Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic Insights into Nickel- and Gold-Catalyzed Diastereoselective [4 + 2 + 1] Cycloadditions between Dienynes and Diazo Compounds: A DFT Study

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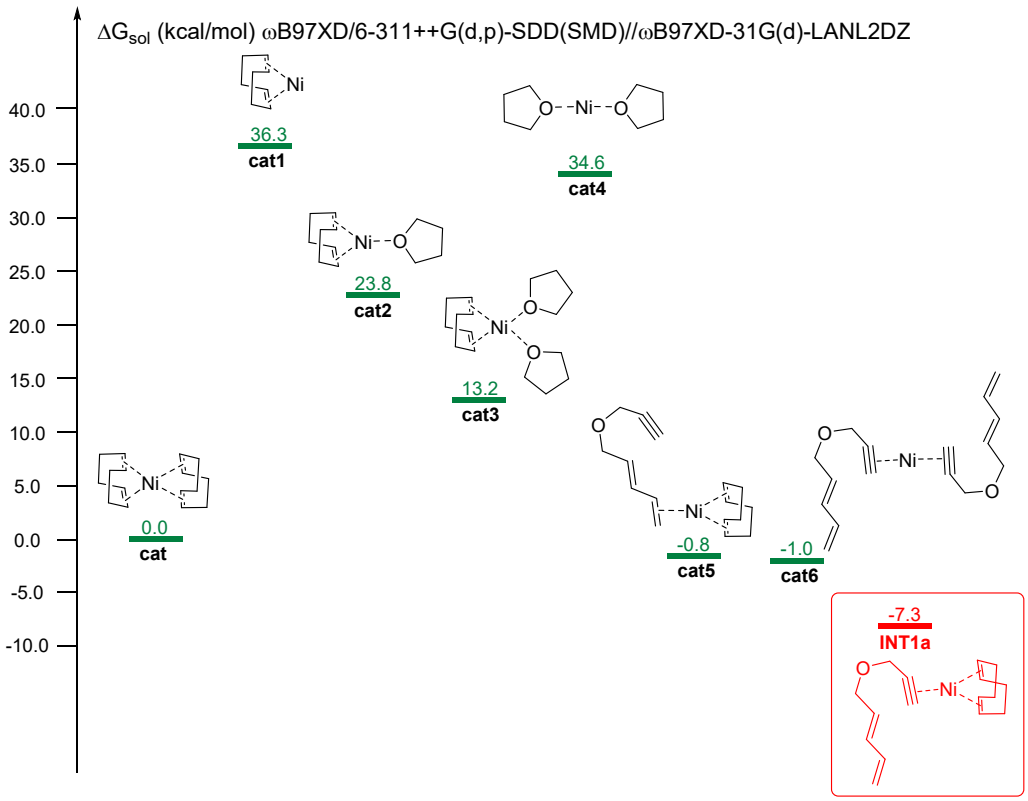


Fig. S1 Energetics of possible L-Ni(0) complexes with different ligands.

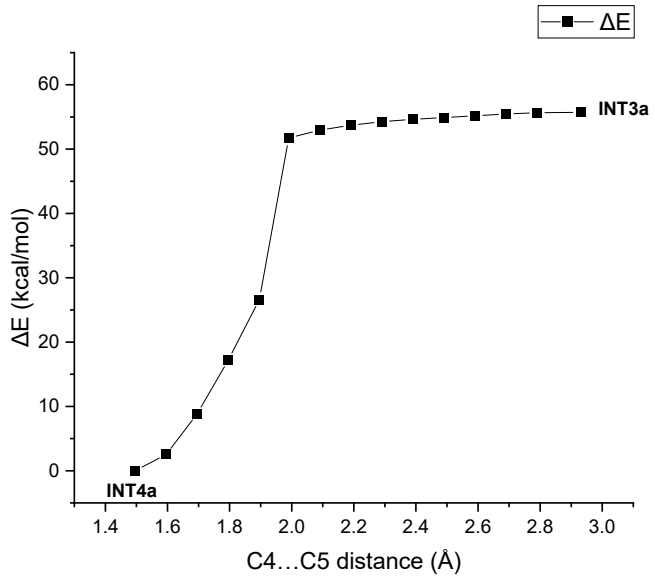


Fig. S2 Potential energy surface scan for the cleavage of C^4–C^5 bond in **INT4a.**

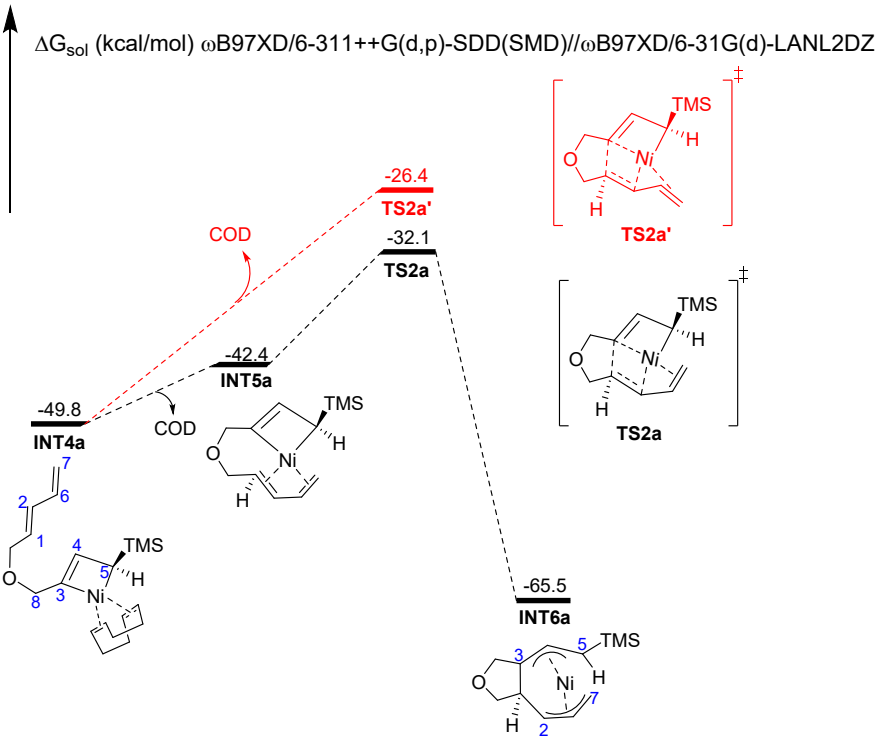


Fig. S3 Free energy profiles for the migratory insertion of C^1=C^2 into Ni–C^3 bond.

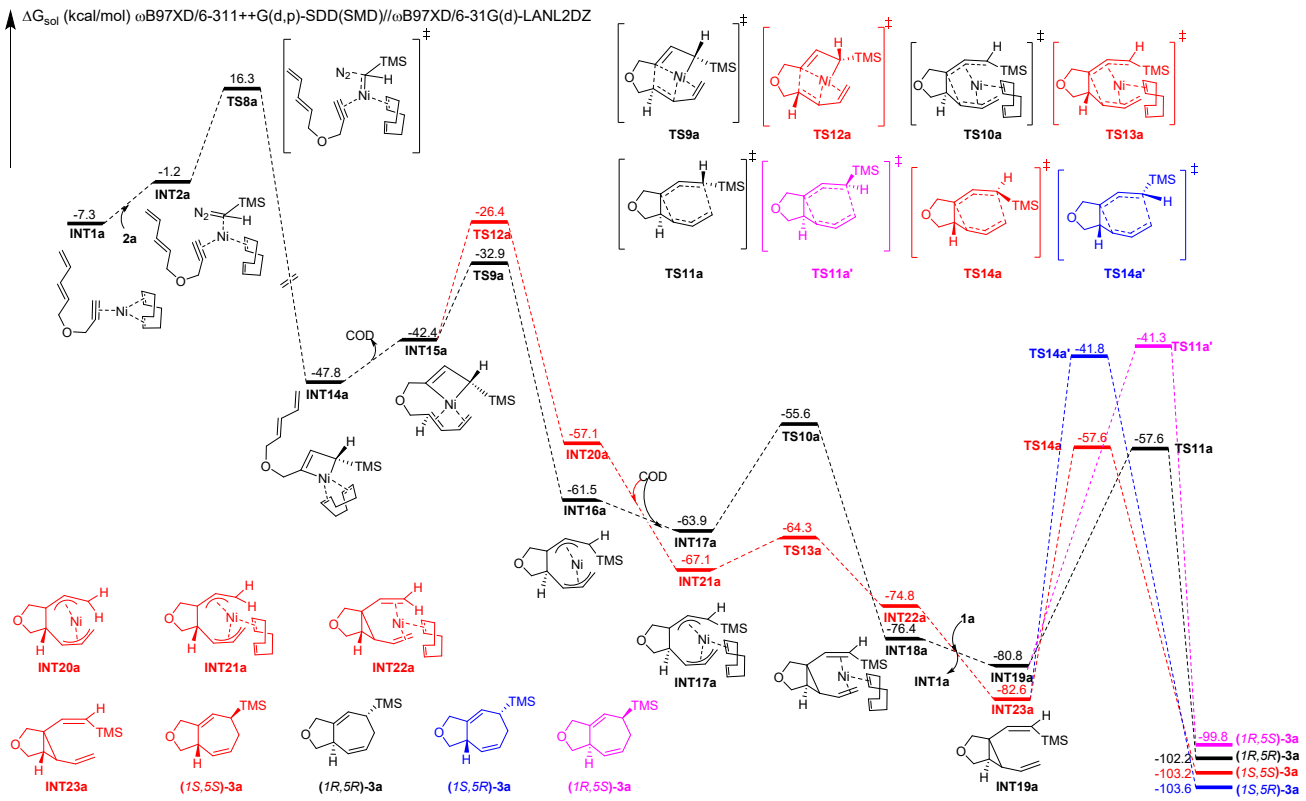


Fig. S4 Free energy profiles for Ni(0)-catalyzed cycloaddition of dienyne **1a** with diazo **2a** to form **3a**.

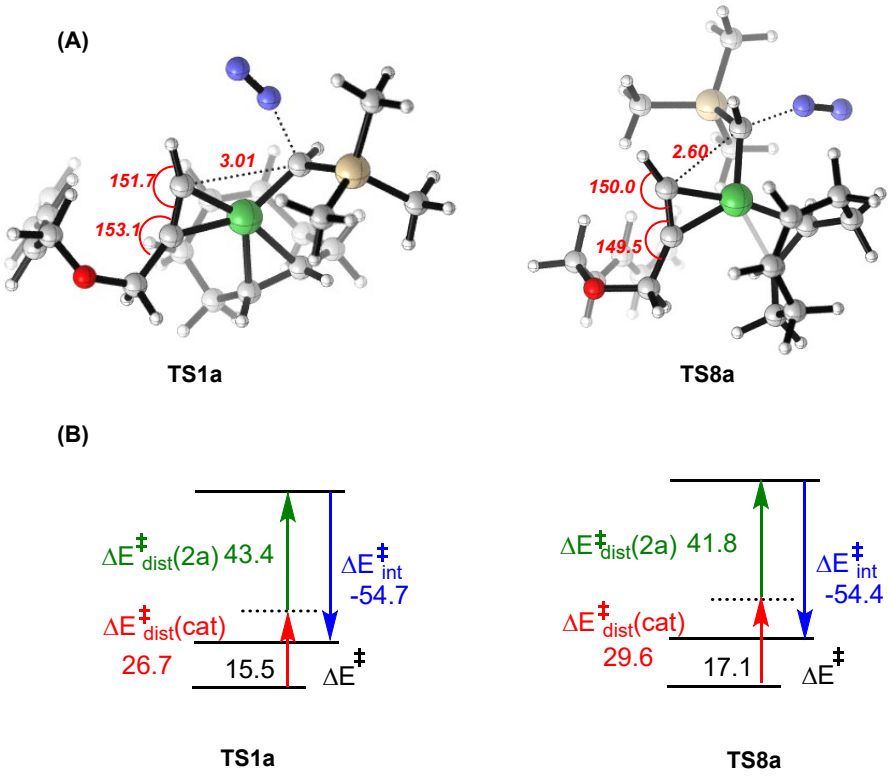


Fig. S5 (A) Geometrical features for **TS1a** and **TS8a** with key bond distance in Å. (B) Distortion, interaction and activation energies for **TS1a** and **TS8a** (green arrow: distortion energy of substrate **2a**; red arrow: distortion energy of the organometallic moiety; blue arrow: interaction energy; black: activation energy, in kcal/mol).

