Supporting Information

Mechanistic differences between aryl iodide electrophiles and pronucleophiles in Pd-catalyzed coupling with cyclopropenes: A DFT study

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Contents

Correction of translational entropy in solution:

In general, entropy can be partitioned into translational (S_{trans}), rotational (S_{rot}), and vibrational (S_{vib}) components.

$$S = S_{trans} + S_{rot} + S_{vib}$$

Although each component has different values in gas and condensed phase, the translational entropy in solution is substantially different from that in gas phase because translational movement is considerably suppressed in solution. In contrast, the rotational and vibrational entropies are only moderately different between in solution and in gas phase. Consequently, we need to evaluate S_{trans} in solution when we discuss Gibbs energy change in solution. In gas phase, S_{trans} could be given by the Sackur-Tetrode equation.[S1] However, the S_{trans} in solution is considerably overestimated using the abovementioned equation since the volume available to the molecule movement in solution is much smaller than in gas phase. According to the method developed by Whitesides et al.,[S2] the free volume is used to correct translational entropy in solution. The rotational entropy is evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy are evaluated with the frequency calculation at 298.15 K and 1 atm.

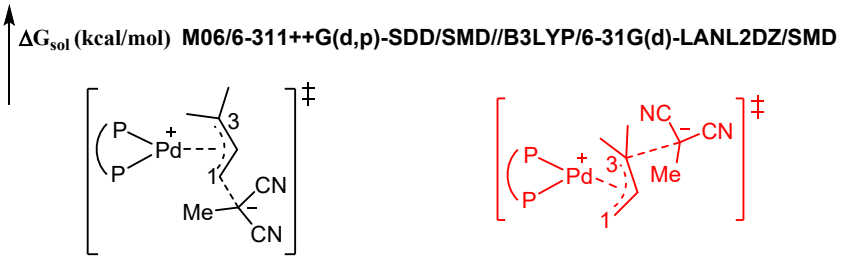


Fig. S1 Comparisons between the transition states of the nucleophilic attack of carbon anion to C^1 and C^3 of allyl group. The numbers in parenthesis are $\Delta\Delta G^{\neq}$ (in kcal/mol).

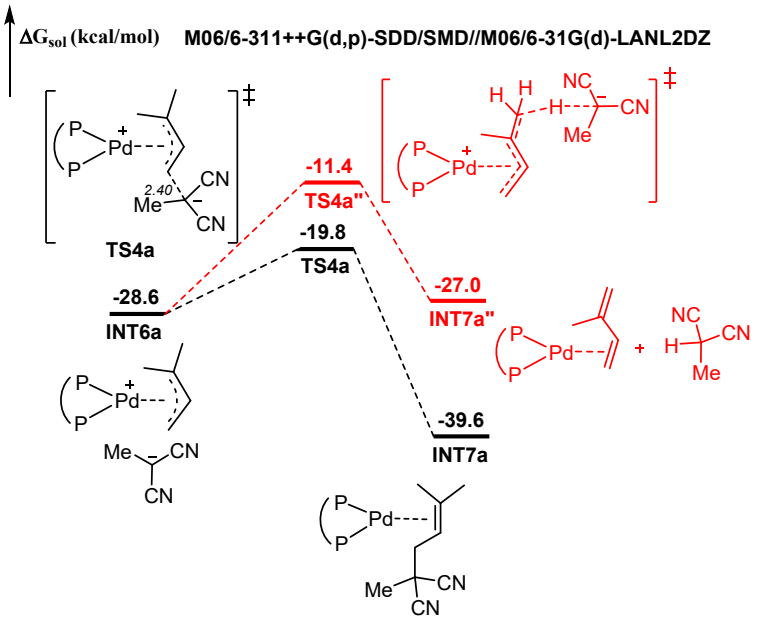


Fig. S2 Energy profile for the deprotonation step by the carbon anion.

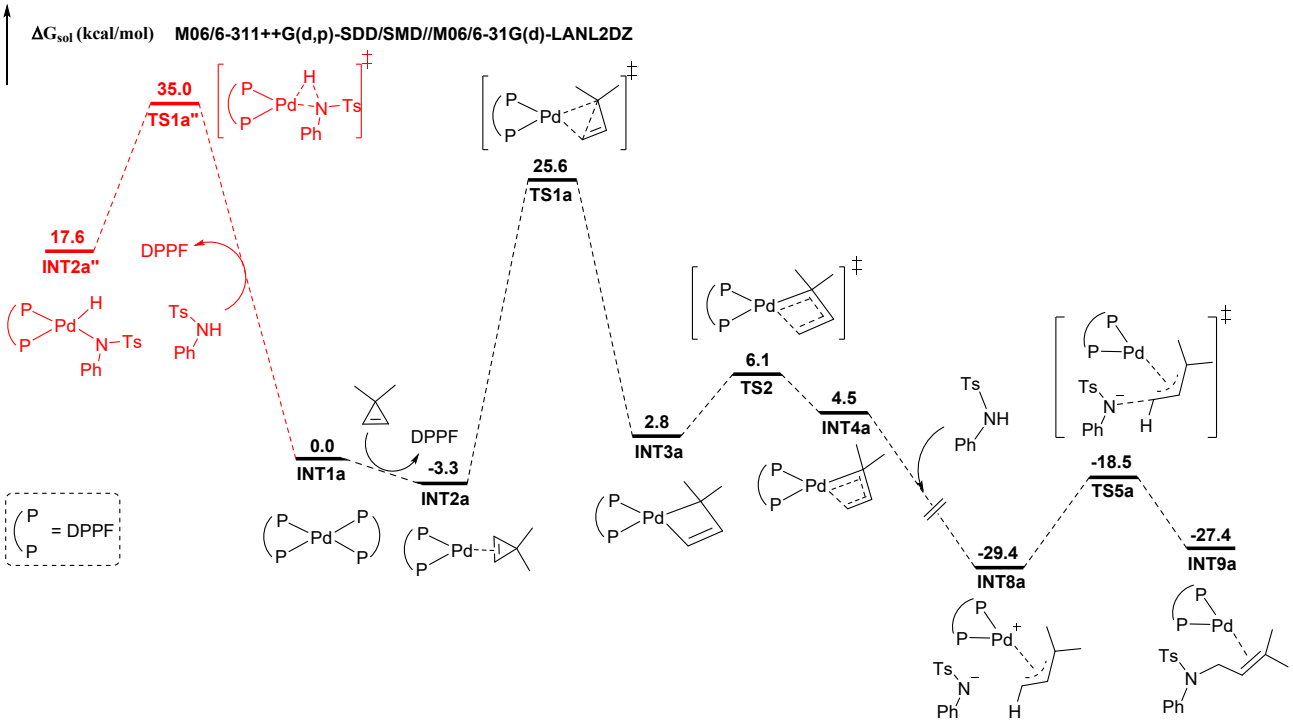


Fig. S3 Energy profiles for the Pd-catalyzed hydroamination of **1a** with secondary amide **2b**.

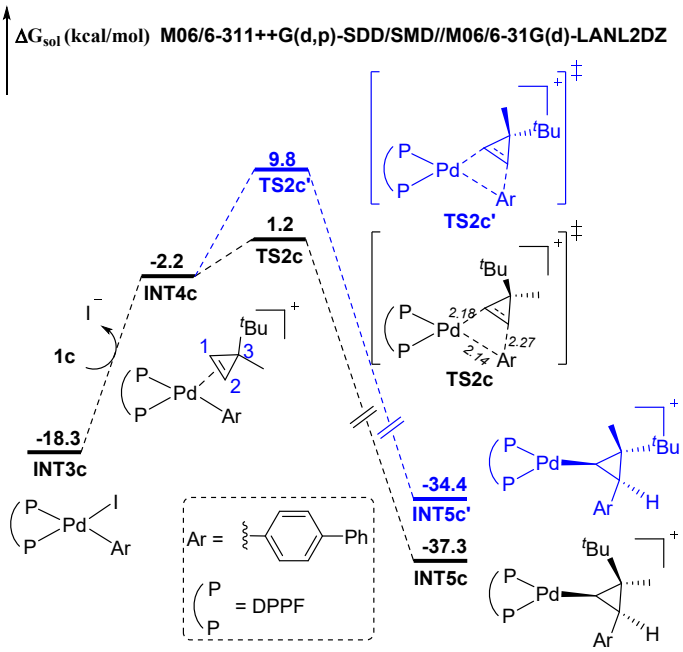


Fig. S4 Energy profiles for two possible migratory insertions of **1c** into **INT3c**.

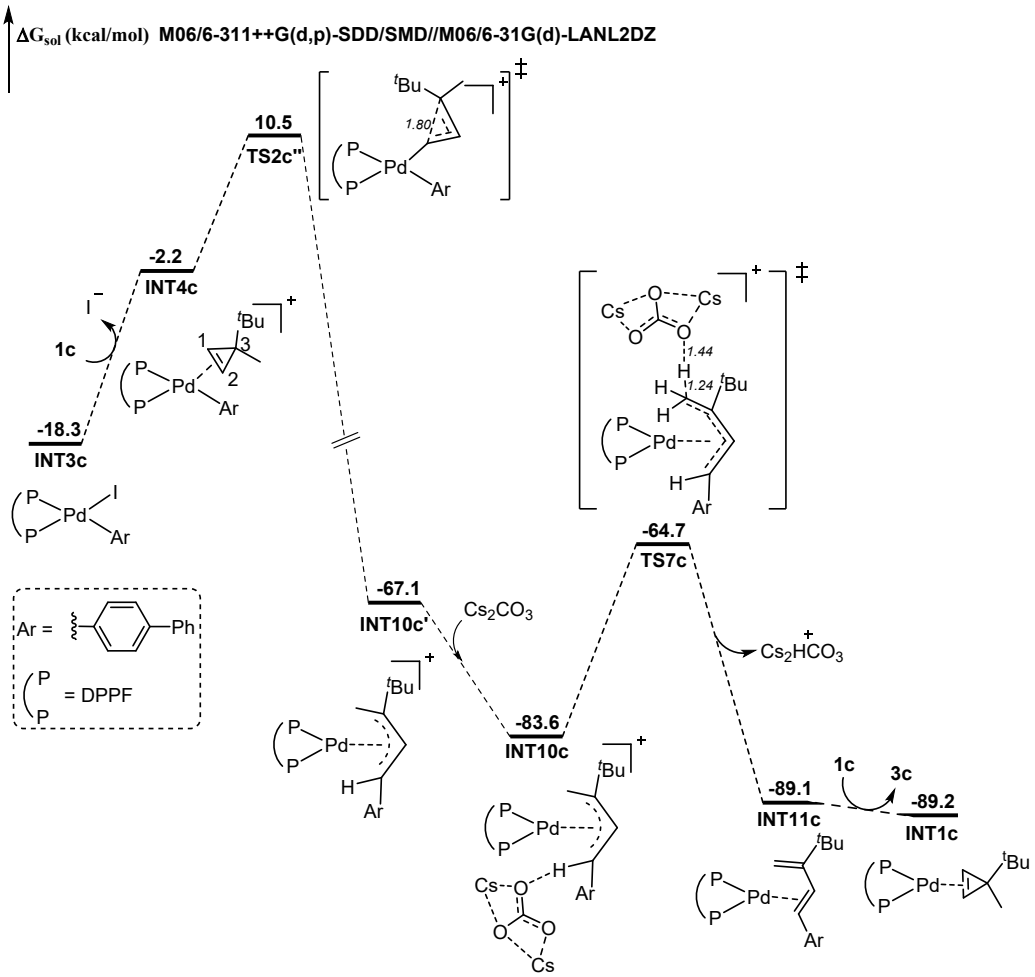
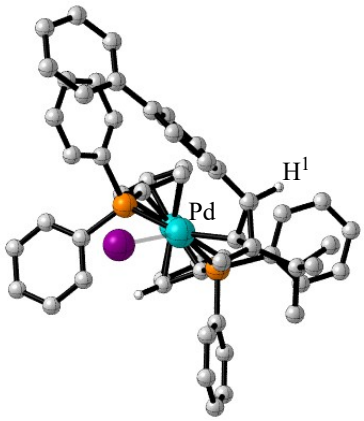


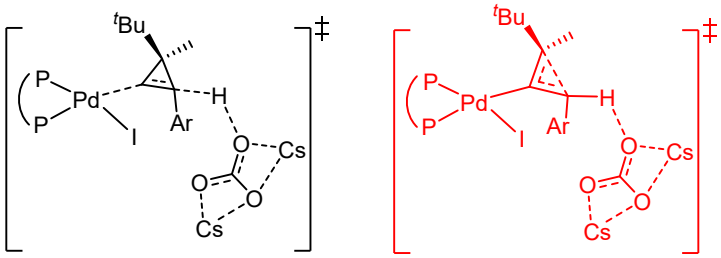
Fig. S5 Energy profiles for ring-opening of **1c** via carbene path to further furnish **3c**.



INT6c

Fig. S6 3D structure of **INT6c**. Some H atoms are omitted for clarity.

Table S1. Comparisons between $\Delta\Delta G^{\neq}$(**TS3c**) and $\Delta\Delta G^{\neq}$(**TS3c′**) using various density functionals (in kcal/mol).



TS3c **TS3c'**

Functional (optimizations in gas phase/ solvation single-point energy calculations)	$\Delta\Delta G^{\neq}$(**TS3c**)	$\Delta\Delta G^{\neq}$(**TS3c′**)
M06/M06	0.0	2.5
B3LYP/M06	0.0	2.3
ω-B97XD/ω-B97XD	0.0	13.5
M06-2X/M06-2X	0.0	3.5

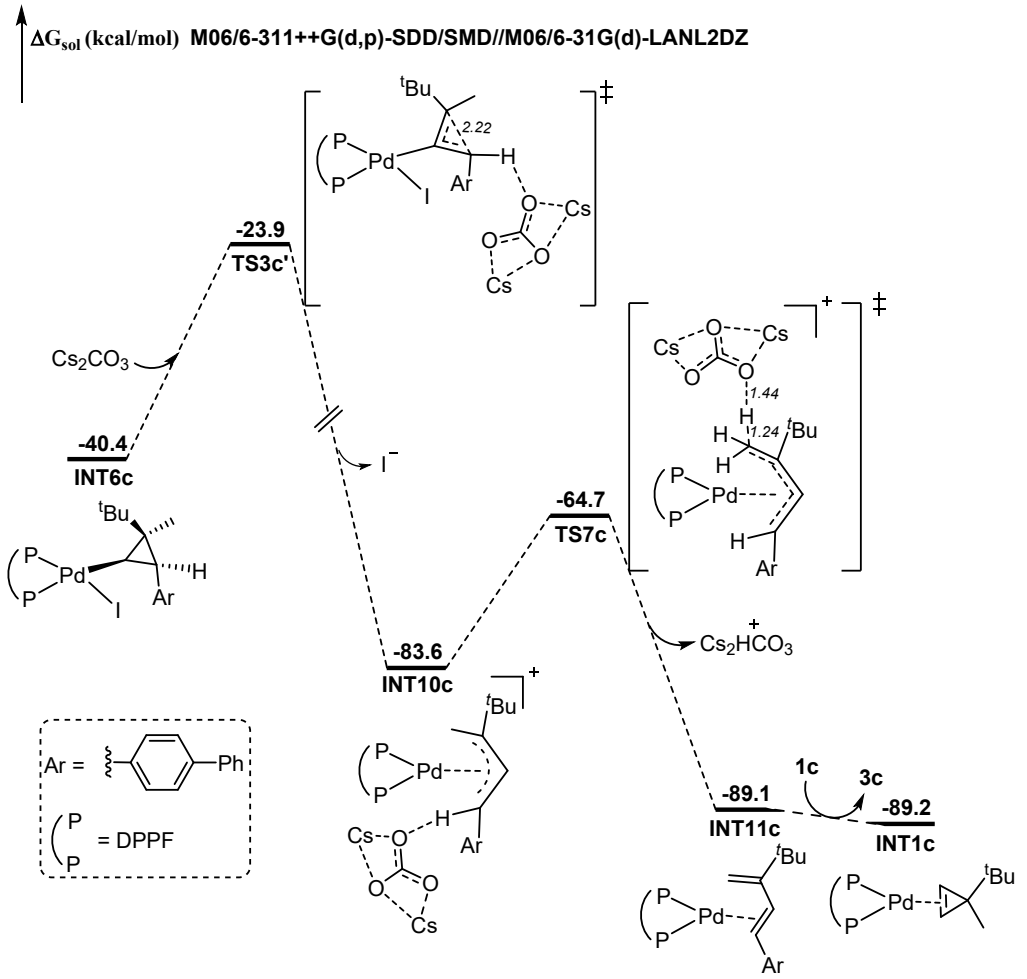


Fig. S7 Energy profiles for the transformation from **INT6c** to product **3c** via cleavage of C^2–C^3 bond followed by *β*-H elimination.

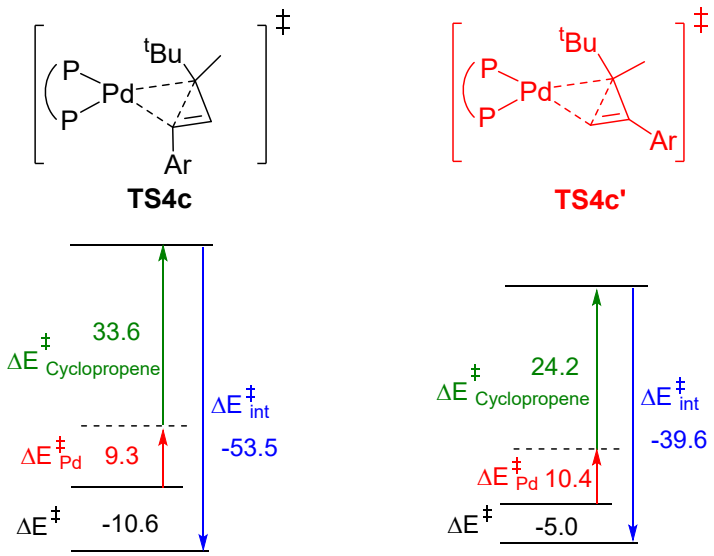


Fig. S8 Distortion, interaction and activation energies for **TS4c** and **TS4c′** (green arrow: distortion energy of aryl cyclopropene; red arrow: distortion energy of the Pd complex; blue arrow: interaction energy; black: activation energy, in kcal/mol).

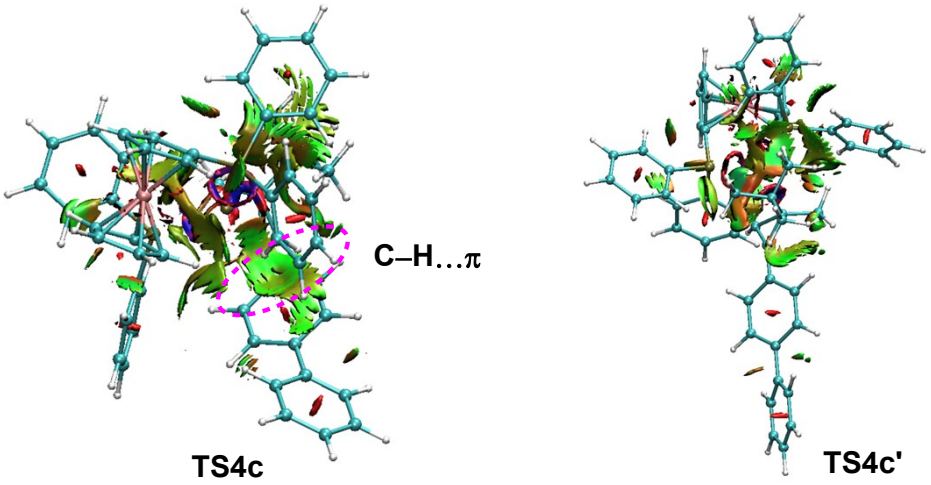


Fig. S9 NCI analysis of **TS4c** and **TS4c′** with C−H…π interactions highlighted by the pink circle.

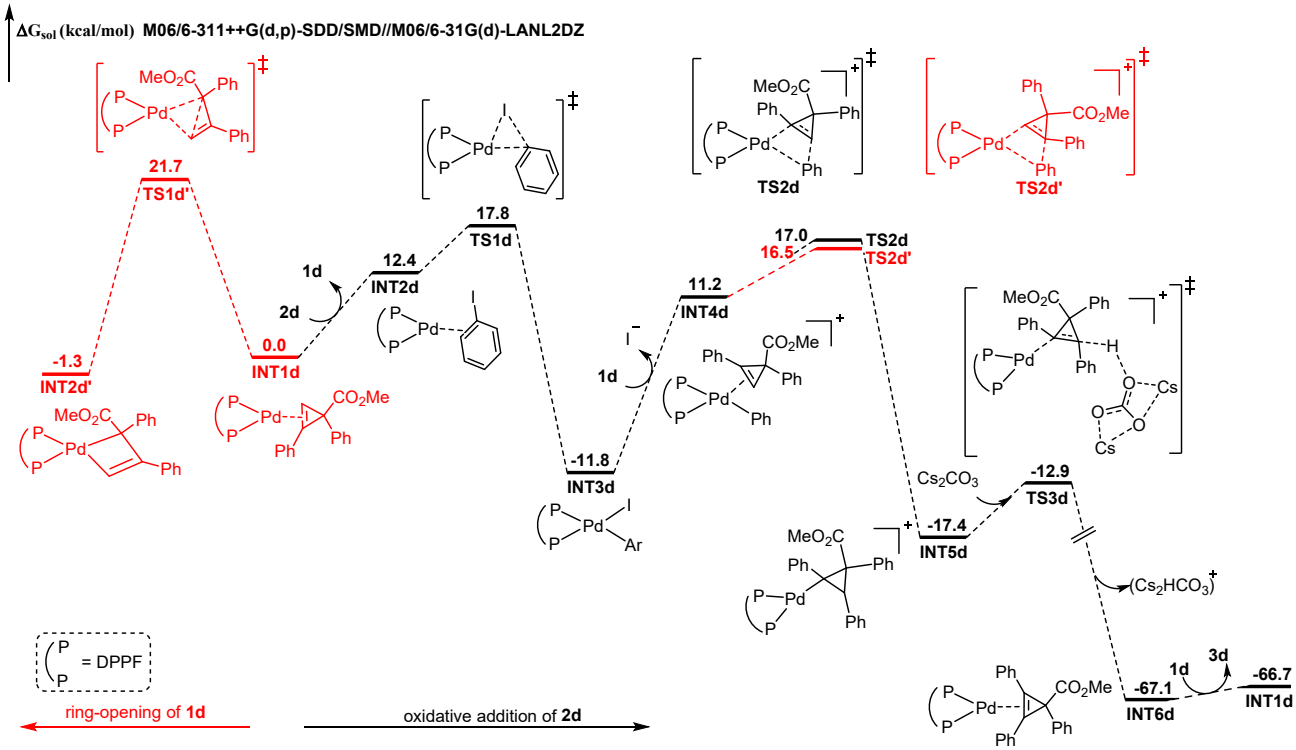


Fig. S10 Energy profiles for the mechanistic pathways of control experiment shown in Scheme 3.

References:

S1) R. W. Gurney, *Introduction to Statistical Mechanics*, 1st ed.; McGraw-Hill Book Company: New York, 1949.

S2) M. Mammen, E. I. Shakhnovich, J. M. Deutch and G. M. Whitesides, *J. Org. Chem.,* 1998, **63**, 3821.

Cartesian Coordinates and Energies

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.258931	0.000154	0.647200
2	6	0	-1.258901	0.000032	-0.647217
3	6	0	0.093226	0.000020	0.000033
4	1	0	-1.805785	-0.000243	1.581646
5	1	0	-1.805512	0.000549	-1.581800
6	6	0	0.933305	-1.261791	-0.000023
7	1	0	1.586890	-1.302924	-0.884273
8	6	0	0.933573	1.261634	0.000043
9	1	0	1.587432	1.302532	0.884096
10	1	0	0.305005	2.160784	0.000352
11	1	0	1.586910	1.302798	-0.884388
12	1	0	1.586911	-1.303005	0.884213
13	1	0	0.304522	-2.160787	-0.000059

Zero-point correction= 0.111802 (Hartree/Particle)
Thermal correction to Energy= 0.117696
Thermal correction to Enthalpy= 0.118640
Thermal correction to Gibbs Free Energy= 0.083633
Sum of electronic and zero-point Energies= -194.983028
Sum of electronic and thermal Energies= -194.977134
Sum of electronic and thermal Enthalpies= -194.976190
Sum of electronic and thermal Free Energies= -195.011197
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -588.069446

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.326321	0.445985
2	1	0	-0.000043	0.444093	1.541092
3	6	0	0.000173	1.714121	-0.214022
4	1	0	0.000147	1.618746	-1.304238
5	1	0	-0.891385	2.270942	0.090585
6	1	0	0.891887	2.270707	0.090564
7	6	0	1.207294	-0.425282	0.084886
8	7	0	2.182934	-0.981893	-0.201983
9	6	0	-1.207457	-0.424942	0.084712
10	7	0	-2.183029	-0.981792	-0.201927

Zero-point correction= 0.073178 (Hartree/Particle)
Thermal correction to Energy= 0.079344
Thermal correction to Enthalpy= 0.080288
Thermal correction to Gibbs Free Energy= 0.043470
Sum of electronic and zero-point Energies= -264.034111
Sum of electronic and thermal Energies= -264.027945
Sum of electronic and thermal Enthalpies= -264.027001
Sum of electronic and thermal Free Energies= -264.063820
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -264.1894569

DPPF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000032	0.000072	2.053489
2	15	0	1.920029	0.157831	-0.846946
3	15	0	-1.919999	-0.157920	-0.846937

4	6	0	4.268344	0.601682	-2.264838
5	6	0	2.185748	-1.668660	-0.860472
6	6	0	1.279359	-3.857354	-1.375160
7	6	0	3.661553	0.749442	-1.011299
8	6	0	2.445588	-4.456097	-0.908686
9	6	0	3.359035	-2.280506	-0.406662
10	6	0	1.153773	-2.470694	-1.358064
11	6	0	3.487096	-3.665463	-0.428789
12	6	0	4.376850	1.380371	0.009296
13	6	0	5.669068	1.849186	-0.218629
14	6	0	-1.638616	-0.457545	0.930841
15	6	0	-2.005573	0.339536	2.061828
16	6	0	-2.185834	1.668582	-0.860528
17	6	0	1.613534	0.349537	3.243129
18	6	0	-1.015407	-1.647592	1.436832
19	6	0	-1.613450	-0.349307	3.243143
20	6	0	5.560579	1.058363	-2.488868
21	6	0	-1.005271	-1.579252	2.857111
22	6	0	-1.153935	2.470672	-1.358188
23	6	0	1.638662	0.457585	0.930835
24	6	0	-3.359103	2.280400	-0.406619
25	6	0	1.005384	1.579467	2.857020
26	6	0	2.005641	-0.339411	2.061871
27	6	0	1.015460	1.647686	1.436746
28	6	0	-3.661488	-0.749572	-1.011188
29	6	0	-4.268324	-0.601597	-2.264667
30	6	0	-3.487198	3.665356	-0.428702
31	6	0	-1.279566	3.857324	-1.375279
32	6	0	-2.445755	4.456036	-0.908674
33	6	0	6.264303	1.687912	-1.464485
34	6	0	-5.668994	-1.849426	-0.218654
35	6	0	-4.376769	-1.380663	0.009321
36	6	0	-6.264284	-1.687926	-1.464460
37	6	0	-5.560588	-1.058185	-2.488743
38	1	0	0.577304	2.437085	0.831177
39	1	0	0.552929	2.303903	3.526838
40	1	0	1.699763	-0.027432	4.257751
41	1	0	2.451730	-1.328171	2.013727
42	1	0	-0.577254	-2.437015	0.831291
43	1	0	-0.552767	-2.303615	3.526975
44	1	0	-1.699658	0.027749	4.257732
45	1	0	-2.451660	1.328299	2.013606
46	1	0	0.243562	-1.996239	-1.731754
47	1	0	0.467909	-4.470370	-1.765094
48	1	0	2.548596	-5.540087	-0.928242
49	1	0	4.405817	-4.130083	-0.072874
50	1	0	4.181088	-1.663605	-0.039812
51	1	0	3.923561	1.507786	0.992728
52	1	0	6.213235	2.340816	0.586879
53	1	0	7.274684	2.054319	-1.639744
54	1	0	6.019539	0.928801	-3.468160
55	1	0	3.718993	0.115698	-3.073741
56	1	0	-4.181170	1.663496	-0.039796
57	1	0	-4.405911	4.129934	-0.072717
58	1	0	-2.548780	5.540024	-0.928167
59	1	0	-0.468164	4.470355	-1.765296
60	1	0	-0.243745	1.996245	-1.731938
61	1	0	-3.923484	-1.508319	0.992714
62	1	0	-6.213110	-2.341224	0.586786
63	1	0	-7.274670	-2.054296	-1.639760
64	1	0	-6.019576	-0.928441	-3.467998
65	1	0	-3.718996	-0.115456	-3.073493

Zero-point correction= 0.514075 (Hartree/Particle)
Thermal correction to Energy= 0.545878
Thermal correction to Enthalpy= 0.546822
Thermal correction to Gibbs Free Energy= 0.448715

Sum of electronic and zero-point Energies= -2116.997467
Sum of electronic and thermal Energies= -2116.965664
Sum of electronic and thermal Enthalpies= -2116.964720
Sum of electronic and thermal Free Energies= -2117.062827
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2118.4181578

INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	4.176823	-0.561376	-1.060719
2	15	0	1.328455	-2.003043	0.204013
3	15	0	1.936658	1.713510	0.404316
4	6	0	-0.375791	-4.204327	0.602801
5	6	0	2.177682	-2.489871	1.775280
6	6	0	2.951119	-1.811233	3.973674
7	6	0	0.554625	-3.613523	-0.264444
8	6	0	3.509958	-3.070155	4.172384
9	6	0	2.727834	-3.757610	1.993856
10	6	0	2.284123	-1.531030	2.784554
11	6	0	3.391299	-4.044465	3.183193
12	6	0	0.750583	-4.187314	-1.524372
13	6	0	0.029617	-5.315004	-1.910829
14	6	0	3.638336	1.152631	-0.054501
15	6	0	4.297404	1.446275	-1.294400
16	6	0	1.800321	3.220594	-0.659935
17	6	0	4.790204	-2.265737	-1.988318
18	6	0	4.547058	0.341768	0.706781
19	6	0	5.597955	0.866263	-1.274456
20	6	0	-1.087178	-5.334757	0.220016
21	6	0	5.753898	0.186659	-0.034595
22	6	0	0.556704	3.495138	-1.221490
23	6	0	2.744287	-1.983923	-0.944798
24	6	0	2.832910	4.151533	-0.832312
25	6	0	3.956183	-1.503831	-2.857422
26	6	0	4.044589	-2.572212	-0.815578
27	6	0	2.699803	-1.328070	-2.218474
28	6	0	2.267544	2.587161	2.020051
29	6	0	2.898151	1.937289	3.087711
30	6	0	2.623191	5.303401	-1.580740
31	6	0	0.337529	4.648936	-1.971953
32	6	0	1.376954	5.552118	-2.157356
33	6	0	-0.890306	-5.892134	-1.042537
34	6	0	1.879918	4.477696	3.500885
35	6	0	1.756902	3.871502	2.254100
36	6	0	2.513717	3.818081	4.547855
37	6	0	3.026450	2.543503	4.332585
38	1	0	1.864649	-0.742678	-2.589519
39	1	0	4.246742	-1.070085	-3.809408
40	1	0	5.833486	-2.513142	-2.160830
41	1	0	4.418923	-3.091593	0.061391
42	1	0	4.343792	-0.140613	1.657442
43	1	0	6.609450	-0.409914	0.266077
44	1	0	6.314062	0.884691	-2.090052
45	1	0	3.855715	1.986141	-2.126183
46	1	0	1.805911	-0.559417	2.634210
47	1	0	3.017519	-1.047951	4.749508
48	1	0	4.028055	-3.298631	5.102715
49	1	0	3.816965	-5.034851	3.339968
50	1	0	2.633315	-4.527427	1.226313
51	1	0	1.472585	-3.749661	-2.213861
52	1	0	0.194080	-5.746985	-2.897201
53	1	0	-1.452183	-6.774690	-1.344912
54	1	0	-1.801618	-5.781338	0.910864
55	1	0	-0.553317	-3.768732	1.588380
56	1	0	3.804031	3.979351	-0.367542

