Energy= 0.553398
Sum of electronic and zero-point Energies= -2007.256466
Sum of electronic and thermal Energies= -2007.216884
Sum of electronic and thermal Enthalpies= -2007.215940
Sum of electronic and thermal Free Energies= -2007.328136
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -2008.77840504

INT25b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.606435	-2.049083	-0.395278
2	6	0	2.529487	-2.283357	1.150117
3	79	0	-0.169761	-0.429228	-0.479218
4	6	0	3.512798	-0.870959	-0.749760
5	8	0	2.992521	-0.078882	-1.683552
6	6	0	2.007727	-1.208652	2.028916
7	6	0	1.479336	-1.631990	3.255942
8	6	0	2.015065	0.159281	1.723095
9	6	0	0.949067	-0.715407	4.151512
10	1	0	1.495945	-2.695191	3.485278
11	6	0	1.513945	1.076583	2.639172
12	1	0	2.430187	0.548790	0.793072
13	6	0	0.970744	0.643292	3.844946
14	1	0	0.534412	-1.059002	5.096877
15	1	0	1.558622	2.137870	2.402825
16	1	0	0.574478	1.369085	4.553809
17	8	0	4.594154	-0.746285	-0.237611
18	6	0	2.240328	-3.765832	-1.892219
19	6	0	1.065485	-2.936626	-1.737584
20	6	0	3.178791	-3.246763	-1.082771
21	1	0	2.313020	-4.637805	-2.531495
22	8	0	2.810571	-3.381730	1.568474
23	7	0	1.239983	-1.952567	-0.907714
24	6	0	3.838346	1.009071	-2.082817
25	1	0	4.792822	0.629156	-2.459116
26	1	0	3.290300	1.531336	-2.869726
27	1	0	4.021504	1.673982	-1.231286
28	6	0	-1.595461	0.994142	-0.269975
29	7	0	-1.467800	2.339050	-0.343854
30	6	0	-3.627275	1.954824	-0.163423
31	6	0	-2.713308	2.946459	-0.282324
32	1	0	-4.706309	1.973723	-0.084589
33	1	0	-2.820456	4.022020	-0.329474
34	7	0	-2.920858	0.763098	-0.158174
35	6	0	-3.502522	-0.547088	-0.033947
36	6	0	-3.515092	-1.148399	1.229110
37	6	0	-4.012620	-1.155000	-1.185549
38	6	0	-4.080125	-2.420381	1.320958
39	6	0	-4.568462	-2.425683	-1.042851
40	6	0	-4.603344	-3.051268	0.198250
41	1	0	-4.112649	-2.914736	2.291030
42	1	0	-4.980043	-2.924141	-1.919712
43	1	0	-5.045932	-4.040990	0.292782
44	6	0	-0.218673	3.050545	-0.327894
45	6	0	0.581367	3.081088	-1.475567
46	6	0	0.133113	3.696382	0.865917
47	6	0	1.778114	3.797229	-1.398659
48	6	0	1.341407	4.391647	0.893829
49	6	0	2.158922	4.441714	-0.229207
50	1	0	2.409267	3.860610	-2.285388
51	1	0	1.638367	4.900310	1.810814
52	1	0	3.093166	4.998846	-0.195463
53	6	0	0.210068	2.373566	-2.743991
54	1	0	-0.874105	2.339297	-2.908756
55	1	0	0.667740	2.868056	-3.609149
56	1	0	0.567866	1.330800	-2.731592

57	6	0	-0.741286	3.632046	2.083273
58	1	0	-1.603600	4.309059	2.011365
59	1	0	-1.137695	2.618970	2.246814
60	1	0	-0.179842	3.926913	2.977907
61	6	0	-2.942220	-0.463205	2.433642
62	1	0	-3.327702	0.559851	2.546198
63	1	0	-3.192709	-1.014901	3.346307
64	1	0	-1.843973	-0.391795	2.383346
65	6	0	-3.953032	-0.472487	-2.518987
66	1	0	-4.570175	0.436264	-2.546915
67	1	0	-2.926914	-0.168295	-2.774436
68	1	0	-4.313718	-1.136545	-3.311687
69	1	0	4.190709	-3.592025	-0.898578
70	1	0	0.108557	-3.076497	-2.238362

Zero-point correction= 0.564421 (Hartree/Particle)
Thermal correction to Energy= 0.600700
Thermal correction to Enthalpy= 0.601644
Thermal correction to Gibbs Free Energy= 0.496034
Sum of electronic and zero-point Energies= -1761.545647
Sum of electronic and thermal Energies= -1761.509369
Sum of electronic and thermal Enthalpies= -1761.508425
Sum of electronic and thermal Free Energies= -1761.614035
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy in DCE solvent = -1762.94259758