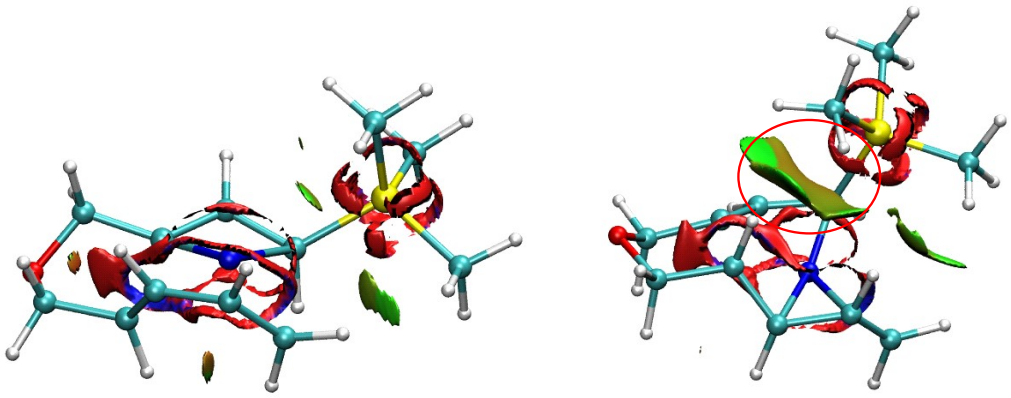


Fig. S6 NCI analysis of **TS2a** and **TS5a** with key steric repulsions highlighted by the red circles.

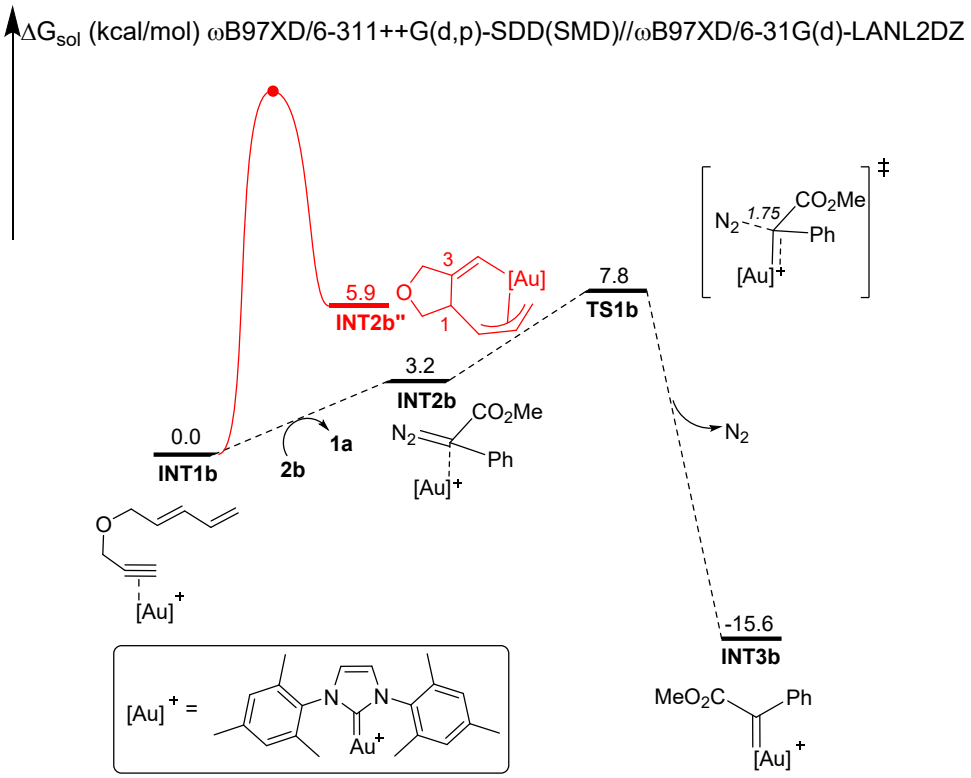


Fig. S7 Free energy profiles for intramolecular cyclization of **INT1b** to form **INT2b″**.

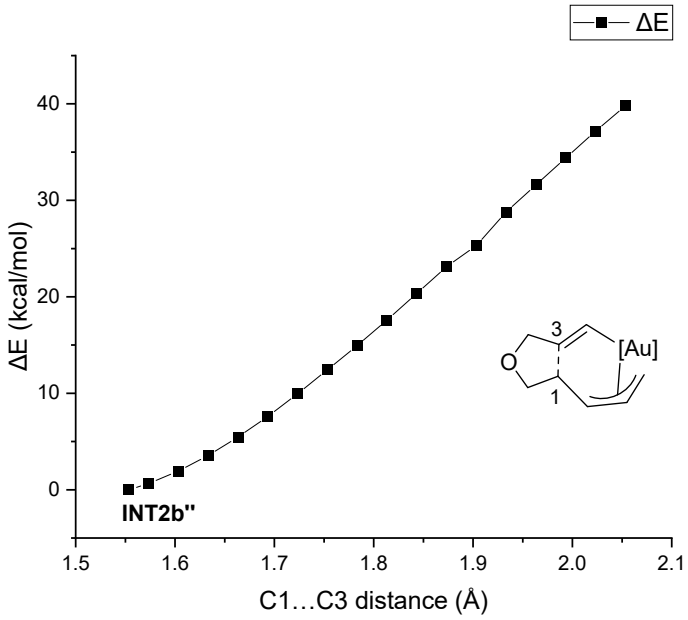


Fig. S8 Potential energy surface scan for the cleavage of C^1–C^3 bond in **INT2b″**.

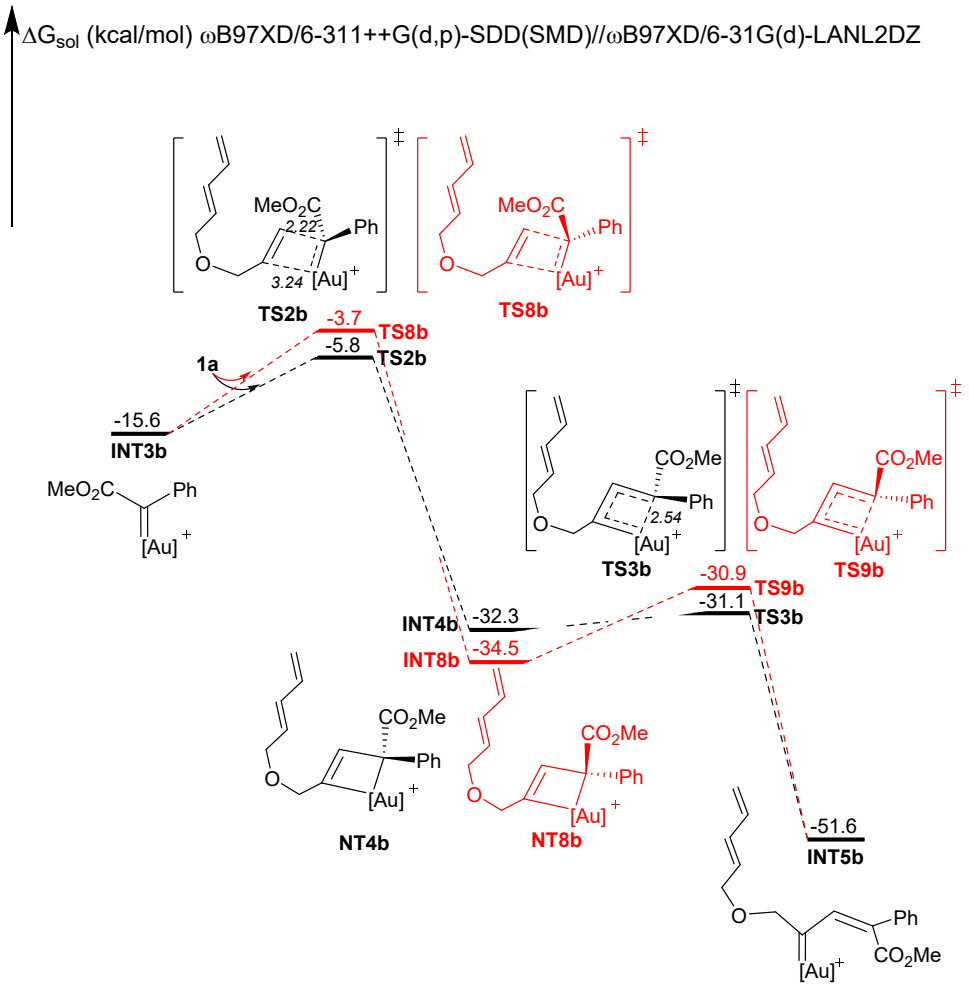
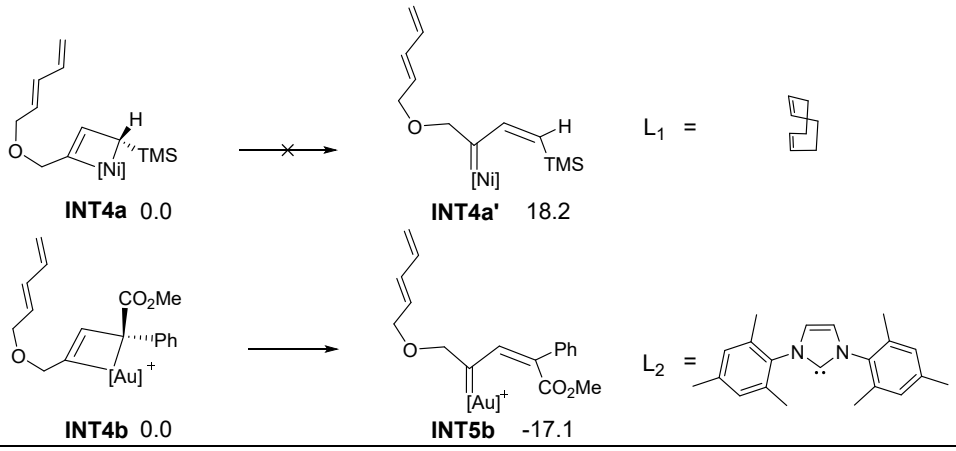


Fig. S9 Free energy profiles for the alkynyl insertion of **1a** from *Si*/*Re* faces followed by cleavage of Au−C bond to form **INT5b**.

Table S1. Comparative calculations of ΔΔG for the vinyl Ni(0)-/Au(I)-carbene intermediates in different systems.



entry	1a	2a/2b	solvent	ligand	transition-metal	ΔΔG(VMC)
1	**1a**	**2a**	THF	L_1	Ni	18.2
2	**1a**	**2b**	$CHCl_3$	L_2	Au	-17.1
3	**1a**	**2b**	THF	L_1	Ni	18.9
4	**1a**	**2a**	$CHCl_3$	L_2	Au	-14.0
5	**1a**	**2a**	$CHCl_3$	L_1	Ni	17.9
6	**1a**	**2b**	THF	L_2	Au	-17.2
7	**1a**	**2a**	THF	L_2	Ni	10.4
8	**1a**	**2b**	$CHCl_3$	L_1	Au	-7.3
9	**1a**	**2a**	THF	L_1	Au	-1.7
10	**1a**	**2b**	$CHCl_3$	L_2	Ni	26.4

Table S2. The calculated $\Delta G^{\neq}$ of key transition states using different combinations of functionals and basis sets.

Entry	Key transition states	$\Delta G^{\neq}$ (kcal/mol) (ωB97XD/ 6-31G(d)-LANL2DZ)	$\Delta G^{\neq}$ (kcal/mol) (ωB97XD/ **6-31G(d,p)**-LANL2DZ)	$\Delta G^{\neq}$ (kcal/mol) (**M06**/ 6-31G(d)-LANL2DZ)
1	**TS1a** (relative to **INT1a**)	21.6	22.0	21.5
2	**TS1a′** (relative to **INT1a**)	36.9	36.9	33.2
3	**TS1a″** (relative to **INT1a**)	43.7	43.2	37.7
4	**TS8a** (relative to **INT1a**)	23.6	23.1	22.9
5	**TS2a** (relative to **INT4a**)	17.7	17.7	15.7
6	**TS5a** (relative to **INT4a**)	22.4	22.0	19.8
7	**TS3a** (relative to **INT7a**)	4.4	4.6	3.5
8	**TS3a′** (relative to **INT7a**)	19.8	19.8	19.8
9	**TS4a** (relative to **INT9a**)	23.0	22.6	22.1
10	**TS4a′** (relative to **INT9a**)	42.5	42.2	39.1
11	**TS1b** (relative to **INT1b**)	7.8	7.7	10.8
12	**TS1b′** (relative to **INT1b**)	16.2	16.3	13.4
13	**TS2b** (relative to **INT3b**)	9.8	11.4	13.9
14	**TS8b** (relative to **INT3b**)	11.9	12.3	15.4
15	**TS4b** (relative to **INT5b**)	8.8	8.3	8.5
16	**TS6b** (relative to **INT5b**)	10.4	9.7	10.4

Cartesian Coordinates and Energies

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.202597	1.062608	0.215453
2	6	0	-2.475160	2.058151	-0.406384
3	1	0	-2.731828	2.941487	-0.946861
4	6	0	-1.842052	-0.153640	0.963300
5	1	0	-0.909990	0.036892	1.515188
6	1	0	-2.624132	-0.385401	1.691636
7	8	0	-1.724611	-1.300790	0.152273
8	6	0	-0.690685	-1.216428	-0.818880
9	1	0	-0.858961	-0.355972	-1.482395
10	1	0	-0.797588	-2.130120	-1.411292
11	6	0	0.675787	-1.140563	-0.202764
12	6	0	1.494505	-0.091108	-0.334246
13	1	0	0.981144	-1.995951	0.400297
14	1	0	1.166871	0.767121	-0.923056
15	6	0	2.822168	-0.004223	0.266731
16	6	0	3.630937	1.050176	0.137174
17	1	0	3.146807	-0.863469	0.852847
18	1	0	4.610258	1.078595	0.603932
19	1	0	3.336893	1.923308	-0.440789