57	1	0	3.434456	6.018619	-1.710724
58	1	0	1.219497	6.456692	-2.743192
59	1	0	-0.646899	4.829756	-2.404982
60	1	0	-0.249327	2.782102	-1.058596
61	1	0	1.253752	4.413177	1.452500
62	1	0	1.481973	5.481736	3.649240
63	1	0	2.610925	4.294341	5.522022
64	1	0	3.534083	2.012954	5.137849
65	1	0	3.309744	0.940807	2.953087
66	26	0	-3.970732	-1.406557	-0.800215
67	15	0	-1.227810	0.279375	-1.970888
68	15	0	-1.993395	0.183941	1.637159
69	6	0	0.635157	1.026736	-3.926607
70	6	0	-2.232088	1.778768	-2.397381
71	6	0	-3.497922	3.692974	-1.602466
72	6	0	-0.280567	0.038928	-3.534949
73	6	0	-3.827703	4.028419	-2.913120
74	6	0	-2.567629	2.128235	-3.709369
75	6	0	-2.701976	2.579193	-1.352418
76	6	0	-3.359203	3.244834	-3.964976
77	6	0	-0.325178	-1.156781	-4.257952
78	6	0	0.529397	-1.363842	-5.338560
79	6	0	-3.592113	-0.487742	1.005198
80	6	0	-4.007505	-1.845375	1.185538
81	6	0	-1.959643	-0.752681	3.236835
82	6	0	-4.468287	-2.147226	-2.628707
83	6	0	-4.635205	0.172500	0.272397
84	6	0	-5.298528	-2.009562	0.607846
85	6	0	1.478501	0.823123	-5.011833
86	6	0	-5.690241	-0.759915	0.048620
87	6	0	-0.962362	-1.712078	3.387713
88	6	0	-2.519544	-0.994251	-2.153249
89	6	0	-2.898643	-0.595129	4.261112
90	6	0	-3.585072	-3.038985	-1.952755
91	6	0	-3.813558	-0.891049	-2.760567
92	6	0	-2.388505	-2.331645	-1.655685
93	6	0	-2.520114	1.855753	2.237547
94	6	0	-3.834383	2.241852	2.525853
95	6	0	-2.835164	-1.389924	5.399854
96	6	0	-0.896204	-2.516955	4.522145
97	6	0	-1.837567	-2.355772	5.531880
98	6	0	1.432805	-0.377733	-5.719332
99	6	0	-1.773546	4.075201	2.877301
100	6	0	-1.497001	2.790651	2.422473
101	6	0	-3.086030	4.452063	3.144628
102	6	0	-4.114462	3.531180	2.970489
103	1	0	-1.543470	-2.704554	-1.087446
104	1	0	-3.811066	-4.056159	-1.648668
105	1	0	-5.488718	-2.366143	-2.928782
106	1	0	-4.242824	0.013065	-3.182050
107	1	0	-4.616155	1.202238	-0.072593
108	1	0	-6.600357	-0.565465	-0.510414
109	1	0	-5.856650	-2.939009	0.551030
110	1	0	-3.413962	-2.621777	1.662002
111	1	0	-2.421394	2.338302	-0.325163
112	1	0	-3.846923	4.303009	-0.769698
113	1	0	-4.444120	4.902846	-3.116881
114	1	0	-3.611557	3.503648	-4.992587
115	1	0	-2.209654	1.517913	-4.539375
116	1	0	-1.025117	-1.940516	-3.967922
117	1	0	0.483562	-2.303453	-5.887735
118	1	0	2.099503	-0.541491	-6.564723
119	1	0	2.178761	1.604864	-5.304509
120	1	0	0.691479	1.964261	-3.368999
121	1	0	-3.684897	0.154616	4.169077
122	1	0	-3.571491	-1.257018	6.191633
123	1	0	-1.796471	-2.976415	6.425972

124	1	0	-0.102644	-3.260269	4.610829
125	1	0	-0.223357	-1.815645	2.595910
126	1	0	-0.467164	2.501202	2.201167
127	1	0	-0.955910	4.780967	3.020908
128	1	0	-3.307713	5.460941	3.489953
129	1	0	-5.144354	3.814525	3.184845
130	1	0	-4.651793	1.533380	2.396492
131	46	0	0.021003	0.085093	0.167612

Zero-point correction= 1.033949 (Hartree/Particle)
Thermal correction to Energy= 1.099739
Thermal correction to Enthalpy= 1.100683
Thermal correction to Gibbs Free Energy= 0.934539
Sum of electronic and zero-point Energies= -4360.864723
Sum of electronic and thermal Energies= -4360.798934
Sum of electronic and thermal Enthalpies= -4360.797990
Sum of electronic and thermal Free Energies= -4360.964134
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -4364.8615782

INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.341595	-2.731906	0.598581
2	15	0	1.932176	-0.239062	-0.043911
3	15	0	-2.053900	0.158190	-0.111911
4	6	0	4.219857	1.283125	0.331636
5	6	0	2.605154	-0.968887	-1.595209
6	6	0	2.380868	-1.281321	-3.987923
7	6	0	3.489580	0.200166	0.836593
8	6	0	3.541717	-2.048055	-4.000861
9	6	0	3.777225	-1.731917	-1.621323
10	6	0	1.919552	-0.740914	-2.790884
11	6	0	4.241000	-2.270084	-2.816709
12	6	0	3.949502	-0.445688	1.986245
13	6	0	5.115645	-0.015101	2.616403
14	6	0	-1.871620	-1.657082	-0.217689
15	6	0	-2.378218	-2.678271	0.648835
16	6	0	-3.015958	0.321304	1.450313
17	6	0	0.993687	-3.880309	1.617575
18	6	0	-1.101299	-2.311113	-1.235019
19	6	0	-1.921367	-3.939937	0.170682
20	6	0	5.387733	1.704188	0.953044
21	6	0	-1.139712	-3.712931	-0.998691
22	6	0	-2.361485	0.808837	2.583996
23	6	0	1.405128	-1.724774	0.875491
24	6	0	-4.364150	-0.037458	1.548083
25	6	0	0.336476	-2.980720	2.505464
26	6	0	1.656006	-3.111195	0.617972
27	6	0	0.584652	-1.657126	2.049559
28	6	0	-3.348947	0.478269	-1.378909
29	6	0	-4.067567	-0.521558	-2.039598
30	6	0	-5.037320	0.077201	2.759406
31	6	0	-3.032365	0.919015	3.798911
32	6	0	-4.371289	0.551901	3.887090
33	6	0	5.836989	1.056515	2.102464
34	6	0	-4.567612	2.152638	-2.635370
35	6	0	-3.601890	1.817791	-1.694202
36	6	0	-5.278461	1.149403	-3.290539
37	6	0	-5.024506	-0.185647	-2.993990
38	1	0	0.178579	-0.743694	2.474749
39	1	0	-0.295129	-3.257652	3.343413
40	1	0	0.944229	-4.964134	1.657025
41	1	0	2.199124	-3.504307	-0.236266
42	1	0	-0.545260	-1.809623	-2.022302
43	1	0	-0.606979	-4.468529	-1.567003

44	1	0	-2.086895	-4.899759	0.650384
45	1	0	-2.957933	-2.505813	1.550767
46	1	0	1.019132	-0.121318	-2.769619
47	1	0	1.838529	-1.093464	-4.913420
48	1	0	3.909943	-2.465159	-4.937079
49	1	0	5.155656	-2.861384	-2.826000
50	1	0	4.334904	-1.897771	-0.698231
51	1	0	3.398223	-1.293173	2.393821
52	1	0	5.462920	-0.526407	3.513363
53	1	0	6.747686	1.390285	2.597417
54	1	0	5.947206	2.544566	0.543600
55	1	0	3.862198	1.800026	-0.562166
56	1	0	-4.892302	-0.407741	0.668183
57	1	0	-6.087953	-0.202629	2.823582
58	1	0	-4.900576	0.643661	4.834420
59	1	0	-2.510812	1.302237	4.674684
60	1	0	-1.317776	1.118731	2.496460
61	1	0	-3.025474	2.600964	-1.194783
62	1	0	-4.759841	3.199209	-2.867483
63	1	0	-6.027185	1.409435	-4.037270
64	1	0	-5.575204	-0.973275	-3.506716
65	1	0	-3.877169	-1.569911	-1.806138
66	46	0	0.059691	1.133681	-0.263600
67	6	0	-0.011147	3.754749	-1.107839
68	6	0	-0.104840	5.019986	-0.831076
69	6	0	0.535159	4.189501	0.231311
70	1	0	-0.157952	2.953804	-1.831367
71	1	0	-0.396600	6.015645	-1.142283
72	6	0	2.039793	4.249571	0.469498
73	6	0	2.872967	4.508669	-0.770241
74	1	0	2.357603	3.297353	0.929352
75	1	0	2.242296	5.027764	1.225608
76	1	0	3.944332	4.520379	-0.530096
77	1	0	2.704813	3.729755	-1.529480
78	6	0	-0.227713	3.870976	1.503065
79	1	0	0.112057	2.910281	1.925345
80	1	0	-1.307787	3.796844	1.317239
81	1	0	2.623638	5.471791	-1.236813
82	1	0	-0.060036	4.643997	2.269545

Zero-point correction= 0.656887 (Hartree/Particle)
Thermal correction to Energy= 0.699293
Thermal correction to Enthalpy= 0.700237
Thermal correction to Gibbs Free Energy= 0.578136
Sum of electronic and zero-point Energies= -2478.053846
Sum of electronic and thermal Energies= -2478.011441
Sum of electronic and thermal Enthalpies= -2478.010497
Sum of electronic and thermal Free Energies= -2478.132597
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.5879472

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.019589	-2.709291	0.549703
2	15	0	1.929741	0.031812	-0.026043
3	15	0	-1.913177	0.087852	-0.112968
4	6	0	3.783577	2.004011	0.588489
5	6	0	2.734618	-0.545849	-1.578959
6	6	0	2.564589	-0.878696	-3.974669
7	6	0	3.367497	0.705019	0.904262
8	6	0	3.844551	-1.423420	-3.993311
9	6	0	4.025917	-1.082013	-1.612111
10	6	0	2.016166	-0.437641	-2.773331
11	6	0	4.575991	-1.520834	-2.811531
12	6	0	4.041176	0.001499	1.906264

13	6	0	5.110806	0.586848	2.579135
14	6	0	-1.572627	-1.704241	-0.201532
15	6	0	-2.009008	-2.766703	0.654667
16	6	0	-2.687885	0.219830	1.554978
17	6	0	1.503022	-3.773227	1.452509
18	6	0	-0.804010	-2.301604	-1.254450
19	6	0	-1.506000	-3.995045	0.138869
20	6	0	4.859286	2.581382	1.252148
21	6	0	-0.766690	-3.708024	-1.044502
22	6	0	-1.944283	0.810306	2.580649
23	6	0	1.648017	-1.543423	0.845088
24	6	0	-3.973945	-0.251000	1.838427
25	6	0	0.780951	-3.010644	2.415318
26	6	0	2.044112	-2.873586	0.490691
27	6	0	0.865915	-1.640436	2.043316
28	6	0	-3.404099	0.170006	-1.200416
29	6	0	-3.980663	-0.944486	-1.816730
30	6	0	-4.496253	-0.144792	3.123079
31	6	0	-2.464035	0.914678	3.867628
32	6	0	-3.741927	0.436239	4.139702
33	6	0	5.522782	1.874431	2.252537
34	6	0	-5.120601	1.565760	-2.193205
35	6	0	-3.984328	1.426461	-1.406477
36	6	0	-5.686884	0.449386	-2.803886
37	6	0	-5.112066	-0.802479	-2.616957
38	1	0	0.372752	-0.810640	2.541984
39	1	0	0.209653	-3.409054	3.247487
40	1	0	1.576676	-4.855822	1.422276
41	1	0	2.602898	-3.144483	-0.400556
42	1	0	-0.297809	-1.760477	-2.049285
43	1	0	-0.213309	-4.425704	-1.641496
44	1	0	-1.613740	-4.970949	0.602301
45	1	0	-2.566953	-2.640431	1.577812
46	1	0	1.019037	0.010861	-2.750176
47	1	0	1.994115	-0.788981	-4.897944
48	1	0	4.278076	-1.765421	-4.931961
49	1	0	5.582527	-1.936615	-2.826428
50	1	0	4.604929	-1.151453	-0.689778
51	1	0	3.728590	-1.011467	2.162528
52	1	0	5.625578	0.031540	3.362232
53	1	0	6.358793	2.331045	2.780330
54	1	0	5.174634	3.591661	0.995328
55	1	0	3.243322	2.566588	-0.176997
56	1	0	-4.571596	-0.702612	1.045167
57	1	0	-5.499751	-0.513483	3.331263
58	1	0	-4.155843	0.523777	5.143184
59	1	0	-1.873502	1.379542	4.655702
60	1	0	-0.946718	1.195321	2.354559
61	1	0	-3.535704	2.304197	-0.940580
62	1	0	-5.563043	2.550778	-2.335451
63	1	0	-6.573452	0.556676	-3.426938
64	1	0	-5.548742	-1.680387	-3.091522
65	1	0	-3.549428	-1.934830	-1.671246
66	46	0	0.020370	1.499759	-0.448987
67	6	0	0.932810	3.126365	-1.509010
68	6	0	0.813697	4.395380	-1.210435
69	6	0	-0.174858	3.849350	-0.265616
70	1	0	1.380213	2.571432	-2.343767
71	1	0	1.113207	5.383497	-1.551414
72	6	0	0.186712	3.911457	1.203852
73	1	0	1.191695	3.515831	1.396512
74	1	0	-0.532570	3.372516	1.836299
75	6	0	-1.614243	4.209783	-0.554399
76	1	0	-2.306967	3.691492	0.123892
77	1	0	-1.889420	3.977401	-1.590303
78	1	0	0.177556	4.969332	1.526976
79	1	0	-1.757275	5.296725	-0.404189

Zero-point correction=	0.626965 (Hartree/Particle)
Thermal correction to Energy=	0.667292
Thermal correction to Enthalpy=	0.668236
Thermal correction to Gibbs Free Energy=	0.552337
Sum of electronic and zero-point Energies=	-2438.787380
Sum of electronic and thermal Energies=	-2438.747052
Sum of electronic and thermal Enthalpies=	-2438.746108
Sum of electronic and thermal Free Energies=	-2438.862007

M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = 2441.5382444

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.342811	2.647912	-0.911867
2	15	0	-1.795015	-0.257035	-0.005129
3	15	0	1.804945	0.157437	-0.003785
4	6	0	-2.407554	-1.889974	2.163840
5	6	0	-3.080015	-0.621147	-1.264673
6	6	0	-3.581101	-1.347006	-3.517699
7	6	0	-2.607765	-0.622563	1.603305
8	6	0	-4.928410	-1.071544	-3.308673
9	6	0	-4.436415	-0.351879	-1.060685
10	6	0	-2.660576	-1.128555	-2.496196
11	6	0	-5.356306	-0.578438	-2.077856
12	6	0	-3.379185	0.313592	2.300082
13	6	0	-3.946188	-0.013401	3.527906
14	6	0	1.393493	1.622627	-1.007365
15	6	0	1.646751	3.020130	-0.809101
16	6	0	1.812820	0.746936	1.733001
17	6	0	-2.036314	3.765341	-0.736907
18	6	0	0.667871	1.498002	-2.240283
19	6	0	1.073003	3.737379	-1.895940
20	6	0	-2.978870	-2.214996	3.389772
21	6	0	0.468876	2.797793	-2.779466
22	6	0	0.957323	0.099488	2.628765
23	6	0	-1.821847	1.571586	-0.028238
24	6	0	2.583378	1.822683	2.188025
25	6	0	-1.307812	3.770322	0.486481
26	6	0	-2.359594	2.415584	-1.052919
27	6	0	-1.165856	2.423657	0.922745
28	6	0	3.586451	-0.066639	-0.379583
29	6	0	4.052657	0.125195	-1.684031
30	6	0	2.449554	2.277693	3.494870
31	6	0	0.821282	0.553410	3.937856
32	6	0	1.557742	1.652988	4.366409
33	6	0	-3.747779	-1.277880	4.074114
34	6	0	5.777908	-0.877163	0.253226
35	6	0	4.462629	-0.570667	0.586375
36	6	0	6.233422	-0.682755	-1.047070
37	6	0	5.368808	-0.177848	-2.013969
38	1	0	-0.624561	2.090585	1.804611
39	1	0	-0.875410	4.641111	0.968862
40	1	0	-2.264566	4.633242	-1.347437
41	1	0	-2.877450	2.070321	-1.943075
42	1	0	0.286171	0.560451	-2.638580
43	1	0	-0.096692	3.036859	-3.674015
44	1	0	1.043048	4.817671	-1.997565
45	1	0	2.121621	3.464868	0.059189
46	1	0	-1.605825	-1.375379	-2.636059
47	1	0	-3.244340	-1.744179	-4.473955
48	1	0	-5.651364	-1.247774	-4.103823
49	1	0	-6.412170	-0.371067	-1.909944
50	1	0	-4.775429	0.036165	-0.099285
51	1	0	-3.529572	1.310172	1.883978

52	1	0	-4.542860	0.725437	4.061066
53	1	0	-4.189756	-1.531369	5.036615
54	1	0	-2.816549	-3.204236	3.815112
55	1	0	-1.786231	-2.616023	1.633869
56	1	0	3.303663	2.295392	1.519191
57	1	0	3.045776	3.121817	3.838368
58	1	0	1.450598	2.018845	5.386454
59	1	0	0.133775	0.046968	4.614083
60	1	0	0.384004	-0.762885	2.280742
61	1	0	4.114309	-0.725260	1.608243
62	1	0	6.450083	-1.270347	1.014365
63	1	0	7.262583	-0.925187	-1.306942
64	1	0	5.719895	-0.022183	-3.032881
65	1	0	3.378201	0.506250	-2.451695
66	46	0	0.203445	-1.615139	-0.318979
67	6	0	-0.763953	-3.411912	-0.630573
68	6	0	0.288831	-4.223694	-0.689353
69	6	0	1.475064	-3.335086	-0.457525
70	1	0	-1.820369	-3.661208	-0.772191
71	1	0	0.352155	-5.311247	-0.873235
72	6	0	2.162958	-3.578742	0.867538
73	1	0	1.448175	-3.574672	1.702085
74	1	0	2.939120	-2.824580	1.072676
75	6	0	2.443697	-3.300423	-1.616530
76	1	0	3.266465	-2.587817	-1.455130
77	1	0	1.940299	-3.039178	-2.557121
78	1	0	2.900925	-4.301266	-1.755059
79	1	0	2.664049	-4.568198	0.865737

Zero-point correction= 0.629481 (Hartree/Particle)
Thermal correction to Energy= 0.669592
Thermal correction to Enthalpy= 0.670536
Thermal correction to Gibbs Free Energy= 0.556990
Sum of electronic and zero-point Energies= -2438.819764
Sum of electronic and thermal Energies= -2438.779654
Sum of electronic and thermal Enthalpies= -2438.778709
Sum of electronic and thermal Free Energies= -2438.892256
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.579118

TS1a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.518578	2.632209	-0.849973
2	15	0	-1.975827	-0.279564	0.147586
3	15	0	1.800795	0.315612	0.011269
4	6	0	-3.351792	-1.859183	1.981487
5	6	0	-2.820187	-0.724962	-1.421304
6	6	0	-2.676666	-1.711770	-3.628000
7	6	0	-3.260511	-0.580677	1.423997
8	6	0	-4.015337	-1.407892	-3.853862
9	6	0	-4.168229	-0.433304	-1.653281
10	6	0	-2.083438	-1.376421	-2.414639
11	6	0	-4.761576	-0.771895	-2.864292
12	6	0	-4.145614	0.413556	1.853071
13	6	0	-5.108965	0.128587	2.815827
14	6	0	1.263634	1.693044	-1.050122
15	6	0	1.453138	3.105549	-0.906157
16	6	0	2.312728	1.129197	1.568982
17	6	0	-2.185358	3.756717	-0.521690
18	6	0	0.450409	1.491963	-2.215054
19	6	0	0.762080	3.758810	-1.964981
20	6	0	-4.320786	-2.145043	2.936016
21	6	0	0.145782	2.762787	-2.774974
22	6	0	1.631897	0.801517	2.743859
23	6	0	-1.938116	1.536206	0.079422

24	6	0	3.368829	2.045557	1.624487
25	6	0	-1.381952	3.708241	0.653218
26	6	0	-2.536832	2.423132	-0.874416
27	6	0	-1.226096	2.345376	1.026387
28	6	0	3.393380	-0.188309	-0.741820
29	6	0	3.612838	-0.068627	-2.115753
30	6	0	3.709934	2.650137	2.828734
31	6	0	1.974543	1.405673	3.950449
32	6	0	3.008104	2.334990	3.990868
33	6	0	-5.199375	-1.150219	3.356465
34	6	0	5.486940	-1.380221	-0.534167
35	6	0	4.341180	-0.850898	0.046947
36	6	0	5.700617	-1.254758	-1.903973
37	6	0	4.763705	-0.595552	-2.691875
38	1	0	-0.623532	1.975813	1.852677
39	1	0	-0.910275	4.555681	1.140063
40	1	0	-2.433500	4.648852	-1.087943
41	1	0	-3.104585	2.118545	-1.748678
42	1	0	0.089103	0.529617	-2.569300
43	1	0	-0.494606	2.943412	-3.632068
44	1	0	0.667057	4.832460	-2.093235
45	1	0	1.968931	3.595003	-0.085973
46	1	0	-1.038360	-1.636304	-2.223535
47	1	0	-2.092698	-2.220941	-4.392660
48	1	0	-4.483151	-1.675599	-4.799972
49	1	0	-5.812825	-0.544617	-3.034876
50	1	0	-4.760794	0.053011	-0.876819
51	1	0	-4.076544	1.418843	1.435807
52	1	0	-5.790057	0.911179	3.146782
53	1	0	-5.951320	-1.369775	4.112685
54	1	0	-4.383492	-3.144885	3.362530
55	1	0	-2.644594	-2.628459	1.666008
56	1	0	3.935384	2.272117	0.719986
57	1	0	4.532987	3.362216	2.864517
58	1	0	3.280769	2.805579	4.934234
59	1	0	1.440538	1.138868	4.860712
60	1	0	0.836491	0.053375	2.707308
61	1	0	4.177413	-0.965681	1.118544
62	1	0	6.215313	-1.896642	0.088902
63	1	0	6.597085	-1.674888	-2.357285
64	1	0	4.922600	-0.496833	-3.764464
65	1	0	2.878823	0.433021	-2.745537
66	46	0	0.082204	-1.423301	0.320665
67	6	0	1.106879	-3.467012	0.395613
68	1	0	-0.419639	-2.946774	0.523227
69	6	0	0.585026	-4.899186	0.601311
70	1	0	1.408484	-5.623526	0.548013
71	1	0	0.104264	-4.987970	1.582115
72	1	0	-0.150020	-5.146309	-0.172895
73	6	0	1.654574	-3.286984	-0.933526
74	7	0	2.031134	-3.169609	-2.031650
75	6	0	2.010320	-3.078517	1.456815
76	7	0	2.698531	-2.795015	2.355446

Zero-point correction= 0.585509 (Hartree/Particle)
Thermal correction to Energy= 0.626010
Thermal correction to Enthalpy= 0.626955
Thermal correction to Gibbs Free Energy= 0.511366
Sum of electronic and zero-point Energies= -2507.829405
Sum of electronic and thermal Energies= -2507.788903
Sum of electronic and thermal Enthalpies= -2507.787959
Sum of electronic and thermal Free Energies= -2507.903548
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2510.5686856

INT2a'

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	26	0	-0.458313	2.257631	-1.536038
2	15	0	-1.883730	-0.330482	0.100693
3	15	0	1.755377	0.199340	0.029706
4	6	0	-2.443746	-1.390780	2.610465
5	6	0	-3.159197	-1.016565	-1.021354
6	6	0	-3.684910	-2.234105	-3.042787
7	6	0	-2.659516	-0.300880	1.759906
8	6	0	-5.032589	-1.932231	-2.875219
9	6	0	-4.514251	-0.715049	-0.859790
10	6	0	-2.751384	-1.783886	-2.113967
11	6	0	-5.447217	-1.177564	-1.780349
12	6	0	-3.439032	0.770225	2.208992
13	6	0	-3.998050	0.745501	3.482842
14	6	0	1.309913	1.316208	-1.334074
15	6	0	1.512715	2.723698	-1.512865
16	6	0	1.618455	1.185346	1.566141
17	6	0	-2.187887	3.325724	-1.689182
18	6	0	0.626392	0.835322	-2.500878
19	6	0	0.940165	3.100904	-2.759360
20	6	0	-3.005888	-1.413741	3.882064
21	6	0	0.393094	1.935545	-3.368129
22	6	0	0.764215	0.723150	2.569912
23	6	0	-1.916284	1.418160	-0.408602
24	6	0	2.305985	2.388799	1.760684
25	6	0	-1.482331	3.687747	-0.506468
26	6	0	-2.462269	1.931392	-1.631902
27	6	0	-1.306662	2.518425	0.283020
28	6	0	3.563739	0.023783	-0.196693
29	6	0	4.106464	0.001375	-1.485143
30	6	0	2.090232	3.141763	2.908589
31	6	0	0.547971	1.475228	3.721512
32	6	0	1.200735	2.692262	3.884115
33	6	0	-3.782636	-0.344774	4.320071
34	6	0	5.767465	-0.353886	0.719579
35	6	0	4.402910	-0.165206	0.906291
36	6	0	6.303203	-0.364277	-0.564641
37	6	0	5.470874	-0.189792	-1.665829
38	1	0	-0.778549	2.455475	1.230149
39	1	0	-1.088592	4.671924	-0.273957
40	1	0	-2.428781	3.985096	-2.516642
41	1	0	-2.956541	1.343292	-2.399422
42	1	0	0.310092	-0.193876	-2.655305
43	1	0	-0.155512	1.902674	-4.303466
44	1	0	0.873636	4.112852	-3.146204
45	1	0	1.953116	3.402167	-0.789741
46	1	0	-1.696335	-2.042235	-2.220997
47	1	0	-3.358509	-2.831071	-3.892588
48	1	0	-5.764677	-2.292767	-3.596079
49	1	0	-6.502814	-0.948790	-1.642931
50	1	0	-4.841771	-0.118477	-0.007589
51	1	0	-3.605773	1.632168	1.563427
52	1	0	-4.602658	1.585061	3.822149
53	1	0	-4.217767	-0.359825	5.318005
54	1	0	-2.828292	-2.266308	4.535075
55	1	0	-1.820104	-2.218587	2.269053
56	1	0	3.028122	2.729411	1.018083
57	1	0	2.622270	4.081474	3.048540
58	1	0	1.030919	3.287000	4.780207
59	1	0	-0.133918	1.105120	4.485878
60	1	0	0.256525	-0.234325	2.440549
61	1	0	3.986831	-0.184714	1.912637
62	1	0	6.411669	-0.503476	1.584118
63	1	0	7.371873	-0.517149	-0.707835
64	1	0	5.882150	-0.210655	-2.673375
65	1	0	3.461725	0.114836	-2.355371

66	46	0	0.084514	-1.632689	0.065130
67	6	0	1.529947	-3.253042	0.002729
68	1	0	-1.001830	-2.807710	0.109966
69	6	0	0.984478	-4.683883	0.058954
70	1	0	1.796557	-5.423957	0.006021
71	1	0	0.433011	-4.838398	0.992486
72	1	0	0.297812	-4.857981	-0.776081
73	6	0	2.133343	-2.944549	-1.270385
74	7	0	2.534084	-2.692466	-2.338054
75	6	0	2.339362	-2.935438	1.152624
76	7	0	2.922067	-2.683431	2.132486

Zero-point correction= 0.587614 (Hartree/Particle)
Thermal correction to Energy= 0.627976
Thermal correction to Enthalpy= 0.628920
Thermal correction to Gibbs Free Energy= 0.515264
Sum of electronic and zero-point Energies= -2507.845942
Sum of electronic and thermal Energies= -2507.805580
Sum of electronic and thermal Enthalpies= -2507.804636
Sum of electronic and thermal Free Energies= -2507.918292
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2510.5907784

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.284816	2.528994	-1.193423
2	15	0	-1.790830	-0.269141	0.028941
3	15	0	1.799887	0.123419	0.007005
4	6	0	-2.473621	-1.661653	2.331054
5	6	0	-3.097778	-0.749083	-1.167641
6	6	0	-3.659783	-1.693796	-3.323374
7	6	0	-2.597754	-0.431414	1.672993
8	6	0	-4.999581	-1.386040	-3.111447
9	6	0	-4.446211	-0.444523	-0.961790
10	6	0	-2.712978	-1.382661	-2.351173
11	6	0	-5.392889	-0.765283	-1.927849
12	6	0	-3.293279	0.611296	2.294087
13	6	0	-3.853240	0.429922	3.555047
14	6	0	1.444318	1.495206	-1.133699
15	6	0	1.699581	2.902555	-1.036399
16	6	0	1.755934	0.870911	1.683225
17	6	0	-1.999365	3.627630	-1.213395
18	6	0	0.771610	1.273818	-2.382706
19	6	0	1.177981	3.532300	-2.201130
20	6	0	-3.039791	-1.837825	3.589567
21	6	0	0.606201	2.526901	-3.032510
22	6	0	0.839978	0.352229	2.602521
23	6	0	-1.781731	1.545459	-0.222052
24	6	0	2.557348	1.953695	2.063514
25	6	0	-1.308516	3.800562	0.019701
26	6	0	-2.295427	2.243843	-1.362145
27	6	0	-1.162539	2.523082	0.629383
28	6	0	3.592257	-0.145510	-0.266681
29	6	0	4.158757	0.053122	-1.528454
30	6	0	2.401091	2.536987	3.315634
31	6	0	0.678821	0.937667	3.855488
32	6	0	1.452131	2.038793	4.207945
33	6	0	-3.725170	-0.794064	4.205225
34	6	0	5.705950	-1.030002	0.514875
35	6	0	4.378646	-0.691753	0.753483
36	6	0	6.262494	-0.829776	-0.745473
37	6	0	5.487117	-0.285384	-1.764835
38	1	0	-0.638456	2.314810	1.559678
39	1	0	-0.904729	4.733476	0.400198
40	1	0	-2.215360	4.405081	-1.939127

41	1	0	-2.784340	1.777042	-2.212483
42	1	0	0.404166	0.308461	-2.723615
43	1	0	0.082077	2.695059	-3.967605
44	1	0	1.159697	4.601085	-2.390141
45	1	0	2.139762	3.410457	-0.184448
46	1	0	-1.664094	-1.650374	-2.494228
47	1	0	-3.350458	-2.189949	-4.241946
48	1	0	-5.742665	-1.636134	-3.867184
49	1	0	-6.442697	-0.532083	-1.756185
50	1	0	-4.756750	0.044310	-0.037535
51	1	0	-3.395303	1.574149	1.793153
52	1	0	-4.389829	1.249402	4.031360
53	1	0	-4.161232	-0.933935	5.193628
54	1	0	-2.938078	-2.797767	4.093972
55	1	0	-1.917356	-2.468804	1.842260
56	1	0	3.317254	2.335027	1.380122
57	1	0	3.023460	3.384278	3.600043
58	1	0	1.327472	2.504680	5.184352
59	1	0	-0.059623	0.530464	4.545317
60	1	0	0.238117	-0.515701	2.323056
61	1	0	3.947398	-0.848073	1.743638
62	1	0	6.308331	-1.452653	1.317451
63	1	0	7.301283	-1.096737	-0.932681
64	1	0	5.918230	-0.123928	-2.751734
65	1	0	3.556211	0.471798	-2.335189
66	46	0	0.203395	-1.621315	-0.165034
67	6	0	-0.869967	-3.458785	-0.186060
68	6	0	0.225393	-3.896343	-0.890833
69	6	0	1.486831	-3.369801	-0.395561
70	1	0	-1.842391	-3.609778	-0.677870
71	1	0	0.215810	-4.422126	-1.865939
72	6	0	1.935550	-3.702376	1.009078
73	1	0	2.599598	-2.927625	1.422039
74	1	0	2.518801	-4.643506	0.993743
75	6	0	2.623356	-3.315547	-1.383739
76	1	0	3.467021	-2.717610	-1.013910
77	1	0	2.309477	-2.899630	-2.351563
78	1	0	1.084484	-3.831354	1.684473
79	1	0	3.007535	-4.335438	-1.566982

Zero-point correction= 0.629624 (Hartree/Particle)
Thermal correction to Energy= 0.669058
Thermal correction to Enthalpy= 0.670002
Thermal correction to Gibbs Free Energy= 0.558496
Sum of electronic and zero-point Energies= -2438.815242
Sum of electronic and thermal Energies= -2438.775809
Sum of electronic and thermal Enthalpies= -2438.774865
Sum of electronic and thermal Free Energies= -2438.886370
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.5754292

TS2a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.005075	-2.473736	-1.354097
2	15	0	1.858753	-0.083786	0.218322
3	15	0	-1.920089	-0.061194	0.091390
4	6	0	3.312518	0.631962	2.472255
5	6	0	2.714910	0.621480	-1.251992
6	6	0	2.587881	2.156365	-3.126479
7	6	0	3.217221	-0.306260	1.441551
8	6	0	3.874978	1.796717	-3.513493
9	6	0	4.012231	0.277576	-1.643052
10	6	0	2.015125	1.573208	-1.999710
11	6	0	4.586814	0.859343	-2.768733
12	6	0	4.131985	-1.364745	1.401524

13	6	0	5.137847	-1.461989	2.357340
14	6	0	-1.611312	-1.230835	-1.277608
15	6	0	-2.029711	-2.595530	-1.412958
16	6	0	-2.887165	-1.054236	1.286645
17	6	0	1.486496	-3.858131	-1.353770
18	6	0	-0.775270	-0.937719	-2.407707
19	6	0	-1.470320	-3.122693	-2.611012
20	6	0	4.321474	0.537552	3.425404
21	6	0	-0.700613	-2.097534	-3.228619
22	6	0	-2.397022	-1.161709	2.590161
23	6	0	1.572187	-1.813315	-0.273652
24	6	0	-4.089804	-1.690010	0.952000
25	6	0	0.717401	-3.962116	-0.159122
26	6	0	2.021978	-2.539235	-1.423015
27	6	0	0.766067	-2.706352	0.505953
28	6	0	-3.163121	1.082812	-0.638235
29	6	0	-2.899682	1.679424	-1.876549
30	6	0	-4.774292	-2.439990	1.900325
31	6	0	-3.084070	-1.915070	3.539489
32	6	0	-4.267515	-2.557486	3.193736
33	6	0	5.237983	-0.507197	3.366008
34	6	0	-5.111616	2.507450	-0.418503
35	6	0	-4.274679	1.519305	0.090480
36	6	0	-4.850981	3.079615	-1.659482
37	6	0	-3.740275	2.662262	-2.386723
38	1	0	0.241197	-2.440217	1.419894
39	1	0	0.138180	-4.825167	0.152678
40	1	0	1.596266	-4.629058	-2.110180
41	1	0	2.610728	-2.125910	-2.237219
42	1	0	-0.229760	-0.012792	-2.573436
43	1	0	-0.105168	-2.198621	-4.130143
44	1	0	-1.562942	-4.147157	-2.957639
45	1	0	-2.617728	-3.148968	-0.687790
46	1	0	1.012350	1.863011	-1.671009
47	1	0	2.031153	2.901917	-3.693303
48	1	0	4.330229	2.255287	-4.390063
49	1	0	5.599535	0.585989	-3.061623
50	1	0	4.585409	-0.439790	-1.054687
51	1	0	4.046691	-2.129800	0.628127
52	1	0	5.842026	-2.292007	2.319177
53	1	0	6.023661	-0.588388	4.115736
54	1	0	4.383397	1.275246	4.223921
55	1	0	2.566666	1.425872	2.535746
56	1	0	-4.497214	-1.584191	-0.054477
57	1	0	-5.708594	-2.931604	1.633096
58	1	0	-4.805858	-3.144554	3.936385
59	1	0	-2.694829	-1.992151	4.553334
60	1	0	-1.480592	-0.628316	2.854561
61	1	0	-4.489711	1.084917	1.066617
62	1	0	-5.974881	2.829958	0.161842
63	1	0	-5.508373	3.851564	-2.055999
64	1	0	-3.524694	3.105646	-3.357934
65	1	0	-2.028485	1.372590	-2.455935
66	46	0	-0.044186	1.120739	0.944491
67	6	0	-1.253758	2.447746	1.954826
68	6	0	-0.917475	3.410314	0.954793
69	6	0	0.377562	3.856458	0.742637
70	1	0	-2.350401	2.322617	2.001389
71	1	0	-1.652988	3.727502	0.192309
72	6	0	1.434697	3.928805	1.801056
73	1	0	2.402140	3.554080	1.433765
74	6	0	0.719450	4.583013	-0.519745
75	1	0	0.908784	5.650527	-0.321239
76	1	0	-0.078859	4.504927	-1.270177
77	1	0	1.648181	4.183893	-0.956596
78	1	0	1.597296	4.987837	2.068818
79	1	0	1.142999	3.377639	2.700188

Zero-point correction=	0.629818 (Hartree/Particle)
Thermal correction to Energy=	0.669219
Thermal correction to Enthalpy=	0.670163
Thermal correction to Gibbs Free Energy=	0.557765
Sum of electronic and zero-point Energies=	-2438.796929
Sum of electronic and thermal Energies=	-2438.757528
Sum of electronic and thermal Enthalpies=	-2438.756584
Sum of electronic and thermal Free Energies=	-2438.868982

M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.5579742

INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.314874	2.523753	-1.152662
2	15	0	-1.803949	-0.304072	0.044008
3	15	0	1.810447	0.142857	0.006360
4	6	0	-2.559070	-1.649293	2.359319
5	6	0	-3.039172	-0.778880	-1.230076
6	6	0	-3.465176	-1.617924	-3.460223
7	6	0	-2.703030	-0.457888	1.638888
8	6	0	-4.825731	-1.379623	-3.292706
9	6	0	-4.407657	-0.546879	-1.068512
10	6	0	-2.576589	-1.326121	-2.429539
11	6	0	-5.296368	-0.849664	-2.093870
12	6	0	-3.498590	0.569017	2.160158
13	6	0	-4.138379	0.408796	3.384843
14	6	0	1.427687	1.511942	-1.128896
15	6	0	1.667223	2.922686	-1.035795
16	6	0	1.823311	0.896833	1.680136
17	6	0	-2.029896	3.621923	-1.113296
18	6	0	0.732229	1.283758	-2.364170
19	6	0	1.114395	3.546517	-2.189248
20	6	0	-3.203058	-1.802830	3.583638
21	6	0	0.537962	2.534919	-3.009533
22	6	0	0.946968	0.375790	2.636514
23	6	0	-1.790807	1.511792	-0.189886
24	6	0	2.638323	1.980566	2.026671
25	6	0	-1.321508	3.759479	0.114455
26	6	0	-2.326983	2.242539	-1.298803
27	6	0	-1.164670	2.465124	0.683156
28	6	0	3.593294	-0.142267	-0.312779
29	6	0	4.123580	0.020243	-1.595449
30	6	0	2.532891	2.565225	3.283392
31	6	0	0.840691	0.959902	3.896189
32	6	0	1.624287	2.064189	4.214597
33	6	0	-3.989136	-0.776562	4.099302
34	6	0	5.724030	-1.022155	0.427588
35	6	0	4.406093	-0.670023	0.696549
36	6	0	6.244906	-0.855319	-0.852554
37	6	0	5.442614	-0.331852	-1.862160
38	1	0	-0.629180	2.230883	1.600915
39	1	0	-0.912587	4.681453	0.515503
40	1	0	-2.259012	4.420803	-1.811309
41	1	0	-2.825384	1.801484	-2.157270
42	1	0	0.367798	0.314809	-2.697151
43	1	0	-0.006838	2.697115	-3.933742
44	1	0	1.079750	4.615070	-2.377161
45	1	0	2.118198	3.436996	-0.193507
46	1	0	-1.511069	-1.538499	-2.542259
47	1	0	-3.094156	-2.043451	-4.391374
48	1	0	-5.523467	-1.615231	-4.094872
49	1	0	-6.362150	-0.672991	-1.956433
50	1	0	-4.780912	-0.130455	-0.132206
51	1	0	-3.613551	1.503822	1.610620

52	1	0	-4.753497	1.214668	3.782948
53	1	0	-4.485899	-0.898871	5.061025
54	1	0	-3.085024	-2.732363	4.138846
55	1	0	-1.930500	-2.445293	1.943963
56	1	0	3.371183	2.360465	1.313736
57	1	0	3.164620	3.413974	3.541440
58	1	0	1.539548	2.529111	5.195687
59	1	0	0.140501	0.549104	4.622194
60	1	0	0.338198	-0.494887	2.379640
61	1	0	4.003090	-0.801955	1.701926
62	1	0	6.347332	-1.429165	1.222262
63	1	0	7.276593	-1.132337	-1.062944
64	1	0	5.845778	-0.196667	-2.864666
65	1	0	3.499934	0.421421	-2.395053
66	46	0	0.217027	-1.609585	-0.098876
67	6	0	-0.860798	-3.464557	0.010511
68	6	0	0.221409	-3.839502	-0.770267
69	6	0	1.509887	-3.380565	-0.311587
70	1	0	-1.828277	-3.589364	-0.502327
71	1	0	0.165458	-4.264103	-1.791427
72	6	0	1.970565	-3.662151	1.098195
73	1	0	2.631747	-2.870440	1.482111
74	1	0	2.562260	-4.597310	1.104667
75	6	0	2.630257	-3.357170	-1.316938
76	1	0	3.465398	-2.723451	-0.990143
77	1	0	2.295618	-2.998982	-2.300459
78	1	0	3.035046	-4.376188	-1.448921
79	1	0	1.123563	-3.777725	1.780842

Zero-point correction= 0.629534 (Hartree/Particle)
Thermal correction to Energy= 0.669760
Thermal correction to Enthalpy= 0.670705
Thermal correction to Gibbs Free Energy= 0.556832
Sum of electronic and zero-point Energies= -2438.815277
Sum of electronic and thermal Energies= -2438.775051
Sum of electronic and thermal Enthalpies= -2438.774107
Sum of electronic and thermal Free Energies= -2438.887980
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.5763382

INT4a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.795630	-2.154478	1.595508
2	15	0	-1.945508	0.464936	-0.237605
3	15	0	1.632509	-0.524608	-0.107833
4	6	0	-3.110285	1.497880	-2.541710
5	6	0	-2.771390	1.443316	1.086724
6	6	0	-2.547543	2.977045	2.949025
7	6	0	-3.195415	0.477578	-1.588808
8	6	0	-3.917772	2.906960	3.177869
9	6	0	-4.149444	1.388770	1.318258
10	6	0	-1.980728	2.253498	1.903722
11	6	0	-4.718811	2.115884	2.357705
12	6	0	-4.212013	-0.475957	-1.701451
13	6	0	-5.133778	-0.402776	-2.741377
14	6	0	1.074371	-1.427462	1.368090
15	6	0	1.116295	-2.824135	1.688536
16	6	0	1.977234	-1.856565	-1.322299
17	6	0	-2.604981	-3.078552	1.738612
18	6	0	0.403510	-0.765317	2.449800
19	6	0	0.469346	-3.013309	2.943130
20	6	0	-4.037638	1.574519	-3.575199
21	6	0	0.032770	-1.741935	3.414519
22	6	0	1.220623	-1.904380	-2.495664
23	6	0	-2.160940	-1.230229	0.414524

24	6	0	2.982629	-2.807159	-1.117806
25	6	0	-1.908819	-3.528118	0.580394
26	6	0	-2.768709	-1.667513	1.635956
27	6	0	-1.631281	-2.394925	-0.233296
28	6	0	3.325827	-0.008048	0.382090
29	6	0	3.838462	-0.180088	1.672055
30	6	0	3.205627	-3.806157	-2.058678
31	6	0	1.444034	-2.904651	-3.438212
32	6	0	2.433490	-3.857527	-3.217312
33	6	0	-5.049448	0.623665	-3.677318
34	6	0	5.342998	1.184915	-0.232454
35	6	0	4.093136	0.678988	-0.566085
36	6	0	5.837689	1.027931	1.060473
37	6	0	5.084966	0.341088	2.008460
38	1	0	-1.063835	-2.399261	-1.160759
39	1	0	-1.586594	-4.545507	0.383170
40	1	0	-2.906018	-3.693466	2.580865
41	1	0	-3.215829	-1.018036	2.382571
42	1	0	0.171642	0.296526	2.483373
43	1	0	-0.538979	-1.557438	4.318112
44	1	0	0.285019	-3.968950	3.424193
45	1	0	1.505361	-3.607577	1.045265
46	1	0	-0.910863	2.326546	1.699046
47	1	0	-1.918434	3.605475	3.577704
48	1	0	-4.365995	3.476850	3.990431
49	1	0	-5.793712	2.068426	2.526454
50	1	0	-4.782902	0.773716	0.677538
51	1	0	-4.281623	-1.283823	-0.971566
52	1	0	-5.919604	-1.152642	-2.822463
53	1	0	-5.770239	0.679513	-4.491864
54	1	0	-3.962180	2.374131	-4.310703
55	1	0	-2.297980	2.224135	-2.467408
56	1	0	3.600159	-2.755322	-0.219455
57	1	0	3.989651	-4.543725	-1.893130
58	1	0	2.612193	-4.637399	-3.956121
59	1	0	0.850200	-2.932159	-4.350448
60	1	0	0.461412	-1.135858	-2.665057
61	1	0	3.691964	0.835926	-1.568771
62	1	0	5.923997	1.722696	-0.981131
63	1	0	6.811105	1.436809	1.327271
64	1	0	5.471977	0.204385	3.017388
65	1	0	3.259206	-0.718624	2.422448
66	46	0	0.228374	1.203708	-0.922922
67	6	0	1.365742	2.500933	-1.947630
68	6	0	2.414935	3.399077	-1.588133
69	6	0	2.748927	3.767769	-0.313161
70	1	0	1.498380	2.216176	-3.007509
71	1	0	3.054739	3.822357	-2.376101
72	6	0	2.010028	3.309327	0.892983
73	1	0	2.469098	2.396066	1.310606
74	6	0	3.937155	4.629545	-0.052563
75	1	0	3.657986	5.524485	0.524997
76	1	0	4.432591	4.949914	-0.977393
77	1	0	4.674735	4.087575	0.562744
78	1	0	2.033804	4.072808	1.684154
79	1	0	0.970947	3.052933	0.631683

Zero-point correction= 0.629719 (Hartree/Particle)
Thermal correction to Energy= 0.670102
Thermal correction to Enthalpy= 0.671046
Thermal correction to Gibbs Free Energy= 0.555199
Sum of electronic and zero-point Energies= -2438.813039
Sum of electronic and thermal Energies= -2438.772656
Sum of electronic and thermal Enthalpies= -2438.771712
Sum of electronic and thermal Free Energies= -2438.887559
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2441.5704737

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.113418	-3.256730	0.212761
2	15	0	1.803721	-0.276868	-0.109211
3	15	0	-1.811401	-0.475774	0.156436
4	6	0	2.729162	1.949489	1.257225
5	6	0	3.033803	-0.521146	-1.454070
6	6	0	3.438401	-1.027868	-3.787495
7	6	0	2.758088	0.551317	1.216700
8	6	0	4.810395	-1.028940	-3.551657
9	6	0	4.411131	-0.530575	-1.224636
10	6	0	2.555874	-0.767014	-2.745048
11	6	0	5.294368	-0.777044	-2.271411
12	6	0	3.500745	-0.145687	2.175420
13	6	0	4.197325	0.546565	3.160449
14	6	0	-1.591238	-2.248599	-0.163946
15	6	0	-1.860903	-3.402355	0.642667
16	6	0	-1.664071	-0.292332	1.973969
17	6	0	1.806111	-4.309193	0.633252
18	6	0	-1.004814	-2.717285	-1.388377
19	6	0	-1.435103	-4.555859	-0.073598
20	6	0	3.433923	2.641045	2.237407
21	6	0	-0.907034	-4.133118	-1.327199
22	6	0	-0.644688	0.516214	2.480290
23	6	0	1.689517	-1.999365	0.513088
24	6	0	-2.508883	-0.960052	2.867330
25	6	0	1.198536	-3.839469	1.832071
26	6	0	2.115324	-3.180861	-0.175575
27	6	0	1.116125	-2.421089	1.760877
28	6	0	-3.602960	-0.225425	-0.116912
29	6	0	-4.377425	-1.135909	-0.839944
30	6	0	-2.292026	-0.867916	4.237384
31	6	0	-0.424289	0.608775	3.851169
32	6	0	-1.240494	-0.095867	4.729902
33	6	0	4.163094	1.937829	3.192095
34	6	0	-5.527325	1.222956	0.090523
35	6	0	-4.186452	0.961445	0.345869
36	6	0	-6.295496	0.311516	-0.631098
37	6	0	-5.719506	-0.866008	-1.095667
38	1	0	0.673801	-1.767624	2.508148
39	1	0	0.803472	-4.456591	2.632592
40	1	0	1.960355	-5.347951	0.359518
41	1	0	2.557655	-3.206249	-1.167134
42	1	0	-0.642125	-2.071333	-2.183987
43	1	0	-0.455088	-4.774945	-2.076347
44	1	0	-1.448609	-5.574913	0.300407
45	1	0	-2.247198	-3.392681	1.656989
46	1	0	1.479615	-0.740043	-2.929172
47	1	0	3.054111	-1.217172	-4.788649
48	1	0	5.504559	-1.220646	-4.368337
49	1	0	6.367115	-0.771856	-2.084631
50	1	0	4.797335	-0.339298	-0.223346
51	1	0	3.535109	-1.234670	2.151281
52	1	0	4.768538	-0.004447	3.906309
53	1	0	4.705449	2.477967	3.966696
54	1	0	3.397573	3.729297	2.254305
55	1	0	2.145820	2.494538	0.508748
56	1	0	-3.349869	-1.544027	2.490548
57	1	0	-2.949749	-1.395562	4.926513
58	1	0	-1.072365	-0.030062	5.803722
59	1	0	0.386495	1.233673	4.223631
60	1	0	-0.019856	1.081699	1.788498
61	1	0	-3.584663	1.683165	0.904449
62	1	0	-5.974146	2.145745	0.457047

63	1	0	-7.345149	0.520967	-0.831453
64	1	0	-6.316856	-1.582645	-1.657398
65	1	0	-3.931045	-2.062723	-1.202926
66	46	0	-0.188181	0.777632	-1.035361
67	6	0	0.835468	2.406819	-2.094016
68	6	0	-0.009607	1.820717	-3.042035
69	6	0	-1.391745	1.623668	-2.708016
70	1	0	1.892673	2.269531	-2.377944
71	1	0	0.355615	1.275869	-3.931944
72	6	0	-2.250077	2.730385	-2.165115
73	1	0	-1.670858	3.464616	-1.601639
74	1	0	-3.051997	2.351538	-1.516771
75	6	0	-2.166309	0.613704	-3.512288
76	1	0	-2.947023	0.126421	-2.909337
77	1	0	-1.515057	-0.165993	-3.931925
78	1	0	-2.682594	1.107920	-4.353032
79	1	0	-2.738923	3.249288	-3.009428
80	1	0	0.414743	3.898606	-0.789029
81	6	0	0.056083	4.704885	-0.052788
82	6	0	-0.507883	5.892726	-0.845678
83	1	0	-0.887394	6.678408	-0.183329
84	1	0	0.283626	6.312786	-1.475271
85	1	0	-1.321620	5.555104	-1.496572
86	6	0	-0.959222	4.037339	0.757053
87	7	0	-1.788599	3.461321	1.332786
88	6	0	1.191058	5.119291	0.763613
89	7	0	2.115644	5.474618	1.370917

Zero-point correction= 0.704301 (Hartree/Particle)
Thermal correction to Energy= 0.751852
Thermal correction to Enthalpy= 0.752797
Thermal correction to Gibbs Free Energy= 0.623681
Sum of electronic and zero-point Energies= -2702.864892
Sum of electronic and thermal Energies= -2702.817341
Sum of electronic and thermal Enthalpies= -2702.816397
Sum of electronic and thermal Free Energies= -2702.945512
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2705.7762699

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.514530	-3.213427	-0.057293
2	15	0	1.686223	-0.568388	-0.094390
3	15	0	-1.896682	-0.151069	0.141059
4	6	0	3.006648	1.330392	1.420863
5	6	0	2.884322	-0.923476	-1.441864
6	6	0	3.256036	-1.301330	-3.804392
7	6	0	2.736411	-0.036526	1.306114
8	6	0	4.595838	-1.581880	-3.550013
9	6	0	4.228075	-1.211548	-1.194372
10	6	0	2.406893	-0.966343	-2.755321
11	6	0	5.080050	-1.533895	-2.246270
12	6	0	3.276921	-0.922987	2.243336
13	6	0	4.067456	-0.442779	3.282470
14	6	0	-2.004850	-1.891007	-0.370105
15	6	0	-2.498412	-3.049508	0.316800
16	6	0	-1.738868	-0.186035	1.966007
17	6	0	0.952379	-4.580471	0.307880
18	6	0	-1.465717	-2.343159	-1.622513
19	6	0	-2.252592	-4.189623	-0.497620
20	6	0	3.806544	1.808489	2.453219
21	6	0	-1.614467	-3.754033	-1.694089
22	6	0	-0.618136	0.402455	2.554851
23	6	0	1.242403	-2.284062	0.377646
24	6	0	-2.688622	-0.809295	2.783257

25	6	0	0.397617	-4.106024	1.529888
26	6	0	1.478729	-3.464300	-0.399532
27	6	0	0.565910	-2.694759	1.576203
28	6	0	-3.601788	0.472125	-0.077929
29	6	0	-4.547907	-0.193776	-0.859907
30	6	0	-2.479106	-0.902902	4.154181
31	6	0	-0.405617	0.308048	3.927076
32	6	0	-1.328801	-0.358677	4.725255
33	6	0	4.330863	0.919979	3.388011
34	6	0	-5.198737	2.241351	0.325303
35	6	0	-3.932211	1.700377	0.509934
36	6	0	-6.140872	1.571055	-0.452848
37	6	0	-5.813687	0.356864	-1.046509
38	1	0	0.219446	-2.034902	2.367201
39	1	0	-0.122955	-4.704699	2.270446
40	1	0	0.932703	-5.605659	-0.047795
41	1	0	1.940798	-3.489143	-1.382021
42	1	0	-0.969791	-1.703617	-2.348530
43	1	0	-1.252116	-4.393512	-2.492067
44	1	0	-2.457466	-5.219982	-0.224350
45	1	0	-2.913664	-3.064840	1.319170
46	1	0	1.359023	-0.726154	-2.950157
47	1	0	2.874106	-1.331972	-4.823674
48	1	0	5.265032	-1.833578	-4.371191
49	1	0	6.128563	-1.748050	-2.045176
50	1	0	4.611750	-1.178016	-0.174613
51	1	0	3.080768	-1.991730	2.159737
52	1	0	4.481421	-1.138966	4.010705
53	1	0	4.950527	1.292164	4.202470
54	1	0	4.013058	2.876046	2.513349
55	1	0	2.586769	2.024436	0.687999
56	1	0	-3.604964	-1.210114	2.347113
57	1	0	-3.219209	-1.395347	4.783151
58	1	0	-1.166218	-0.439305	5.798933
59	1	0	0.486978	0.757923	4.360422
60	1	0	0.090437	0.950702	1.935334
61	1	0	-3.186917	2.235406	1.103926
62	1	0	-5.450471	3.193592	0.789263
63	1	0	-7.131682	1.999187	-0.596797
64	1	0	-6.547639	-0.170122	-1.654275
65	1	0	-4.297179	-1.149676	-1.321648
66	46	0	-0.061335	0.896816	-0.947087
67	6	0	1.242832	2.408839	-1.892219
68	6	0	0.284424	2.054071	-2.849426
69	6	0	-1.110601	2.092402	-2.527546
70	1	0	2.255195	2.103422	-2.200235
71	1	0	0.548774	1.493542	-3.762701
72	6	0	-1.774484	3.265782	-1.866655
73	1	0	-1.131901	3.785793	-1.155066
74	1	0	-2.683563	2.958492	-1.331816
75	6	0	-2.047015	1.308272	-3.407043
76	1	0	-2.890199	0.902297	-2.829189
77	1	0	-1.540572	0.475973	-3.915195
78	1	0	-2.483578	1.961860	-4.181105
79	1	0	-2.087899	3.984719	-2.644469
80	1	0	1.246349	3.598992	-0.768417
81	6	0	1.155664	4.530341	0.086082
82	6	0	0.762476	5.798083	-0.676806
83	1	0	0.550346	6.643182	-0.011186
84	1	0	1.584840	6.080699	-1.344087
85	1	0	-0.121877	5.609400	-1.296353
86	6	0	0.126114	3.990004	0.942119
87	7	0	-0.738977	3.449722	1.508282
88	6	0	2.422774	4.674371	0.763292
89	7	0	3.473224	4.787359	1.254238

Zero-point correction= 0.700962 (Hartree/Particle)

Thermal correction to Energy= 0.747939
Thermal correction to Enthalpy= 0.748884
Thermal correction to Gibbs Free Energy= 0.621127
Sum of electronic and zero-point Energies= -2702.866226
Sum of electronic and thermal Energies= -2702.819248
Sum of electronic and thermal Enthalpies= -2702.818304
Sum of electronic and thermal Free Energies= -2702.946061
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2705.7744974

INT6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.367233	-3.256111	-0.115347
2	15	0	1.742265	-0.540163	-0.071336
3	15	0	-1.867044	-0.271594	0.167599
4	6	0	3.014976	1.381043	1.443415
5	6	0	2.944054	-0.769058	-1.442744
6	6	0	3.329258	-1.291211	-3.778619
7	6	0	2.781593	0.008138	1.323329
8	6	0	4.698242	-1.104460	-3.597484
9	6	0	4.316502	-0.582588	-1.271006
10	6	0	2.458424	-1.114295	-2.710478
11	6	0	5.186728	-0.747122	-2.346365
12	6	0	3.397573	-0.877253	2.214590
13	6	0	4.225468	-0.384139	3.217562
14	6	0	-1.914066	-1.990956	-0.410227
15	6	0	-2.362382	-3.188266	0.238482
16	6	0	-1.939487	-0.391043	1.992671
17	6	0	1.137983	-4.580757	0.259268
18	6	0	-1.337680	-2.382615	-1.665172
19	6	0	-2.056858	-4.293036	-0.604832
20	6	0	3.858058	1.871242	2.434999
21	6	0	-1.424469	-3.796126	-1.780403
22	6	0	-0.868814	0.074177	2.759708
23	6	0	1.355032	-2.277778	0.346463
24	6	0	-3.049162	-0.955034	2.630859
25	6	0	0.554815	-4.132339	1.477491
26	6	0	1.636523	-3.444501	-0.436024
27	6	0	0.680043	-2.717616	1.534383
28	6	0	-3.516656	0.393036	-0.248961
29	6	0	-4.445731	-0.310307	-1.017987
30	6	0	-3.063157	-1.100611	4.013452
31	6	0	-0.884765	-0.072104	4.143680
32	6	0	-1.975261	-0.668230	4.769194
33	6	0	4.455970	0.985540	3.326822
34	6	0	-5.021871	2.283459	-0.177879
35	6	0	-3.811051	1.697778	0.171493
36	6	0	-5.946012	1.578536	-0.947670
37	6	0	-5.657597	0.283533	-1.364655
38	1	0	0.300976	-2.073421	2.322432
39	1	0	0.044816	-4.751352	2.208416
40	1	0	1.154514	-5.603549	-0.103297
41	1	0	2.112226	-3.450075	-1.411819
42	1	0	-0.862634	-1.698154	-2.364188
43	1	0	-1.024446	-4.396255	-2.590888
44	1	0	-2.218031	-5.338692	-0.362247
45	1	0	-2.786992	-3.247672	1.235725
46	1	0	1.384225	-1.245324	-2.856882
47	1	0	2.938914	-1.566399	-4.757282
48	1	0	5.382018	-1.231541	-4.434912
49	1	0	6.254481	-0.592407	-2.200936
50	1	0	4.710245	-0.300664	-0.295253
51	1	0	3.236585	-1.951032	2.120590
52	1	0	4.697977	-1.075624	3.913915
53	1	0	5.110100	1.363528	4.111222

54	1	0	4.028192	2.946356	2.485744
55	1	0	2.546178	2.083123	0.752383
56	1	0	-3.913811	-1.266686	2.041856
57	1	0	-3.928290	-1.544064	4.504073
58	1	0	-1.988131	-0.779978	5.852284
59	1	0	-0.043334	0.291519	4.730964
60	1	0	-0.034463	0.576057	2.269902
61	1	0	-3.075403	2.250029	0.761570
62	1	0	-5.245430	3.297013	0.151619
63	1	0	-6.892977	2.041048	-1.221341
64	1	0	-6.378890	-0.271413	-1.962694
65	1	0	-4.223934	-1.325146	-1.349620
66	46	0	-0.020997	0.932212	-0.749452
67	6	0	1.276564	2.212506	-1.918086
68	6	0	0.207195	1.843339	-2.771388
69	6	0	-1.115322	2.252388	-2.565280
70	1	0	2.271977	1.825230	-2.138152
71	1	0	0.378720	1.037026	-3.490628
72	6	0	-1.487791	3.571344	-1.966581
73	1	0	-0.650957	4.084595	-1.482138
74	1	0	-2.299390	3.461589	-1.233264
75	6	0	-2.221293	1.575775	-3.314743
76	1	0	-3.109203	1.449181	-2.677895
77	1	0	-1.926159	0.589530	-3.695951
78	1	0	-2.536108	2.195471	-4.169972
79	1	0	-1.872429	4.218875	-2.772016
80	1	0	1.251793	3.150993	-1.353598
81	6	0	0.711637	4.838821	0.717714
82	6	0	0.018032	6.157788	0.475930
83	1	0	0.019675	6.814816	1.359536
84	1	0	0.484933	6.717815	-0.346773
85	1	0	-1.031790	5.985903	0.202722
86	6	0	-0.000197	3.674330	0.918973
87	7	0	-0.606258	2.661581	1.037311
88	6	0	2.102519	4.773661	0.897899
89	7	0	3.268321	4.706030	1.026388

Zero-point correction= 0.705685 (Hartree/Particle)
Thermal correction to Energy= 0.753333
Thermal correction to Enthalpy= 0.754277
Thermal correction to Gibbs Free Energy= 0.623492
Sum of electronic and zero-point Energies= -2702.908185
Sum of electronic and thermal Energies= -2702.860537
Sum of electronic and thermal Enthalpies= -2702.859593
Sum of electronic and thermal Free Energies= -2702.990378
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2705.8283024

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.966681	-2.687096	-0.597486
2	15	0	1.087085	-1.284167	-0.029910
3	15	0	-2.118768	0.662506	-0.002153
4	6	0	2.387655	-0.412388	2.296432
5	6	0	2.223284	-1.717196	-1.397903
6	6	0	2.557417	-2.178153	-3.753263
7	6	0	2.105087	-1.505615	1.475381
8	6	0	3.934939	-2.039815	-3.590616
9	6	0	3.605757	-1.564894	-1.248499
10	6	0	1.705391	-1.998123	-2.670438
11	6	0	4.453817	-1.717302	-2.342395
12	6	0	2.652447	-2.755204	1.791019
13	6	0	3.477303	-2.896115	2.898896
14	6	0	-2.744841	-0.830256	-0.829147
15	6	0	-3.762854	-1.759319	-0.435000

16	6	0	-2.552867	0.451562	1.762687
17	6	0	-1.334845	-4.593334	-0.243008
18	6	0	-2.193423	-1.306787	-2.065389
19	6	0	-3.831922	-2.787743	-1.416127
20	6	0	3.228783	-0.548164	3.397570
21	6	0	-2.864446	-2.508277	-2.423209
22	6	0	-1.509278	0.424619	2.691642
23	6	0	-0.057046	-2.697609	0.102028
24	6	0	-3.870762	0.315804	2.214038
25	6	0	-1.777927	-3.983355	0.964387
26	6	0	-0.269605	-3.810885	-0.771412
27	6	0	-0.996853	-2.815958	1.178984
28	6	0	-3.270336	1.972266	-0.564749
29	6	0	-3.728912	1.987720	-1.885564
30	6	0	-4.131112	0.120353	3.565533
31	6	0	-1.768990	0.227634	4.044795
32	6	0	-3.080408	0.068272	4.480059
33	6	0	3.773562	-1.791171	3.696584
34	6	0	-4.304626	4.133977	-0.210738
35	6	0	-3.559879	3.060150	0.266654
36	6	0	-4.761624	4.138454	-1.525365
37	6	0	-4.472454	3.062956	-2.360208
38	1	0	-1.112346	-2.109034	1.996507
39	1	0	-2.607698	-4.313174	1.580933
40	1	0	-1.766094	-5.473597	-0.709090
41	1	0	0.262424	-3.998221	-1.698606
42	1	0	-1.370622	-0.836260	-2.599456
43	1	0	-2.637538	-3.132606	-3.281405
44	1	0	-4.466077	-3.667472	-1.370135
45	1	0	-4.329331	-1.722650	0.490482
46	1	0	0.626033	-2.068022	-2.816357
47	1	0	2.142560	-2.410901	-4.733159
48	1	0	4.599806	-2.163267	-4.443787
49	1	0	5.519586	-1.549250	-2.201492
50	1	0	4.041798	-1.288700	-0.288085
51	1	0	2.439385	-3.615548	1.154703
52	1	0	3.903675	-3.869613	3.135648
53	1	0	4.437619	-1.902248	4.552112
54	1	0	3.464987	0.328268	3.997809
55	1	0	1.953329	0.563904	2.078172
56	1	0	-4.696303	0.383038	1.504122
57	1	0	-5.158552	0.013857	3.909887
58	1	0	-3.288320	-0.085476	5.537649
59	1	0	-0.945283	0.204217	4.755904
60	1	0	-0.483457	0.554118	2.338679
61	1	0	-3.207903	3.065842	1.299240
62	1	0	-4.528616	4.970924	0.448660
63	1	0	-5.343108	4.979529	-1.898638
64	1	0	-4.828868	3.059297	-3.389058
65	1	0	-3.502830	1.152860	-2.549717
66	46	0	0.207847	0.935307	-0.404245
67	6	0	2.509475	1.745078	-0.478208
68	6	0	1.587003	2.477869	-1.250727
69	6	0	0.482888	3.178032	-0.718633
70	1	0	3.139794	1.000033	-0.956545
71	1	0	1.650863	2.384971	-2.338008
72	6	0	0.477731	3.729201	0.681640
73	1	0	1.162886	3.220974	1.371787
74	1	0	-0.536282	3.702924	1.107504
75	6	0	-0.455723	3.870349	-1.663017
76	1	0	-1.469736	3.931646	-1.244310
77	1	0	-0.514965	3.360587	-2.633312
78	1	0	-0.121540	4.906165	-1.839340
79	1	0	0.784582	4.788831	0.657423
80	1	0	2.477038	1.754692	0.603102
81	6	0	4.550334	2.909253	0.033436
82	6	0	4.491644	4.103334	-0.881553

83	1	0	5.308681	4.824043	-0.728068
84	1	0	4.528881	3.775198	-1.929093
85	1	0	3.543055	4.643099	-0.736957
86	6	0	4.177608	3.042792	1.386425
87	7	0	3.739982	3.089836	2.474716
88	6	0	5.339108	1.787945	-0.297450
89	7	0	5.896227	0.804815	-0.611612

Zero-point correction= 0.705022 (Hartree/Particle)
Thermal correction to Energy= 0.752399
Thermal correction to Enthalpy= 0.753343
Thermal correction to Gibbs Free Energy= 0.623475
Sum of electronic and zero-point Energies= -2702.889518
Sum of electronic and thermal Energies= -2702.842141
Sum of electronic and thermal Enthalpies= -2702.841197
Sum of electronic and thermal Free Energies= -2702.971065
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2705.814311