Zero-point correction= 0.158819 (Hartree/Particle)
Thermal correction to Energy= 0.168840
Thermal correction to Enthalpy= 0.169784
Thermal correction to Gibbs Free Energy= 0.122177
Sum of electronic and zero-point Energies= -385.666385
Sum of electronic and thermal Energies= -385.656365
Sum of electronic and thermal Enthalpies= -385.655420
Sum of electronic and thermal Free Energies= -385.703027
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -385.9433636

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.902123	0.998777	0.002306
2	7	0	-2.059507	0.414648	0.000879
3	7	0	-3.055431	-0.136438	-0.000497
4	1	0	-0.959462	2.083332	0.004858
5	14	0	0.670974	-0.010347	-0.000087
6	6	0	1.683448	0.400287	-1.534077
7	1	0	2.633280	-0.147343	-1.534994
8	1	0	1.139818	0.137704	-2.447799
9	1	0	1.917785	1.469805	-1.581314
10	6	0	1.684684	0.395568	1.534357
11	1	0	1.141857	0.129512	2.447578
12	1	0	2.634867	-0.151434	1.532684
13	1	0	1.918330	1.465066	1.585101
14	6	0	0.165319	-1.823012	-0.002422
15	1	0	1.052307	-2.466479	-0.002419
16	1	0	-0.428534	-2.077072	0.882668
17	1	0	-0.427293	-2.075426	-0.888806

Zero-point correction= 0.137025 (Hartree/Particle)
Thermal correction to Energy= 0.147684
Thermal correction to Enthalpy= 0.148628
Thermal correction to Gibbs Free Energy= 0.100780
Sum of electronic and zero-point Energies= -557.181216

Sum of electronic and thermal Energies= -557.170558
Sum of electronic and thermal Enthalpies= -557.169614
Sum of electronic and thermal Free Energies= -557.217461
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -557.4181792

(1R, 5S)-3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.549245	-0.714075	0.044601
2	6	0	0.246106	-0.762944	0.297989
3	1	0	-0.138962	-1.565996	0.928452
4	6	0	2.632071	-1.646779	0.534943
5	1	0	2.500064	-1.964259	1.572625
6	1	0	2.694057	-2.547857	-0.100547
7	8	0	3.827975	-0.896189	0.446218
8	6	0	3.701094	-0.087522	-0.707404
9	1	0	3.929562	-0.674751	-1.611851
10	1	0	4.428674	0.724341	-0.628211
11	6	0	2.233576	0.388977	-0.742915
12	6	0	2.024384	1.760781	-0.133506
13	1	0	1.875369	0.400693	-1.782144
14	1	0	2.899671	2.410135	-0.149508
15	6	0	0.909131	2.257381	0.404746
16	6	0	-0.458465	1.632810	0.553063
17	1	0	0.971969	3.269237	0.806388
18	1	0	-0.651991	1.488888	1.626952
19	1	0	-1.193425	2.380867	0.222309
20	6	0	-0.704736	0.306045	-0.194659
21	1	0	-0.497612	0.491590	-1.261125
22	14	0	-2.517185	-0.257171	-0.103881
23	6	0	-2.995055	-0.546761	1.698337
24	1	0	-2.953512	0.384026	2.275312
25	1	0	-4.014912	-0.940052	1.777092
26	1	0	-2.325360	-1.266998	2.181946
27	6	0	-2.688309	-1.860491	-1.081122
28	1	0	-3.702555	-2.268396	-1.004784
29	1	0	-2.473349	-1.697512	-2.143423
30	1	0	-1.992591	-2.624607	-0.716753
31	6	0	-3.634978	1.064567	-0.852776
32	1	0	-3.349146	1.286620	-1.887357
33	1	0	-4.678901	0.730605	-0.862533
34	1	0	-3.594643	2.001388	-0.286028

Zero-point correction= 0.297023 (Hartree/Particle)
Thermal correction to Energy= 0.313248
Thermal correction to Enthalpy= 0.314193
Thermal correction to Gibbs Free Energy= 0.253588
Sum of electronic and zero-point Energies= -833.541725
Sum of electronic and thermal Energies= -833.525500
Sum of electronic and thermal Enthalpies= -833.524556
Sum of electronic and thermal Free Energies= -833.585160
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -834.0183352

COD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.185621	1.245584	-0.501056
2	6	0	-0.040590	1.693928	-0.224375
3	6	0	-1.095441	1.085551	0.669446
4	6	0	-1.915647	-0.020086	-0.016410
5	6	0	-1.185624	-1.245540	-0.501157
6	6	0	0.040592	-1.693906	-0.224529
7	6	0	1.095443	-1.085605	0.669342

8	6	0	1.915646	0.020078	-0.016444
9	1	0	1.778508	1.853202	-1.185382
10	1	0	-0.344226	2.611636	-0.727405
11	1	0	-1.794923	1.875969	0.965010
12	1	0	-0.664974	0.712772	1.601029
13	1	0	-2.718396	-0.338862	0.665018
14	1	0	-2.429271	0.420059	-0.882334
15	1	0	-1.778513	-1.853092	-1.185539
16	1	0	0.344234	-2.611560	-0.727653
17	1	0	1.794922	-1.876049	0.964847
18	1	0	0.664980	-0.712888	1.600950
19	1	0	2.718423	0.338788	0.664982
20	1	0	2.429235	-0.419999	-0.882424

Zero-point correction= 0.183377 (Hartree/Particle)
Thermal correction to Energy= 0.190717
Thermal correction to Enthalpy= 0.191661
Thermal correction to Gibbs Free Energy= 0.151932
Sum of electronic and zero-point Energies= -311.749877
Sum of electronic and thermal Energies= -311.742536
Sum of electronic and thermal Enthalpies= -311.741592
Sum of electronic and thermal Free Energies= -311.781321
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -312.0220746

Ni(0)(COD)$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.350070	-1.531629	-0.605797
2	6	0	1.493749	-0.468158	-1.471218
3	6	0	2.594468	0.578166	-1.415075
4	6	0	2.202404	1.829266	-0.606834
5	6	0	1.350460	1.531209	0.606285
6	6	0	1.494002	0.467610	1.471450
7	6	0	2.594575	-0.578749	1.415273
8	6	0	2.202110	-1.829843	0.607212
9	1	0	0.741672	-2.365854	-0.951085
10	1	0	0.965470	-0.539145	-2.418568
11	1	0	2.844487	0.883095	-2.437384
12	1	0	3.507875	0.132144	-1.010075
13	1	0	3.105599	2.388666	-0.318348
14	1	0	1.625392	2.498082	-1.256916
15	1	0	0.741918	2.365348	0.951491
16	1	0	0.965268	0.538323	2.418728
17	1	0	2.844817	-0.883404	2.437770
18	1	0	3.507910	-0.132784	1.009932
19	1	0	3.105150	-2.389373	0.318640
20	1	0	1.625161	-2.498490	1.257359
21	6	0	-1.350939	-1.531641	0.606617
22	6	0	-1.494280	-0.468047	1.471752
23	6	0	-2.594170	0.579093	1.415390
24	6	0	-2.201259	1.829826	0.606856
25	6	0	-1.349265	1.531167	-0.606195
26	6	0	-1.493105	0.467387	-1.471498
27	6	0	-2.594395	-0.578361	-1.414952
28	6	0	-2.202256	-1.829550	-0.607021
29	1	0	-0.742425	-2.365817	0.951816
30	1	0	-0.965583	-0.538824	2.418886
31	1	0	-2.843886	0.884333	2.437789
32	1	0	-3.507911	0.133643	1.010550
33	1	0	-3.104135	2.389836	0.318410
34	1	0	-1.623841	2.498356	1.256982
35	1	0	-0.741427	2.365574	-0.952017
36	1	0	-0.965628	0.538344	-2.419117
37	1	0	-2.845114	-0.883171	-2.437151
38	1	0	-3.507417	-0.132080	-1.009477

39	1	0	-3.105319	-2.389593	-0.319300
40	1	0	-1.624543	-2.497741	-1.257204
41	28	0	-0.000589	0.000502	-0.000542

Zero-point correction= 0.370756 (Hartree/Particle)
Thermal correction to Energy= 0.386672
Thermal correction to Enthalpy= 0.387617
Thermal correction to Gibbs Free Energy= 0.329870
Sum of electronic and zero-point Energies= -792.850510
Sum of electronic and thermal Energies= -792.834594
Sum of electronic and thermal Enthalpies= -792.833650
Sum of electronic and thermal Free Energies= -792.891396
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -795.0322277

INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448510	-0.286601	1.623121
2	6	0	-0.836444	0.810187	1.069684
3	6	0	-1.539845	1.972190	0.398676
4	6	0	-1.693113	1.787024	-1.128207
5	6	0	-1.986550	0.367903	-1.562880
6	6	0	-2.803756	-0.529848	-0.927489
7	6	0	-3.646761	-0.240044	0.298467
8	6	0	-2.928729	-0.597946	1.618287
9	1	0	-0.847329	-0.918305	2.274920
10	1	0	0.220343	0.958821	1.284526
11	1	0	-0.956754	2.881340	0.579486
12	1	0	-2.515025	2.138523	0.864771
13	1	0	-2.462873	2.474175	-1.508728
14	1	0	-0.754077	2.083178	-1.609569
15	1	0	-1.619722	0.100367	-2.551471
16	1	0	-3.003096	-1.470248	-1.437673
17	1	0	-4.574185	-0.819623	0.237518
18	1	0	-3.950895	0.810222	0.300179
19	1	0	-3.429206	-0.098266	2.460664
20	1	0	-3.036830	-1.674131	1.793624
21	28	0	-0.758021	-0.813290	-0.301127
22	6	0	0.831996	-1.782072	-0.149452
23	6	0	0.338105	-1.955124	-1.314427
24	1	0	0.442959	-2.420727	-2.282691
25	6	0	1.902081	-1.947217	0.867946
26	1	0	1.835511	-1.127705	1.599077
27	1	0	1.746470	-2.885828	1.409253
28	8	0	3.214883	-2.026140	0.346787
29	6	0	3.572405	-0.931986	-0.477892
30	1	0	2.984488	-0.942504	-1.406477
31	1	0	4.621938	-1.109578	-0.734715
32	6	0	3.415532	0.399285	0.201645
33	6	0	2.600330	1.362250	-0.243318
34	1	0	3.992325	0.552101	1.114581
35	1	0	2.007719	1.180723	-1.140962
36	6	0	2.430485	2.659382	0.405204
37	6	0	1.653872	3.636941	-0.072244
38	1	0	2.980768	2.815794	1.332761
39	1	0	1.552819	4.589264	0.438599
40	1	0	1.103580	3.517704	-1.003124

Zero-point correction= 0.346705 (Hartree/Particle)
Thermal correction to Energy= 0.365548
Thermal correction to Enthalpy= 0.366492
Thermal correction to Gibbs Free Energy= 0.299967
Sum of electronic and zero-point Energies= -866.770351
Sum of electronic and thermal Energies= -866.751508
Sum of electronic and thermal Enthalpies= -866.750564

Sum of electronic and thermal Free Energies= -866.817089
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -868.964955

INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.250617	1.416969	-1.521219
2	6	0	-0.044553	1.052056	-1.883430
3	6	0	-1.314298	1.868789	-1.668947
4	6	0	-1.932416	1.856756	-0.259708
5	6	0	-1.056110	2.152645	0.930426
6	6	0	0.059223	2.883018	1.002922
7	6	0	0.740180	3.595466	-0.135198
8	6	0	1.732800	2.732707	-0.939377
9	1	0	2.038318	0.922067	-2.094702
10	1	0	-0.114641	0.339965	-2.704166
11	1	0	-2.082308	1.475186	-2.345625
12	1	0	-1.144836	2.897264	-2.005032
13	1	0	-2.790733	2.545017	-0.246855
14	1	0	-2.359657	0.863226	-0.093850
15	1	0	-1.413707	1.702828	1.856746
16	1	0	0.547303	2.959991	1.975139
17	1	0	1.299021	4.450227	0.264528
18	1	0	-0.004029	4.022052	-0.811447
19	1	0	2.103213	3.349492	-1.772096
20	1	0	2.620865	2.544331	-0.319503
21	6	0	-0.859946	-1.379475	-0.595518
22	6	0	-0.306978	-1.588889	0.520129
23	1	0	-0.241127	-2.149694	1.441658
24	6	0	-1.876307	-1.633935	-1.641870
25	1	0	-2.506497	-0.737401	-1.743377
26	1	0	-1.384784	-1.797008	-2.605803
27	8	0	-2.676863	-2.780376	-1.434114
28	6	0	-3.413908	-2.770247	-0.225207
29	1	0	-2.737465	-2.776343	0.640428
30	1	0	-3.966237	-3.715739	-0.231045
31	6	0	-4.361353	-1.609018	-0.122364
32	6	0	-4.283866	-0.674788	0.831968
33	1	0	-5.127809	-1.537056	-0.894632
34	1	0	-3.492446	-0.747040	1.579966
35	6	0	-5.179167	0.473621	0.936416
36	6	0	-5.057571	1.429245	1.862111
37	1	0	-5.976384	0.537918	0.196481
38	1	0	-5.736759	2.274943	1.901680
39	1	0	-4.270759	1.395125	2.612380
40	28	0	0.566258	-0.092214	-0.301973
41	6	0	2.181370	0.100200	1.004946
42	7	0	1.775300	-0.412005	2.167748
43	7	0	1.425292	-0.905252	3.116876
44	1	0	2.340941	1.170121	1.135575
45	14	0	3.562396	-0.895655	0.137486
46	6	0	4.448014	-1.906637	1.460988
47	1	0	3.778496	-2.639005	1.927666
48	1	0	5.280803	-2.465026	1.017886
49	1	0	4.855236	-1.270025	2.254668
50	6	0	2.944264	-2.067579	-1.191882
51	1	0	2.484051	-1.531371	-2.027358
52	1	0	3.781786	-2.662298	-1.579130
53	1	0	2.188451	-2.751559	-0.792792
54	6	0	4.727055	0.393229	-0.584217
55	1	0	4.237423	0.998744	-1.353908
56	1	0	5.104473	1.070670	0.189861
57	1	0	5.589490	-0.099420	-1.048162

Zero-point correction= 0.485326 (Hartree/Particle)

Thermal correction to Energy= 0.516260
Thermal correction to Enthalpy= 0.517204
Thermal correction to Gibbs Free Energy= 0.422680
Sum of electronic and zero-point Energies= -1423.947430
Sum of electronic and thermal Energies= -1423.916496
Sum of electronic and thermal Enthalpies= -1423.915552
Sum of electronic and thermal Free Energies= -1424.010076
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1426.383797

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.243152	1.458856	-1.393361
2	6	0	-0.044983	1.092597	-1.796157
3	6	0	-1.321838	1.898950	-1.583086
4	6	0	-1.972102	1.858957	-0.188481
5	6	0	-1.123502	2.123789	1.028744
6	6	0	-0.010724	2.850740	1.143510
7	6	0	0.686387	3.596813	0.038544
8	6	0	1.703145	2.762244	-0.763464
9	1	0	2.038072	1.003599	-1.986454
10	1	0	-0.084883	0.428540	-2.657916
11	1	0	-2.074266	1.519294	-2.284709
12	1	0	-1.147868	2.934707	-1.893873
13	1	0	-2.828780	2.549282	-0.183432
14	1	0	-2.407376	0.864163	-0.054194
15	1	0	-1.495609	1.642714	1.933292
16	1	0	0.465801	2.892256	2.122831
17	1	0	1.230823	4.445256	0.470416
18	1	0	-0.047253	4.034814	-0.642077
19	1	0	2.081670	3.399695	-1.576564
20	1	0	2.576753	2.563610	-0.129308
21	6	0	-0.933239	-1.345904	-0.643068
22	6	0	-0.363327	-1.638186	0.443051
23	1	0	-0.257722	-2.251108	1.327416
24	6	0	-1.959935	-1.544861	-1.690561
25	1	0	-2.587026	-0.643097	-1.748808
26	1	0	-1.475031	-1.667900	-2.663783
27	8	0	-2.763742	-2.696080	-1.527500
28	6	0	-3.503431	-2.727947	-0.320427
29	1	0	-2.828598	-2.754934	0.546267
30	1	0	-4.048728	-3.676739	-0.355845
31	6	0	-4.458262	-1.575926	-0.187027
32	6	0	-4.381893	-0.660874	0.785812
33	1	0	-5.226387	-1.490414	-0.956238
34	1	0	-3.589354	-0.745776	1.531420
35	6	0	-5.279978	0.482877	0.914167
36	6	0	-5.155916	1.423950	1.854289
37	1	0	-6.081025	0.557081	0.179307
38	1	0	-5.837083	2.267098	1.910564
39	1	0	-4.364748	1.380772	2.599501
40	28	0	0.559781	-0.122821	-0.255160
41	6	0	2.109406	0.053746	0.768477
42	7	0	1.900737	-0.911633	2.304243
43	7	0	1.496022	-1.704281	2.964787
44	1	0	2.295595	0.975651	1.332716
45	14	0	3.698694	-0.746371	0.055294
46	6	0	4.743930	-1.592117	1.382522
47	1	0	4.235316	-2.457879	1.820907
48	1	0	5.680861	-1.953933	0.942459
49	1	0	5.002127	-0.902557	2.194367
50	6	0	3.207065	-2.008311	-1.247190
51	1	0	2.693106	-1.525272	-2.085378
52	1	0	4.080703	-2.542050	-1.639857
53	1	0	2.511118	-2.743411	-0.827614

54	6	0	4.730981	0.640124	-0.702501
55	1	0	4.205757	1.165777	-1.505914
56	1	0	5.020068	1.380364	0.052142
57	1	0	5.651402	0.221511	-1.127243

Zero-point correction= 0.482668 (Hartree/Particle)
Thermal correction to Energy= 0.513751
Thermal correction to Enthalpy= 0.514695
Thermal correction to Gibbs Free Energy= 0.419985
Sum of electronic and zero-point Energies= -1423.919761
Sum of electronic and thermal Energies= -1423.888678
Sum of electronic and thermal Enthalpies= -1423.887734
Sum of electronic and thermal Free Energies= -1423.982444
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1426.3563317

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460837	1.169865	-1.407839
2	6	0	0.183692	0.829472	-1.872101
3	6	0	-1.049140	1.726630	-1.848394
4	6	0	-1.799915	1.892262	-0.512599
5	6	0	-1.027868	2.238908	0.734708
6	6	0	0.118427	2.908792	0.859996
7	6	0	0.940804	3.482313	-0.260950
8	6	0	1.958685	2.501182	-0.869175
9	1	0	2.273516	0.598384	-1.858587
10	1	0	0.172132	0.080592	-2.661528
11	1	0	-1.772358	1.308745	-2.558908
12	1	0	-0.786859	2.706359	-2.261956
13	1	0	-2.596723	2.637683	-0.655645
14	1	0	-2.319984	0.952992	-0.300946
15	1	0	-1.499522	1.882283	1.649307
16	1	0	0.527634	3.028926	1.862677
17	1	0	1.506277	4.343636	0.114208
18	1	0	0.291380	3.875261	-1.046483
19	1	0	2.449555	3.013551	-1.710476
20	1	0	2.751141	2.310506	-0.136126
21	6	0	-0.930320	-1.426368	-0.544095
22	6	0	-0.385090	-1.740464	0.548691
23	1	0	-0.282781	-2.337955	1.436015
24	6	0	-1.970420	-1.617389	-1.581168
25	1	0	-2.534036	-0.679961	-1.690010
26	1	0	-1.492418	-1.821230	-2.544258
27	8	0	-2.853950	-2.698078	-1.365953
28	6	0	-3.538067	-2.664653	-0.126265
29	1	0	-2.837845	-2.835523	0.703160
30	1	0	-4.226472	-3.514997	-0.168637
31	6	0	-4.292607	-1.386520	0.106760
32	6	0	-4.027048	-0.551715	1.117819
33	1	0	-5.073845	-1.141019	-0.613251
34	1	0	-3.220285	-0.800123	1.808838
35	6	0	-4.724999	0.707982	1.356538
36	6	0	-4.435050	1.535864	2.364347
37	1	0	-5.513293	0.970737	0.651816
38	1	0	-4.963199	2.473323	2.505407
39	1	0	-3.655986	1.297591	3.085132
40	28	0	0.620154	-0.268722	-0.175410
41	6	0	2.000330	-0.076081	0.903445
42	1	0	1.969035	0.646841	1.734483
43	14	0	3.648796	-0.951468	0.656252
44	6	0	4.122572	-1.825862	2.263108
45	1	0	3.365198	-2.562885	2.552146
46	1	0	5.075703	-2.355460	2.148082
47	1	0	4.230724	-1.111581	3.086908

48	6	0	3.508081	-2.205930	-0.739573
49	1	0	3.248348	-1.713342	-1.683674
50	1	0	4.446398	-2.752593	-0.890683
51	1	0	2.715960	-2.931071	-0.522864
52	6	0	4.958796	0.341491	0.215731
53	1	0	4.717550	0.847631	-0.726051
54	1	0	5.048810	1.105922	0.995671
55	1	0	5.940171	-0.132505	0.093890

Zero-point correction= 0.474998 (Hartree/Particle)
Thermal correction to Energy= 0.504014
Thermal correction to Enthalpy= 0.504959
Thermal correction to Gibbs Free Energy= 0.414405
Sum of electronic and zero-point Energies= -1314.462190
Sum of electronic and thermal Energies= -1314.433174
Sum of electronic and thermal Enthalpies= -1314.432229
Sum of electronic and thermal Free Energies= -1314.522783
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.8630004

INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432590	1.331743	-1.855417
2	6	0	-1.473269	1.320379	-0.976797
3	6	0	-1.910121	2.465496	-0.092719
4	6	0	-1.277503	2.387315	1.308597
5	6	0	0.185922	2.015788	1.314218
6	6	0	1.137166	2.353732	0.397980
7	6	0	0.956027	3.235378	-0.818870
8	6	0	0.556319	2.448350	-2.087185
9	1	0	-0.354200	0.499927	-2.551322
10	1	0	-2.139652	0.460982	-0.990617
11	1	0	-2.997245	2.415877	0.020907
12	1	0	-1.688803	3.423429	-0.569010
13	1	0	-1.426747	3.336677	1.842510
14	1	0	-1.812656	1.624287	1.885686
15	1	0	0.534221	1.524561	2.220383
16	1	0	2.162178	2.083322	0.634589
17	1	0	1.902569	3.747943	-1.019134
18	1	0	0.226347	4.020694	-0.607217
19	1	0	0.165996	3.145116	-2.842368
20	1	0	1.455889	1.999273	-2.520423
21	6	0	0.072160	-1.472499	-0.589017
22	6	0	0.694307	-1.984399	0.475898
23	1	0	0.640731	-2.998057	0.891217
24	6	0	-0.882883	-2.132267	-1.532286
25	1	0	-1.645288	-1.414335	-1.874639
26	1	0	-0.346406	-2.466086	-2.428116
27	8	0	-1.525629	-3.307430	-1.051324
28	6	0	-2.333029	-3.112599	0.089087
29	1	0	-1.726630	-2.845794	0.965308
30	1	0	-2.790117	-4.090919	0.277595
31	6	0	-3.407625	-2.078893	-0.099377
32	6	0	-3.599319	-1.054373	0.739678
33	1	0	-4.057976	-2.204039	-0.966248
34	1	0	-2.926519	-0.936399	1.590838
35	6	0	-4.661034	-0.061846	0.599632
36	6	0	-4.877457	0.930552	1.469181
37	1	0	-5.306709	-0.160602	-0.272809
38	1	0	-5.680836	1.647258	1.330976
39	1	0	-4.261714	1.048839	2.358419
40	28	0	0.325874	0.336232	-0.058607
41	6	0	1.479173	-0.839827	1.032414
42	1	0	1.360909	-0.676146	2.114732
43	14	0	3.263566	-0.757283	0.476687

44	6	0	4.023658	-2.489716	0.466687
45	1	0	3.491586	-3.136359	-0.240736
46	1	0	5.080648	-2.468015	0.175419
47	1	0	3.955823	-2.956914	1.456232
48	6	0	3.444682	-0.048241	-1.268352
49	1	0	3.246045	1.030040	-1.287035
50	1	0	4.453897	-0.210479	-1.665863
51	1	0	2.726359	-0.532770	-1.939723
52	6	0	4.260043	0.310804	1.685465
53	1	0	3.841835	1.317401	1.807707
54	1	0	4.281588	-0.154818	2.677997
55	1	0	5.297749	0.423751	1.349802

Zero-point correction= 0.478107 (Hartree/Particle)
Thermal correction to Energy= 0.506039
Thermal correction to Enthalpy= 0.506984
Thermal correction to Gibbs Free Energy= 0.420279
Sum of electronic and zero-point Energies= -1314.547855
Sum of electronic and thermal Energies= -1314.519922
Sum of electronic and thermal Enthalpies= -1314.518978
Sum of electronic and thermal Free Energies= -1314.605683
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9453197