INT7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.059985	-1.962177	-1.643164
2	15	0	0.878608	-1.493647	0.046611
3	15	0	-2.029008	0.893889	0.237666
4	6	0	1.734254	-1.723605	2.676894
5	6	0	2.288377	-1.703960	-1.116892
6	6	0	3.230660	-1.164612	-3.288810
7	6	0	1.407109	-2.442478	1.524543
8	6	0	4.449201	-1.725687	-2.908544
9	6	0	3.515630	-2.258717	-0.744732
10	6	0	2.166067	-1.143250	-2.396367
11	6	0	4.588547	-2.267025	-1.635707
12	6	0	1.502926	-3.838479	1.539355
13	6	0	1.926763	-4.499481	2.685830
14	6	0	-2.585245	-0.045285	-1.219746
15	6	0	-3.747826	-0.855785	-1.427847
16	6	0	-3.051522	0.199098	1.597004
17	6	0	-1.708201	-3.931890	-2.018513
18	6	0	-1.811827	-0.102047	-2.425944
19	6	0	-3.682617	-1.403669	-2.740572
20	6	0	2.163149	-2.385672	3.824703
21	6	0	-2.486736	-0.936626	-3.358240
22	6	0	-2.414771	-0.533876	2.601921
23	6	0	-0.390018	-2.607911	-0.654493
24	6	0	-4.436255	0.385856	1.664446
25	6	0	-2.387903	-3.772601	-0.777617
26	6	0	-0.476289	-3.220147	-1.943700
27	6	0	-1.584734	-2.950983	0.060353
28	6	0	-2.821432	2.528769	-0.026817
29	6	0	-3.434688	2.903810	-1.223472
30	6	0	-5.171921	-0.176463	2.701532
31	6	0	-3.150855	-1.097661	3.640814
32	6	0	-4.530244	-0.922616	3.687992
33	6	0	2.259632	-3.772749	3.828001
34	6	0	-3.153623	4.773509	0.823087
35	6	0	-2.685914	3.478000	0.994279
36	6	0	-3.755262	5.143233	-0.379070
37	6	0	-3.895668	4.207508	-1.397660
38	1	0	-1.843991	-2.604603	1.057648
39	1	0	-3.374103	-4.155070	-0.535061
40	1	0	-2.084991	-4.458183	-2.889914
41	1	0	0.252822	-3.121149	-2.742000
42	1	0	-0.851430	0.390369	-2.563486
43	1	0	-2.126418	-1.217140	-4.342700
44	1	0	-4.388383	-2.108227	-3.169827

45	1	0	-4.508099	-1.070536	-0.682813
46	1	0	1.221707	-0.678643	-2.688155
47	1	0	3.113198	-0.733214	-4.282016
48	1	0	5.287769	-1.734924	-3.602846
49	1	0	5.537798	-2.703471	-1.328097
50	1	0	3.639682	-2.688923	0.248937
51	1	0	1.245814	-4.406389	0.643710
52	1	0	1.999648	-5.585938	2.690682
53	1	0	2.591828	-4.293171	4.724950
54	1	0	2.419392	-1.816253	4.716590
55	1	0	1.640767	-0.635122	2.665688
56	1	0	-4.938093	0.985053	0.902848
57	1	0	-6.249769	-0.027197	2.745702
58	1	0	-5.107262	-1.359266	4.501695
59	1	0	-2.643405	-1.665227	4.419287
60	1	0	-1.329547	-0.655644	2.563715
61	1	0	-2.197452	3.192719	1.929078
62	1	0	-3.041632	5.502088	1.624663
63	1	0	-4.113530	6.161705	-0.519459
64	1	0	-4.369809	4.490545	-2.336458
65	1	0	-3.550675	2.174681	-2.025970
66	46	0	0.343754	0.828422	0.238135
67	6	0	3.320495	1.555012	0.643657
68	6	0	2.193771	1.869034	-0.295500
69	6	0	1.224796	2.868089	-0.117311
70	1	0	3.521247	0.471985	0.686165
71	1	0	2.360711	1.532267	-1.325913
72	6	0	1.126969	3.721354	1.118894
73	1	0	1.500239	3.223483	2.022746
74	1	0	0.079729	4.003652	1.302298
75	6	0	0.584921	3.495957	-1.328347
76	1	0	-0.468351	3.756944	-1.146861
77	1	0	0.628334	2.833739	-2.204630
78	1	0	1.111630	4.431779	-1.586347
79	1	0	1.695435	4.657597	0.989049
80	1	0	3.096395	1.882093	1.667946
81	6	0	4.674260	2.207564	0.207025
82	6	0	5.162235	1.636251	-1.136030
83	1	0	6.163982	2.006964	-1.378197
84	1	0	5.187063	0.539538	-1.078415
85	1	0	4.477983	1.930313	-1.938966
86	6	0	4.501067	3.663923	0.090537
87	7	0	4.326612	4.805175	-0.031433
88	6	0	5.675987	1.915727	1.243210
89	7	0	6.447254	1.629088	2.062255

Zero-point correction= 0.708258 (Hartree/Particle)
Thermal correction to Energy= 0.755170
Thermal correction to Enthalpy= 0.756115
Thermal correction to Gibbs Free Energy= 0.627277
Sum of electronic and zero-point Energies= -2702.935695
Sum of electronic and thermal Energies= -2702.888783
Sum of electronic and thermal Enthalpies= -2702.887839
Sum of electronic and thermal Free Energies= -2703.016676
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -2705.8495523

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.259173	0.681903	-0.895228
2	6	0	-1.080247	0.990336	-0.306847
3	6	0	-2.148870	0.181887	-0.280469
4	1	0	0.692217	1.576289	-1.367033
5	1	0	-1.180054	1.977027	0.152965
6	6	0	-2.198313	-1.200197	-0.852576

7	1	0	-1.303293	-1.480584	-1.416946
8	1	0	-3.069691	-1.310388	-1.513877
9	6	0	-3.425488	0.627611	0.363283
10	1	0	-4.251464	0.627387	-0.363096
11	1	0	-3.346843	1.633300	0.792191
12	1	0	-3.719744	-0.065454	1.164964
13	1	0	-2.313981	-1.939301	-0.047028
14	1	0	0.198908	-0.086290	-1.676690
15	6	0	1.297510	0.206661	0.167857
16	6	0	1.509592	1.262040	1.264717
17	1	0	2.272714	0.936932	1.979093
18	1	0	1.832971	2.204478	0.806801
19	1	0	0.569965	1.426132	1.802475
20	6	0	0.822493	-1.044837	0.780196
21	7	0	0.412202	-2.014200	1.267770
22	6	0	2.576456	-0.045099	-0.514941
23	7	0	3.579863	-0.194565	-1.077739

Zero-point correction= 0.191288 (Hartree/Particle)
Thermal correction to Energy= 0.203608
Thermal correction to Enthalpy= 0.204552
Thermal correction to Gibbs Free Energy= 0.153293
Sum of electronic and zero-point Energies= -459.101977
Sum of electronic and thermal Energies= -459.089657
Sum of electronic and thermal Enthalpies= -459.088713
Sum of electronic and thermal Free Energies= -459.139972
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in ethanol solvent = -459.4262488

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.697627	-0.806294	-0.650774
2	6	0	1.688672	-0.820304	0.643573
3	6	0	0.774503	0.180481	0.001598
4	1	0	2.093031	-1.186405	-1.584462
5	1	0	2.069967	-1.220896	1.574606
6	6	0	-0.749903	-0.068981	-0.000791
7	6	0	-1.402480	0.676582	-1.166560
8	1	0	-2.474514	0.439616	-1.225196
9	1	0	-1.314839	1.766164	-1.063089
10	6	0	1.188585	1.643422	0.008519
11	1	0	0.915446	2.152155	-0.926670
12	1	0	2.276424	1.725501	0.120754
13	1	0	0.727884	2.205971	0.832724
14	1	0	-0.941693	0.388682	-2.123381
15	6	0	-1.360174	0.410844	1.317933
16	1	0	-1.251512	1.494511	1.457618
17	1	0	-2.436014	0.185521	1.352385
18	1	0	-0.885327	-0.089827	2.174500
19	6	0	-1.060034	-1.555582	-0.154189
20	1	0	-0.646730	-1.960813	-1.089051
21	1	0	-0.645492	-2.148476	0.672721
22	1	0	-2.147408	-1.712699	-0.169323

Zero-point correction= 0.196559 (Hartree/Particle)
Thermal correction to Energy= 0.206225
Thermal correction to Enthalpy= 0.207169
Thermal correction to Gibbs Free Energy= 0.163080
Sum of electronic and zero-point Energies= -312.743918
Sum of electronic and thermal Energies= -312.734252
Sum of electronic and thermal Enthalpies= -312.733308
Sum of electronic and thermal Free Energies= -312.777397
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -313.0312482

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.467631	0.000002	0.000001
2	6	0	-0.747726	-1.137297	0.382000
3	6	0	0.641625	-1.145806	0.384339
4	6	0	1.328436	0.000003	0.000000
5	6	0	0.641625	1.145810	-0.384338
6	6	0	-0.747727	1.137301	-0.381998
7	6	0	-2.943743	0.000001	0.000000
8	6	0	-3.660831	-1.139183	-0.383693
9	6	0	-5.050030	-1.139678	-0.383693
10	6	0	-5.750473	-0.000002	-0.000001
11	6	0	-5.050034	1.139674	0.383692
12	6	0	-3.660834	1.139183	0.383693
13	1	0	-1.285220	-2.026562	0.710429
14	1	0	1.182329	-2.038317	0.692245
15	1	0	1.182328	2.038322	-0.692245
16	1	0	-1.285220	2.026566	-0.710429
17	1	0	-3.119003	-2.025768	-0.712782
18	1	0	-5.589482	-2.033533	-0.693118
19	1	0	-6.839039	-0.000005	-0.000003
20	1	0	-5.589487	2.033529	0.693116
21	1	0	-3.119010	2.025769	0.712784
22	53	0	3.457846	-0.000001	0.000000

Zero-point correction= 0.170957 (Hartree/Particle)
Thermal correction to Energy= 0.181463
Thermal correction to Enthalpy= 0.182407
Thermal correction to Gibbs Free Energy= 0.132506
Sum of electronic and zero-point Energies= -473.503432
Sum of electronic and thermal Energies= -473.492927
Sum of electronic and thermal Enthalpies= -473.491983
Sum of electronic and thermal Free Energies= -473.541884
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -473.8437278

INT1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.046332	-3.118403	0.394221
2	15	0	1.884757	-0.299840	0.000700
3	15	0	-1.872635	-0.341979	-0.096579
4	6	0	3.672892	1.701765	0.689910
5	6	0	2.765843	-0.754272	-1.550352
6	6	0	2.758539	-0.854199	-3.970211
7	6	0	3.258075	0.401448	1.000025
8	6	0	4.027703	-1.423451	-3.953452
9	6	0	4.048899	-1.311514	-1.544858
10	6	0	2.132947	-0.516696	-2.772876
11	6	0	4.674654	-1.647508	-2.739795
12	6	0	3.894759	-0.288677	2.033517
13	6	0	4.928728	0.313953	2.746460
14	6	0	-1.556969	-2.119242	-0.333906
15	6	0	-1.978916	-3.242292	0.449573
16	6	0	-2.641422	-0.301125	1.575638
17	6	0	1.540654	-4.184281	1.278698
18	6	0	-0.749452	-2.628682	-1.403908
19	6	0	-1.429223	-4.421972	-0.128580
20	6	0	4.710805	2.297046	1.395568
21	6	0	-0.674316	-4.043021	-1.275529
22	6	0	-1.935445	0.294455	2.623141
23	6	0	1.631370	-1.922823	0.788255
24	6	0	-3.908479	-0.837205	1.830949
25	6	0	0.774986	-3.493781	2.261276

26	6	0	2.075112	-3.221420	0.376556
27	6	0	0.825774	-2.104362	1.962084
28	6	0	-3.342293	-0.082217	-1.171286
29	6	0	-3.989941	-1.113760	-1.855063
30	6	0	-4.444413	-0.796517	3.113033
31	6	0	-2.471201	0.336879	3.907418
32	6	0	-3.725703	-0.211417	4.153238
33	6	0	5.338515	1.604097	2.428719
34	6	0	-4.942608	1.492985	-2.076917
35	6	0	-3.825467	1.225248	-1.295858
36	6	0	-5.581155	0.459212	-2.758460
37	6	0	-5.101784	-0.841329	-2.648726
38	1	0	0.295594	-1.318351	2.493686
39	1	0	0.198987	-3.951355	3.059008
40	1	0	1.648241	-5.261148	1.195179
41	1	0	2.658199	-3.432960	-0.514842
42	1	0	-0.240318	-2.022476	-2.148751
43	1	0	-0.088101	-4.707134	-1.902341
44	1	0	-1.517738	-5.426467	0.273260
45	1	0	-2.559905	-3.186929	1.365558
46	1	0	1.146960	-0.043982	-2.771608
47	1	0	2.256761	-0.663296	-4.917654
48	1	0	4.521450	-1.682982	-4.888793
49	1	0	5.674587	-2.078753	-2.726010
50	1	0	4.563614	-1.472921	-0.596198
51	1	0	3.584522	-1.304008	2.282359
52	1	0	5.417812	-0.230636	3.553082
53	1	0	6.146464	2.073682	2.987771
54	1	0	5.025200	3.309174	1.145046
55	1	0	3.161523	2.246524	-0.107592
56	1	0	-4.481778	-1.283021	1.016709
57	1	0	-5.431749	-1.216339	3.300302
58	1	0	-4.150926	-0.173983	5.155037
59	1	0	-1.911585	0.809167	4.713193
60	1	0	-0.958125	0.736728	2.420617
61	1	0	-3.306705	2.036319	-0.780374
62	1	0	-5.312736	2.513650	-2.161370
63	1	0	-6.451433	0.670583	-3.377954
64	1	0	-5.597436	-1.652948	-3.179820
65	1	0	-3.626169	-2.137983	-1.767676
66	46	0	-0.006955	1.085494	-0.474077
67	6	0	-0.662871	2.829110	-1.493873
68	6	0	0.729499	2.867290	-1.435551
69	6	0	-0.025519	4.050838	-0.886966
70	1	0	-1.393430	2.760568	-2.300602
71	1	0	1.519883	2.827101	-2.186401
72	6	0	-0.145472	4.431928	0.611617
73	6	0	0.653148	5.710806	0.897496
74	1	0	0.647123	5.926164	1.975783
75	1	0	1.702827	5.593650	0.587691
76	6	0	-0.052319	5.254897	-1.822593
77	1	0	-0.888955	5.935371	-1.604982
78	1	0	-0.162220	4.920158	-2.862230
79	1	0	0.872296	5.847084	-1.766360
80	1	0	0.244917	6.593517	0.388426
81	6	0	-1.621611	4.669067	0.938538
82	1	0	-1.743484	5.054309	1.962147
83	1	0	-2.083156	5.395422	0.254163
84	1	0	-2.185275	3.726688	0.862518
85	6	0	0.390811	3.375311	1.570470
86	1	0	-0.111147	2.404921	1.434907
87	1	0	1.470361	3.215763	1.441985
88	1	0	0.215720	3.696735	2.608572

Zero-point correction= 0.715355 (Hartree/Particle)
Thermal correction to Energy= 0.758827
Thermal correction to Enthalpy= 0.759772

Thermal correction to Gibbs Free Energy= 0.638618
Sum of electronic and zero-point Energies= -2556.585122
Sum of electronic and thermal Energies= -2556.541650
Sum of electronic and thermal Enthalpies= -2556.540706
Sum of electronic and thermal Free Energies= -2556.661860
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2559.4657995

INT2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.513149	3.421422	-0.870848
2	15	0	1.700215	0.893220	-0.386413
3	15	0	-2.089390	0.738553	0.527606
4	6	0	4.044919	-0.435547	-1.369387
5	6	0	2.930250	1.802476	0.635932
6	6	0	3.581095	2.568725	2.844234
7	6	0	2.720205	-0.054389	-1.599021
8	6	0	4.711876	3.174731	2.305207
9	6	0	4.066138	2.424144	0.105152
10	6	0	2.698653	1.885746	2.011574
11	6	0	4.953490	3.100975	0.934963
12	6	0	2.078323	-0.540433	-2.746154
13	6	0	2.749537	-1.349389	-3.653706
14	6	0	-1.834312	2.540044	0.384990
15	6	0	-2.490773	3.516219	-0.434462
16	6	0	-3.126733	0.371334	-0.947906
17	6	0	0.564394	4.324946	-2.344594
18	6	0	-0.816676	3.229749	1.123962
19	6	0	-1.874859	4.780220	-0.207262
20	6	0	4.716473	-1.252064	-2.276994
21	6	0	-0.843275	4.603752	0.759076
22	6	0	-2.602916	-0.455525	-1.944312
23	6	0	1.052638	2.250941	-1.429944
24	6	0	-4.423072	0.875580	-1.097072
25	6	0	-0.342439	3.379864	-2.900759
26	6	0	1.424232	3.635219	-1.443802
27	6	0	-0.052052	2.107908	-2.334839
28	6	0	-3.350582	0.658465	1.866421
29	6	0	-3.715566	1.758666	2.645200
30	6	0	-5.165373	0.585193	-2.236215
31	6	0	-3.346203	-0.750169	-3.084370
32	6	0	-4.624967	-0.224126	-3.233475
33	6	0	4.076840	-1.705611	-3.424059
34	6	0	-4.859589	-0.725842	3.161704
35	6	0	-3.929334	-0.587402	2.140188
36	6	0	-5.214180	0.376262	3.937584
37	6	0	-4.639830	1.615026	3.677932
38	1	0	-0.621034	1.198962	-2.510629
39	1	0	-1.157387	3.597904	-3.583431
40	1	0	0.564025	5.394709	-2.528878
41	1	0	2.188754	4.091801	-0.823758
42	1	0	-0.112177	2.757134	1.803589
43	1	0	-0.156459	5.367997	1.108296
44	1	0	-2.106946	5.702528	-0.730786
45	1	0	-3.267355	3.308841	-1.164229
46	1	0	1.816659	1.392304	2.428512
47	1	0	3.386548	2.624374	3.914190
48	1	0	5.407260	3.706748	2.952688
49	1	0	5.837588	3.574725	0.510717
50	1	0	4.259783	2.369636	-0.966885
51	1	0	1.034540	-0.285918	-2.934617
52	1	0	2.233161	-1.704236	-4.544656
53	1	0	4.605729	-2.339275	-4.134395
54	1	0	5.749284	-1.533357	-2.074687
55	1	0	4.566523	-0.103680	-0.472489

56	1	0	-4.857252	1.490054	-0.306599
57	1	0	-6.173269	0.983865	-2.343490
58	1	0	-5.210572	-0.458226	-4.121371
59	1	0	-2.931097	-1.407591	-3.846956
60	1	0	-1.608846	-0.891463	-1.803579
61	1	0	-3.655297	-1.454524	1.533415
62	1	0	-5.308371	-1.699075	3.355653
63	1	0	-5.938908	0.266816	4.742937
64	1	0	-4.915557	2.481485	4.277855
65	1	0	-3.279979	2.737551	2.443961
66	6	0	2.102612	-2.774289	0.757010
67	6	0	1.042645	-2.334045	1.592014
68	6	0	-0.303363	-2.655938	1.305890
69	6	0	-0.566033	-3.377402	0.122080
70	6	0	0.449303	-3.754890	-0.732994
71	6	0	1.781862	-3.458951	-0.406792
72	1	0	1.277935	-1.930818	2.577924
73	1	0	-1.070500	-2.536919	2.068601
74	1	0	0.226224	-4.299442	-1.648574
75	1	0	2.568103	-3.749042	-1.102815
76	53	0	-2.572363	-3.945435	-0.304932
77	46	0	-0.006853	-0.427073	0.646684
78	6	0	3.499959	-2.480158	1.124802
79	6	0	3.808965	-1.358280	1.903787
80	6	0	4.557998	-3.292092	0.696583
81	6	0	5.124082	-1.032862	2.212080
82	1	0	3.006194	-0.697331	2.227414
83	6	0	5.873520	-2.976097	1.011436
84	1	0	4.344422	-4.192460	0.121088
85	6	0	6.165494	-1.839758	1.763131
86	1	0	5.331166	-0.133353	2.792150
87	1	0	6.678683	-3.625877	0.670756
88	1	0	7.198141	-1.590539	2.002256

Zero-point correction= 0.688296 (Hartree/Particle)
Thermal correction to Energy= 0.733467
Thermal correction to Enthalpy= 0.734411
Thermal correction to Gibbs Free Energy= 0.608835
Sum of electronic and zero-point Energies= -2717.344454
Sum of electronic and thermal Energies= -2717.299283
Sum of electronic and thermal Enthalpies= -2717.298338
Sum of electronic and thermal Free Energies= -2717.423914
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2720.2661986

TS1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.810787	3.059683	-0.590112
2	15	0	0.955940	1.067303	-0.645807
3	15	0	-2.505443	-0.092601	0.465766
4	6	0	3.743687	1.185680	-1.288516
5	6	0	1.600606	1.757503	0.932135
6	6	0	1.793933	1.498813	3.337905
7	6	0	2.430060	1.082187	-1.751528
8	6	0	2.559155	2.658924	3.407805
9	6	0	2.371588	2.923531	1.017265
10	6	0	1.322059	1.050481	2.106384
11	6	0	2.849009	3.369792	2.245081
12	6	0	2.217448	0.815566	-3.109374
13	6	0	3.289649	0.685074	-3.983593
14	6	0	-2.743832	1.709266	0.603958
15	6	0	-3.704603	2.536783	-0.062043
16	6	0	-3.968697	-0.573464	-0.535475
17	6	0	-1.072161	4.416508	-1.918747
18	6	0	-1.895270	2.575234	1.371304

19	6	0	-3.446442	3.892083	0.289208
20	6	0	4.818897	1.055145	-2.163363
21	6	0	-2.335846	3.914411	1.181006
22	6	0	-3.755129	-1.027221	-1.838912
23	6	0	-0.049797	2.414309	-1.355440
24	6	0	-5.277754	-0.480379	-0.051614
25	6	0	-1.753351	3.371885	-2.605876
26	6	0	-0.025668	3.833373	-1.149930
27	6	0	-1.127461	2.142633	-2.263208
28	6	0	-2.961778	-0.656478	2.156834
29	6	0	-3.589452	0.156769	3.104796
30	6	0	-6.352401	-0.819226	-0.864808
31	6	0	-4.831840	-1.362849	-2.655282
32	6	0	-6.130269	-1.257019	-2.169281
33	6	0	4.595979	0.807493	-3.513440
34	6	0	-2.973241	-2.480314	3.751324
35	6	0	-2.651333	-1.978308	2.495969
36	6	0	-3.595083	-1.661877	4.690810
37	6	0	-3.900542	-0.344106	4.366066
38	1	0	-1.442055	1.148748	-2.572064
39	1	0	-2.632905	3.485487	-3.230933
40	1	0	-1.345864	5.466937	-1.924203
41	1	0	0.627876	4.366754	-0.467412
42	1	0	-1.035049	2.262445	1.958670
43	1	0	-1.866081	4.801659	1.593548
44	1	0	-3.969814	4.760314	-0.098668
45	1	0	-4.458368	2.184738	-0.759909
46	1	0	0.732371	0.132140	2.043907
47	1	0	1.565297	0.936546	4.242062
48	1	0	2.933977	3.010090	4.368118
49	1	0	3.452960	4.274643	2.293871
50	1	0	2.625045	3.474042	0.110802
51	1	0	1.199762	0.696513	-3.487099
52	1	0	3.104872	0.482596	-5.037713
53	1	0	5.435200	0.701670	-4.199128
54	1	0	5.833181	1.132473	-1.771670
55	1	0	3.944547	1.350842	-0.230745
56	1	0	-5.454743	-0.140467	0.970000
57	1	0	-7.368196	-0.744999	-0.479224
58	1	0	-6.974112	-1.524919	-2.803362
59	1	0	-4.653465	-1.718449	-3.668815
60	1	0	-2.731502	-1.136424	-2.203267
61	1	0	-2.152885	-2.615223	1.761733
62	1	0	-2.730594	-3.512505	3.999341
63	1	0	-3.838705	-2.051177	5.678171
64	1	0	-4.385154	0.300831	5.097840
65	1	0	-3.834376	1.190274	2.857836
66	6	0	3.810876	-1.777992	0.513123
67	6	0	2.811055	-2.034335	1.455742
68	6	0	1.531418	-2.414322	1.064018
69	6	0	1.222098	-2.447563	-0.303371
70	6	0	2.242972	-2.346494	-1.256227
71	6	0	3.518622	-2.005469	-0.842538
72	1	0	3.036975	-1.925708	2.517801
73	1	0	0.761454	-2.614609	1.809212
74	1	0	2.013067	-2.436426	-2.317300
75	1	0	4.284784	-1.814105	-1.595160
76	53	0	-0.686009	-3.700957	-0.938442
77	46	0	-0.395405	-1.004977	-0.319110
78	6	0	5.098464	-1.183893	0.908958
79	6	0	5.123246	-0.151457	1.857680
80	6	0	6.303551	-1.557706	0.302816
81	6	0	6.312449	0.488593	2.184364
82	1	0	4.184890	0.181247	2.307375
83	6	0	7.494464	-0.921853	0.634799
84	1	0	6.302206	-2.367163	-0.427418
85	6	0	7.504484	0.105747	1.574542

86	1	0	6.302388	1.301835	2.909508
87	1	0	8.423154	-1.233576	0.158415
88	1	0	8.437016	0.607559	1.827958

Zero-point correction= 0.687140 (Hartree/Particle)
Thermal correction to Energy= 0.732087
Thermal correction to Enthalpy= 0.733031
Thermal correction to Gibbs Free Energy= 0.607085
Sum of electronic and zero-point Energies= -2717.335120
Sum of electronic and thermal Energies= -2717.290173
Sum of electronic and thermal Enthalpies= -2717.289229
Sum of electronic and thermal Free Energies= -2717.415175
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2720.2568489

INT3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.669785	2.401659	-1.239514
2	15	0	0.411232	1.558806	-0.064420
3	15	0	-2.445890	-0.713078	0.116923
4	6	0	3.083784	2.197695	0.467515
5	6	0	0.062034	2.271801	1.580703
6	6	0	-0.802997	1.942976	3.819478
7	6	0	2.063699	2.210394	-0.488584
8	6	0	-0.670683	3.304644	4.070570
9	6	0	0.228060	3.633889	1.855526
10	6	0	-0.429336	1.429127	2.580635
11	6	0	-0.143628	4.147221	3.092643
12	6	0	2.357013	2.597323	-1.799099
13	6	0	3.653196	2.962285	-2.147650
14	6	0	-3.388499	0.830198	-0.183797
15	6	0	-4.238052	1.104496	-1.304603
16	6	0	-3.345058	-1.828541	-1.024962
17	6	0	-1.979862	3.960102	-2.366438
18	6	0	-3.355351	2.017422	0.623301
19	6	0	-4.707944	2.442628	-1.193453
20	6	0	4.378930	2.552437	0.112525
21	6	0	-4.170633	3.002264	-0.000048
22	6	0	-2.800864	-2.035542	-2.294720
23	6	0	-0.663961	2.432032	-1.233172
24	6	0	-4.586542	-2.383252	-0.710266
25	6	0	-1.960350	2.754458	-3.124063
26	6	0	-1.179702	3.770371	-1.205664
27	6	0	-1.147224	1.814188	-2.435351
28	6	0	-3.019930	-1.151145	1.807788
29	6	0	-4.241059	-0.696983	2.320408
30	6	0	-5.282116	-3.122490	-1.661357
31	6	0	-3.503368	-2.763126	-3.248673
32	6	0	-4.745682	-3.305488	-2.932534
33	6	0	4.666771	2.933263	-1.195394
34	6	0	-2.585867	-2.266489	3.913133
35	6	0	-2.194948	-1.938188	2.618829
36	6	0	-3.801937	-1.811258	4.413042
37	6	0	-4.629694	-1.027669	3.614073
38	1	0	-0.957843	0.782421	-2.721792
39	1	0	-2.516091	2.565404	-4.036410
40	1	0	-2.559785	4.847635	-2.598751
41	1	0	-1.046277	4.487084	-0.401107
42	1	0	-2.782317	2.148425	1.537752
43	1	0	-4.306297	4.022128	0.345461
44	1	0	-5.326049	2.960592	-1.919582
45	1	0	-4.439180	0.419185	-2.123127
46	1	0	-0.530338	0.361048	2.377131
47	1	0	-1.199537	1.273898	4.581865
48	1	0	-0.965831	3.712330	5.036040

49	1	0	-0.017579	5.208994	3.298365
50	1	0	0.661280	4.292306	1.101588
51	1	0	1.571697	2.607648	-2.555268
52	1	0	3.872153	3.263207	-3.170907
53	1	0	5.684802	3.202437	-1.471523
54	1	0	5.171307	2.522362	0.859002
55	1	0	2.869678	1.888919	1.490701
56	1	0	-5.011851	-2.241544	0.283489
57	1	0	-6.246856	-3.558931	-1.407608
58	1	0	-5.292510	-3.883007	-3.676208
59	1	0	-3.069998	-2.922616	-4.234537
60	1	0	-1.809294	-1.643229	-2.523834
61	1	0	-1.244325	-2.304009	2.226152
62	1	0	-1.935323	-2.883541	4.530631
63	1	0	-4.105783	-2.066802	5.427082
64	1	0	-5.582640	-0.668369	3.999787
65	1	0	-4.891867	-0.075545	1.705114
66	6	0	4.887933	-0.974824	0.015570
67	6	0	4.130293	-1.103006	1.184681
68	6	0	2.738378	-1.088114	1.145399
69	6	0	2.070591	-0.938085	-0.069219
70	6	0	2.813588	-0.833505	-1.242632
71	6	0	4.202813	-0.849412	-1.198729
72	1	0	4.637041	-1.246108	2.140218
73	1	0	2.174978	-1.208354	2.073158
74	1	0	2.310625	-0.706700	-2.203251
75	1	0	4.768065	-0.717164	-2.122308
76	53	0	0.050582	-3.474500	-0.216191
77	46	0	0.033173	-0.771128	-0.084673
78	6	0	6.362728	-0.946686	0.057902
79	6	0	7.041480	-0.325452	1.114049
80	6	0	7.126763	-1.529514	-0.960863
81	6	0	8.430041	-0.285494	1.149959
82	1	0	6.466255	0.149588	1.909216
83	6	0	8.515085	-1.487647	-0.928667
84	1	0	6.619442	-2.047175	-1.774640
85	6	0	9.174552	-0.864426	0.126724
86	1	0	8.934311	0.208886	1.979499
87	1	0	9.086209	-1.956491	-1.728968
88	1	0	10.262563	-0.832825	0.153362

Zero-point correction= 0.688665 (Hartree/Particle)
Thermal correction to Energy= 0.733931
Thermal correction to Enthalpy= 0.734875
Thermal correction to Gibbs Free Energy= 0.607666
Sum of electronic and zero-point Energies= -2717.368508
Sum of electronic and thermal Energies= -2717.323242
Sum of electronic and thermal Enthalpies= -2717.322298
Sum of electronic and thermal Free Energies= -2717.449507
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2720.2568489

TS1c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.474693	-3.016786	0.006983
2	15	0	1.959300	0.040074	0.027745
3	15	0	-1.818797	-0.460362	-0.066170
4	6	0	3.407691	2.131607	1.122628
5	6	0	2.996710	-0.115244	-1.489330
6	6	0	3.084909	-0.193595	-3.912718
7	6	0	3.166745	0.755860	1.218526
8	6	0	4.459280	-0.400190	-3.860610
9	6	0	4.380313	-0.316840	-1.449991
10	6	0	2.360436	-0.047117	-2.732921
11	6	0	5.105951	-0.459046	-2.627712

12	6	0	3.831366	0.019803	2.202724
13	6	0	4.716669	0.649163	3.074745
14	6	0	-1.263860	-2.133586	-0.545189
15	6	0	-1.517317	-3.403282	0.069358
16	6	0	-2.299117	-0.709161	1.697734
17	6	0	2.114608	-4.004304	0.700019
18	6	0	-0.434287	-2.380723	-1.688720
19	6	0	-0.845147	-4.408858	-0.680995
20	6	0	4.299852	2.756106	1.984920
21	6	0	-0.177588	-3.777420	-1.769137
22	6	0	-1.538542	-0.081759	2.688837
23	6	0	1.913066	-1.701577	0.569110
24	6	0	-3.391433	-1.494093	2.082942
25	6	0	1.296972	-3.574954	1.784800
26	6	0	2.502121	-2.854093	-0.044267
27	6	0	1.166038	-2.161021	1.703986
28	6	0	-3.478434	-0.418311	-0.868085
29	6	0	-3.809112	-1.243332	-1.946147
30	6	0	-3.696415	-1.668949	3.428702
31	6	0	-1.841246	-0.256320	4.036552
32	6	0	-2.919391	-1.053519	4.407334
33	6	0	4.953482	2.015384	2.967363
34	6	0	-5.643753	0.656150	-1.073087
35	6	0	-4.411204	0.537911	-0.443485
36	6	0	-5.962787	-0.171490	-2.147417
37	6	0	-5.042066	-1.118226	-2.581736
38	1	0	0.559390	-1.537288	2.354858
39	1	0	0.804274	-4.218357	2.506788
40	1	0	2.353149	-5.033615	0.450479
41	1	0	3.089698	-2.845834	-0.957958
42	1	0	-0.030139	-1.613659	-2.343552
43	1	0	0.466359	-4.265363	-2.493534
44	1	0	-0.795683	-5.463396	-0.428051
45	1	0	-2.063386	-3.557559	0.994950
46	1	0	1.283859	0.137421	-2.765338
47	1	0	2.575416	-0.135905	-4.873492
48	1	0	5.030239	-0.508142	-4.781585
49	1	0	6.182845	-0.615846	-2.583919
50	1	0	4.891763	-0.367828	-0.487607
51	1	0	3.661395	-1.053865	2.286409
52	1	0	5.227421	0.065380	3.839498
53	1	0	5.646276	2.504545	3.650395
54	1	0	4.479552	3.826582	1.896149
55	1	0	2.883286	2.711895	0.360599
56	1	0	-4.014386	-1.963521	1.320087
57	1	0	-4.549424	-2.282610	3.715315
58	1	0	-3.162118	-1.188251	5.460364
59	1	0	-1.239578	0.240136	4.796298
60	1	0	-0.700871	0.554754	2.389639
61	1	0	-4.171266	1.189204	0.399589
62	1	0	-6.360101	1.397961	-0.722450
63	1	0	-6.927854	-0.076758	-2.642748
64	1	0	-5.285157	-1.771967	-3.418391
65	1	0	-3.101017	-1.997481	-2.290347
66	46	0	-0.123387	1.210203	-0.451588
67	6	0	0.609378	2.941734	-1.626150
68	6	0	0.133113	4.145043	-1.792483
69	6	0	-0.931742	3.501473	-1.007036
70	1	0	1.418166	2.373937	-2.099671
71	1	0	0.286507	5.066052	-2.347783
72	6	0	-1.148230	4.062536	0.424053
73	6	0	-1.541804	5.540815	0.274757
74	1	0	-1.737428	5.984141	1.261963
75	1	0	-0.737789	6.122735	-0.197325
76	6	0	-2.190164	3.214078	-1.808256
77	1	0	-2.890109	2.530353	-1.315433
78	1	0	-1.922867	2.771208	-2.774700