TS1a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.558914	-1.124719	-0.110722
2	6	0	1.393849	0.661743	-1.294117
3	6	0	1.038598	-0.377668	-1.931896
4	1	0	0.511753	-0.657032	-2.829763
5	6	0	1.179416	2.119206	-1.016677
6	1	0	1.638666	2.689144	-1.843364
7	1	0	0.112074	2.353037	-0.982333
8	8	0	1.718890	2.510096	0.216136
9	6	0	3.043089	1.995531	0.334958
10	1	0	3.327161	2.161520	1.377397
11	1	0	3.723629	2.571684	-0.309820
12	6	0	3.050333	0.541022	-0.052532
13	6	0	2.561268	-0.428223	0.823143
14	1	0	3.730942	0.227737	-0.838512
15	1	0	2.097356	-0.098158	1.754719
16	6	0	2.391042	-1.783666	0.429759
17	6	0	1.369693	-2.566537	1.015522
18	1	0	2.944799	-2.153978	-0.428138
19	1	0	1.224302	-3.588605	0.672979
20	1	0	1.070599	-2.381041	2.046405
21	6	0	-1.137520	-0.746540	1.034173
22	6	0	-1.505924	-1.211578	-0.214335
23	6	0	-2.111488	-0.414921	-1.345352
24	6	0	-3.638479	-0.260785	-1.202688
25	6	0	-4.177293	0.312714	0.086059
26	6	0	-3.583828	1.103366	0.983240
27	6	0	-2.178111	1.644901	0.940723
28	6	0	-1.120830	0.689058	1.534289
29	1	0	-1.076127	-1.495206	1.820308
30	1	0	-1.679207	-2.286965	-0.285580
31	1	0	-1.920660	-0.942747	-2.287236
32	1	0	-1.625669	0.556247	-1.451415
33	1	0	-4.011744	0.337784	-2.047075
34	1	0	-4.091461	-1.253261	-1.331382
35	1	0	-5.210106	0.031014	0.291106
36	1	0	-4.167007	1.380489	1.861015
37	1	0	-2.134640	2.577756	1.514582
38	1	0	-1.907727	1.918206	-0.081583
39	1	0	-0.133616	1.146771	1.382430

40	1	0	-1.266921	0.651225	2.620801

Zero-point correction= 0.160826 (Hartree/Particle)
Thermal correction to Energy= 0.169860
Thermal correction to Enthalpy= 0.170804
Thermal correction to Gibbs Free Energy= 0.126461
Sum of electronic and zero-point Energies= -554.943198
Sum of electronic and thermal Energies= -554.934164
Sum of electronic and thermal Enthalpies= -554.933219
Sum of electronic and thermal Free Energies= -554.977562
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -868.9072278

INT3a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.969292	-0.167023	0.145980
2	6	0	0.831035	0.570400	0.682100
3	1	0	1.188475	1.405782	1.305465
4	6	0	1.724531	-1.421878	-0.680876
5	1	0	0.888211	-1.976326	-0.226263
6	1	0	1.490209	-1.221853	-1.731387
7	8	0	2.924404	-2.178001	-0.648441
8	6	0	3.547222	-1.942370	0.601770
9	1	0	4.616097	-2.140847	0.475184
10	1	0	3.150491	-2.614141	1.379646
11	6	0	3.225529	-0.502733	0.950425
12	6	0	3.342660	0.480657	-0.165531
13	1	0	3.318659	-0.166515	1.978678
14	1	0	3.797405	0.103876	-1.081206
15	6	0	3.600926	1.909810	0.105628
16	6	0	4.273326	2.711516	-0.718912
17	1	0	3.226592	2.310469	1.046674
18	1	0	4.451722	3.754807	-0.477776
19	1	0	4.671697	2.350131	-1.664333
20	6	0	-2.317803	1.529527	-0.753586
21	6	0	-1.903201	0.466411	-1.509361
22	6	0	-2.655891	-0.834136	-1.695888
23	6	0	-2.293627	-1.912721	-0.642519
24	6	0	-2.049216	-1.382522	0.752486
25	6	0	-2.745878	-0.376028	1.367381
26	6	0	-3.959946	0.333183	0.808006
27	6	0	-3.588356	1.630733	0.058889
28	1	0	-1.757611	2.457585	-0.860708
29	1	0	-1.034141	0.616608	-2.145828
30	1	0	-2.428691	-1.236697	-2.688404
31	1	0	-3.732350	-0.642903	-1.689076
32	1	0	-3.081923	-2.678597	-0.625093
33	1	0	-1.379323	-2.422842	-0.964443
34	1	0	-1.356174	-1.963594	1.356544
35	1	0	-2.515245	-0.181945	2.414102
36	1	0	-4.636289	0.587212	1.631412
37	1	0	-4.524131	-0.340564	0.157299
38	1	0	-4.426843	1.951946	-0.576277
39	1	0	-3.442429	2.428161	0.796459
40	28	0	-0.924402	0.374546	0.412176

Zero-point correction= 0.727161 (Hartree/Particle)
Thermal correction to Energy= 0.777482
Thermal correction to Enthalpy= 0.778426
Thermal correction to Gibbs Free Energy= 0.641933
Sum of electronic and zero-point Energies= -3770.251861
Sum of electronic and thermal Energies= -3770.201540
Sum of electronic and thermal Enthalpies= -3770.200596
Sum of electronic and thermal Free Energies= -3770.337089

ω B97XD /6-311++G(2d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chlorobenzene solvent = -3773.2743528

TS1a″

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.571195	-0.872434	-0.595246
2	6	0	-0.727638	-0.925647	-1.627119
3	1	0	-0.803189	-0.510539	-2.627663
4	6	0	-1.886542	-1.822734	0.569803
5	1	0	-1.898687	-2.838082	0.148261
6	1	0	-1.177175	-1.804218	1.400347
7	8	0	-3.147560	-1.482698	1.105047
8	6	0	-3.899757	-0.881099	0.074883
9	1	0	-4.762226	-0.397030	0.538605
10	1	0	-4.251390	-1.629183	-0.652835
11	6	0	-2.945087	0.097762	-0.599468
12	6	0	-2.469143	1.172105	0.200601
13	1	0	-3.176701	0.335419	-1.637888
14	1	0	-2.507129	1.059873	1.282504
15	6	0	-1.853157	2.332266	-0.353947
16	6	0	-1.375006	3.384798	0.345029
17	1	0	-1.773036	2.358024	-1.441923
18	1	0	-0.947790	4.249717	-0.151905
19	1	0	-1.441722	3.422497	1.430128
20	6	0	2.316030	-1.017138	-1.121390
21	6	0	2.178864	0.332575	-1.370265
22	6	0	2.789332	1.443267	-0.541087
23	6	0	1.873812	1.928504	0.610138
24	6	0	1.055807	0.840640	1.269315
25	6	0	1.490654	-0.413601	1.598594
26	6	0	2.893467	-0.941522	1.387142
27	6	0	3.058432	-1.661153	0.029865
28	1	0	2.034944	-1.698925	-1.920705
29	1	0	1.769598	0.618756	-2.336856
30	1	0	3.004840	2.296722	-1.192252
31	1	0	3.755138	1.114301	-0.145952
32	1	0	2.481035	2.451942	1.363435
33	1	0	1.164736	2.660688	0.213252
34	1	0	0.082129	1.152636	1.642454
35	1	0	0.829723	-1.033273	2.203294
36	1	0	3.136675	-1.647990	2.187736
37	1	0	3.614167	-0.124104	1.477756
38	1	0	4.127175	-1.756598	-0.211659
39	1	0	2.674899	-2.682917	0.128501
40	28	0	0.488258	-0.418417	-0.349932

Zero-point correction= 0.344231 (Hartree/Particle)
Thermal correction to Energy= 0.362283
Thermal correction to Enthalpy= 0.363228
Thermal correction to Gibbs Free Energy= 0.298902
Sum of electronic and zero-point Energies= -866.705862
Sum of electronic and thermal Energies= -866.687810
Sum of electronic and thermal Enthalpies= -866.686866
Sum of electronic and thermal Free Energies= -866.751192
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -868.8943343

INT3a″

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.242245	-0.884048	-0.243297
2	6	0	-2.057089	1.139727	0.292534
3	6	0	-0.782230	0.956590	-0.088641
4	1	0	-0.184401	1.850432	-0.305119

5	6	0	-2.958507	2.349190	0.384501
6	1	0	-2.846278	2.906708	1.322708
7	1	0	-2.792663	3.046654	-0.449521
8	8	0	-4.288889	1.830328	0.348892
9	6	0	-4.252982	0.482147	-0.095725
10	1	0	-4.252948	0.428579	-1.198211
11	1	0	-5.154509	-0.010373	0.278125
12	6	0	-2.938721	-0.071554	0.458641
13	6	0	-2.221194	-1.174664	-0.282572
14	1	0	-3.071151	-0.335982	1.517415
15	1	0	-2.360338	-1.192102	-1.365975
16	6	0	-1.608552	-2.282784	0.334233
17	6	0	-0.586155	-2.963269	-0.342341
18	1	0	-1.690601	-2.389319	1.416270
19	1	0	0.002709	-3.709567	0.182700
20	1	0	-0.628373	-3.071520	-1.426406
21	6	0	1.729941	-0.635457	-1.055945
22	6	0	1.836592	-1.003338	0.259779
23	6	0	2.110171	-0.128581	1.457407
24	6	0	3.613579	0.054109	1.722132
25	6	0	4.443212	0.683355	0.632223
26	6	0	4.074685	1.392451	-0.437587
27	6	0	2.687879	1.782424	-0.892288
28	6	0	1.995362	0.693109	-1.726888
29	1	0	1.666558	-1.466382	-1.760941
30	1	0	1.915181	-2.071475	0.453193
31	1	0	1.668026	-0.612349	2.336241
32	1	0	1.604592	0.831745	1.364857
33	1	0	3.737235	0.637177	2.646070
34	1	0	4.050705	-0.929900	1.942258
35	1	0	5.513801	0.523432	0.761275
36	1	0	4.877085	1.723193	-1.096637
37	1	0	2.771229	2.671872	-1.527336
38	1	0	2.056135	2.078133	-0.053364
39	1	0	1.060669	1.088130	-2.140507
40	1	0	2.635369	0.472898	-2.592686

Zero-point correction= 0.347921 (Hartree/Particle)
Thermal correction to Energy= 0.365754
Thermal correction to Enthalpy= 0.366698
Thermal correction to Gibbs Free Energy= 0.301258
Sum of electronic and zero-point Energies= -866.742897
Sum of electronic and thermal Energies= -866.725064
Sum of electronic and thermal Enthalpies= -866.724120
Sum of electronic and thermal Free Energies= -866.789560
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -868.934295

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.854521	-1.433214	-0.285862
2	6	0	-0.289548	-1.829950	-0.823288
3	1	0	-0.641295	-2.837225	-1.074055
4	6	0	2.083434	-2.147705	0.173438
5	1	0	2.060265	-2.272678	1.270497
6	1	0	2.142571	-3.143553	-0.279484
7	8	0	3.298672	-1.507124	-0.188227
8	6	0	3.496272	-0.267406	0.445740
9	1	0	4.536923	0.003522	0.238845
10	1	0	3.375060	-0.363477	1.537982
11	6	0	2.570879	0.799226	-0.078957
12	6	0	1.854159	1.642122	0.749240
13	1	0	2.654438	0.989435	-1.148178
14	1	0	1.973620	1.535226	1.825933
15	6	0	0.730765	2.443292	0.305138

16	6	0	0.232724	2.434315	-0.974878
17	1	0	0.125494	2.891190	1.089880
18	1	0	-0.727064	2.895367	-1.178211
19	1	0	0.826979	2.169929	-1.845535
20	28	0	0.497662	0.411980	-0.181007
21	6	0	-1.040400	-0.526656	-0.964632
22	1	0	-1.173116	-0.198575	-2.003738
23	14	0	-2.527854	-0.255467	0.133050
24	6	0	-3.884637	-1.526236	-0.227521
25	1	0	-3.496120	-2.546564	-0.125921
26	1	0	-4.728298	-1.421119	0.465255
27	1	0	-4.271595	-1.417725	-1.247395
28	6	0	-2.004685	-0.444551	1.940342
29	1	0	-1.281911	0.331645	2.223875
30	1	0	-2.858087	-0.377537	2.625289
31	1	0	-1.517616	-1.414215	2.095014
32	6	0	-3.234779	1.480516	-0.127628
33	1	0	-2.556359	2.245214	0.268497
34	1	0	-3.390573	1.688125	-1.193154
35	1	0	-4.199514	1.598577	0.379149

Zero-point correction= 0.293202 (Hartree/Particle)
Thermal correction to Energy= 0.311757
Thermal correction to Enthalpy= 0.312701
Thermal correction to Gibbs Free Energy= 0.247641
Sum of electronic and zero-point Energies= -1002.774310
Sum of electronic and thermal Energies= -1002.755755
Sum of electronic and thermal Enthalpies= -1002.754811
Sum of electronic and thermal Free Energies= -1002.819871
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.902548