79	1	0	-2.728981	4.155777	-2.018122
80	1	0	-2.452460	5.666392	-0.327711
81	6	0	-2.271299	3.350386	1.177168
82	1	0	-2.339233	3.735871	2.204973
83	1	0	-3.251586	3.508033	0.705438
84	1	0	-2.086430	2.268356	1.234255
85	6	0	0.122024	4.001409	1.268915
86	1	0	0.438291	2.960771	1.443142
87	1	0	0.956034	4.525477	0.783399
88	1	0	-0.054509	4.476979	2.244779

Zero-point correction= 0.712292 (Hartree/Particle)
Thermal correction to Energy= 0.756221
Thermal correction to Enthalpy= 0.757165
Thermal correction to Gibbs Free Energy= 0.634899
Sum of electronic and zero-point Energies= -2556.544667
Sum of electronic and thermal Energies= -2556.500738
Sum of electronic and thermal Enthalpies= -2556.499794
Sum of electronic and thermal Free Energies= -2556.622060
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2559.4204818

INT2c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.055463	-2.823123	-0.623358
2	15	0	1.875263	0.370988	-0.025763
3	15	0	-1.587242	-0.722707	0.028745
4	6	0	2.192190	2.423672	1.818518
5	6	0	3.111825	0.827126	-1.304842
6	6	0	3.575226	1.311668	-3.629578
7	6	0	2.549222	1.102192	1.520655
8	6	0	4.937913	1.347010	-3.352919
9	6	0	4.482329	0.870716	-1.033596
10	6	0	2.664641	1.058866	-2.607366
11	6	0	5.390837	1.131509	-2.052977
12	6	0	3.355556	0.398067	2.420056
13	6	0	3.792148	1.001386	3.596237
14	6	0	-0.835476	-2.156080	-0.821104
15	6	0	-0.828485	-3.552773	-0.497112
16	6	0	-1.515036	-1.162940	1.807734
17	6	0	2.927899	-3.571298	-0.331213
18	6	0	-0.121160	-2.009599	-2.057640
19	6	0	-0.107757	-4.244511	-1.510301
20	6	0	2.636043	3.025507	2.990542
21	6	0	0.328823	-3.291848	-2.474397
22	6	0	-0.780180	-0.312113	2.639095
23	6	0	2.272430	-1.405087	0.163936
24	6	0	-2.080871	-2.319978	2.355633
25	6	0	2.183985	-3.606004	0.882027
26	6	0	2.990199	-2.219994	-0.772328
27	6	0	1.771625	-2.279288	1.188408
28	6	0	-3.346037	-0.977436	-0.444552
29	6	0	-3.633729	-1.162533	-1.801785
30	6	0	-1.873659	-2.638391	3.693196
31	6	0	-0.570582	-0.629384	3.978229
32	6	0	-1.108814	-1.800200	4.502777
33	6	0	3.432430	2.314097	3.884267
34	6	0	-5.722022	-0.963689	0.017668
35	6	0	-4.404974	-0.878306	0.460818
36	6	0	-5.997049	-1.144951	-1.333276
37	6	0	-4.948037	-1.246952	-2.243243
38	1	0	1.151826	-1.983454	2.032039
39	1	0	1.920005	-4.495608	1.445027
40	1	0	3.334676	-4.430104	-0.855491
41	1	0	3.451999	-1.866231	-1.689549

42	1	0	0.081183	-1.057244	-2.543679
43	1	0	0.945850	-3.500157	-3.342278
44	1	0	0.126361	-5.304459	-1.511349
45	1	0	-1.232550	-4.000597	0.404620
46	1	0	1.591515	1.065605	-2.807674
47	1	0	3.216517	1.493452	-4.641418
48	1	0	5.651518	1.550103	-4.150077
49	1	0	6.456820	1.166494	-1.833137
50	1	0	4.840505	0.695632	-0.018152
51	1	0	3.641055	-0.631171	2.203053
52	1	0	4.416674	0.440137	4.289958
53	1	0	3.772013	2.782734	4.806790
54	1	0	2.349737	4.052855	3.210442
55	1	0	1.548487	2.971861	1.127246
56	1	0	-2.698359	-2.970441	1.735149
57	1	0	-2.312190	-3.544866	4.108050
58	1	0	-0.943729	-2.056845	5.548078
59	1	0	0.020584	0.037887	4.603743
60	1	0	-0.357856	0.603925	2.218386
61	1	0	-4.204808	-0.721619	1.520670
62	1	0	-6.536595	-0.882295	0.735798
63	1	0	-7.027943	-1.205962	-1.678120
64	1	0	-5.153800	-1.389142	-3.302982
65	1	0	-2.819913	-1.230445	-2.525575
66	46	0	-0.332445	1.297651	-0.502556
67	6	0	0.395651	3.081906	-1.221612
68	6	0	-0.739600	3.714320	-1.497020
69	6	0	-1.829047	2.799196	-1.012899
70	1	0	1.420388	3.401871	-1.435149
71	1	0	-0.908239	4.688421	-1.990527
72	6	0	-2.615317	3.373982	0.190091
73	6	0	-3.484435	4.544809	-0.300800
74	1	0	-3.974504	5.041596	0.549971
75	1	0	-2.883593	5.302124	-0.824531
76	6	0	-2.690615	2.306349	-2.160510
77	1	0	-3.494329	1.625027	-1.846487
78	1	0	-2.076472	1.773735	-2.899581
79	1	0	-3.162659	3.152936	-2.696238
80	1	0	-4.274744	4.206432	-0.984622
81	6	0	-3.532855	2.342998	0.840405
82	1	0	-4.125884	2.812124	1.640518
83	1	0	-4.236637	1.892747	0.127427
84	1	0	-2.944550	1.533034	1.296667
85	6	0	-1.678593	3.906138	1.274506
86	1	0	-1.010772	3.110261	1.637631
87	1	0	-1.043270	4.722434	0.906429
88	1	0	-2.264034	4.283249	2.126726

Zero-point correction= 0.715319 (Hartree/Particle)
Thermal correction to Energy= 0.758748
Thermal correction to Enthalpy= 0.759693
Thermal correction to Gibbs Free Energy= 0.640633
Sum of electronic and zero-point Energies= -2556.575402
Sum of electronic and thermal Energies= -2556.531972
Sum of electronic and thermal Enthalpies= -2556.531028
Sum of electronic and thermal Free Energies= -2556.650087
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -2559.4593806

INT4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.785056	-2.913063	1.432205
2	15	0	0.429697	-1.502698	-0.664229
3	15	0	-2.475879	0.282469	0.476318
4	6	0	2.485883	-1.763430	-2.538193

5	6	0	-0.610982	-1.961445	-2.094476
6	6	0	-2.349267	-1.378271	-3.680031
7	6	0	2.107952	-1.956105	-1.204877
8	6	0	-2.314866	-2.669316	-4.194664
9	6	0	-0.551228	-3.246424	-2.650371
10	6	0	-1.490889	-1.026122	-2.641818
11	6	0	-1.405240	-3.597759	-3.688409
12	6	0	3.049605	-2.405892	-0.275547
13	6	0	4.355559	-2.662143	-0.677427
14	6	0	-3.016771	-1.398174	0.927321
15	6	0	-3.311142	-1.850608	2.257761
16	6	0	-2.873641	1.173881	2.028331
17	6	0	-0.562799	-4.476334	1.951556
18	6	0	-3.201896	-2.516922	0.044267
19	6	0	-3.660313	-3.225897	2.189609
20	6	0	3.789407	-2.033259	-2.937579
21	6	0	-3.601336	-3.632782	0.827987
22	6	0	-1.864787	1.336267	2.983945
23	6	0	0.048671	-2.645381	0.680916
24	6	0	-4.166744	1.619645	2.313968
25	6	0	-0.363529	-3.380103	2.836072
26	6	0	-0.304856	-4.035566	0.625803
27	6	0	0.019976	-2.253034	2.062903
28	6	0	-3.738438	0.816064	-0.737138
29	6	0	-4.990317	0.195439	-0.816014
30	6	0	-4.444539	2.212682	3.541844
31	6	0	-2.146707	1.920739	4.213505
32	6	0	-3.438790	2.358740	4.492575
33	6	0	4.724190	-2.481563	-2.007806
34	6	0	-4.383834	2.299487	-2.540051
35	6	0	-3.444455	1.869770	-1.609605
36	6	0	-5.625991	1.674994	-2.613387
37	6	0	-5.927296	0.625509	-1.750291
38	1	0	0.216203	-1.250903	2.433124
39	1	0	-0.528797	-3.389157	3.908021
40	1	0	-0.915212	-5.463473	2.231789
41	1	0	-0.429636	-4.630420	-0.272236
42	1	0	-3.042167	-2.514251	-1.030145
43	1	0	-3.770216	-4.637483	0.454862
44	1	0	-3.884943	-3.863930	3.037686
45	1	0	-3.234695	-1.252951	3.161168
46	1	0	-1.520161	-0.012617	-2.242818
47	1	0	-3.044310	-0.639128	-4.076330
48	1	0	-2.984461	-2.952908	-5.004262
49	1	0	-1.357195	-4.599565	-4.110866
50	1	0	0.177207	-3.969471	-2.283073
51	1	0	2.765796	-2.552958	0.766510
52	1	0	5.088448	-3.004913	0.050893
53	1	0	5.745062	-2.694994	-2.321158
54	1	0	4.075740	-1.893704	-3.978238
55	1	0	1.760470	-1.402484	-3.268577
56	1	0	-4.960370	1.502651	1.576038
57	1	0	-5.452822	2.561512	3.756241
58	1	0	-3.659973	2.821649	5.452256
59	1	0	-1.356954	2.041436	4.952561
60	1	0	-0.847048	1.008801	2.758428
61	1	0	-2.471260	2.358103	-1.560820
62	1	0	-4.141448	3.124035	-3.208688
63	1	0	-6.361089	2.007627	-3.343688
64	1	0	-6.898012	0.136374	-1.804337
65	1	0	-5.234747	-0.628488	-0.145935
66	6	0	4.797072	0.727129	0.548444
67	6	0	4.261794	0.985863	-0.718512
68	6	0	2.886956	1.057511	-0.923535
69	6	0	2.016244	0.858028	0.141466
70	6	0	2.529304	0.638951	1.418610
71	6	0	3.906218	0.570988	1.616000

72	1	0	4.935665	1.146454	-1.560319
73	1	0	2.506756	1.240457	-1.929084
74	1	0	1.866808	0.503623	2.276819
75	1	0	4.294861	0.358032	2.612097
76	46	0	-0.071641	0.734017	0.003326
77	6	0	6.253599	0.602594	0.751403
78	6	0	7.057436	-0.013061	-0.215797
79	6	0	6.862555	1.082185	1.916608
80	6	0	8.427061	-0.145900	-0.022969
81	1	0	6.592070	-0.417296	-1.115967
82	6	0	8.231864	0.949207	2.110201
83	1	0	6.257867	1.590838	2.667503
84	6	0	9.019278	0.333989	1.141377
85	1	0	9.035227	-0.633399	-0.783130
86	1	0	8.688240	1.336929	3.019324
87	1	0	10.092086	0.230514	1.292466
88	6	0	-0.803261	2.903172	0.164268
89	6	0	0.532330	2.965597	0.312669
90	6	0	-0.030816	3.587129	-0.935801
91	1	0	-1.707487	3.040344	0.750977
92	1	0	1.302447	3.119508	1.058931
93	6	0	-0.128091	5.132964	-0.979502
94	6	0	-1.456655	5.529809	-1.629682
95	1	0	-1.556549	6.623744	-1.654453
96	1	0	-1.538014	5.176184	-2.666380
97	6	0	0.172535	2.934045	-2.288970
98	1	0	-0.581476	3.262456	-3.018044
99	1	0	0.111515	1.838649	-2.218067
100	1	0	1.159136	3.180253	-2.701926
101	1	0	-2.314138	5.132924	-1.064816
102	6	0	1.038980	5.710021	-1.783901
103	1	0	0.984892	5.452125	-2.849083
104	1	0	1.036364	6.806314	-1.716368
105	1	0	2.004055	5.353589	-1.393950
106	6	0	-0.081820	5.744341	0.421863
107	1	0	-0.909129	5.405489	1.060307
108	1	0	0.862341	5.517953	0.937633
109	1	0	-0.156328	6.836700	0.345938

Zero-point correction= 0.888156 (Hartree/Particle)
Thermal correction to Energy= 0.941576
Thermal correction to Enthalpy= 0.942520
Thermal correction to Gibbs Free Energy= 0.801220
Sum of electronic and zero-point Energies= -3018.531164
Sum of electronic and thermal Energies= -3018.477744
Sum of electronic and thermal Enthalpies= -3018.476800
Sum of electronic and thermal Free Energies= -3018.618100
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.7535142

TS2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.845411	-2.909577	-1.413241
2	15	0	-0.401109	-1.520121	0.657008
3	15	0	2.468519	0.314050	-0.488452
4	6	0	-2.500707	-1.813435	2.487273
5	6	0	0.613585	-1.974784	2.107419
6	6	0	2.339377	-1.368674	3.700438
7	6	0	-2.096315	-1.961756	1.155964
8	6	0	2.306436	-2.655232	4.226890
9	6	0	0.556489	-3.254642	2.674428
10	6	0	1.487007	-1.031171	2.652784
11	6	0	1.404447	-3.592196	3.722320
12	6	0	-3.021092	-2.380085	0.195174
13	6	0	-4.332189	-2.656950	0.564393

14	6	0	3.038513	-1.361323	-0.918433
15	6	0	3.349531	-1.820122	-2.243171
16	6	0	2.851796	1.203781	-2.042683
17	6	0	0.663973	-4.506611	-1.921309
18	6	0	3.244728	-2.466981	-0.022931
19	6	0	3.731141	-3.185780	-2.159323
20	6	0	-3.809830	-2.103354	2.854233
21	6	0	3.674917	-3.580411	-0.793991
22	6	0	1.838850	1.357338	-2.994773
23	6	0	0.002795	-2.680533	-0.668299
24	6	0	4.142642	1.651461	-2.334967
25	6	0	0.440881	-3.423433	-2.816371
26	6	0	0.390338	-4.060248	-0.600246
27	6	0	0.027612	-2.299354	-2.053723
28	6	0	3.706224	0.880163	0.732971
29	6	0	4.964446	0.276745	0.836421
30	6	0	4.413584	2.240512	-3.566145
31	6	0	2.114082	1.937488	-4.228054
32	6	0	3.403460	2.379175	-4.513514
33	6	0	-4.724762	-2.527297	1.893912
34	6	0	4.304975	2.394145	2.524446
35	6	0	3.385413	1.942528	1.584738
36	6	0	5.553874	1.786538	2.623712
37	6	0	5.882574	0.731369	1.777580
38	1	0	-0.186278	-1.303850	-2.432418
39	1	0	0.610606	-3.437915	-3.887584
40	1	0	1.041699	-5.487116	-2.191736
41	1	0	0.530717	-4.641891	0.304261
42	1	0	3.078397	-2.459098	1.050607
43	1	0	3.864663	-4.577364	-0.410237
44	1	0	3.974386	-3.826772	-3.000002
45	1	0	3.263638	-1.233280	-3.152807
46	1	0	1.517797	-0.021507	2.243452
47	1	0	3.028284	-0.621163	4.092179
48	1	0	2.971322	-2.928995	5.043766
49	1	0	1.358572	-4.590449	4.153449
50	1	0	-0.165218	-3.984167	2.306015
51	1	0	-2.718273	-2.491496	-0.846118
52	1	0	-5.050304	-2.978053	-0.188163
53	1	0	-5.748902	-2.760707	2.181696
54	1	0	-4.114834	-2.002383	3.894090
55	1	0	-1.789325	-1.478562	3.243253
56	1	0	4.939531	1.539151	-1.599731
57	1	0	5.419745	2.592029	-3.785988
58	1	0	3.619364	2.838940	-5.475922
59	1	0	1.321509	2.051742	-4.965140
60	1	0	0.823867	1.026559	-2.761425
61	1	0	2.407853	2.417742	1.504856
62	1	0	4.044233	3.223829	3.180027
63	1	0	6.273461	2.137691	3.360829
64	1	0	6.859147	0.256729	1.851442
65	1	0	5.228666	-0.552860	0.181101
66	6	0	-4.768810	0.732993	-0.533097
67	6	0	-4.247769	0.987374	0.740324
68	6	0	-2.879638	1.136503	0.950253
69	6	0	-1.997422	1.036228	-0.120562
70	6	0	-2.501585	0.812425	-1.403695
71	6	0	-3.866797	0.649381	-1.602533
72	1	0	-4.928768	1.100463	1.583545
73	1	0	-2.514464	1.326406	1.958942
74	1	0	-1.830988	0.774262	-2.265214
75	1	0	-4.239595	0.435506	-2.604174
76	46	0	0.115409	0.736189	0.005825
77	6	0	-6.217103	0.550290	-0.747514
78	6	0	-7.009504	-0.082896	0.218227
79	6	0	-6.832449	0.997020	-1.923059
80	6	0	-8.371025	-0.267875	0.012597

81	1	0	-6.541462	-0.458915	1.128528
82	6	0	-8.193665	0.812147	-2.129350
83	1	0	-6.242056	1.523146	-2.673080
84	6	0	-8.968214	0.177331	-1.162908
85	1	0	-8.968745	-0.768853	0.772234
86	1	0	-8.654106	1.175095	-3.046546
87	1	0	-10.034702	0.032333	-1.324216
88	6	0	0.662705	2.840203	-0.175877
89	6	0	-0.706581	2.899757	-0.262566
90	6	0	-0.074943	3.522631	0.950154
91	1	0	1.479394	3.107786	-0.842814
92	1	0	-1.432195	3.204748	-1.005714
93	6	0	-0.001951	5.071184	0.983395
94	6	0	1.355336	5.486682	1.558918
95	1	0	1.426395	6.581940	1.610122
96	1	0	1.512364	5.104782	2.576684
97	6	0	-0.200594	2.877464	2.316717
98	1	0	0.595622	3.212916	2.995739
99	1	0	-0.133462	1.782558	2.254165
100	1	0	-1.159461	3.125673	2.788702
101	1	0	2.184949	5.131036	0.929114
102	6	0	-1.130930	5.629752	1.853025
103	1	0	-1.005307	5.386533	2.915396
104	1	0	-1.158389	6.724892	1.773804
105	1	0	-2.109101	5.246706	1.525635
106	6	0	-0.136450	5.689499	-0.409578
107	1	0	0.635591	5.340481	-1.108266
108	1	0	-1.120909	5.489793	-0.855654
109	1	0	-0.034017	6.779533	-0.332904

Zero-point correction= 0.888458 (Hartree/Particle)
Thermal correction to Energy= 0.940939
Thermal correction to Enthalpy= 0.941883
Thermal correction to Gibbs Free Energy= 0.803148
Sum of electronic and zero-point Energies= -3018.529226
Sum of electronic and thermal Energies= -3018.476744
Sum of electronic and thermal Enthalpies= -3018.475800
Sum of electronic and thermal Free Energies= -3018.614536
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.7499951

TS2c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.740452	-2.925076	1.257963
2	15	0	0.402506	-1.323698	-0.751861
3	15	0	-2.499018	0.335514	0.563336
4	6	0	2.466163	-1.374976	-2.635526
5	6	0	-0.617659	-1.744314	-2.209987
6	6	0	-2.386657	-1.139461	-3.753761
7	6	0	2.094274	-1.689503	-1.323628
8	6	0	-2.287662	-2.387014	-4.359409
9	6	0	-0.495004	-2.981734	-2.855381
10	6	0	-1.548942	-0.820790	-2.688441
11	6	0	-1.333513	-3.302811	-3.915773
12	6	0	3.038866	-2.231038	-0.448456
13	6	0	4.338573	-2.464882	-0.885130
14	6	0	-2.993066	-1.393165	0.871926
15	6	0	-3.278348	-1.949765	2.165355
16	6	0	-2.921324	1.069036	2.187666
17	6	0	-0.494158	-4.503992	1.651396
18	6	0	-3.164697	-2.448070	-0.091154
19	6	0	-3.609387	-3.319932	1.996256
20	6	0	3.762046	-1.622992	-3.071654
21	6	0	-3.548159	-3.624218	0.608482
22	6	0	-1.930970	1.167513	3.170267

23	6	0	0.079196	-2.578915	0.507688
24	6	0	-4.235567	1.426873	2.499597
25	6	0	-0.298005	-3.471537	2.610147
26	6	0	-0.255583	-3.966245	0.357955
27	6	0	0.062617	-2.287101	1.915269
28	6	0	-3.786752	0.955711	-0.581193
29	6	0	-4.936141	0.217289	-0.881401
30	6	0	-4.551966	1.871723	3.779291
31	6	0	-2.251021	1.605177	4.450776
32	6	0	-3.563430	1.957144	4.755216
33	6	0	4.697642	-2.170749	-2.197616
34	6	0	-4.576245	2.731374	-2.026063
35	6	0	-3.619726	2.220607	-1.156883
36	6	0	-5.711838	1.984757	-2.329791
37	6	0	-5.891689	0.732185	-1.752379
38	1	0	0.253141	-1.311999	2.354544
39	1	0	-0.450567	-3.559416	3.680399
40	1	0	-0.831507	-5.513150	1.863424
41	1	0	-0.387618	-4.494897	-0.579984
42	1	0	-3.009645	-2.367132	-1.162872
43	1	0	-3.704400	-4.600585	0.161727
44	1	0	-3.819624	-4.023071	2.795104
45	1	0	-3.209313	-1.423572	3.112138
46	1	0	-1.633274	0.156113	-2.214635
47	1	0	-3.113052	-0.407813	-4.105045
48	1	0	-2.940909	-2.644867	-5.190713
49	1	0	-1.236892	-4.269616	-4.406189
50	1	0	0.270960	-3.690171	-2.539616
51	1	0	2.764236	-2.471660	0.578842
52	1	0	5.073247	-2.880351	-0.197280
53	1	0	5.711187	-2.372255	-2.541543
54	1	0	4.040609	-1.392241	-4.098211
55	1	0	1.736472	-0.946492	-3.324183
56	1	0	-5.017064	1.350543	1.743641
57	1	0	-5.577097	2.150585	4.015057
58	1	0	-3.815277	2.303146	5.755722
59	1	0	-1.474957	1.678839	5.210282
60	1	0	-0.899033	0.906221	2.925518
61	1	0	-2.733270	2.810056	-0.918384
62	1	0	-4.435598	3.716067	-2.468935
63	1	0	-6.458335	2.382198	-3.014725
64	1	0	-6.782028	0.148843	-1.979451
65	1	0	-5.092327	-0.761713	-0.431149
66	6	0	4.737911	0.736619	0.705113
67	6	0	4.246879	1.130278	-0.543128
68	6	0	2.885070	1.324858	-0.759937
69	6	0	1.976883	1.134872	0.276427
70	6	0	2.453965	0.755920	1.534191
71	6	0	3.812166	0.551076	1.741040
72	1	0	4.944681	1.304720	-1.362118
73	1	0	2.551722	1.614666	-1.755715
74	1	0	1.765596	0.630197	2.373379
75	1	0	4.160665	0.221474	2.719889
76	46	0	-0.154217	0.876353	0.071499
77	6	0	6.179261	0.514383	0.927456
78	6	0	6.978716	-0.056015	-0.070949
79	6	0	6.779644	0.865459	2.142135
80	6	0	8.334552	-0.272867	0.141561
81	1	0	6.518986	-0.357433	-1.013163
82	6	0	8.135741	0.651238	2.353928
83	1	0	6.181220	1.341240	2.919007
84	6	0	8.918025	0.079297	1.354929
85	1	0	8.939006	-0.724971	-0.643001
86	1	0	8.586569	0.941119	3.301369
87	1	0	9.980334	-0.089365	1.520763
88	6	0	-0.705266	2.912886	0.592206
89	6	0	0.674112	2.936922	0.702978

90	6	0	0.048741	3.924305	-0.238654
91	1	0	-1.488625	3.039025	1.337467
92	1	0	1.367597	3.076701	1.523769
93	6	0	0.000609	5.307311	0.407321
94	6	0	0.175655	3.967332	-1.776603
95	6	0	-0.847170	4.966813	-2.334829
96	1	0	-1.869237	4.720377	-2.007954
97	1	0	-0.637680	6.000824	-2.035442
98	1	0	-0.833391	4.939649	-3.432794
99	6	0	1.585670	4.439722	-2.148012
100	1	0	1.698287	4.480021	-3.240370
101	1	0	1.799428	5.445760	-1.766021
102	1	0	2.353158	3.764168	-1.748411
103	6	0	-0.100467	2.637051	-2.472185
104	1	0	0.070599	2.749397	-3.552006
105	1	0	0.547843	1.819348	-2.128043
106	1	0	-1.147175	2.329279	-2.341930
107	1	0	0.742037	5.993665	-0.018534
108	1	0	-0.990497	5.763739	0.280049
109	1	0	0.188834	5.245383	1.486331

Zero-point correction= 0.890249 (Hartree/Particle)
Thermal correction to Energy= 0.942253
Thermal correction to Enthalpy= 0.943197
Thermal correction to Gibbs Free Energy= 0.807373
Sum of electronic and zero-point Energies= -3018.518845
Sum of electronic and thermal Energies= -3018.466842
Sum of electronic and thermal Enthalpies= -3018.465897
Sum of electronic and thermal Free Energies= -3018.601722
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.7405424

TS2c''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.637564	-2.209892	-1.782610
2	15	0	0.057584	-1.812143	0.347329
3	15	0	2.530131	0.791364	-0.199258
4	6	0	-1.934725	-3.147259	1.828514
5	6	0	1.099977	-2.332391	1.750506
6	6	0	2.528899	-1.700132	3.603179
7	6	0	-1.511355	-2.711601	0.570256
8	6	0	2.819307	-3.039942	3.836765
9	6	0	1.364603	-3.681072	2.020758
10	6	0	1.666315	-1.350580	2.567712
11	6	0	2.226552	-4.029879	3.053103
12	6	0	-2.359275	-2.855154	-0.533032
13	6	0	-3.617547	-3.419540	-0.376234
14	6	0	3.477560	-0.602125	-0.890996
15	6	0	3.955821	-0.721974	-2.237348
16	6	0	2.792090	2.091920	-1.467865
17	6	0	1.833965	-3.834750	-2.736483
18	6	0	3.832424	-1.813374	-0.202084
19	6	0	4.585347	-1.988136	-2.373630
20	6	0	-3.189200	-3.731074	1.977311
21	6	0	4.517352	-2.655783	-1.119661
22	6	0	2.013829	2.053551	-2.632209
23	6	0	0.757476	-2.527198	-1.162454
24	6	0	3.711147	3.128809	-1.298871
25	6	0	1.420113	-2.634755	-3.378910
26	6	0	1.425571	-3.778978	-1.376294
27	6	0	0.751054	-1.830742	-2.418922
28	6	0	3.555059	1.345325	1.214332
29	6	0	4.854421	0.880464	1.436670
30	6	0	3.846718	4.111277	-2.277258
31	6	0	2.157633	3.028685	-3.612011

32	6	0	3.073015	4.063769	-3.431606
33	6	0	-4.031731	-3.863075	0.878296
34	6	0	3.747187	2.755304	3.176258
35	6	0	3.012309	2.290872	2.092221
36	6	0	5.035442	2.275045	3.398803
37	6	0	5.587058	1.342577	2.526519
38	1	0	0.327910	-0.841353	-2.577605
39	1	0	1.625882	-2.360259	-4.407926
40	1	0	2.418298	-4.629189	-3.188803
41	1	0	1.643166	-4.527137	-0.621574
42	1	0	3.596466	-2.050739	0.831990
43	1	0	4.869674	-3.660915	-0.912745
44	1	0	4.998785	-2.393719	-3.291017
45	1	0	3.821586	0.013798	-3.024086
46	1	0	1.439602	-0.299448	2.379372
47	1	0	2.972408	-0.922906	4.223678
48	1	0	3.495950	-3.319084	4.642083
49	1	0	2.432979	-5.079427	3.254067
50	1	0	0.878987	-4.462367	1.436323
51	1	0	-2.043575	-2.501942	-1.515450
52	1	0	-4.281992	-3.508954	-1.233820
53	1	0	-5.015708	-4.314191	0.997032
54	1	0	-3.509475	-4.080284	2.957179
55	1	0	-1.286751	-3.031035	2.697114
56	1	0	4.324329	3.172333	-0.399395
57	1	0	4.566783	4.915047	-2.135634
58	1	0	3.183961	4.831930	-4.194507
59	1	0	1.552693	2.984988	-4.515992
60	1	0	1.289181	1.248238	-2.774051
61	1	0	2.011224	2.683060	1.910740
62	1	0	3.314925	3.492783	3.850060
63	1	0	5.611306	2.632146	4.250388
64	1	0	6.597417	0.972399	2.689989
65	1	0	5.301683	0.157518	0.756685
66	6	0	-4.793458	0.132359	-0.278840
67	6	0	-4.175145	-0.071501	0.960871
68	6	0	-2.798261	0.064524	1.111360
69	6	0	-1.996883	0.408973	0.024517
70	6	0	-2.603123	0.635457	-1.211505
71	6	0	-3.983098	0.497682	-1.359780
72	1	0	-4.784573	-0.335985	1.825546
73	1	0	-2.352652	-0.137780	2.088217
74	1	0	-2.004254	0.906406	-2.085516
75	1	0	-4.433430	0.641291	-2.342513
76	46	0	0.048929	0.549806	0.118412
77	6	0	-6.247824	-0.061681	-0.441864
78	6	0	-6.909890	-1.083809	0.249124
79	6	0	-6.997481	0.760957	-1.290178
80	6	0	-8.277771	-1.275086	0.099148
81	1	0	-6.336233	-1.751709	0.892708
82	6	0	-8.365491	0.569877	-1.441292
83	1	0	-6.504563	1.578802	-1.816127
84	6	0	-9.011149	-0.448752	-0.746786
85	1	0	-8.773836	-2.079553	0.639765
86	1	0	-8.933548	1.226184	-2.098342
87	1	0	-10.082834	-0.597594	-0.864328
88	6	0	-0.119795	2.661485	-0.214175
89	6	0	0.066585	3.919593	0.243964
90	6	0	-1.042703	3.566189	1.044224
91	1	0	-0.161812	2.622051	-1.315025
92	1	0	0.314504	4.845057	-0.279349
93	6	0	-2.339874	4.363005	0.823611
94	6	0	-2.125931	5.750759	1.442988
95	1	0	-3.036519	6.351684	1.318908
96	1	0	-1.914300	5.691522	2.519278
97	6	0	-0.928878	2.799388	2.328628
98	1	0	0.052088	2.327735	2.440790

99	1	0	-1.700848	2.028682	2.414425
100	1	0	-1.071052	3.508184	3.159776
101	1	0	-1.301992	6.295629	0.961891
102	6	0	-3.545953	3.690984	1.481886
103	1	0	-3.452775	3.633864	2.573743
104	1	0	-4.446631	4.280031	1.264534
105	1	0	-3.708750	2.676003	1.092833
106	6	0	-2.635815	4.504682	-0.670684
107	1	0	-1.846578	5.044251	-1.211558
108	1	0	-2.766091	3.517209	-1.138712
109	1	0	-3.568990	5.065518	-0.808537

Zero-point correction= 0.887077 (Hartree/Particle)
Thermal correction to Energy= 0.940332
Thermal correction to Enthalpy= 0.941276
Thermal correction to Gibbs Free Energy= 0.800081
Sum of electronic and zero-point Energies= -3018.511888
Sum of electronic and thermal Energies= -3018.458634
Sum of electronic and thermal Enthalpies= -3018.457690
Sum of electronic and thermal Free Energies= -3018.598884
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.7321124

INT5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.099599	-3.178370	1.455913
2	15	0	0.921615	-1.409852	-0.517090
3	15	0	-2.399343	-0.149226	0.382533
4	6	0	3.161222	-0.499892	-1.855635
5	6	0	0.294465	-2.186080	-2.048502
6	6	0	-1.278463	-2.134592	-3.891054
7	6	0	2.716873	-1.343238	-0.830342
8	6	0	-0.788327	-3.355795	-4.341876
9	6	0	0.812443	-3.391780	-2.535202
10	6	0	-0.727954	-1.549763	-2.754238
11	6	0	0.265980	-3.975815	-3.671678
12	6	0	3.640037	-2.102584	-0.110736
13	6	0	4.995270	-2.031681	-0.426908
14	6	0	-2.551031	-1.893331	0.870940
15	6	0	-2.831389	-2.394121	2.186961
16	6	0	-3.255448	0.729082	1.734653
17	6	0	0.312374	-4.538398	2.046259
18	6	0	-2.479975	-3.025207	-0.013302
19	6	0	-2.934979	-3.808259	2.107131
20	6	0	4.510065	-0.445048	-2.177142
21	6	0	-2.725577	-4.195139	0.754298
22	6	0	-2.602474	0.857896	2.967160
23	6	0	0.717519	-2.636390	0.795170
24	6	0	-4.499741	1.332250	1.548548
25	6	0	0.302431	-3.426275	2.933457
26	6	0	0.575167	-4.061478	0.732815
27	6	0	0.554791	-2.254919	2.171847
28	6	0	-3.489797	-0.021592	-1.070675
29	6	0	-4.626484	-0.828613	-1.199542
30	6	0	-5.090931	2.043137	2.591296
31	6	0	-3.199778	1.558648	4.005902
32	6	0	-4.445827	2.155107	3.817125
33	6	0	5.428093	-1.214832	-1.464445
34	6	0	-4.023827	1.050026	-3.172694
35	6	0	-3.198414	0.918410	-2.061062
36	6	0	-5.145946	0.237172	-3.301688
37	6	0	-5.447429	-0.698140	-2.313979
38	1	0	0.578517	-1.235731	2.549559
39	1	0	0.081431	-3.460764	3.994795
40	1	0	0.092472	-5.567090	2.312500

41	1	0	0.580741	-4.663685	-0.169502
42	1	0	-2.261727	-2.991088	-1.077212
43	1	0	-2.693765	-5.213146	0.380451
44	1	0	-3.092964	-4.479497	2.944561
45	1	0	-2.927198	-1.796502	3.087545
46	1	0	-1.102231	-0.587777	-2.403115
47	1	0	-2.087596	-1.630196	-4.418031
48	1	0	-1.214269	-3.820684	-5.229050
49	1	0	0.667409	-4.916753	-4.043510
50	1	0	1.655569	-3.867996	-2.032479
51	1	0	3.302557	-2.759054	0.692026
52	1	0	5.714154	-2.623194	0.137207
53	1	0	6.487209	-1.165962	-1.709300
54	1	0	4.850468	0.202834	-2.983539
55	1	0	2.442116	0.103460	-2.416331
56	1	0	-5.008677	1.255515	0.588257
57	1	0	-6.061177	2.512151	2.439703
58	1	0	-4.910144	2.712575	4.628019
59	1	0	-2.688560	1.652747	4.962041
60	1	0	-1.609598	0.423477	3.106088
61	1	0	-2.315297	1.547861	-1.955542
62	1	0	-3.788799	1.789679	-3.936541
63	1	0	-5.790932	0.332665	-4.172971
64	1	0	-6.328214	-1.329687	-2.410504
65	1	0	-4.871468	-1.559719	-0.429436
66	6	0	4.132997	1.928319	0.669941
67	6	0	3.826544	3.127270	-0.001798
68	6	0	2.537106	3.626881	-0.049904
69	6	0	1.486442	2.966075	0.597071
70	6	0	1.786835	1.779566	1.284150
71	6	0	3.085110	1.262345	1.303063
72	1	0	4.630631	3.695524	-0.467236
73	1	0	2.336886	4.565738	-0.567274
74	1	0	1.024456	1.341173	1.940318
75	1	0	3.279477	0.324623	1.823419
76	46	0	-0.237501	0.669703	0.074703
77	6	0	5.518376	1.421890	0.727283
78	6	0	6.431631	1.705982	-0.295212
79	6	0	5.954669	0.642555	1.805249
80	6	0	7.734005	1.225058	-0.245236
81	1	0	6.109829	2.285473	-1.160467
82	6	0	7.253981	0.153054	1.853416
83	1	0	5.278152	0.440658	2.635006
84	6	0	8.148948	0.440692	0.827189
85	1	0	8.426819	1.458392	-1.052020
86	1	0	7.573625	-0.443162	2.706314
87	1	0	9.169333	0.064445	0.868545
88	6	0	-1.032804	2.562783	0.416334
89	6	0	0.104611	3.517637	0.627532
90	6	0	-0.749609	3.590828	-0.637574
91	1	0	-1.921797	2.668025	1.035763
92	1	0	-0.031071	4.327192	1.349129
93	6	0	-1.714639	4.793942	-0.787316
94	6	0	-2.885264	4.421200	-1.700039
95	1	0	-3.573774	5.271479	-1.797202
96	1	0	-2.564212	4.150846	-2.715442
97	6	0	-0.092789	3.141699	-1.931561
98	1	0	-0.839806	2.902534	-2.700325
99	1	0	0.517996	2.235916	-1.797620
100	1	0	0.569527	3.911716	-2.348562
101	1	0	-3.455252	3.577219	-1.282593
102	6	0	-0.948761	5.976148	-1.389951
103	1	0	-0.631986	5.787887	-2.423873
104	1	0	-1.583433	6.872870	-1.405622
105	1	0	-0.054140	6.214011	-0.794548
106	6	0	-2.320151	5.261978	0.540655
107	1	0	-2.902830	4.477280	1.043699

108	1	0	-1.568382	5.642883	1.243832
109	1	0	-3.010592	6.092314	0.342440

Zero-point correction= 0.891654 (Hartree/Particle)
Thermal correction to Energy= 0.944054
Thermal correction to Enthalpy= 0.944998
Thermal correction to Gibbs Free Energy= 0.806015
Sum of electronic and zero-point Energies= -3018.594461
Sum of electronic and thermal Energies= -3018.542061
Sum of electronic and thermal Enthalpies= -3018.541117
Sum of electronic and thermal Free Energies= -3018.680100
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.8142319

INT5c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.275137	-2.848481	1.053765
2	15	0	0.301227	-1.614148	-0.659845
3	15	0	-2.488087	0.555979	0.510977
4	6	0	2.883961	-1.315803	-1.659773
5	6	0	-0.251919	-2.156876	-2.311414
6	6	0	-1.530723	-1.733651	-4.321727
7	6	0	2.099922	-1.938088	-0.681280
8	6	0	-1.114567	-2.955370	-4.841617
9	6	0	0.181460	-3.372822	-2.852262
10	6	0	-1.097323	-1.333149	-3.060714
11	6	0	-0.256210	-3.772935	-4.108887
12	6	0	2.716305	-2.729150	0.292146
13	6	0	4.100253	-2.885030	0.289698
14	6	0	-3.192580	-1.104516	0.666898
15	6	0	-3.732300	-1.691700	1.862800
16	6	0	-2.755503	1.246434	2.179245
17	6	0	-1.378443	-4.630754	1.516263
18	6	0	-3.409275	-2.034142	-0.406953
19	6	0	-4.265042	-2.964160	1.522091
20	6	0	4.263172	-1.479134	-1.661296
21	6	0	-4.070915	-3.171938	0.127754
22	6	0	-1.720739	1.182671	3.116209
23	6	0	-0.347883	-2.824055	0.511382
24	6	0	-4.002988	1.747414	2.561335
25	6	0	-1.109749	-3.666483	2.527755
26	6	0	-0.903905	-4.123476	0.275486
27	6	0	-0.474935	-2.552107	1.916659
28	6	0	-3.682619	1.374909	-0.602023
29	6	0	-5.009399	0.928889	-0.675271
30	6	0	-4.210519	2.168768	3.870515
31	6	0	-1.932878	1.599624	4.425083
32	6	0	-3.179454	2.091434	4.802665
33	6	0	4.874762	-2.256257	-0.679290
34	6	0	-4.198503	3.120369	-2.195025
35	6	0	-3.286961	2.472441	-1.369830
36	6	0	-5.515639	2.677228	-2.259184
37	6	0	-5.919071	1.582924	-1.498427
38	1	0	-0.176496	-1.629498	2.408934
39	1	0	-1.395572	-3.741392	3.571435
40	1	0	-1.909150	-5.566736	1.655573
41	1	0	-1.015310	-4.598922	-0.694292
42	1	0	-3.091726	-1.905065	-1.438828
43	1	0	-4.325218	-4.071156	-0.423503
44	1	0	-4.693125	-3.676928	2.219042
45	1	0	-3.697438	-1.251578	2.855052
46	1	0	-1.416732	-0.369865	-2.652512
47	1	0	-2.187369	-1.087754	-4.901385
48	1	0	-1.451204	-3.269130	-5.827849
49	1	0	0.081229	-4.720822	-4.523722

50	1	0	0.874803	-3.999640	-2.289395
51	1	0	2.117068	-3.228400	1.053532
52	1	0	4.576952	-3.498423	1.052812
53	1	0	5.958540	-2.360679	-0.661887
54	1	0	4.867832	-0.987632	-2.421452
55	1	0	2.410289	-0.705389	-2.431029
56	1	0	-4.814946	1.809608	1.836992
57	1	0	-5.182157	2.561762	4.163046
58	1	0	-3.345770	2.423309	5.825584
59	1	0	-1.122037	1.548197	5.149007
60	1	0	-0.739268	0.816994	2.810450
61	1	0	-2.255562	2.812732	-1.322338
62	1	0	-3.875398	3.971751	-2.792664
63	1	0	-6.230164	3.181357	-2.906858
64	1	0	-6.947731	1.231582	-1.549174
65	1	0	-5.333375	0.068218	-0.090083
66	6	0	4.575440	1.311825	1.069457
67	6	0	4.523562	2.681365	0.763582
68	6	0	3.315457	3.354888	0.685019
69	6	0	2.100187	2.688127	0.887986
70	6	0	2.161077	1.346866	1.279973
71	6	0	3.372409	0.664953	1.354748
72	1	0	5.454002	3.224069	0.599176
73	1	0	3.302655	4.418900	0.446474
74	1	0	1.240862	0.827859	1.576817
75	1	0	3.376987	-0.395859	1.606465
76	46	0	-0.261948	0.712354	-0.130742
77	6	0	5.854602	0.576508	1.078629
78	6	0	6.835013	0.852433	0.118566
79	6	0	6.103352	-0.432866	2.015617
80	6	0	8.024834	0.134621	0.089521
81	1	0	6.648423	1.619606	-0.633144
82	6	0	7.294190	-1.148789	1.990236
83	1	0	5.362191	-0.641313	2.787345
84	6	0	8.258351	-0.869860	1.024923
85	1	0	8.772774	0.357815	-0.669320
86	1	0	7.475675	-1.920996	2.736120
87	1	0	9.191983	-1.428977	1.006472
88	6	0	-0.456748	2.733031	0.262826
89	6	0	0.812348	3.406584	0.703905
90	6	0	0.181869	3.731456	-0.669859
91	1	0	-1.362435	3.086943	0.761921
92	1	0	0.683882	4.219374	1.427876
93	6	0	-0.523194	5.079168	-0.664418
94	6	0	0.838410	3.374573	-2.027701
95	6	0	-0.230815	3.338454	-3.129942
96	1	0	-0.959230	2.531053	-2.965175
97	1	0	-0.778042	4.284271	-3.224213
98	1	0	0.250040	3.151557	-4.100312
99	6	0	1.876314	4.438485	-2.406363
100	1	0	2.366976	4.167871	-3.351318
101	1	0	1.421037	5.426043	-2.551480
102	1	0	2.657128	4.528989	-1.640620
103	6	0	1.545961	2.018088	-2.084315
104	1	0	1.897283	1.841870	-3.112148
105	1	0	2.411665	1.926941	-1.420923
106	1	0	0.845879	1.175309	-1.879943
107	1	0	0.173739	5.902239	-0.872753
108	1	0	-1.336150	5.138850	-1.400084
109	1	0	-0.966718	5.277323	0.319165

Zero-point correction= 0.892129 (Hartree/Particle)
Thermal correction to Energy= 0.944478
Thermal correction to Enthalpy= 0.945422
Thermal correction to Gibbs Free Energy= 0.805946
Sum of electronic and zero-point Energies= -3018.589235
Sum of electronic and thermal Energies= -3018.536887

Sum of electronic and thermal Enthalpies= -3018.535942
Sum of electronic and thermal Free Energies= -3018.675419
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.8094869

INT6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.375850	-3.061735	-1.310663
2	15	0	-0.506829	-1.896341	0.100422
3	15	0	2.561256	0.118762	-0.185560
4	6	0	-3.308659	-1.966672	0.435690
5	6	0	-0.371382	-2.938527	1.598896
6	6	0	0.583040	-3.285718	3.794054
7	6	0	-2.243519	-2.158455	-0.454342
8	6	0	-0.038996	-4.528287	3.870649
9	6	0	-1.009825	-4.179172	1.691833
10	6	0	0.410858	-2.490171	2.665981
11	6	0	-0.840560	-4.972125	2.821955
12	6	0	-2.524847	-2.515519	-1.777005
13	6	0	-3.840763	-2.686608	-2.199780
14	6	0	3.312422	-1.519545	-0.430459
15	6	0	4.070815	-1.978935	-1.558866
16	6	0	3.302223	1.035116	-1.598026
17	6	0	1.448726	-4.563488	-2.338126
18	6	0	3.195271	-2.619111	0.483440
19	6	0	4.396600	-3.347302	-1.343492
20	6	0	-4.620635	-2.132854	0.008104
21	6	0	3.860134	-3.739724	-0.084231
22	6	0	2.547335	1.168732	-2.768014
23	6	0	0.380808	-2.884546	-1.152396
24	6	0	4.595033	1.561436	-1.558489
25	6	0	1.498614	-3.377828	-3.124518
26	6	0	0.756248	-4.267592	-1.130435
27	6	0	0.841306	-2.345291	-2.399668
28	6	0	3.451803	0.681955	1.318266
29	6	0	4.766390	0.271620	1.581973
30	6	0	5.130732	2.190901	-2.678491
31	6	0	3.084886	1.791786	-3.888370
32	6	0	4.380775	2.300517	-3.845091
33	6	0	-4.890450	-2.499191	-1.308004
34	6	0	3.462411	1.950001	3.378693
35	6	0	2.800516	1.513719	2.234548
36	6	0	4.773242	1.556156	3.621666
37	6	0	5.423918	0.712690	2.723583
38	1	0	0.743807	-1.306099	-2.702358
39	1	0	2.002856	-3.264017	-4.078573
40	1	0	1.914916	-5.511928	-2.585206
41	1	0	0.607135	-4.947930	-0.297712
42	1	0	2.645240	-2.610079	1.420744
43	1	0	3.899004	-4.735745	0.344297
44	1	0	4.918501	-3.991735	-2.043395
45	1	0	4.302565	-1.394649	-2.444576
46	1	0	0.863910	-1.497968	2.616251
47	1	0	1.189358	-2.924369	4.622724
48	1	0	0.088150	-5.147126	4.757481
49	1	0	-1.342719	-5.936075	2.888056
50	1	0	-1.652691	-4.519611	0.878792
51	1	0	-1.717041	-2.675240	-2.489484
52	1	0	-4.040975	-2.973219	-3.231336
53	1	0	-5.920721	-2.626432	-1.636251
54	1	0	-5.440016	-1.967941	0.706263
55	1	0	-3.107854	-1.673167	1.465142
56	1	0	5.184633	1.489382	-0.645053
57	1	0	6.137922	2.601952	-2.635617
58	1	0	4.801229	2.795271	-4.718964

59	1	0	2.485905	1.892953	-4.791665
60	1	0	1.514747	0.814716	-2.782201
61	1	0	1.766682	1.810746	2.047862
62	1	0	2.941619	2.597538	4.082433
63	1	0	5.288730	1.896652	4.518361
64	1	0	6.445771	0.390511	2.917522
65	1	0	5.276366	-0.405339	0.895303
66	6	0	-4.407866	1.770213	-1.013097
67	6	0	-4.110987	3.038383	-0.506262
68	6	0	-2.815620	3.539153	-0.543215
69	6	0	-1.764769	2.769531	-1.041201
70	6	0	-2.077194	1.526005	-1.603939
71	6	0	-3.373342	1.034381	-1.599661
72	1	0	-4.913576	3.645823	-0.087064
73	1	0	-2.611943	4.535286	-0.152116
74	1	0	-1.271935	0.921175	-2.032923
75	1	0	-3.577476	0.039310	-1.998452
76	46	0	0.256300	0.440770	0.233255
77	6	0	-5.764534	1.202561	-0.900330
78	6	0	-6.478483	1.316134	0.298365
79	6	0	-6.354409	0.510285	-1.963207
80	6	0	-7.739831	0.747524	0.433009
81	1	0	-6.014121	1.827595	1.141605
82	6	0	-7.617534	-0.054934	-1.831529
83	1	0	-5.813565	0.425550	-2.906305
84	6	0	-8.314239	0.057423	-0.631242
85	1	0	-8.273353	0.835938	1.378514
86	1	0	-8.064658	-0.582055	-2.674051
87	1	0	-9.302663	-0.387692	-0.526533
88	6	0	0.707838	2.468094	-0.237442
89	6	0	-0.342090	3.220506	-1.025877
90	6	0	0.343072	3.866944	0.174862
91	1	0	1.667034	2.472135	-0.750038
92	1	0	-0.005753	3.560239	-2.011151
93	6	0	1.418320	4.958971	-0.108455
94	6	0	2.598784	4.769880	0.847210
95	1	0	3.329593	5.582820	0.722703
96	1	0	2.283436	4.768996	1.899766
97	6	0	-0.447561	4.110487	1.437912
98	1	0	0.212422	4.092614	2.319056
99	1	0	-1.198590	3.335659	1.594354
100	1	0	-0.960841	5.080900	1.429166
101	1	0	3.119236	3.819755	0.653715
102	6	0	0.817983	6.353849	0.099808
103	1	0	0.601911	6.565979	1.154234
104	1	0	1.519007	7.124498	-0.252014
105	1	0	-0.117403	6.465190	-0.470510
106	6	0	1.973745	4.942538	-1.538250
107	1	0	2.371548	3.965490	-1.847194
108	1	0	1.220725	5.257776	-2.273570
109	1	0	2.804878	5.658975	-1.604951
110	53	0	-1.573466	0.745000	2.317086

Zero-point correction= 0.892420 (Hartree/Particle)
Thermal correction to Energy= 0.946911
Thermal correction to Enthalpy= 0.947855
Thermal correction to Gibbs Free Energy= 0.804171
Sum of electronic and zero-point Energies= -3030.164180
Sum of electronic and thermal Energies= -3030.109689
Sum of electronic and thermal Enthalpies= -3030.108744
Sum of electronic and thermal Free Energies= -3030.252429
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3033.3944547

TS3c

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

1	26	0	4.595738	-1.046174	-1.742117
2	15	0	1.956546	-2.160194	0.077831
3	15	0	3.043259	1.436816	-0.026471
4	6	0	-0.552073	-3.395378	0.356275
5	6	0	2.902687	-3.265999	1.196143
6	6	0	4.294684	-3.490299	3.161353
7	6	0	0.568860	-3.257465	-0.474585
8	6	0	4.430010	-4.852422	2.913036
9	6	0	3.027381	-4.639043	0.964354
10	6	0	3.526943	-2.700679	2.311220
11	6	0	3.790900	-5.428171	1.817548
12	6	0	0.583202	-3.934018	-1.702714
13	6	0	-0.504409	-4.710506	-2.100568
14	6	0	4.561546	0.631485	-0.632324
15	6	0	5.271050	0.859333	-1.858132
16	6	0	2.658525	2.570893	-1.423481
17	6	0	4.572276	-2.603573	-3.062686
18	6	0	5.250819	-0.411517	0.068157
19	6	0	6.366274	-0.048214	-1.913877
20	6	0	-1.631199	-4.181477	-0.039336
21	6	0	6.354279	-0.830256	-0.723868
22	6	0	1.534002	2.311456	-2.212081
23	6	0	2.969726	-2.184753	-1.439509
24	6	0	3.438500	3.696376	-1.709915
25	6	0	3.750387	-1.538335	-3.530047
26	6	0	4.091666	-3.008806	-1.785098
27	6	0	2.762295	-1.279329	-2.537690
28	6	0	3.745182	2.513201	1.286884
29	6	0	5.071993	2.961466	1.256204
30	6	0	3.114106	4.522180	-2.780384
31	6	0	1.195368	3.148185	-3.270555
32	6	0	1.992698	4.249219	-3.561602
33	6	0	-1.617166	-4.832826	-1.271403
34	6	0	3.420331	3.695003	3.372904
35	6	0	2.928788	2.874587	2.361869
36	6	0	4.734055	4.148170	3.327829
37	6	0	5.560954	3.777231	2.270249
38	1	0	2.042011	-0.462686	-2.560851
39	1	0	3.894053	-0.975467	-4.446859
40	1	0	5.451424	-2.995355	-3.564182
41	1	0	4.536943	-3.759998	-1.139708
42	1	0	4.944423	-0.846210	1.015767
43	1	0	7.030805	-1.645081	-0.487452
44	1	0	7.057875	-0.159363	-2.742942
45	1	0	4.974156	1.558980	-2.633734
46	1	0	3.373167	-1.642668	2.530550
47	1	0	4.770043	-3.040951	4.031430
48	1	0	5.024114	-5.472199	3.582973
49	1	0	3.881261	-6.497454	1.631892
50	1	0	2.520034	-5.098677	0.114597
51	1	0	1.453343	-3.861030	-2.356163
52	1	0	-0.470933	-5.238877	-3.053280
53	1	0	-2.462311	-5.449028	-1.575554
54	1	0	-2.485161	-4.289324	0.628604
55	1	0	-0.577395	-2.874720	1.317893
56	1	0	4.300071	3.935554	-1.086026
57	1	0	3.729044	5.394860	-2.995370
58	1	0	1.726846	4.913745	-4.382210
59	1	0	0.276642	2.957322	-3.822382
60	1	0	0.857835	1.495643	-1.952447
61	1	0	1.905719	2.497300	2.405642
62	1	0	2.769160	3.970517	4.201744
63	1	0	5.119952	4.784498	4.122808
64	1	0	6.594426	4.119183	2.237948
65	1	0	5.731432	2.661837	0.440350
66	6	0	-4.799795	-0.673789	1.385552

67	6	0	-4.763401	0.644013	1.874303
68	6	0	-3.643187	1.442886	1.727550
69	6	0	-2.469491	0.964034	1.111505
70	6	0	-2.483658	-0.384918	0.705588
71	6	0	-3.619213	-1.170909	0.810673
72	1	0	-5.659048	1.068851	2.333930
73	1	0	-3.674626	2.481709	2.052961
74	1	0	-1.551628	-0.816910	0.334545
75	1	0	-3.580532	-2.212866	0.483506
76	46	0	1.236975	0.116686	0.867178
77	6	0	-6.044036	-1.459885	1.412722
78	6	0	-6.976263	-1.319827	2.452646
79	6	0	-6.366479	-2.340548	0.366454
80	6	0	-8.173693	-2.023587	2.444568
81	1	0	-6.736710	-0.672832	3.296067
82	6	0	-7.561736	-3.051325	0.361869
83	1	0	-5.664985	-2.460904	-0.462016
84	6	0	-8.476235	-2.892720	1.399348
85	1	0	-8.873223	-1.902369	3.270618
86	1	0	-7.783180	-3.729248	-0.461993
87	1	0	-9.412691	-3.447691	1.397598
88	6	0	0.064312	1.887425	0.818173
89	6	0	-1.396855	1.864794	0.756557
90	6	0	-0.721420	2.880759	1.653251
91	1	0	0.522713	2.336300	-0.061429
92	1	0	-1.564346	2.065621	-0.514189
93	6	0	-0.797919	4.371978	1.231133
94	6	0	0.009096	5.258458	2.182997
95	1	0	-0.028398	6.304169	1.843528
96	1	0	-0.373674	5.234616	3.212319
97	6	0	-0.826363	2.641016	3.145279
98	1	0	0.096890	2.920327	3.676804
99	1	0	-1.017810	1.586164	3.365407
100	1	0	-1.642649	3.229979	3.589552
101	1	0	1.068128	4.957793	2.205011
102	6	0	-2.270952	4.798136	1.248384
103	1	0	-2.736180	4.641411	2.234310
104	1	0	-2.358597	5.871327	1.017767
105	1	0	-2.835295	4.238351	0.485926
106	6	0	-0.279893	4.625573	-0.185699
107	1	0	0.806049	4.456604	-0.264446
108	1	0	-0.794351	4.005022	-0.932957
109	1	0	-0.459993	5.678210	-0.450952
110	53	0	0.292380	-0.961277	3.249167
111	6	0	-2.934065	1.917033	-2.073908
112	8	0	-3.432492	1.047768	-2.877746
113	8	0	-3.613325	2.786706	-1.462297
114	8	0	-1.622509	1.834163	-1.820526
115	55	0	-5.983465	1.174367	-1.324882
116	55	0	-1.272024	-0.948869	-2.678398

Zero-point correction= 0.903834 (Hartree/Particle)
Thermal correction to Energy= 0.967241
Thermal correction to Enthalpy= 0.968185
Thermal correction to Gibbs Free Energy= 0.800431
Sum of electronic and zero-point Energies= -3333.609440
Sum of electronic and thermal Energies= -3333.546033
Sum of electronic and thermal Enthalpies= -3333.545089
Sum of electronic and thermal Free Energies= -3333.712843
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3337.5601546

TS3c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	4.243615	1.263684	2.509773

2	15	0	2.509429	1.848517	-0.345131
3	15	0	3.114154	-1.667445	1.055177
4	6	0	0.429522	2.846118	-1.904842
5	6	0	3.868208	2.540068	-1.366531
6	6	0	5.800176	2.130964	-2.762013
7	6	0	1.121134	3.014173	-0.695754
8	6	0	6.013440	3.500774	-2.872608
9	6	0	4.078919	3.916555	-1.496733
10	6	0	4.727475	1.650616	-2.015897
11	6	0	5.149157	4.395247	-2.243832
12	6	0	0.685369	3.992601	0.203044
13	6	0	-0.423638	4.784713	-0.091133
14	6	0	4.346524	-0.711151	2.001356
15	6	0	4.525591	-0.546376	3.411117
16	6	0	2.174566	-2.546103	2.358447
17	6	0	4.148432	3.181457	3.180567
18	6	0	5.376865	0.043503	1.351640
19	6	0	5.649929	0.301913	3.623045
20	6	0	-0.665362	3.649969	-2.203101
21	6	0	6.179659	0.660076	2.350307
22	6	0	1.417551	-1.792056	3.266469
23	6	0	3.008630	2.370977	1.331725
24	6	0	2.031170	-3.936908	2.362735
25	6	0	3.027027	2.439891	3.651267
26	6	0	4.136512	3.146391	1.756878
27	6	0	2.328804	1.937209	2.518649
28	6	0	4.190477	-2.971295	0.339497
29	6	0	5.179799	-3.620939	1.088264
30	6	0	1.170140	-4.557353	3.264344
31	6	0	0.571195	-2.412489	4.177385
32	6	0	0.441414	-3.799143	4.175829
33	6	0	-1.101441	4.617491	-1.294773
34	6	0	4.817322	-4.280925	-1.594169
35	6	0	4.017150	-3.303407	-1.005625
36	6	0	5.792718	-4.926483	-0.843343
37	6	0	5.975015	-4.595464	0.499467
38	1	0	1.437316	1.314848	2.537051
39	1	0	2.782409	2.241000	4.689943
40	1	0	4.914130	3.640221	3.798471
41	1	0	4.890840	3.567776	1.099276
42	1	0	5.493912	0.153116	0.276157
43	1	0	7.006173	1.339856	2.169867
44	1	0	6.004484	0.659834	4.584767
45	1	0	3.882610	-0.962769	4.180597
46	1	0	4.525235	0.578842	-1.963944
47	1	0	6.458503	1.430250	-3.272459
48	1	0	6.848871	3.875811	-3.462235
49	1	0	5.306868	5.468555	-2.341668
50	1	0	3.398203	4.617109	-1.009559
51	1	0	1.214107	4.136286	1.146127
52	1	0	-0.755274	5.539908	0.621288
53	1	0	-1.953795	5.254566	-1.534110
54	1	0	-1.168877	3.530998	-3.164769
55	1	0	0.756797	2.074755	-2.609402
56	1	0	2.598656	-4.541301	1.655031
57	1	0	1.071556	-5.641924	3.253883
58	1	0	-0.231050	-4.286568	4.879997
59	1	0	-0.006653	-1.807923	4.874966
60	1	0	1.491559	-0.703369	3.256532
61	1	0	3.263387	-2.773557	-1.594958
62	1	0	4.677741	-4.526031	-2.645818
63	1	0	6.421146	-5.687492	-1.304153
64	1	0	6.743937	-5.097145	1.085539
65	1	0	5.323345	-3.358788	2.138148
66	6	0	-3.139399	1.429981	1.696416
67	6	0	-3.588281	0.101766	1.701714
68	6	0	-2.732963	-0.953578	1.434584

69	6	0	-1.387228	-0.722732	1.105081
70	6	0	-0.929130	0.607156	1.124225
71	6	0	-1.783656	1.659749	1.410428
72	1	0	-4.646093	-0.115161	1.834242
73	1	0	-3.161354	-1.950337	1.328154
74	1	0	0.115037	0.795152	0.861940
75	1	0	-1.394806	2.678702	1.353043
76	46	0	1.810032	-0.507144	-0.568691
77	6	0	-4.087323	2.547561	1.869240
78	6	0	-5.419810	2.409670	1.440085
79	6	0	-3.681541	3.780562	2.397907
80	6	0	-6.306004	3.476966	1.545936
81	1	0	-5.734631	1.470469	0.967835
82	6	0	-4.573635	4.841442	2.503632
83	1	0	-2.658225	3.899509	2.754663
84	6	0	-5.891076	4.695777	2.078245
85	1	0	-7.332172	3.357530	1.197872
86	1	0	-4.238050	5.787063	2.927772
87	1	0	-6.590218	5.526559	2.161680
88	6	0	0.285118	-2.068453	-0.412819
89	6	0	-0.561334	-1.850373	0.725779
90	6	0	-0.649467	-1.942366	-1.493336
91	1	0	0.764245	-3.049913	-0.362463
92	1	0	-0.709873	-2.738059	1.350018
93	6	0	-1.081035	-3.192071	-2.249390
94	6	0	0.105162	-4.096138	-2.600920
95	1	0	-0.265316	-4.949376	-3.185255
96	1	0	0.848159	-3.555860	-3.205082
97	6	0	-1.363614	-0.697138	-1.815504
98	1	0	-1.205926	-0.500095	-2.886297
99	1	0	-0.975640	0.164215	-1.267533
100	1	0	-2.463421	-0.851160	-1.685476
101	1	0	0.609987	-4.509728	-1.717065
102	6	0	-1.850556	-2.857793	-3.532774
103	1	0	-1.232773	-2.280295	-4.235572
104	1	0	-2.121840	-3.800409	-4.027947
105	1	0	-2.781895	-2.317334	-3.309833
106	6	0	-2.060025	-3.938511	-1.314452
107	1	0	-1.554843	-4.273622	-0.397185
108	1	0	-2.939786	-3.325001	-1.046791
109	1	0	-2.419778	-4.832784	-1.845567
110	53	0	1.943602	-0.611107	-3.480273
111	6	0	-5.001520	-1.211613	-0.864691
112	8	0	-5.809652	-0.269332	-0.437461
113	8	0	-4.339171	-1.024457	-1.951828
114	8	0	-4.875263	-2.296019	-0.182464
115	55	0	-3.914706	1.816073	-1.655297
116	55	0	-7.503969	-2.191453	0.905250

Zero-point correction= 0.907942 (Hartree/Particle)
Thermal correction to Energy= 0.971220
Thermal correction to Enthalpy= 0.972165
Thermal correction to Gibbs Free Energy= 0.804697
Sum of electronic and zero-point Energies= -3333.596025
Sum of electronic and thermal Energies= -3333.532746
Sum of electronic and thermal Enthalpies= -3333.531802
Sum of electronic and thermal Free Energies= -3333.699270
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3337.5604321

INT7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-3.207532	-1.751880	-1.187219
2	15	0	-1.925252	1.121641	0.134929
3	15	0	-0.113940	-2.190789	0.141084