INT4a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.455218	1.169255	-0.691894
2	6	0	0.484536	1.871820	-1.371523
3	6	0	0.095257	3.309620	-1.088155
4	6	0	-1.116643	3.426186	-0.140640
5	6	0	-1.165284	2.350819	0.921063
6	6	0	-0.115111	1.893452	1.671488
7	6	0	1.309648	2.406046	1.572335
8	6	0	2.188746	1.651232	0.539281
9	1	0	1.869044	0.278870	-1.156449
10	1	0	0.144868	1.455462	-2.319429
11	1	0	-0.146129	3.808384	-2.033183
12	1	0	0.955032	3.849119	-0.678996
13	1	0	-1.138315	4.423868	0.322252
14	1	0	-2.033997	3.344553	-0.732850
15	1	0	-2.162658	2.030358	1.219123
16	1	0	-0.341276	1.245003	2.514906
17	1	0	1.785382	2.319487	2.554671
18	1	0	1.290688	3.475160	1.340473
19	1	0	3.036057	2.288700	0.248985
20	1	0	2.632435	0.771920	1.017794
21	6	0	-0.308317	-1.289244	0.314510
22	6	0	-1.091856	-2.328038	-0.352515
23	1	0	-0.567181	-3.259517	-0.586574
24	6	0	0.775227	-1.862124	1.203997
25	1	0	1.572364	-1.126840	1.377952
26	1	0	0.295349	-2.044247	2.176823
27	8	0	1.352596	-3.108331	0.830620
28	6	0	2.269104	-2.996311	-0.237672
29	1	0	1.796338	-2.544021	-1.125131
30	1	0	2.537664	-4.028118	-0.492775
31	6	0	3.501271	-2.220308	0.138124
32	6	0	4.072208	-1.286465	-0.629701

33	1	0	3.932328	-2.467236	1.108992
34	1	0	3.630190	-1.049696	-1.598827
35	6	0	5.259699	-0.523540	-0.257779
36	6	0	5.775418	0.459058	-1.001851
37	1	0	5.723575	-0.779281	0.694494
38	1	0	6.653039	1.013804	-0.685727
39	1	0	5.334122	0.738208	-1.956127
40	28	0	-0.357518	0.499159	0.062147
41	6	0	-2.413514	-2.265259	-0.628022
42	1	0	-2.844197	-3.159513	-1.086557
43	14	0	-3.604639	-0.858467	-0.263879
44	6	0	-5.328184	-1.456119	-0.754364
45	1	0	-5.626725	-2.333665	-0.168915
46	1	0	-6.079082	-0.675005	-0.586693
47	1	0	-5.368242	-1.732587	-1.814599
48	6	0	-3.630472	-0.412903	1.569322
49	1	0	-2.616139	-0.221629	1.932968
50	1	0	-4.245902	0.476355	1.754666
51	1	0	-4.051596	-1.238126	2.155103
52	6	0	-3.186539	0.637199	-1.338927
53	1	0	-3.775338	1.516057	-1.048823
54	1	0	-2.123218	0.908359	-1.268405
55	1	0	-3.396286	0.418282	-2.392369

Zero-point correction= 0.476486 (Hartree/Particle)
Thermal correction to Energy= 0.504688
Thermal correction to Enthalpy= 0.505632
Thermal correction to Gibbs Free Energy= 0.417509
Sum of electronic and zero-point Energies= -1314.520926
Sum of electronic and thermal Energies= -1314.492724
Sum of electronic and thermal Enthalpies= -1314.491780
Sum of electronic and thermal Free Energies= -1314.579903
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9136005

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.205298	-1.236847	-0.159887
2	6	0	-0.115703	-1.573746	-0.136519
3	1	0	-0.481336	-2.446659	0.424049
4	6	0	2.366701	-2.021216	0.344395
5	1	0	2.525972	-1.873667	1.428120
6	1	0	2.216388	-3.088156	0.158571
7	8	0	3.539024	-1.651928	-0.355582
8	6	0	3.732566	-0.275197	-0.178249
9	1	0	4.535569	0.020456	-0.859368
10	1	0	4.063198	-0.075217	0.855620
11	6	0	2.493350	0.558907	-0.465424
12	6	0	2.130350	1.532268	0.529213
13	1	0	2.323019	0.778259	-1.516491
14	1	0	2.640642	1.475223	1.488108
15	6	0	1.023349	2.422697	0.437029
16	6	0	0.110982	2.377122	-0.628045
17	1	0	0.771140	2.985845	1.332624
18	1	0	-0.818265	2.930586	-0.543042
19	1	0	0.429089	2.163723	-1.646088
20	28	0	0.445047	0.496143	0.121362
21	6	0	-1.014982	-0.554797	-0.672842
22	1	0	-0.856457	-0.337999	-1.731196
23	14	0	-2.748611	-0.316675	-0.023338
24	6	0	-3.775563	-1.892018	-0.233998
25	1	0	-3.297986	-2.748150	0.257248
26	1	0	-4.775668	-1.776277	0.200754
27	1	0	-3.897068	-2.143790	-1.293758
28	6	0	-2.658305	0.102895	1.816491

29	1	0	-2.104384	1.037124	1.969318
30	1	0	-3.652647	0.220440	2.262833
31	1	0	-2.134467	-0.686028	2.370209
32	6	0	-3.582585	1.088784	-0.966573
33	1	0	-3.070308	2.041623	-0.794146
34	1	0	-3.574852	0.896434	-2.045884
35	1	0	-4.627293	1.209990	-0.657765

Zero-point correction= 0.293033 (Hartree/Particle)
Thermal correction to Energy= 0.310843
Thermal correction to Enthalpy= 0.311787
Thermal correction to Gibbs Free Energy= 0.247730
Sum of electronic and zero-point Energies= -1002.759370
Sum of electronic and thermal Energies= -1002.741560
Sum of electronic and thermal Enthalpies= -1002.740616
Sum of electronic and thermal Free Energies= -1002.804673
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.886101

INT6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.370438	-0.977454	-0.053946
2	6	0	-0.016734	-1.190970	0.029005
3	1	0	-0.330352	-1.906331	0.792806
4	6	0	2.390295	-1.866701	0.642850
5	1	0	2.349327	-1.825819	1.734693
6	1	0	2.235166	-2.910679	0.327315
7	8	0	3.668631	-1.412504	0.236569
8	6	0	3.521421	-0.773500	-1.018589
9	1	0	3.465483	-1.511598	-1.834126
10	1	0	4.392329	-0.130668	-1.169749
11	6	0	2.205040	-0.006807	-0.909735
12	6	0	2.303905	1.134788	0.107018
13	1	0	1.773544	0.270415	-1.874568
14	1	0	3.108499	0.996748	0.825874
15	6	0	1.525288	2.303403	0.237362
16	6	0	0.288656	2.524215	-0.422703
17	1	0	1.771682	2.937054	1.088648
18	1	0	-0.303808	3.381116	-0.115437
19	1	0	0.149798	2.232202	-1.461504
20	28	0	0.347675	0.720181	0.477734
21	6	0	-0.996908	-0.345906	-0.571989
22	1	0	-0.757322	0.055757	-1.559948
23	14	0	-2.805324	-0.375921	-0.115730
24	6	0	-3.726998	-1.751496	-1.029420
25	1	0	-3.311887	-2.735470	-0.781836
26	1	0	-4.792657	-1.762223	-0.770976
27	1	0	-3.647715	-1.622995	-2.115184
28	6	0	-2.967423	-0.653049	1.744022
29	1	0	-2.465351	0.150724	2.295033
30	1	0	-4.018794	-0.672608	2.053577
31	1	0	-2.516302	-1.603261	2.054320
32	6	0	-3.539602	1.291915	-0.594681
33	1	0	-3.032413	2.098137	-0.053299
34	1	0	-3.411486	1.480357	-1.667317
35	1	0	-4.611442	1.346369	-0.372358

Zero-point correction= 0.295098 (Hartree/Particle)
Thermal correction to Energy= 0.313075
Thermal correction to Enthalpy= 0.314020
Thermal correction to Gibbs Free Energy= 0.249358
Sum of electronic and zero-point Energies= -1002.815334
Sum of electronic and thermal Energies= -1002.797357
Sum of electronic and thermal Enthalpies= -1002.796413
Sum of electronic and thermal Free Energies= -1002.861074

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.9409709

INT7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.422863	1.902165	-0.710165
2	6	0	-1.301621	0.847125	-0.991741
3	1	0	-1.136160	0.331283	-1.939513
4	6	0	0.532994	2.511962	-1.723126
5	1	0	1.352326	1.857184	-2.031537
6	1	0	-0.030006	2.808545	-2.623265
7	8	0	1.105028	3.648500	-1.100306
8	6	0	0.197162	4.099054	-0.109840
9	1	0	-0.612589	4.695768	-0.559159
10	1	0	0.755981	4.719384	0.595791
11	6	0	-0.366847	2.821556	0.503963
12	6	0	0.675818	2.054548	1.294997
13	1	0	-1.315438	2.962461	1.028598
14	1	0	1.705367	2.307399	1.049930
15	6	0	0.457716	1.139298	2.338377
16	6	0	-0.788195	0.540567	2.618930
17	1	0	1.349532	0.713533	2.790589
18	1	0	-0.812268	-0.264225	3.348796
19	1	0	-1.711192	1.106762	2.541923
20	28	0	-0.231400	0.274662	0.637520
21	6	0	-2.190804	0.274371	-0.047133
22	1	0	-2.623585	0.955559	0.685606
23	14	0	-3.143811	-1.301359	-0.348901
24	6	0	-4.993450	-0.968676	-0.155933
25	1	0	-5.341603	-0.230769	-0.887635
26	1	0	-5.579885	-1.884608	-0.294156
27	1	0	-5.218648	-0.577828	0.843535
28	6	0	-2.814407	-1.932515	-2.101037
29	1	0	-1.750340	-2.116841	-2.290321
30	1	0	-3.344451	-2.876271	-2.274149
31	1	0	-3.164321	-1.212145	-2.849824
32	6	0	-2.645092	-2.621451	0.904576
33	1	0	-1.610376	-2.946125	0.747031
34	1	0	-2.708398	-2.216285	1.920968
35	1	0	-3.290909	-3.505763	0.845784
36	6	0	4.292702	-2.205707	-0.242041
37	6	0	4.037175	-1.461506	-1.320517
38	6	0	2.965198	-0.420436	-1.555149
39	6	0	1.576873	-1.041215	-1.760728
40	6	0	0.837968	-1.516142	-0.538213
41	6	0	1.214380	-1.594377	0.760409
42	6	0	2.531391	-1.228298	1.409581
43	6	0	3.671202	-2.214910	1.127101
44	1	0	5.097958	-2.934265	-0.343542
45	1	0	4.651926	-1.670253	-2.195614
46	1	0	3.225528	0.127786	-2.467684
47	1	0	2.918721	0.331379	-0.762249
48	1	0	0.934520	-0.326506	-2.290109
49	1	0	1.673360	-1.897850	-2.443036
50	1	0	-0.109249	-1.996354	-0.777520
51	1	0	0.528431	-2.131276	1.414256
52	1	0	2.369962	-1.222956	2.493280
53	1	0	2.847308	-0.214549	1.151479
54	1	0	4.474498	-2.028288	1.854857
55	1	0	3.322527	-3.235869	1.339538

Zero-point correction= 0.480626 (Hartree/Particle)
Thermal correction to Energy= 0.507427
Thermal correction to Enthalpy= 0.508372
Thermal correction to Gibbs Free Energy= 0.424876

Sum of electronic and zero-point Energies= -1314.583561
Sum of electronic and thermal Energies= -1314.556760
Sum of electronic and thermal Enthalpies= -1314.555815
Sum of electronic and thermal Free Energies= -1314.639311
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9796196