4	6	0	-1.471089	3.851235	0.381902
5	6	0	-2.997214	1.133403	1.624398
6	6	0	-3.352907	0.401974	3.905841
7	6	0	-2.049986	2.864793	-0.425484
8	6	0	-4.562248	1.088933	3.939102
9	6	0	-4.204459	1.837924	1.674617
10	6	0	-2.571179	0.431284	2.754243
11	6	0	-4.984648	1.811571	2.825020
12	6	0	-2.623103	3.233917	-1.644662
13	6	0	-2.609481	4.565891	-2.053005
14	6	0	-1.791270	-2.824841	-0.210206
15	6	0	-2.325374	-3.588592	-1.297198
16	6	0	0.963255	-3.001511	-1.100111
17	6	0	-4.572266	-0.792505	-2.354017
18	6	0	-2.887164	-2.509565	0.660499
19	6	0	-3.729551	-3.722740	-1.102916
20	6	0	-1.463479	5.179501	-0.025553
21	6	0	-4.074822	-3.061656	0.109133
22	6	0	0.645187	-2.966705	-2.464295
23	6	0	-2.919898	0.250726	-1.113677
24	6	0	2.206110	-3.513676	-0.712755
25	6	0	-3.340183	-0.934928	-3.056471
26	6	0	-4.318771	-0.058117	-1.159890
27	6	0	-2.323236	-0.293639	-2.297591
28	6	0	0.252316	-3.120797	1.681996
29	6	0	0.094413	-4.509025	1.764314
30	6	0	3.093129	-4.010034	-1.662957
31	6	0	1.526858	-3.479834	-3.409032
32	6	0	2.753863	-4.004618	-3.011820
33	6	0	-2.028711	5.539325	-1.247271
34	6	0	0.937611	-3.080053	4.002892
35	6	0	0.670844	-2.414281	2.808581
36	6	0	0.780483	-4.458887	4.075128
37	6	0	0.358363	-5.173756	2.954295
38	1	0	-1.262862	-0.237827	-2.538423
39	1	0	-3.192842	-1.485580	-3.980362
40	1	0	-5.525329	-1.222948	-2.645330
41	1	0	-5.039286	0.163083	-0.377535
42	1	0	-2.824199	-1.906379	1.562487
43	1	0	-5.075264	-2.943919	0.512746
44	1	0	-4.421175	-4.200433	-1.789634
45	1	0	-1.766468	-3.965721	-2.146878
46	1	0	-1.611001	-0.089531	2.719716
47	1	0	-3.012874	-0.151139	4.779955
48	1	0	-5.173578	1.073203	4.840134
49	1	0	-5.922745	2.363832	2.856823
50	1	0	-4.522652	2.424307	0.811049
51	1	0	-3.077132	2.478153	-2.285866
52	1	0	-3.057412	4.841591	-3.007135
53	1	0	-2.016014	6.579388	-1.569762
54	1	0	-1.000604	5.931248	0.612445
55	1	0	-1.004843	3.575152	1.330383
56	1	0	2.492220	-3.518167	0.339979
57	1	0	4.056636	-4.401798	-1.339330
58	1	0	3.446105	-4.400785	-3.753035
59	1	0	1.256191	-3.461308	-4.464422
60	1	0	-0.293502	-2.520898	-2.796804
61	1	0	0.792797	-1.331563	2.732625
62	1	0	1.271144	-2.518334	4.874696
63	1	0	0.987752	-4.983111	5.006956
64	1	0	0.235092	-6.254168	3.012047
65	1	0	-0.231644	-5.069426	0.886653
66	6	0	1.315826	4.950684	3.263673
67	6	0	1.109793	3.638307	3.687926
68	6	0	1.280552	2.583043	2.802954
69	6	0	1.660849	2.814859	1.472062
70	6	0	1.856512	4.136630	1.056256

71	6	0	1.694102	5.191911	1.946095
72	1	0	0.810714	3.437421	4.715850
73	1	0	1.090821	1.557086	3.125170
74	1	0	2.135674	4.332151	0.021046
75	1	0	1.858815	6.213124	1.603620
76	46	0	0.266653	0.161549	0.299289
77	6	0	1.783387	1.709280	0.537423
78	6	0	2.399299	0.489217	0.349316
79	6	0	2.482711	1.500506	-0.785654
80	1	0	1.181621	5.778122	3.958375
81	6	0	3.845778	2.122091	-0.892784
82	8	0	4.531004	2.453092	0.047671
83	8	0	4.253079	2.236503	-2.172040
84	6	0	5.564126	2.759650	-2.330665
85	1	0	5.743944	2.801250	-3.407199
86	1	0	5.642492	3.760076	-1.890419
87	1	0	6.300197	2.109709	-1.843452
88	6	0	1.701796	1.351852	-2.059305
89	6	0	1.846199	0.226183	-2.873259
90	6	0	0.830625	2.366033	-2.465808
91	6	0	1.147751	0.122995	-4.072126
92	1	0	2.507385	-0.583016	-2.554851
93	6	0	0.126626	2.263661	-3.661332
94	1	0	0.693308	3.239033	-1.824610
95	6	0	0.288293	1.143715	-4.472835
96	1	0	1.278704	-0.760220	-4.697115
97	1	0	-0.554455	3.062686	-3.953411
98	1	0	-0.257178	1.064300	-5.412517
99	6	0	3.402127	-0.401006	0.912873
100	6	0	3.485599	-0.625240	2.293808
101	6	0	4.299612	-1.071158	0.071903
102	6	0	4.418751	-1.511620	2.812278
103	1	0	2.815034	-0.080442	2.959493
104	6	0	5.245033	-1.945658	0.594184
105	1	0	4.246654	-0.895835	-1.004167
106	6	0	5.300885	-2.180408	1.964857
107	1	0	4.466600	-1.675754	3.888291
108	1	0	5.938764	-2.451943	-0.076601
109	1	0	6.033685	-2.874043	2.374113

Zero-point correction= 0.877350 (Hartree/Particle)
Thermal correction to Energy= 0.930258
Thermal correction to Enthalpy= 0.931202
Thermal correction to Gibbs Free Energy= 0.789957
Sum of electronic and zero-point Energies= -3018.179805
Sum of electronic and thermal Energies= -3018.126897
Sum of electronic and thermal Enthalpies= -3018.125953
Sum of electronic and thermal Free Energies= -3018.267197
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.3485601

Cs_2CO_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.217357	-0.000795
2	8	0	-0.000001	0.112214	-0.001171
3	8	0	-1.118309	-1.842261	-0.000076
4	8	0	1.118313	-1.842257	-0.000138
5	55	0	-2.854397	0.326205	0.000137
6	55	0	2.854397	0.326205	0.000151

Zero-point correction= 0.016375 (Hartree/Particle)
Thermal correction to Energy= 0.023451
Thermal correction to Enthalpy= 0.024395
Thermal correction to Gibbs Free Energy= -0.020998
Sum of electronic and zero-point Energies= -303.402709

Sum of electronic and thermal Energies= -303.395632
Sum of electronic and thermal Enthalpies= -303.394688
Sum of electronic and thermal Free Energies= -303.440081
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -304.1833035

$Cs_2HCO_3^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.094749	1.182734	0.000056
2	8	0	-0.061932	-0.060551	0.000151
3	8	0	-1.107151	1.905966	-0.000230
4	8	0	1.133017	1.857826	0.000243
5	1	0	-0.830445	2.835529	-0.000319
6	55	0	-3.031319	-0.365283	0.000001
7	55	0	3.041328	-0.353951	-0.000025

Zero-point correction= 0.028937 (Hartree/Particle)
Thermal correction to Energy= 0.036653
Thermal correction to Enthalpy= 0.037597
Thermal correction to Gibbs Free Energy= -0.009146
Sum of electronic and zero-point Energies= -303.901216
Sum of electronic and thermal Energies= -303.893499
Sum of electronic and thermal Enthalpies= -303.892555
Sum of electronic and thermal Free Energies= -303.939299
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -304.6942572

I^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	0.000000	0.000000

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.016848
Sum of electronic and zero-point Energies= -11.435014
Sum of electronic and thermal Energies= -11.433598
Sum of electronic and thermal Enthalpies= -11.432654
Sum of electronic and thermal Free Energies= -11.451862
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -11.5728444

TS4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.194775	0.783179	-3.033663
2	15	0	-0.939513	2.046067	0.115450
3	15	0	-0.920222	-1.738832	-0.749997
4	6	0	-0.222200	3.885532	2.080486
5	6	0	-2.673148	2.670210	0.165325
6	6	0	-5.024307	2.199444	0.527741
7	6	0	-0.024598	3.516974	0.743354
8	6	0	-5.337739	3.526126	0.249066
9	6	0	-2.999414	4.004107	-0.101118
10	6	0	-3.698170	1.777977	0.490846
11	6	0	-4.323418	4.428515	-0.062315
12	6	0	0.958996	4.177465	0.002330
13	6	0	1.734224	5.175395	0.589943
14	6	0	-1.648109	-1.054223	-2.286567
15	6	0	-1.184932	-1.157437	-3.639611
16	6	0	0.675796	-2.388394	-1.402852
17	6	0	-0.561695	2.491826	-3.950054

18	6	0	-2.806312	-0.208339	-2.307331
19	6	0	-2.045371	-0.386681	-4.471210
20	6	0	0.541418	4.889126	2.661063
21	6	0	-3.049880	0.197078	-3.648573
22	6	0	1.867444	-1.782633	-1.000932
23	6	0	-0.554859	2.130651	-1.663342
24	6	0	0.730221	-3.445075	-2.320850
25	6	0	0.550200	1.655113	-3.643292
26	6	0	-1.238644	2.793254	-2.734317
27	6	0	0.558373	1.432177	-2.239346
28	6	0	-1.898070	-3.293227	-0.561546
29	6	0	-3.255941	-3.341179	-0.890714
30	6	0	1.949130	-3.870011	-2.835884
31	6	0	3.090204	-2.202788	-1.521601
32	6	0	3.130611	-3.244373	-2.441440
33	6	0	1.529870	5.532365	1.917923
34	6	0	-2.091795	-5.517934	0.385527
35	6	0	-1.327808	-4.396677	0.084157
36	6	0	-3.443923	-5.554044	0.054294
37	6	0	-4.021900	-4.462484	-0.585732
38	1	0	1.252464	0.797875	-1.693068
39	1	0	1.232774	1.211316	-4.360814
40	1	0	-0.875425	2.794382	-4.944421
41	1	0	-2.158593	3.362265	-2.637757
42	1	0	-3.367905	0.114524	-1.435357
43	1	0	-3.826021	0.882404	-3.973694
44	1	0	-1.918094	-0.220929	-5.536472
45	1	0	-0.287850	-1.677619	-3.960250
46	1	0	-3.439137	0.741463	0.724486
47	1	0	-5.811928	1.492647	0.784713
48	1	0	-6.373353	3.861054	0.283448
49	1	0	-4.564936	5.469838	-0.271030
50	1	0	-2.206494	4.716841	-0.333097
51	1	0	1.129119	3.906665	-1.039926
52	1	0	2.500729	5.678270	0.001557
53	1	0	2.139619	6.309263	2.376209
54	1	0	0.373805	5.163902	3.701388
55	1	0	-0.979528	3.368961	2.673736
56	1	0	-0.191257	-3.940256	-2.630030
57	1	0	1.978419	-4.694164	-3.547488
58	1	0	4.085205	-3.577419	-2.846273
59	1	0	4.010942	-1.717915	-1.195994
60	1	0	1.833398	-0.979543	-0.261654
61	1	0	-0.270150	-4.380654	0.350878
62	1	0	-1.627345	-6.368321	0.883549
63	1	0	-4.043690	-6.431010	0.292619
64	1	0	-5.077091	-4.483106	-0.855184
65	1	0	-3.723254	-2.494982	-1.394797
66	6	0	4.427894	0.010800	1.041262
67	6	0	3.600218	1.141127	1.029882
68	6	0	2.358710	1.128255	1.647908
69	6	0	1.891893	-0.024054	2.299053
70	6	0	2.735805	-1.144635	2.344126
71	6	0	3.977270	-1.124700	1.726865
72	1	0	3.944608	2.057073	0.547943
73	1	0	1.744704	2.026302	1.652612
74	1	0	2.388084	-2.046685	2.846802
75	1	0	4.595025	-2.023428	1.736290
76	46	0	-0.619615	-0.183292	1.119544
77	6	0	5.721697	0.007747	0.332643
78	6	0	5.855065	0.647701	-0.906491
79	6	0	6.840659	-0.642962	0.866460
80	6	0	7.067610	0.643595	-1.585265
81	1	0	4.982979	1.129734	-1.350502
82	6	0	8.053226	-0.647806	0.188034
83	1	0	6.761074	-1.126130	1.840196
84	6	0	8.172629	-0.003387	-1.040018

85	1	0	7.147253	1.141301	-2.550695
86	1	0	8.913990	-1.151265	0.625883
87	1	0	9.123169	-0.006974	-1.570891
88	6	0	0.126160	-0.292331	4.154370
89	6	0	0.575101	-0.077198	2.942980
90	6	0	-1.129474	-0.640624	3.474324
91	1	0	0.513757	-0.367566	5.170322
92	6	0	-1.574884	-2.109975	3.602663
93	6	0	-2.222598	0.402023	3.581606
94	1	0	-3.038929	0.278384	2.860964
95	1	0	-2.665257	0.359375	4.594197
96	1	0	-1.804774	1.407253	3.455953
97	6	0	-1.918971	-2.363959	5.081240
98	1	0	-2.742551	-1.725226	5.428660
99	1	0	-2.234630	-3.408488	5.217296
100	1	0	-1.053646	-2.192530	5.736964
101	6	0	-0.452394	-3.071690	3.219548
102	1	0	-0.802404	-4.111879	3.291152
103	1	0	-0.114864	-2.885562	2.189277
104	1	0	0.413937	-2.962262	3.887015
105	6	0	-2.819783	-2.408810	2.767248
106	1	0	-3.701507	-1.875342	3.149169
107	1	0	-2.671709	-2.119435	1.717792
108	1	0	-3.050789	-3.483856	2.791536

Zero-point correction= 0.872796 (Hartree/Particle)
Thermal correction to Energy= 0.926510
Thermal correction to Enthalpy= 0.927455
Thermal correction to Gibbs Free Energy= 0.783079
Sum of electronic and zero-point Energies= -3018.136549
Sum of electronic and thermal Energies= -3018.082834
Sum of electronic and thermal Enthalpies= -3018.081890
Sum of electronic and thermal Free Energies= -3018.226265
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.2990583

TS4c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	4.201823	0.985445	-1.275744
2	15	0	1.322923	1.948364	0.267530
3	15	0	2.275596	-1.658299	-0.304487
4	6	0	-0.170168	2.915314	2.382551
5	6	0	0.585479	2.996506	-1.057781
6	6	0	-0.473480	3.100478	-3.238512
7	6	0	1.075374	3.004871	1.750575
8	6	0	-0.495005	4.489349	-3.166819
9	6	0	0.549346	4.393000	-0.993150
10	6	0	0.059249	2.360117	-2.186702
11	6	0	0.014218	5.133754	-2.041570
12	6	0	2.036807	3.880109	2.262913
13	6	0	1.754534	4.652986	3.386247
14	6	0	3.434027	-0.885322	-1.486785
15	6	0	4.866817	-0.914900	-1.522799
16	6	0	3.399481	-2.128282	1.073671
17	6	0	5.130465	2.778206	-1.012731
18	6	0	3.007946	-0.032395	-2.558559
19	6	0	5.307473	-0.096444	-2.600561
20	6	0	-0.454252	3.695360	3.496893
21	6	0	4.158773	0.447484	-3.242430
22	6	0	3.211110	-1.508539	2.312426
23	6	0	3.098242	2.193809	-0.069546
24	6	0	4.430076	-3.065613	0.937901
25	6	0	5.392866	1.916704	0.090977
26	6	0	3.721394	2.957534	-1.108598
27	6	0	4.146102	1.550448	0.669537

28	6	0	1.919997	-3.271812	-1.116631
29	6	0	1.575171	-3.286781	-2.473190
30	6	0	5.262346	-3.360717	2.012254
31	6	0	4.045235	-1.800030	3.388356
32	6	0	5.072744	-2.725670	3.237666
33	6	0	0.510266	4.563857	4.002550
34	6	0	1.311931	-5.615410	-0.982189
35	6	0	1.775668	-4.450889	-0.376920
36	6	0	0.979600	-5.619611	-2.332871
37	6	0	1.113851	-4.450110	-3.076717
38	1	0	4.006670	0.858243	1.495986
39	1	0	6.366663	1.548441	0.397733
40	1	0	5.870250	3.179595	-1.698348
41	1	0	3.195858	3.520128	-1.874614
42	1	0	1.977943	0.243162	-2.766727
43	1	0	4.161084	1.152772	-4.067083
44	1	0	6.340883	0.127956	-2.846054
45	1	0	5.505082	-1.416465	-0.801943
46	1	0	0.059071	1.268343	-2.226353
47	1	0	-0.881406	2.590330	-4.109834
48	1	0	-0.916722	5.071818	-3.984515
49	1	0	-0.006945	6.220868	-1.979620
50	1	0	0.947464	4.903905	-0.115436
51	1	0	3.009420	3.964081	1.776626
52	1	0	2.510108	5.332339	3.778819
53	1	0	0.291441	5.169515	4.880731
54	1	0	-1.428255	3.618387	3.977967
55	1	0	-0.915432	2.220786	1.987381
56	1	0	4.571133	-3.577173	-0.015140
57	1	0	6.059237	-4.093722	1.894743
58	1	0	5.722666	-2.961331	4.079001
59	1	0	3.885436	-1.310219	4.347589
60	1	0	2.394637	-0.790064	2.426152
61	1	0	2.022458	-4.461066	0.684949
62	1	0	1.210779	-6.524986	-0.391621
63	1	0	0.614424	-6.530461	-2.804489
64	1	0	0.855132	-4.443067	-4.134629
65	1	0	1.662149	-2.374789	-3.065051
66	46	0	0.368913	-0.295592	0.239441
67	6	0	-1.736563	0.127632	0.055585
68	6	0	-2.823903	-0.535547	0.399653
69	6	0	-1.761931	-1.541247	0.613445
70	1	0	-1.622320	0.949187	-0.667646
71	6	0	-1.509627	-1.976594	2.084538
72	6	0	-2.790693	-2.656660	2.594347
73	1	0	-2.648000	-2.999131	3.629713
74	1	0	-3.643865	-1.965144	2.583339
75	6	0	-1.731550	-2.652600	-0.424929
76	1	0	-0.780673	-3.196933	-0.456845
77	1	0	-1.906336	-2.234539	-1.424389
78	1	0	-2.527498	-3.394225	-0.236779
79	1	0	-3.056758	-3.539840	1.995455
80	6	0	-0.368625	-2.984380	2.216572
81	1	0	-0.202346	-3.225582	3.276814
82	1	0	-0.587962	-3.926389	1.694958
83	1	0	0.569795	-2.579951	1.812408
84	6	0	-1.230354	-0.786438	2.999544
85	1	0	-0.305753	-0.260695	2.709678
86	1	0	-2.050218	-0.056205	2.969763
87	1	0	-1.121470	-1.131111	4.038259
88	6	0	-4.254987	-0.433768	0.223529
89	6	0	-4.834661	0.827488	0.016385
90	6	0	-5.099505	-1.552623	0.233369
91	6	0	-6.198162	0.961822	-0.177795
92	1	0	-4.193242	1.709242	0.028970
93	6	0	-6.464124	-1.414157	0.028346
94	1	0	-4.671253	-2.542315	0.388188

95	6	0	-7.044195	-0.156601	-0.178184
96	1	0	-6.628598	1.955477	-0.302603
97	1	0	-7.093663	-2.303607	0.004064
98	6	0	-8.496889	-0.010640	-0.386788
99	6	0	-9.003671	0.954291	-1.266523
100	6	0	-9.409334	-0.831807	0.287764
101	6	0	-10.371664	1.094471	-1.463321
102	1	0	-8.310805	1.583640	-1.824821
103	6	0	-10.777487	-0.694227	0.090046
104	1	0	-9.037429	-1.568202	0.999893
105	6	0	-11.265801	0.270289	-0.786460
106	1	0	-10.742089	1.846122	-2.159079
107	1	0	-11.467628	-1.338444	0.633040
108	1	0	-12.338032	0.379628	-0.940669

Zero-point correction= 0.874557 (Hartree/Particle)
Thermal correction to Energy= 0.927815
Thermal correction to Enthalpy= 0.928759
Thermal correction to Gibbs Free Energy= 0.784830
Sum of electronic and zero-point Energies= -3018.132326
Sum of electronic and thermal Energies= -3018.079068
Sum of electronic and thermal Enthalpies= -3018.078124
Sum of electronic and thermal Free Energies= -3018.222053
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.2979675

INT8c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.213693	-2.707172	-1.307720
2	15	0	-0.600868	-0.937798	-0.717291
3	15	0	2.764577	0.021637	0.615652
4	6	0	-3.332056	-0.766927	-1.579538
5	6	0	-1.330923	-2.212169	0.384042
6	6	0	-1.664940	-3.003472	2.653251
7	6	0	-1.993124	-0.457531	-1.824199
8	6	0	-2.423315	-4.067745	2.176283
9	6	0	-2.094056	-3.289099	-0.082844
10	6	0	-1.125283	-2.082439	1.760164
11	6	0	-2.636560	-4.210012	0.807361
12	6	0	-1.678715	0.346146	-2.926318
13	6	0	-2.676580	0.807987	-3.774692
14	6	0	3.072221	-1.748802	0.245173
15	6	0	4.077719	-2.374135	-0.562643
16	6	0	4.352914	0.779605	0.089248
17	6	0	1.570607	-3.552223	-3.047805
18	6	0	2.204612	-2.789707	0.713505
19	6	0	3.810225	-3.771472	-0.608474
20	6	0	-4.332636	-0.300721	-2.428115
21	6	0	2.656205	-4.028186	0.183184
22	6	0	4.732100	0.680142	-1.256850
23	6	0	0.447803	-1.904358	-1.863196
24	6	0	5.124974	1.566942	0.946435
25	6	0	2.215778	-2.310580	-3.310968
26	6	0	0.482382	-3.307609	-2.162582
27	6	0	1.527472	-1.297970	-2.587806
28	6	0	2.889832	-0.056157	2.450421
29	6	0	3.956368	-0.704562	3.084559
30	6	0	6.253361	2.231060	0.472074
31	6	0	5.866729	1.330275	-1.725061
32	6	0	6.629490	2.112004	-0.860792
33	6	0	-4.008400	0.482923	-3.528831
34	6	0	1.892183	0.366328	4.616346
35	6	0	1.856526	0.472049	3.227723
36	6	0	2.961057	-0.269905	5.236777
37	6	0	3.993766	-0.806442	4.469252

38	1	0	1.798338	-0.245110	-2.531948
39	1	0	3.109032	-2.168116	-3.911145
40	1	0	1.891466	-4.525140	-3.406142
41	1	0	-0.161727	-4.066304	-1.729995
42	1	0	1.322664	-2.650503	1.331386
43	1	0	2.171291	-4.989479	0.319116
44	1	0	4.365374	-4.504123	-1.185524
45	1	0	4.880862	-1.866895	-1.085917
46	1	0	-0.529092	-1.244900	2.129409
47	1	0	-1.494387	-2.886343	3.722058
48	1	0	-2.851376	-4.787521	2.872192
49	1	0	-3.232517	-5.040191	0.431281
50	1	0	-2.285779	-3.396063	-1.150938
51	1	0	-0.642588	0.627459	-3.118185
52	1	0	-2.412012	1.429346	-4.629133
53	1	0	-4.791906	0.849960	-4.190008
54	1	0	-5.373044	-0.539605	-2.208691
55	1	0	-3.609313	-1.355396	-0.705807
56	1	0	4.843755	1.666442	1.994504
57	1	0	6.841987	2.844656	1.152268
58	1	0	7.512421	2.631537	-1.229012
59	1	0	6.147610	1.240403	-2.773240
60	1	0	4.119160	0.103083	-1.952590
61	1	0	1.016828	0.963840	2.728163
62	1	0	1.081967	0.784595	5.211427
63	1	0	2.991295	-0.353139	6.322111
64	1	0	4.828358	-1.311050	4.953740
65	1	0	4.761401	-1.133946	2.486157
66	6	0	-5.169053	1.154706	0.768802
67	6	0	-4.179401	0.539787	1.547263
68	6	0	-2.852536	0.922422	1.443039
69	6	0	-2.451162	1.933284	0.557784
70	6	0	-3.446954	2.570772	-0.196954
71	6	0	-4.776657	2.189904	-0.089327
72	1	0	-4.456207	-0.249365	2.248372
73	1	0	-2.092856	0.429692	2.050324
74	1	0	-3.150973	3.344894	-0.906194
75	1	0	-5.523623	2.664295	-0.727239
76	46	0	0.592248	1.075719	0.092542
77	6	0	-6.568221	0.692327	0.816059
78	6	0	-6.863947	-0.670600	0.952417
79	6	0	-7.637047	1.591115	0.710763
80	6	0	-8.178753	-1.118565	0.987030
81	1	0	-6.044859	-1.388967	1.008623
82	6	0	-8.952254	1.144142	0.742673
83	1	0	-7.427753	2.657618	0.628529
84	6	0	-9.230102	-0.212736	0.881789
85	1	0	-8.383497	-2.183743	1.087489
86	1	0	-9.767034	1.863073	0.667079
87	1	0	-10.261044	-0.561993	0.907194
88	6	0	-0.440720	3.460085	0.585353
89	6	0	-1.052454	2.292438	0.403495
90	6	0	1.006574	3.233219	0.275710
91	1	0	-0.877794	4.410510	0.942222
92	6	0	1.438067	3.885599	-1.067235
93	6	0	1.907064	3.573108	1.445442
94	1	0	2.930295	3.186121	1.335475
95	1	0	1.987579	4.669151	1.582180
96	1	0	1.496980	3.173850	2.381716
97	6	0	1.123058	5.390588	-1.016589
98	1	0	1.625315	5.891241	-0.176741
99	1	0	1.466672	5.878759	-1.940750
100	1	0	0.044099	5.575796	-0.926596
101	6	0	0.685594	3.299164	-2.261875
102	1	0	0.964840	3.833947	-3.183170
103	1	0	0.935972	2.234222	-2.392555
104	1	0	-0.403543	3.367664	-2.137591

105	6	0	2.931625	3.721605	-1.334087
106	1	0	3.556030	4.203432	-0.569053
107	1	0	3.209227	2.661320	-1.373569
108	1	0	3.194309	4.173175	-2.302709

Zero-point correction= 0.877055 (Hartree/Particle)
Thermal correction to Energy= 0.929890
Thermal correction to Enthalpy= 0.930834
Thermal correction to Gibbs Free Energy= 0.791368
Sum of electronic and zero-point Energies= -3018.158121
Sum of electronic and thermal Energies= -3018.105286
Sum of electronic and thermal Enthalpies= -3018.104342
Sum of electronic and thermal Free Energies= -3018.243809
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.3314067

TS5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.913376	-2.301386	2.203876
2	15	0	0.575441	-1.303492	-0.649986
3	15	0	-2.544805	0.301117	0.507551
4	6	0	2.474735	-1.487385	-2.688055
5	6	0	-0.330032	-2.556597	-1.650358
6	6	0	-2.269160	-3.123907	-2.991762
7	6	0	2.272366	-1.540855	-1.303978
8	6	0	-1.795964	-4.423886	-3.133715
9	6	0	0.155538	-3.856654	-1.832963
10	6	0	-1.533268	-2.195537	-2.259432
11	6	0	-0.577732	-4.786109	-2.561463
12	6	0	3.362773	-1.767131	-0.463640
13	6	0	4.633575	-1.960067	-0.997464
14	6	0	-2.493660	-1.181160	1.593748
15	6	0	-2.456568	-1.250095	3.024379
16	6	0	-2.776764	1.604801	1.782882
17	6	0	0.628735	-3.480186	2.831717
18	6	0	-2.602206	-2.526965	1.109244
19	6	0	-2.526141	-2.617815	3.409154
20	6	0	3.742807	-1.686489	-3.219017
21	6	0	-2.623376	-3.404923	2.227154
22	6	0	-1.670610	1.898352	2.590804
23	6	0	0.685095	-2.067678	0.997464
24	6	0	-3.945660	2.349214	1.942949
25	6	0	0.802541	-2.150767	3.310852
26	6	0	0.563075	-3.434721	1.411110
27	6	0	0.844536	-1.281950	2.187738
28	6	0	-4.229315	0.029824	-0.188157
29	6	0	-5.294500	-0.398008	0.614519
30	6	0	-4.007194	3.365144	2.894683
31	6	0	-1.738253	2.899776	3.550495
32	6	0	-2.909006	3.640341	3.700820
33	6	0	4.824175	-1.927895	-2.374648
34	6	0	-5.688039	-0.058424	-2.120878
35	6	0	-4.439106	0.191167	-1.557981
36	6	0	-6.741188	-0.470751	-1.312984
37	6	0	-6.543262	-0.639237	0.056478
38	1	0	0.952300	-0.200565	2.210804
39	1	0	0.842014	-1.848382	4.352122
40	1	0	0.500618	-4.366701	3.444859
41	1	0	0.365642	-4.278586	0.757996
42	1	0	-2.629041	-2.821214	0.062917
43	1	0	-2.641845	-4.489106	2.180527
44	1	0	-2.459207	-2.995820	4.424410
45	1	0	-2.349971	-0.405598	3.697149
46	1	0	-1.889077	-1.169101	-2.149306
47	1	0	-3.211144	-2.825691	-3.450535

48	1	0	-2.367351	-5.154276	-3.704486
49	1	0	-0.191914	-5.795901	-2.693632
50	1	0	1.125482	-4.134433	-1.418489
51	1	0	3.225138	-1.783887	0.617902
52	1	0	5.477911	-2.126514	-0.328926
53	1	0	5.818732	-2.082497	-2.792358
54	1	0	3.888583	-1.648422	-4.297635
55	1	0	1.632075	-1.284876	-3.350845
56	1	0	-4.814374	2.144102	1.318225
57	1	0	-4.923339	3.943499	3.003493
58	1	0	-2.961710	4.434306	4.443771
59	1	0	-0.870034	3.116022	4.170827
60	1	0	-0.743872	1.338856	2.451733
61	1	0	-3.611074	0.522487	-2.184904
62	1	0	-5.835791	0.072238	-3.191686
63	1	0	-7.719756	-0.664765	-1.749467
64	1	0	-7.365922	-0.966510	0.690348
65	1	0	-5.139534	-0.547328	1.684026
66	6	0	5.002679	1.418848	0.096460
67	6	0	4.857654	1.490089	-1.295807
68	6	0	3.610688	1.597357	-1.889194
69	6	0	2.440799	1.665927	-1.117750
70	6	0	2.594155	1.642928	0.280923
71	6	0	3.841566	1.508313	0.873525
72	1	0	5.746704	1.454868	-1.926631
73	1	0	3.520507	1.608915	-2.975568
74	1	0	1.695781	1.719148	0.898951
75	1	0	3.916523	1.444735	1.960422
76	46	0	-0.587113	0.829016	-0.852700
77	6	0	6.329298	1.228325	0.710992
78	6	0	7.300152	0.433892	0.085174
79	6	0	6.661301	1.827024	1.933455
80	6	0	8.554138	0.250103	0.654328
81	1	0	7.051341	-0.064556	-0.852717
82	6	0	7.913454	1.640514	2.506077
83	1	0	5.932979	2.472444	2.424398
84	6	0	8.867788	0.852353	1.869300
85	1	0	9.289256	-0.375556	0.149479
86	1	0	8.149811	2.124800	3.452873
87	1	0	9.850048	0.709337	2.317083
88	6	0	0.422082	2.905863	-1.741945
89	6	0	1.125166	1.734508	-1.741610
90	6	0	-1.002474	2.770201	-1.965773
91	1	0	0.851930	3.862790	-1.395102
92	6	0	-1.873352	3.943676	-1.486216
93	6	0	-1.424698	2.154025	-3.288512
94	1	0	-2.383385	1.621134	-3.242211
95	1	0	-1.545747	2.943823	-4.053333
96	1	0	-0.665132	1.453984	-3.649634
97	6	0	-1.665263	5.136102	-2.437362
98	1	0	-2.014153	4.920127	-3.456067
99	1	0	-2.228791	6.008173	-2.074155
100	1	0	-0.606386	5.423440	-2.495777
101	6	0	-1.486970	4.402142	-0.077912
102	1	0	-2.187598	5.174107	0.274461
103	1	0	-1.512347	3.571115	0.636530
104	1	0	-0.479004	4.835180	-0.045776
105	6	0	-3.358315	3.585762	-1.487914
106	1	0	-3.730485	3.354136	-2.495746
107	1	0	-3.560233	2.717222	-0.847001
108	1	0	-3.952487	4.427999	-1.102992

Zero-point correction= 0.874834 (Hartree/Particle)
Thermal correction to Energy= 0.927704
Thermal correction to Enthalpy= 0.928649
Thermal correction to Gibbs Free Energy= 0.788678
Sum of electronic and zero-point Energies= -3018.152779

Sum of electronic and thermal Energies= -3018.099909
Sum of electronic and thermal Enthalpies= -3018.098964
Sum of electronic and thermal Free Energies= -3018.238935
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.3256137

INT9c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.843356	-2.220134	2.266347
2	15	0	0.578665	-1.324172	-0.674390
3	15	0	-2.526152	0.303586	0.517145
4	6	0	2.465872	-1.583440	-2.717100
5	6	0	-0.340529	-2.621346	-1.603181
6	6	0	-2.327683	-3.272878	-2.830999
7	6	0	2.270609	-1.585732	-1.330972
8	6	0	-1.832114	-4.566406	-2.955256
9	6	0	0.164335	-3.916571	-1.766434
10	6	0	-1.579532	-2.305787	-2.164346
11	6	0	-0.580611	-4.884209	-2.430436
12	6	0	3.366498	-1.776044	-0.488557
13	6	0	4.635913	-1.981238	-1.020856
14	6	0	-2.447123	-1.133555	1.660414
15	6	0	-2.360383	-1.135664	3.090788
16	6	0	-2.756570	1.652298	1.746986
17	6	0	0.726320	-3.366516	2.885592
18	6	0	-2.567757	-2.500487	1.242874
19	6	0	-2.412247	-2.484276	3.540858
20	6	0	3.732810	-1.795558	-3.246015
21	6	0	-2.547594	-3.325425	2.400437
22	6	0	-1.645218	1.989933	2.530039
23	6	0	0.714471	-2.020111	1.001664
24	6	0	-3.934525	2.384416	1.897565
25	6	0	0.904198	-2.019718	3.311641
26	6	0	0.616713	-3.372244	1.467074
27	6	0	0.903211	-1.191107	2.157792
28	6	0	-4.218235	-0.002160	-0.145591
29	6	0	-5.265498	-0.433923	0.678500
30	6	0	-4.000299	3.430439	2.816007
31	6	0	-1.716227	3.022361	3.456387
32	6	0	-2.896462	3.749544	3.597702
33	6	0	4.820030	-1.998476	-2.399002
34	6	0	-5.709231	-0.121998	-2.052767
35	6	0	-4.453654	0.144985	-1.512915
36	6	0	-6.743845	-0.539349	-1.223809
37	6	0	-6.520602	-0.694114	0.143308
38	1	0	0.999682	-0.108610	2.138772
39	1	0	0.972531	-1.679987	4.339844
40	1	0	0.625751	-4.231409	3.533734
41	1	0	0.405382	-4.240563	0.851365
42	1	0	-2.633788	-2.844840	0.214092
43	1	0	-2.565135	-4.410594	2.405020
44	1	0	-2.310408	-2.814674	4.569731
45	1	0	-2.233548	-0.258357	3.716908
46	1	0	-1.954120	-1.284472	-2.069982
47	1	0	-3.296698	-3.009988	-3.253593
48	1	0	-2.412516	-5.326727	-3.475633
49	1	0	-0.178746	-5.889441	-2.548956
50	1	0	1.157240	-4.161627	-1.387234
51	1	0	3.235660	-1.756171	0.593392
52	1	0	5.483159	-2.119827	-0.349715
53	1	0	5.813383	-2.162036	-2.816065
54	1	0	3.873103	-1.796965	-4.326029
55	1	0	1.619915	-1.408938	-3.383051
56	1	0	-4.808684	2.144214	1.293117
57	1	0	-4.924418	3.997265	2.918307

58	1	0	-2.951942	4.566797	4.314775
59	1	0	-0.843989	3.271135	4.058733
60	1	0	-0.712908	1.437112	2.401700
61	1	0	-3.640178	0.478761	-2.157221
62	1	0	-5.876150	-0.002085	-3.122006
63	1	0	-7.727337	-0.748152	-1.641946
64	1	0	-7.328440	-1.025405	0.793958
65	1	0	-5.092537	-0.571184	1.746897
66	6	0	4.964018	1.438792	0.044562
67	6	0	4.848954	1.450515	-1.352446
68	6	0	3.613140	1.516257	-1.974698
69	6	0	2.423837	1.612040	-1.234752
70	6	0	2.551428	1.658248	0.166487
71	6	0	3.785979	1.552513	0.792167
72	1	0	5.751471	1.396407	-1.962491
73	1	0	3.543364	1.479163	-3.061935
74	1	0	1.642559	1.760474	0.765167
75	1	0	3.837572	1.533208	1.882225
76	46	0	-0.600744	0.789756	-0.883334
77	6	0	6.277759	1.284424	0.696081
78	6	0	7.269766	0.473806	0.126718
79	6	0	6.574976	1.934589	1.901132
80	6	0	8.509931	0.321935	0.734478
81	1	0	7.048963	-0.062865	-0.797003
82	6	0	7.813196	1.780360	2.512152
83	1	0	5.830997	2.594506	2.347189
84	6	0	8.788147	0.973847	1.932253
85	1	0	9.261434	-0.318348	0.274018
86	1	0	8.022791	2.303959	3.444247
87	1	0	9.759490	0.855154	2.409943
88	6	0	0.357367	2.782497	-1.726694
89	6	0	1.128471	1.642182	-1.915342
90	6	0	-1.032478	2.739169	-2.047752
91	1	0	0.741970	3.652984	-1.167515
92	6	0	-1.913800	3.912009	-1.595707
93	6	0	-1.441881	2.072546	-3.345584
94	1	0	-2.366054	1.484274	-3.279196
95	1	0	-1.622016	2.843096	-4.116233
96	1	0	-0.642836	1.415028	-3.701087
97	6	0	-1.717122	5.076479	-2.583501
98	1	0	-2.071692	4.832807	-3.593565
99	1	0	-2.281552	5.955701	-2.239742
100	1	0	-0.658264	5.361843	-2.653484
101	6	0	-1.542600	4.428113	-0.202612
102	1	0	-2.302584	5.142930	0.146214
103	1	0	-1.481245	3.614173	0.529578
104	1	0	-0.579330	4.954013	-0.198876
105	6	0	-3.393269	3.529059	-1.591821
106	1	0	-3.746637	3.222744	-2.586192
107	1	0	-3.588976	2.703042	-0.894826
108	1	0	-4.005073	4.385863	-1.273357

Zero-point correction= 0.876214 (Hartree/Particle)
Thermal correction to Energy= 0.929404
Thermal correction to Enthalpy= 0.930348
Thermal correction to Gibbs Free Energy= 0.790396
Sum of electronic and zero-point Energies= -3018.151856
Sum of electronic and thermal Energies= -3018.098667
Sum of electronic and thermal Enthalpies= -3018.097723
Sum of electronic and thermal Free Energies= -3018.237675
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.327666

TS6c

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

1	26	0	2.842797	1.928043	-2.582562
2	15	0	0.166949	0.253811	-1.276361
3	15	0	3.573543	0.230186	0.334364
4	6	0	-2.506906	-0.569502	-1.380756
5	6	0	0.518686	-1.240619	-2.306556
6	6	0	1.712386	-3.345096	-2.542243
7	6	0	-1.625391	0.482146	-1.652235
8	6	0	1.179587	-3.511562	-3.819451
9	6	0	-0.031210	-1.432541	-3.580569
10	6	0	1.372598	-2.220527	-1.790846
11	6	0	0.299488	-2.557461	-4.333043
12	6	0	-2.127486	1.652212	-2.225983
13	6	0	-3.478381	1.751982	-2.554415
14	6	0	4.029883	0.894833	-1.309958
15	6	0	4.632087	2.154864	-1.629235
16	6	0	4.392715	1.456578	1.429969
17	6	0	1.709175	3.013167	-3.890833
18	6	0	3.862861	0.181304	-2.544043
19	6	0	4.813526	2.219378	-3.037916
20	6	0	-3.849727	-0.477490	-1.727372
21	6	0	4.345252	1.000057	-3.601437
22	6	0	3.841647	2.743798	1.488645
23	6	0	0.889033	1.611605	-2.240818
24	6	0	5.472659	1.147336	2.257715
25	6	0	1.811639	3.697737	-2.647112
26	6	0	1.136976	1.733702	-3.649026
27	6	0	1.302204	2.844354	-1.632254
28	6	0	4.674208	-1.239536	0.371403
29	6	0	5.992658	-1.195391	-0.097988
30	6	0	5.986603	2.103044	3.131612
31	6	0	4.367163	3.701732	2.346427
32	6	0	5.438479	3.379453	3.177410
33	6	0	-4.339128	0.683278	-2.324431
34	6	0	4.955404	-3.593236	0.873532
35	6	0	4.164312	-2.447939	0.848083
36	6	0	6.266951	-3.536246	0.415155
37	6	0	6.784277	-2.336770	-0.071710
38	1	0	1.247434	3.061962	-0.568697
39	1	0	2.252703	4.677156	-2.494361
40	1	0	2.070197	3.376314	-4.847798
41	1	0	0.990090	0.958387	-4.394624
42	1	0	3.415986	-0.803531	-2.654259
43	1	0	4.305943	0.759639	-4.658867
44	1	0	5.192717	3.073588	-3.589286
45	1	0	4.864696	2.943316	-0.920812
46	1	0	1.778757	-2.086886	-0.785086
47	1	0	2.409355	-4.076908	-2.133214
48	1	0	1.456821	-4.376738	-4.420620
49	1	0	-0.120000	-2.684161	-5.330205
50	1	0	-0.730046	-0.698234	-3.983582
51	1	0	-1.465848	2.493465	-2.429764
52	1	0	-3.854948	2.672975	-2.997658
53	1	0	-5.387938	0.759408	-2.612780
54	1	0	-4.499481	-1.329822	-1.517129
55	1	0	-2.151634	-1.447737	-0.842311
56	1	0	5.915420	0.152205	2.229905
57	1	0	6.824847	1.844932	3.776520
58	1	0	5.842610	4.123764	3.860909
59	1	0	3.931103	4.698724	2.378245
60	1	0	2.985991	2.993688	0.858697
61	1	0	3.133610	-2.477891	1.204285
62	1	0	4.549350	-4.528226	1.256978
63	1	0	6.890721	-4.428233	0.434360
64	1	0	7.809926	-2.292832	-0.433563
65	1	0	6.399335	-0.259762	-0.484344
66	6	0	-3.219229	3.346518	0.734507
67	6	0	-3.781642	2.092875	1.005574

68	6	0	-2.999120	1.014550	1.389093
69	6	0	-1.611291	1.136396	1.548410
70	6	0	-1.058991	2.410267	1.326790
71	6	0	-1.835969	3.481664	0.909694
72	1	0	-4.863741	1.973100	0.907848
73	1	0	-3.429063	0.034331	1.597350
74	1	0	0.019830	2.543000	1.446177
75	1	0	-1.358213	4.436487	0.685902
76	46	0	1.227434	-0.015549	0.922899
77	6	0	-4.045617	4.474192	0.264331
78	6	0	-5.141665	4.260850	-0.582695
79	6	0	-3.756250	5.789855	0.647612
80	6	0	-5.919687	5.322612	-1.028362
81	1	0	-5.363140	3.247309	-0.920300
82	6	0	-4.531795	6.852355	0.201226
83	1	0	-2.928697	5.977235	1.331302
84	6	0	-5.617500	6.624085	-0.639166
85	1	0	-6.761625	5.134575	-1.693382
86	1	0	-4.292293	7.865709	0.519236
87	1	0	-6.225666	7.456673	-0.987906
88	6	0	0.128577	0.164176	2.926385
89	6	0	-0.805467	-0.055068	1.888827
90	6	0	1.140896	-0.749494	3.266369
91	1	0	0.169572	1.144990	3.419252
92	6	0	2.149925	-0.378934	4.357973
93	6	0	0.961073	-2.224111	3.020694
94	1	0	1.904581	-2.732053	2.790174
95	1	0	0.578651	-2.689811	3.943668
96	1	0	0.232507	-2.441161	2.236824
97	6	0	1.540286	-0.798115	5.710309
98	1	0	1.415861	-1.885060	5.796959
99	1	0	2.203512	-0.476853	6.525829
100	1	0	0.559825	-0.326806	5.865771
101	6	0	2.430382	1.124204	4.431679
102	1	0	3.281400	1.310517	5.101099
103	1	0	2.678758	1.544355	3.449279
104	1	0	1.577296	1.684460	4.835855
105	6	0	3.474763	-1.123818	4.175646
106	1	0	3.360341	-2.210639	4.282166
107	1	0	3.919341	-0.925826	3.190655
108	1	0	4.195147	-0.796134	4.937896
109	6	0	-3.028730	-2.573998	1.238178
110	8	0	-3.726676	-3.167348	0.360385
111	8	0	-1.695420	-2.451872	0.946019
112	8	0	-3.443451	-2.062780	2.298772
113	1	0	-1.339313	-1.542489	1.399656
114	55	0	-1.625498	-4.429024	-1.304861
115	55	0	-6.119109	-1.466985	1.416911

Zero-point correction= 0.907346 (Hartree/Particle)
Thermal correction to Energy= 0.968133
Thermal correction to Enthalpy= 0.969077
Thermal correction to Gibbs Free Energy= 0.809870
Sum of electronic and zero-point Energies= -3322.097139
Sum of electronic and thermal Energies= -3322.036352
Sum of electronic and thermal Enthalpies= -3322.035408
Sum of electronic and thermal Free Energies= -3322.194615
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3326.0353435

INT10c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-4.921803	0.398045	-0.453883
2	15	0	-2.267813	0.673842	1.636303
3	15	0	-2.515128	-2.027161	-0.900361

4	6	0	-0.630196	1.896355	3.531500
5	6	0	-3.108270	-0.182947	3.023743
6	6	0	-3.682165	-2.281055	4.091839
7	6	0	-1.546432	2.127624	2.497818
8	6	0	-4.381207	-1.590510	5.076625
9	6	0	-3.797085	0.503391	4.029715
10	6	0	-3.042639	-1.577506	3.075415
11	6	0	-4.433323	-0.198048	5.047863
12	6	0	-1.843348	3.443428	2.139226
13	6	0	-1.250498	4.507941	2.815747
14	6	0	-4.261080	-1.467759	-0.912365
15	6	0	-5.017971	-0.927538	-2.001206
16	6	0	-2.192877	-2.137350	-2.707811
17	6	0	-5.638434	2.269026	-0.061610
18	6	0	-5.126134	-1.496895	0.231755
19	6	0	-6.324405	-0.619942	-1.528383
20	6	0	-0.044183	2.958182	4.208851
21	6	0	-6.392960	-0.977904	-0.152455
22	6	0	-1.892722	-0.941351	-3.372785
23	6	0	-3.617088	1.428286	0.687513
24	6	0	-2.159334	-3.332868	-3.426103
25	6	0	-4.720012	2.310700	-1.149110
26	6	0	-4.963111	1.735667	1.071383
27	6	0	-3.476090	1.795890	-0.693089
28	6	0	-2.752657	-3.764388	-0.356932
29	6	0	-3.833986	-4.543459	-0.787285
30	6	0	-1.826563	-3.334536	-4.778826
31	6	0	-1.572968	-0.941537	-4.725132
32	6	0	-1.531844	-2.142772	-5.430716
33	6	0	-0.356239	4.270214	3.853521
34	6	0	-2.007884	-5.609905	1.026443
35	6	0	-1.848509	-4.308095	0.557979
36	6	0	-3.078133	-6.378810	0.582448
37	6	0	-3.991338	-5.843998	-0.324215
38	1	0	-2.572473	1.663427	-1.282916
39	1	0	-4.948901	2.621033	-2.163381
40	1	0	-6.689484	2.536073	-0.105784
41	1	0	-5.410006	1.523408	2.037901
42	1	0	-4.848069	-1.826471	1.229384
43	1	0	-7.239715	-0.820907	0.507610
44	1	0	-7.111985	-0.143709	-2.103400
45	1	0	-4.641755	-0.742436	-3.002701
46	1	0	-2.486332	-2.112376	2.302651
47	1	0	-3.626794	-3.368374	4.114005
48	1	0	-4.880129	-2.135685	5.876099
49	1	0	-4.968151	0.342821	5.826894
50	1	0	-3.822181	1.594252	4.021056
51	1	0	-2.551423	3.645150	1.335669
52	1	0	-1.507819	5.529656	2.537903
53	1	0	0.094507	5.103629	4.390422
54	1	0	0.651582	2.763780	5.024054
55	1	0	-0.387637	0.869597	3.815366
56	1	0	-2.371628	-4.276740	-2.925134
57	1	0	-1.796305	-4.276564	-5.323954
58	1	0	-1.271494	-2.146964	-6.487685
59	1	0	-1.352744	-0.002608	-5.231744
60	1	0	-1.913170	-0.000814	-2.817003
61	1	0	-1.021903	-3.689951	0.914024
62	1	0	-1.296728	-6.020478	1.741400
63	1	0	-3.207724	-7.395723	0.948892
64	1	0	-4.834787	-6.442023	-0.665058
65	1	0	-4.560041	-4.125675	-1.486416
66	6	0	0.846364	4.505910	-0.732980
67	6	0	1.372586	4.055636	0.484727
68	6	0	1.405826	2.705002	0.803031
69	6	0	0.925836	1.725337	-0.081093
70	6	0	0.404179	2.178654	-1.307078

71	6	0	0.360863	3.530749	-1.618592
72	1	0	1.776463	4.776954	1.195401
73	1	0	1.809291	2.390363	1.767014
74	1	0	0.004923	1.454511	-2.019373
75	1	0	-0.092135	3.844665	-2.559561
76	46	0	-0.851243	-0.652806	0.205210
77	6	0	0.792611	5.943883	-1.057738
78	6	0	0.600788	6.895161	-0.047690
79	6	0	0.930797	6.398962	-2.375103
80	6	0	0.552841	8.251613	-0.342537
81	1	0	0.458490	6.560161	0.979597
82	6	0	0.879391	7.755380	-2.671987
83	1	0	1.100217	5.680385	-3.177558
84	6	0	0.692212	8.688256	-1.656502
85	1	0	0.394698	8.973082	0.457348
86	1	0	0.992866	8.086920	-3.702861
87	1	0	0.652340	9.750685	-1.888932
88	6	0	1.187736	-0.750291	-0.662048
89	6	0	1.070027	0.305570	0.273313
90	6	0	2.208581	-1.866763	-0.409968
91	1	0	1.067964	-0.485314	-1.718291
92	6	0	2.374593	-2.787459	-1.669163
93	6	0	1.884430	-2.642082	0.857000
94	1	0	0.975317	-3.233517	0.698892
95	1	0	2.707597	-3.297704	1.146371
96	1	0	1.689975	-1.953162	1.689121
97	6	0	3.214601	-4.031954	-1.367990
98	1	0	2.698222	-4.711850	-0.677726
99	1	0	3.386723	-4.586692	-2.301597
100	1	0	4.181803	-3.779193	-0.922661
101	6	0	3.073050	-2.028582	-2.805405
102	1	0	3.105746	-2.661102	-3.703213
103	1	0	2.537260	-1.109044	-3.087641
104	1	0	4.108730	-1.769421	-2.541586
105	6	0	1.016763	-3.265245	-2.185550
106	1	0	0.442437	-3.797922	-1.413499
107	1	0	0.390191	-2.448212	-2.562996
108	1	0	1.168428	-3.970386	-3.016333
109	6	0	4.652530	-1.453168	0.308981
110	8	0	5.524745	-0.557467	0.144383
111	8	0	4.783374	-2.538449	0.899793
112	8	0	3.441845	-1.084978	-0.254935
113	1	0	1.545716	0.157525	1.249139
114	55	0	7.544495	-2.173123	1.754711
115	55	0	4.050213	1.597071	-1.448728

Zero-point correction= 0.911254 (Hartree/Particle)
Thermal correction to Energy= 0.972297
Thermal correction to Enthalpy= 0.973241
Thermal correction to Gibbs Free Energy= 0.810096
Sum of electronic and zero-point Energies= -3322.151448
Sum of electronic and thermal Energies= -3322.090405
Sum of electronic and thermal Enthalpies= -3322.089460
Sum of electronic and thermal Free Energies= -3322.252605
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3326.0837798

TS7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-4.602150	2.006129	-0.409523
2	15	0	-1.929166	1.294314	1.573376
3	15	0	-3.297887	-1.134653	-0.857903
4	6	0	0.111084	1.869085	3.391107
5	6	0	-2.943750	0.827937	3.024130
6	6	0	-4.226484	-0.866051	4.185914

7	6	0	-0.639282	2.364051	2.317682
8	6	0	-4.549161	0.055329	5.176994
9	6	0	-3.259446	1.743716	4.034362
10	6	0	-3.420299	-0.481397	3.118206
11	6	0	-4.060485	1.358551	5.103271
12	6	0	-0.322415	3.616734	1.788792
13	6	0	0.715910	4.367638	2.334168
14	6	0	-4.712400	0.020948	-0.852980
15	6	0	-5.220916	0.803537	-1.937648
16	6	0	-3.125438	-1.500808	-2.649883
17	6	0	-4.567516	4.004645	0.008251
18	6	0	-5.497850	0.335737	0.305822
19	6	0	-6.304543	1.587413	-1.451525
20	6	0	1.138199	2.625633	3.942225
21	6	0	-6.480025	1.293082	-0.070131
22	6	0	-2.465923	-0.549436	-3.439177
23	6	0	-2.959129	2.478630	0.665270
24	6	0	-3.554168	-2.689427	-3.242707
25	6	0	-3.747638	3.723215	-1.121179
26	6	0	-4.084481	3.246210	1.110203
27	6	0	-2.756831	2.785049	-0.722305
28	6	0	-4.055878	-2.635320	-0.131268
29	6	0	-5.386170	-2.999464	-0.369768
30	6	0	-3.323738	-2.924138	-4.596363
31	6	0	-2.261375	-0.772438	-4.795371
32	6	0	-2.683769	-1.967097	-5.375491
33	6	0	1.443156	3.878943	3.413950
34	6	0	-3.802484	-4.572690	1.299512
35	6	0	-3.271586	-3.428464	0.710801
36	6	0	-5.124267	-4.929199	1.052531
37	6	0	-5.915704	-4.142667	0.217920
38	1	0	-1.991282	2.340096	-1.353381
39	1	0	-3.891156	4.112623	-2.123765
40	1	0	-5.449735	4.636800	0.011849
41	1	0	-4.534653	3.195233	2.096853
42	1	0	-5.346249	-0.067732	1.304340
43	1	0	-7.195979	1.761357	0.597371
44	1	0	-6.863430	2.320626	-2.023740
45	1	0	-4.822240	0.822494	-2.947213
46	1	0	-3.153975	-1.203559	2.344517
47	1	0	-4.594318	-1.889462	4.242617
48	1	0	-5.174966	-0.242815	6.016345
49	1	0	-4.301309	2.076349	5.885511
50	1	0	-2.864115	2.759517	3.988147
51	1	0	-0.890829	4.015829	0.949069
52	1	0	0.947077	5.345355	1.912831
53	1	0	2.245357	4.474639	3.848002
54	1	0	1.699434	2.238799	4.791666
55	1	0	-0.124761	0.888005	3.808784
56	1	0	-4.061167	-3.445812	-2.644100
57	1	0	-3.654396	-3.860167	-5.043154
58	1	0	-2.510284	-2.150921	-6.434191
59	1	0	-1.758687	-0.019058	-5.399901
60	1	0	-2.106527	0.374399	-2.979925
61	1	0	-2.235044	-3.140707	0.904119
62	1	0	-3.182037	-5.185334	1.951674
63	1	0	-5.542709	-5.822588	1.512975
64	1	0	-6.950840	-4.419856	0.026447
65	1	0	-6.008909	-2.380245	-1.017209
66	6	0	2.794516	3.418389	-0.720561
67	6	0	3.079726	2.734241	0.468540
68	6	0	2.453217	1.535475	0.778910
69	6	0	1.511221	0.954411	-0.083093
70	6	0	1.202662	1.656566	-1.261902
71	6	0	1.829953	2.854605	-1.572123
72	1	0	3.822368	3.137312	1.157923
73	1	0	2.707571	1.018528	1.704718

74	1	0	0.446376	1.258302	-1.940367
75	1	0	1.543454	3.386396	-2.479962
76	46	0	-1.205644	-0.456922	0.124322
77	6	0	3.503739	4.663083	-1.073966
78	6	0	3.910652	5.569884	-0.086226
79	6	0	3.811160	4.959933	-2.408538
80	6	0	4.601409	6.727564	-0.421258
81	1	0	3.660272	5.375351	0.956941
82	6	0	4.500343	6.118880	-2.745136
83	1	0	3.513569	4.266121	-3.196462
84	6	0	4.900420	7.007156	-1.751561
85	1	0	4.900404	7.422162	0.361862
86	1	0	4.730397	6.327340	-3.788775
87	1	0	5.440788	7.914801	-2.013046
88	6	0	0.644619	-1.313741	-0.756254
89	6	0	0.942632	-0.354364	0.252040
90	6	0	0.685810	-2.721948	-0.541031
91	1	0	0.699828	-0.980773	-1.792069
92	6	0	0.535126	-3.690401	-1.709201
93	6	0	0.956428	-3.265843	0.749618
94	1	0	0.689014	-4.316582	0.889129
95	1	0	2.192945	-3.202629	0.810519
96	1	0	0.637280	-2.657720	1.601669
97	6	0	1.699649	-4.694300	-1.699936
98	1	0	1.684754	-5.339034	-0.812236
99	1	0	1.615833	-5.345299	-2.581715
100	1	0	2.653546	-4.153770	-1.721215
101	6	0	0.516467	-2.997789	-3.070715
102	1	0	0.384822	-3.752443	-3.858169
103	1	0	-0.314405	-2.284153	-3.165690
104	1	0	1.463850	-2.475466	-3.260693
105	6	0	-0.784165	-4.463032	-1.548758
106	1	0	-0.818640	-5.039207	-0.614758
107	1	0	-1.654055	-3.792943	-1.569790
108	1	0	-0.891207	-5.171658	-2.382608
109	6	0	4.059940	-2.245825	-0.001327
110	8	0	5.211097	-1.696782	0.130603
111	8	0	3.597919	-2.958581	1.007999
112	8	0	3.359447	-2.121288	-1.057904
113	1	0	1.266162	-0.727287	1.227526
114	55	0	6.154554	-3.351602	2.339623
115	55	0	4.643120	0.376939	-1.933536

Zero-point correction= 0.904397 (Hartree/Particle)
Thermal correction to Energy= 0.965541
Thermal correction to Enthalpy= 0.966486
Thermal correction to Gibbs Free Energy= 0.804092
Sum of electronic and zero-point Energies= -3322.115739
Sum of electronic and thermal Energies= -3322.054594
Sum of electronic and thermal Enthalpies= -3322.053650
Sum of electronic and thermal Free Energies= -3322.216044
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3326.0476385

INT11c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.728849	-2.354960	2.305168
2	15	0	0.599371	-1.580934	-0.749565
3	15	0	-2.373027	0.183071	0.669657
4	6	0	2.554538	-1.574009	-2.737604
5	6	0	-0.228539	-2.974479	-1.614860
6	6	0	-2.204425	-3.800281	-2.748111
7	6	0	2.323650	-1.736255	-1.366289
8	6	0	-1.598132	-5.042340	-2.906706
9	6	0	0.380486	-4.220450	-1.798770

10	6	0	-1.518805	-2.769898	-2.110105
11	6	0	-0.303114	-5.249961	-2.435972
12	6	0	3.411849	-1.947334	-0.517811
13	6	0	4.703820	-2.012752	-1.033741
14	6	0	-2.377909	-1.260312	1.799016
15	6	0	-2.209806	-1.286261	3.219081
16	6	0	-2.749540	1.548775	1.844466
17	6	0	0.884941	-3.449397	2.894876
18	6	0	-2.499253	-2.620545	1.360964
19	6	0	-2.230544	-2.643744	3.648697
20	6	0	3.841302	-1.656383	-3.253667
21	6	0	-2.417471	-3.466842	2.501891
22	6	0	-1.684712	2.042559	2.609707
23	6	0	0.772473	-2.189756	0.956177
24	6	0	-3.999252	2.161475	1.956132
25	6	0	1.061853	-2.081754	3.252116
26	6	0	0.713627	-3.520770	1.483507
27	6	0	0.993416	-1.305518	2.063213
28	6	0	-3.956252	-0.075670	-0.223213
29	6	0	-5.085151	-0.654034	0.368926
30	6	0	-4.179212	3.243452	2.815200
31	6	0	-1.870386	3.106726	3.483298
32	6	0	-3.120313	3.714860	3.582748
33	6	0	4.921216	-1.877291	-2.400618
34	6	0	-5.197266	0.176539	-2.287801
35	6	0	-4.020958	0.332266	-1.558625
36	6	0	-6.314034	-0.397807	-1.691105
37	6	0	-6.256980	-0.813383	-0.361751
38	1	0	1.063870	-0.223545	1.984882
39	1	0	1.168869	-1.694941	4.260302
40	1	0	0.824991	-4.285137	3.585153
41	1	0	0.493989	-4.417775	0.911810
42	1	0	-2.598577	-2.946255	0.328379
43	1	0	-2.429200	-4.551986	2.488550
44	1	0	-2.077341	-2.990808	4.665730
45	1	0	-2.052414	-0.418377	3.851916
46	1	0	-1.982635	-1.787344	-1.991488
47	1	0	-3.210281	-3.627443	-3.128022
48	1	0	-2.129810	-5.849146	-3.409028
49	1	0	0.177905	-6.217518	-2.572942
50	1	0	1.401710	-4.379176	-1.448503
51	1	0	3.253290	-2.069218	0.553658
52	1	0	5.543213	-2.177093	-0.358498
53	1	0	5.932102	-1.938320	-2.802804
54	1	0	4.004114	-1.542094	-4.324661
55	1	0	1.710523	-1.386589	-3.405794
56	1	0	-4.838085	1.801430	1.360652
57	1	0	-5.156968	3.717978	2.884912
58	1	0	-3.264608	4.559336	4.254518
59	1	0	-1.033940	3.474223	4.075926
60	1	0	-0.697045	1.587826	2.506062
61	1	0	-3.144187	0.790830	-2.024541
62	1	0	-5.235178	0.507076	-3.325187
63	1	0	-7.234040	-0.523951	-2.260079
64	1	0	-7.130668	-1.264095	0.106964
65	1	0	-5.044006	-0.978728	1.409691
66	6	0	4.739430	1.748560	-0.003818
67	6	0	4.532765	1.513754	-1.367394
68	6	0	3.268025	1.599956	-1.926825
69	6	0	2.143289	1.923833	-1.156703
70	6	0	2.353070	2.167207	0.211525
71	6	0	3.617914	2.080332	0.770338
72	1	0	5.383770	1.284382	-2.008761
73	1	0	3.139628	1.414723	-2.994044
74	1	0	1.501765	2.406671	0.850395
75	1	0	3.737803	2.242051	1.842074
76	46	0	-0.477775	0.543708	-0.738201

77	6	0	6.083867	1.651147	0.592879
78	6	0	7.019310	0.720723	0.120084
79	6	0	6.468837	2.490766	1.646314
80	6	0	8.288635	0.633964	0.678574
81	1	0	6.732377	0.040486	-0.682723
82	6	0	7.736087	2.401795	2.208465
83	1	0	5.771159	3.245092	2.009495
84	6	0	8.653818	1.472973	1.727334
85	1	0	8.996457	-0.100576	0.296097
86	1	0	8.012735	3.071331	3.021846
87	1	0	9.647983	1.403488	2.165918
88	6	0	-0.277261	2.694719	-1.316017
89	6	0	0.827296	1.978555	-1.803680
90	6	0	-1.430522	3.112751	-2.137059
91	1	0	-0.134886	3.234451	-0.380413
92	6	0	-2.325916	4.259167	-1.623087
93	6	0	-1.689933	2.566229	-3.339342
94	1	0	-2.517607	2.903701	-3.961462
95	1	0	-1.087351	1.757590	-3.751412
96	6	0	-2.104329	5.479194	-2.524947
97	1	0	-2.394760	5.271616	-3.563084
98	1	0	-2.695889	6.335477	-2.167169
99	1	0	-1.045428	5.774761	-2.527529
100	6	0	-2.017523	4.674757	-0.183246
101	1	0	-2.755682	5.419754	0.146837
102	1	0	-2.076820	3.823849	0.509291
103	1	0	-1.025000	5.136097	-0.086390
104	6	0	-3.803656	3.856767	-1.666859
105	1	0	-4.125020	3.540712	-2.667749
106	1	0	-4.007364	3.026988	-0.974020
107	1	0	-4.433705	4.706883	-1.366008
108	1	0	0.846897	1.718163	-2.866038

Zero-point correction= 0.877316 (Hartree/Particle)
Thermal correction to Energy= 0.930391
Thermal correction to Enthalpy= 0.931335
Thermal correction to Gibbs Free Energy= 0.789514
Sum of electronic and zero-point Energies= -3018.209091
Sum of electronic and thermal Energies= -3018.156016
Sum of electronic and thermal Enthalpies= -3018.155072
Sum of electronic and thermal Free Energies= -3018.296893
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -3021.3810415

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.541911	-0.186945	-0.001852
2	6	0	-2.012193	-1.357081	0.551925
3	6	0	-0.647870	-1.599191	0.536298
4	6	0	0.250250	-0.684224	-0.027394
5	6	0	-0.283802	0.482974	-0.592258
6	6	0	-1.645841	0.726250	-0.575035
7	1	0	-2.680600	-2.075025	1.026204
8	1	0	-0.256679	-2.513985	0.982902
9	1	0	0.378418	1.201296	-1.074387
10	1	0	-2.033919	1.627563	-1.048956
11	6	0	-3.993626	0.073170	0.008636
12	6	0	-4.911468	-0.971537	-0.152624
13	6	0	-4.491277	1.370091	0.181630
14	6	0	-6.278645	-0.728568	-0.140079
15	1	0	-4.542995	-1.983540	-0.318524
16	6	0	-5.858355	1.614447	0.193337
17	1	0	-3.793574	2.192381	0.338017
18	6	0	-6.758553	0.565803	0.033014
19	1	0	-6.974971	-1.554587	-0.275769

20	1	0	-6.223851	2.629919	0.337730
21	1	0	-7.830184	0.756785	0.042455
22	6	0	2.681893	-0.145013	-0.309014
23	6	0	1.677593	-0.983949	-0.005684
24	6	0	4.103711	-0.512862	-0.302503
25	1	0	2.441264	0.894892	-0.546507
26	6	0	5.086553	0.561773	0.155715
27	6	0	4.481587	-1.735502	-0.700561
28	1	0	5.515058	-2.070632	-0.678364
29	1	0	3.752082	-2.447103	-1.083785
30	6	0	4.660479	1.087044	1.530575
31	1	0	4.654241	0.276717	2.272595
32	1	0	5.358992	1.861844	1.877394
33	1	0	3.654785	1.526854	1.510630
34	6	0	5.087270	1.715568	-0.855118
35	1	0	5.798990	2.491693	-0.539371
36	1	0	5.386948	1.362427	-1.851211
37	1	0	4.103909	2.195079	-0.947621
38	6	0	6.511616	0.028144	0.265115
39	1	0	6.578298	-0.801754	0.981851
40	1	0	6.891372	-0.323370	-0.703874
41	1	0	7.181605	0.825684	0.613982
42	1	0	1.936348	-1.995499	0.319879

Zero-point correction= 0.360530 (Hartree/Particle)
Thermal correction to Energy= 0.379302
Thermal correction to Enthalpy= 0.380246
Thermal correction to Gibbs Free Energy= 0.312317
Sum of electronic and zero-point Energies= -774.379070
Sum of electronic and thermal Energies= -774.360298
Sum of electronic and thermal Enthalpies= -774.359353
Sum of electronic and thermal Free Energies= -774.427283
M06/6-311++G(d,p)-SDD/SMD//m06/6-31G(d)-LANL2DZ energy in acetonitrile solvent = -774.9450768