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.491740	-1.940141	0.536831
2	6	0	-1.255815	-0.766730	0.831953
3	1	0	-1.048577	-0.305397	1.797240
4	6	0	0.318279	-2.671064	1.595872
5	1	0	1.231371	-2.156334	1.907544
6	1	0	-0.316736	-2.824966	2.483211
7	8	0	0.693306	-3.911841	1.025784
8	6	0	-0.259804	-4.240192	0.028896
9	1	0	-1.147445	-4.719201	0.470063
10	1	0	0.216407	-4.934213	-0.668659
11	6	0	-0.644296	-2.905666	-0.592681
12	6	0	0.516506	-2.143140	-1.137921
13	1	0	-1.567011	-2.883770	-1.171909
14	1	0	1.492207	-2.517302	-0.840882
15	6	0	0.485400	-1.144018	-2.162503
16	6	0	-0.660052	-0.506381	-2.637708
17	1	0	1.455514	-0.834177	-2.539337
18	1	0	-0.549826	0.250928	-3.408351
19	1	0	-1.638024	-0.971043	-2.583055
20	28	0	-0.135205	0.016621	-0.647399
21	6	0	-2.175996	-0.163717	-0.031925
22	1	0	-2.597034	-0.782327	-0.822214
23	14	0	-3.072009	1.428699	0.360039
24	6	0	-4.931073	1.158170	0.161882
25	1	0	-5.296835	0.391443	0.854272
26	1	0	-5.488676	2.081927	0.356406
27	1	0	-5.174793	0.832794	-0.856540
28	6	0	-2.706134	1.946246	2.139751
29	1	0	-1.635047	2.096518	2.316939
30	1	0	-3.212584	2.889428	2.375461
31	1	0	-3.059635	1.191311	2.851744
32	6	0	-2.534535	2.795237	-0.823959
33	1	0	-1.473957	3.032724	-0.686081
34	1	0	-2.663735	2.472952	-1.863547
35	1	0	-3.113610	3.714562	-0.675669
36	6	0	4.386777	1.987478	0.332520
37	6	0	4.091169	1.193326	1.364656
38	6	0	2.973471	0.188948	1.543671
39	6	0	1.612150	0.860844	1.776035
40	6	0	0.887564	1.414825	0.569389
41	6	0	1.298068	1.539602	-0.745347
42	6	0	2.620186	1.158189	-1.380328
43	6	0	3.779862	2.100365	-1.038779
44	1	0	5.221295	2.673622	0.483172
45	1	0	4.708487	1.326665	2.252792
46	1	0	3.207314	-0.411942	2.430300
47	1	0	2.900084	-0.522656	0.715984
48	1	0	0.950895	0.154468	2.295166
49	1	0	1.759512	1.686356	2.487055
50	1	0	0.053408	2.057205	0.850172
51	1	0	0.737205	2.264858	-1.336345
52	1	0	2.478491	1.188626	-2.467551
53	1	0	2.914331	0.131837	-1.148375
54	1	0	4.586661	1.938767	-1.769192
55	1	0	3.457853	3.140824	-1.191298

Zero-point correction= 0.479978 (Hartree/Particle)
Thermal correction to Energy= 0.505960
Thermal correction to Enthalpy= 0.506904
Thermal correction to Gibbs Free Energy= 0.425716
Sum of electronic and zero-point Energies= -1314.580274
Sum of electronic and thermal Energies= -1314.554291
Sum of electronic and thermal Enthalpies= -1314.553347
Sum of electronic and thermal Free Energies= -1314.634536
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9734142

INT8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.336812	1.773811	-0.486158
2	6	0	-1.222931	0.306747	-0.677992
3	1	0	-0.740601	0.008696	-1.608346
4	6	0	-1.387925	2.684915	-1.703847
5	1	0	-0.414918	2.850972	-2.177211
6	1	0	-2.078182	2.258971	-2.450128
7	8	0	-1.854716	3.934864	-1.231639
8	6	0	-2.731333	3.692990	-0.142291
9	1	0	-3.757984	3.503028	-0.492637
10	1	0	-2.729769	4.592339	0.480502
11	6	0	-2.185319	2.456472	0.546815
12	6	0	-0.699326	2.452542	0.757270
13	1	0	-2.830502	1.895331	1.215761
14	1	0	-0.186529	3.387251	0.537820
15	6	0	-0.023852	1.611870	1.775301
16	6	0	-0.583521	0.672145	2.596917
17	1	0	1.015502	1.877776	1.944851
18	1	0	0.012161	0.233457	3.392805
19	1	0	-1.655454	0.515401	2.663057
20	28	0	0.135582	-0.302342	0.795278
21	6	0	-1.844080	-0.641131	0.107355
22	1	0	-2.526647	-0.262727	0.870775
23	14	0	-2.036089	-2.469452	-0.260359
24	6	0	-3.888725	-2.807201	-0.422986
25	1	0	-4.317772	-2.260113	-1.270204
26	1	0	-4.081807	-3.875057	-0.580609
27	1	0	-4.430542	-2.502367	0.480153
28	6	0	-1.193559	-2.960401	-1.873176
29	1	0	-0.106526	-3.027374	-1.775414
30	1	0	-1.559901	-3.941336	-2.198293
31	1	0	-1.418241	-2.245031	-2.672950
32	6	0	-1.378917	-3.483857	1.188102
33	1	0	-0.309628	-3.309434	1.349094
34	1	0	-1.900087	-3.210698	2.113467
35	1	0	-1.529804	-4.557351	1.024590
36	6	0	4.872173	0.059258	-0.543460
37	6	0	4.144374	0.211813	-1.653150
38	6	0	2.647730	0.342006	-1.841539
39	6	0	1.907477	-0.982665	-1.595203
40	6	0	1.580273	-1.335684	-0.157587
41	6	0	2.054023	-0.764752	1.038562
42	6	0	3.020116	0.389336	1.241038
43	6	0	4.482463	0.072668	0.909303
44	1	0	5.943064	-0.084483	-0.693719
45	1	0	4.701056	0.163628	-2.588989
46	1	0	2.471372	0.641365	-2.880764
47	1	0	2.204956	1.131422	-1.226080
48	1	0	0.979654	-0.985079	-2.180977
49	1	0	2.516855	-1.793534	-2.019676
50	1	0	1.267511	-2.377730	-0.060435
51	1	0	2.040236	-1.444557	1.896282
52	1	0	2.970696	0.665137	2.302409

53	1	0	2.725255	1.286204	0.689609
54	1	0	5.123428	0.813916	1.409502
55	1	0	4.755845	-0.894312	1.356447

Zero-point correction= 0.481460 (Hartree/Particle)
Thermal correction to Energy= 0.507688
Thermal correction to Enthalpy= 0.508632
Thermal correction to Gibbs Free Energy= 0.426269
Sum of electronic and zero-point Energies= -1314.595321
Sum of electronic and thermal Energies= -1314.569093
Sum of electronic and thermal Enthalpies= -1314.568149
Sum of electronic and thermal Free Energies= -1314.650512
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9872713

TS3a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.063700	2.068943	0.375012
2	6	0	1.083324	1.363170	0.700096
3	1	0	1.295655	1.165017	1.749161
4	6	0	-1.021014	2.708078	1.360155
5	1	0	-1.433057	2.013553	2.096852
6	1	0	-0.518111	3.531585	1.895386
7	8	0	-2.088952	3.216070	0.580012
8	6	0	-1.528047	3.591579	-0.666428
9	1	0	-0.995164	4.551716	-0.576356
10	1	0	-2.345352	3.702698	-1.383600
11	6	0	-0.548081	2.471011	-1.016680
12	6	0	-1.262867	1.222323	-1.503114
13	1	0	0.245735	2.807484	-1.693231
14	1	0	-2.346510	1.220120	-1.423189
15	6	0	-0.631781	0.099217	-1.990174
16	6	0	0.828605	0.010767	-2.021513
17	1	0	-1.240408	-0.756941	-2.265203
18	1	0	1.223172	-0.971227	-2.272100
19	1	0	1.314816	0.791457	-2.596452
20	28	0	-0.076410	-0.057406	-0.051918
21	6	0	1.931320	0.795692	-0.354618
22	1	0	2.235096	1.550979	-1.076116
23	14	0	3.362276	-0.331209	0.148141
24	6	0	4.965855	0.655529	-0.007510
25	1	0	4.945281	1.547287	0.629721
26	1	0	5.832260	0.052517	0.289084
27	1	0	5.130120	0.986899	-1.039715
28	6	0	3.154363	-0.887727	1.938026
29	1	0	2.189441	-1.377236	2.106766
30	1	0	3.941134	-1.602827	2.204949
31	1	0	3.228487	-0.043917	2.633727
32	6	0	3.479922	-1.844532	-0.969329
33	1	0	2.569303	-2.451181	-0.916382
34	1	0	3.635497	-1.561818	-2.016852
35	1	0	4.323721	-2.476636	-0.668425
36	6	0	-3.557696	-0.929046	-0.295278
37	6	0	-3.241937	-2.095303	-0.860230
38	6	0	-2.412623	-3.220397	-0.297142
39	6	0	-0.894280	-3.039343	-0.442682
40	6	0	-0.215240	-2.020776	0.454550
41	6	0	-0.740969	-1.209213	1.467244
42	6	0	-2.180811	-1.055063	1.947716
43	6	0	-3.200363	-0.349322	1.043954
44	1	0	-4.182998	-0.260029	-0.889402
45	1	0	-3.617845	-2.263430	-1.869839
46	1	0	-2.686300	-4.139609	-0.828594
47	1	0	-2.652008	-3.402660	0.753626
48	1	0	-0.430573	-4.012464	-0.225712

49	1	0	-0.654591	-2.836295	-1.496602
50	1	0	0.842284	-2.259021	0.580107
51	1	0	-0.025523	-0.955914	2.251493
52	1	0	-2.139312	-0.456983	2.866735
53	1	0	-2.578190	-2.026747	2.265375
54	1	0	-4.134389	-0.241713	1.616587
55	1	0	-2.856313	0.677533	0.865512

Zero-point correction= 0.481385 (Hartree/Particle)
Thermal correction to Energy= 0.506619
Thermal correction to Enthalpy= 0.507563
Thermal correction to Gibbs Free Energy= 0.429103
Sum of electronic and zero-point Energies= -1314.560713
Sum of electronic and thermal Energies= -1314.535478
Sum of electronic and thermal Enthalpies= -1314.534534
Sum of electronic and thermal Free Energies= -1314.612995
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9522827

INT9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.536075	-0.420715	0.314428
2	6	0	0.070480	-0.571023	0.456721
3	1	0	-0.236078	-1.086311	1.369787
4	6	0	2.423869	-1.600079	0.695986
5	1	0	2.582353	-1.713042	1.773419
6	1	0	1.980298	-2.529725	0.304081
7	8	0	3.685634	-1.347909	0.105583
8	6	0	3.467915	-0.627933	-1.098757
9	1	0	3.270006	-1.312153	-1.938761
10	1	0	4.382761	-0.065832	-1.307975
11	6	0	2.249476	0.235235	-0.837122
12	6	0	2.233836	0.941756	0.485821
13	1	0	1.703496	0.638754	-1.683869
14	1	0	3.159319	0.887353	1.059937
15	6	0	1.437511	2.168433	0.727865
16	6	0	0.882328	2.947176	-0.197489
17	1	0	1.299443	2.422257	1.778493
18	1	0	0.299069	3.820849	0.076761
19	1	0	0.994966	2.751551	-1.260683
20	6	0	-0.867457	-0.111622	-0.380226
21	1	0	-0.526459	0.398684	-1.283826
22	14	0	-2.710884	-0.246310	-0.083760
23	6	0	-3.503709	-1.250432	-1.470274
24	1	0	-3.080638	-2.259922	-1.517135
25	1	0	-4.585325	-1.345558	-1.319578
26	1	0	-3.344459	-0.776918	-2.445766
27	6	0	-3.028733	-1.090114	1.571544
28	1	0	-2.605746	-0.515397	2.402961
29	1	0	-4.105269	-1.190409	1.750112
30	1	0	-2.594139	-2.095651	1.602118
31	6	0	-3.452757	1.487715	-0.071847
32	1	0	-3.004664	2.100233	0.718121
33	1	0	-3.279147	1.997243	-1.026524
34	1	0	-4.535480	1.455233	0.096397

Zero-point correction= 0.294277 (Hartree/Particle)
Thermal correction to Energy= 0.311615
Thermal correction to Enthalpy= 0.312559
Thermal correction to Gibbs Free Energy= 0.247995
Sum of electronic and zero-point Energies= -833.513648
Sum of electronic and thermal Energies= -833.496310
Sum of electronic and thermal Enthalpies= -833.495366
Sum of electronic and thermal Free Energies= -833.559930
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.986429

INT10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.378981	-0.734495	-0.471978
2	6	0	0.262485	-0.892594	-1.333125
3	1	0	0.573360	-1.170929	-2.343043
4	6	0	2.769642	-1.073134	-0.984289
5	1	0	2.752542	-1.813715	-1.787746
6	1	0	3.314407	-0.183175	-1.341702
7	8	0	3.430769	-1.645994	0.124393
8	6	0	3.033497	-0.933870	1.280853
9	1	0	3.764596	-0.148585	1.524382
10	1	0	2.998593	-1.644742	2.110711
11	6	0	1.653745	-0.307921	0.981108
12	6	0	1.635574	1.191567	0.717813
13	1	0	0.893856	-0.604374	1.703980
14	1	0	2.534218	1.657595	0.317024
15	6	0	0.451711	1.941033	0.994010
16	6	0	-0.056387	2.871137	0.077474
17	1	0	-0.231846	1.559131	1.754517
18	1	0	-1.018188	3.340484	0.258157
19	1	0	0.615552	3.408409	-0.594220
20	28	0	0.288961	1.001372	-0.724145
21	6	0	-1.085649	-0.437466	-1.210263
22	1	0	-1.596261	-0.475048	-2.176811
23	14	0	-2.346751	-0.627727	0.161585
24	6	0	-3.636464	-1.864121	-0.459440
25	1	0	-3.180169	-2.841269	-0.655457
26	1	0	-4.436754	-2.007004	0.276736
27	1	0	-4.099440	-1.520105	-1.391876
28	6	0	-1.642175	-1.311799	1.777623
29	1	0	-1.155959	-0.543902	2.389084
30	1	0	-2.457234	-1.731957	2.378802
31	1	0	-0.918953	-2.114159	1.593044
32	6	0	-3.230155	1.003904	0.508959
33	1	0	-2.597201	1.690094	1.081779
34	1	0	-3.493301	1.505404	-0.429212
35	1	0	-4.153207	0.842107	1.078085

Zero-point correction= 0.295621 (Hartree/Particle)
Thermal correction to Energy= 0.313211
Thermal correction to Enthalpy= 0.314155
Thermal correction to Gibbs Free Energy= 0.251631
Sum of electronic and zero-point Energies= -1002.796716
Sum of electronic and thermal Energies= -1002.779125
Sum of electronic and thermal Enthalpies= -1002.778181
Sum of electronic and thermal Free Energies= -1002.840705
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.9242715

INT11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.396854	1.480168	-0.726049
2	6	0	0.405504	0.157476	-1.220868
3	1	0	-0.440516	-0.035474	-1.882565
4	6	0	-0.523999	2.551730	-1.273913
5	1	0	-0.893005	2.322616	-2.277020
6	1	0	-1.389989	2.745086	-0.622456
7	8	0	0.288809	3.707297	-1.348748
8	6	0	1.086302	3.707844	-0.181031
9	1	0	0.546253	4.179713	0.655950
10	1	0	1.983835	4.294047	-0.389179
11	6	0	1.389784	2.230094	0.137428

12	6	0	0.850191	1.684624	1.429399
13	1	0	2.432945	1.965342	-0.033340
14	1	0	0.027745	2.210601	1.910195
15	6	0	1.431039	0.525046	1.996252
16	6	0	0.662020	-0.410815	2.708489
17	1	0	2.423046	0.239864	1.662204
18	1	0	1.121960	-1.349054	3.006529
19	1	0	-0.170614	-0.084204	3.326655
20	28	0	-0.054255	-0.091680	0.800131
21	6	0	1.166118	-0.967055	-0.843724
22	1	0	0.726698	-1.872082	-1.276857
23	14	0	2.976275	-1.337405	-0.589112
24	6	0	3.493803	-2.384409	-2.078788
25	1	0	3.370048	-1.828223	-3.015132
26	1	0	4.544881	-2.688676	-2.002745
27	1	0	2.889324	-3.296357	-2.153228
28	6	0	4.165906	0.134508	-0.546519
29	1	0	4.171512	0.685043	0.400023
30	1	0	5.183824	-0.243862	-0.701822
31	1	0	3.954084	0.843173	-1.355329
32	6	0	3.249823	-2.410971	0.943583
33	1	0	3.183970	-1.849065	1.881351
34	1	0	2.496387	-3.206268	0.983202
35	1	0	4.237569	-2.886054	0.910864
36	6	0	-4.624246	-1.578576	-0.745926
37	6	0	-4.616751	-0.248496	-0.868303
38	6	0	-3.477454	0.741821	-0.760439
39	6	0	-3.023240	0.959251	0.689448
40	6	0	-2.147696	-0.098948	1.312436
41	6	0	-1.753087	-1.336144	0.840437
42	6	0	-2.078488	-2.022883	-0.468992
43	6	0	-3.509115	-2.568367	-0.544688
44	1	0	-5.602345	-2.055995	-0.817720
45	1	0	-5.591891	0.216472	-1.010994
46	1	0	-3.828844	1.702777	-1.152608
47	1	0	-2.621338	0.466010	-1.381350
48	1	0	-2.514672	1.927287	0.779300
49	1	0	-3.921838	1.048200	1.316604
50	1	0	-2.057113	0.036786	2.388822
51	1	0	-1.414564	-2.031881	1.607286
52	1	0	-1.386901	-2.866243	-0.569296
53	1	0	-1.894507	-1.388383	-1.336325
54	1	0	-3.560262	-3.293691	-1.369849
55	1	0	-3.724450	-3.150535	0.363329

Zero-point correction= 0.481506 (Hartree/Particle)
Thermal correction to Energy= 0.507580
Thermal correction to Enthalpy= 0.508524
Thermal correction to Gibbs Free Energy= 0.427893
Sum of electronic and zero-point Energies= -1314.572456
Sum of electronic and thermal Energies= -1314.546381
Sum of electronic and thermal Enthalpies= -1314.545437
Sum of electronic and thermal Free Energies= -1314.626068

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9713836

TS6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.889625	1.566268	-0.602956
2	6	0	0.426590	0.319910	-1.143553
3	1	0	-0.472655	0.435060	-1.750855
4	6	0	0.337769	2.914337	-1.034406
5	1	0	-0.235321	2.854573	-1.963299
6	1	0	-0.298461	3.372807	-0.259586
7	8	0	1.477010	3.719221	-1.264497

8	6	0	2.447084	3.365292	-0.294334
9	1	0	2.361607	4.009726	0.594212
10	1	0	3.433521	3.516316	-0.739188
11	6	0	2.187724	1.895817	0.063977
12	6	0	1.373361	1.604821	1.275307
13	1	0	3.018378	1.217588	-0.106920
14	1	0	0.830761	2.433562	1.725781
15	6	0	1.467263	0.343654	1.961482
16	6	0	0.429613	-0.108296	2.785440
17	1	0	2.316920	-0.297449	1.753952
18	1	0	0.518577	-1.081885	3.261103
19	1	0	-0.230097	0.597786	3.286808
20	28	0	-0.139461	0.079927	0.825352
21	6	0	0.880455	-0.980583	-0.916079
22	1	0	0.197534	-1.700347	-1.379720
23	14	0	2.436034	-1.948365	-0.572801
24	6	0	2.688183	-3.053308	-2.088591
25	1	0	2.911247	-2.456855	-2.980855
26	1	0	3.517336	-3.754702	-1.935482
27	1	0	1.789503	-3.644061	-2.302476
28	6	0	4.077700	-1.035560	-0.331764
29	1	0	4.175506	-0.505500	0.621243
30	1	0	4.877966	-1.785640	-0.361821
31	1	0	4.271338	-0.325801	-1.144285
32	6	0	2.143895	-3.095438	0.900577
33	1	0	2.069044	-2.550738	1.847691
34	1	0	1.200715	-3.638001	0.764828
35	1	0	2.946987	-3.836080	0.995656
36	6	0	-4.856833	-1.127238	-0.432456
37	6	0	-4.759478	0.140122	-0.841205
38	6	0	-3.531066	0.937017	-1.212602
39	6	0	-2.805496	1.532047	0.005878
40	6	0	-2.196127	0.572720	1.011093
41	6	0	-2.008711	-0.795676	0.920756
42	6	0	-2.330132	-1.722399	-0.228344
43	6	0	-3.796203	-2.178193	-0.235919
44	1	0	-5.862236	-1.484511	-0.207408
45	1	0	-5.691619	0.703052	-0.886501
46	1	0	-3.846558	1.776099	-1.844024
47	1	0	-2.839813	0.354456	-1.825286
48	1	0	-2.050013	2.239916	-0.349876
49	1	0	-3.534261	2.143537	0.555495
50	1	0	-2.184242	0.977766	2.022346
51	1	0	-1.905220	-1.318434	1.871293
52	1	0	-1.700089	-2.612938	-0.122691
53	1	0	-2.065541	-1.287643	-1.192568
54	1	0	-3.922181	-2.949135	-1.010875
55	1	0	-4.005581	-2.689028	0.714836

Zero-point correction= 0.481065 (Hartree/Particle)
Thermal correction to Energy= 0.506589
Thermal correction to Enthalpy= 0.507533
Thermal correction to Gibbs Free Energy= 0.427880
Sum of electronic and zero-point Energies= -1314.571429
Sum of electronic and thermal Energies= -1314.545905
Sum of electronic and thermal Enthalpies= -1314.544961
Sum of electronic and thermal Free Energies= -1314.624613
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9680168

INT12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.530020	1.538049	-0.641587
2	6	0	0.768791	0.346325	-1.109106
3	1	0	0.014004	0.622396	-1.848708

4	6	0	1.432631	2.814077	-1.463523
5	1	0	1.596289	2.584782	-2.530048
6	1	0	0.473574	3.333238	-1.360034
7	8	0	2.437458	3.673667	-0.963912
8	6	0	3.521312	2.869934	-0.524799
9	1	0	4.061157	3.442203	0.235515
10	1	0	4.210081	2.643353	-1.354127
11	6	0	2.896724	1.588860	-0.007865
12	6	0	1.687162	1.759796	0.861350
13	1	0	3.511471	0.703826	0.086681
14	1	0	1.472469	2.762708	1.230771
15	6	0	1.238924	0.610903	1.711896
16	6	0	0.078839	0.644007	2.467889
17	1	0	1.977569	-0.156483	1.934649
18	1	0	-0.080673	-0.090517	3.253719
19	1	0	-0.513851	1.552866	2.549089
20	28	0	-0.303695	-0.174159	0.621018
21	6	0	0.941805	-1.009545	-0.911248
22	1	0	0.237523	-1.587123	-1.520968
23	14	0	2.117850	-2.267048	-0.154115
24	6	0	2.338733	-3.571253	-1.504093
25	1	0	2.819483	-3.145441	-2.392389
26	1	0	2.962099	-4.400905	-1.150310
27	1	0	1.375028	-3.990508	-1.816126
28	6	0	3.854409	-1.745077	0.372495
29	1	0	3.881948	-1.089891	1.248429
30	1	0	4.404748	-2.657472	0.635016
31	1	0	4.401905	-1.260557	-0.443606
32	6	0	1.249880	-3.084587	1.309309
33	1	0	1.126862	-2.395004	2.151104
34	1	0	0.249952	-3.427422	1.018783
35	1	0	1.815012	-3.955788	1.662027
36	6	0	-4.989829	-0.656534	-0.794608
37	6	0	-5.103399	0.312323	0.116769
38	6	0	-4.162463	1.473125	0.299748
39	6	0	-2.929062	1.188432	1.200800
40	6	0	-2.304612	-0.196569	1.080565
41	6	0	-2.057672	-0.873020	-0.108838
42	6	0	-2.480251	-0.390064	-1.474039
43	6	0	-3.910446	-0.851547	-1.836791
44	1	0	-5.766373	-1.420644	-0.804642
45	1	0	-5.947132	0.261730	0.803911
46	1	0	-4.708060	2.316027	0.739941
47	1	0	-3.823419	1.823393	-0.679493
48	1	0	-2.192826	1.974555	0.991572
49	1	0	-3.218629	1.326040	2.248633
50	1	0	-2.379667	-0.806090	1.979022
51	1	0	-1.940131	-1.957432	-0.034733
52	1	0	-1.802361	-0.790953	-2.240235
53	1	0	-2.394246	0.697869	-1.539451
54	1	0	-4.212801	-0.367788	-2.777524
55	1	0	-3.866078	-1.925019	-2.062025

Zero-point correction= 0.481738 (Hartree/Particle)
Thermal correction to Energy= 0.507683
Thermal correction to Enthalpy= 0.508627
Thermal correction to Gibbs Free Energy= 0.427146
Sum of electronic and zero-point Energies= -1314.592007
Sum of electronic and thermal Energies= -1314.566062
Sum of electronic and thermal Enthalpies= -1314.565118
Sum of electronic and thermal Free Energies= -1314.646600
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9840196

INT13a

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

1	6	0	-1.434457	-0.407150	0.312928
2	6	0	0.027836	-0.289237	0.541734
3	1	0	0.307214	-0.160867	1.589714
4	6	0	-2.183789	-1.541121	1.007512
5	1	0	-1.593215	-2.467933	0.927730
6	1	0	-2.403201	-1.351355	2.062975
7	8	0	-3.420988	-1.662728	0.329601
8	6	0	-3.210709	-1.309728	-1.029263
9	1	0	-4.170699	-0.968791	-1.427975
10	1	0	-2.869620	-2.177086	-1.616517
11	6	0	-2.133740	-0.244772	-1.003073
12	6	0	-2.306877	0.821162	0.059202
13	1	0	-1.598720	-0.003823	-1.916516
14	1	0	-3.267061	0.830906	0.573674
15	6	0	-1.684566	2.147261	-0.132992
16	6	0	-2.235465	3.294813	0.257725
17	1	0	-0.713464	2.159303	-0.626494
18	1	0	-1.741229	4.246964	0.091594
19	1	0	-3.201483	3.323935	0.756484
20	6	0	0.981613	-0.315236	-0.396424
21	1	0	0.657153	-0.451491	-1.431853
22	14	0	2.814295	-0.113343	-0.056298
23	6	0	3.096502	0.085217	1.795993
24	1	0	2.746853	-0.790910	2.353444
25	1	0	4.164483	0.208835	2.008339
26	1	0	2.577028	0.965660	2.190290
27	6	0	3.738152	-1.630845	-0.688522
28	1	0	3.568496	-1.782726	-1.760519
29	1	0	4.818240	-1.523640	-0.535352
30	1	0	3.413145	-2.538107	-0.167648
31	6	0	3.439085	1.416274	-0.966292
32	1	0	3.270082	1.332974	-2.045939
33	1	0	2.927593	2.319845	-0.616511
34	1	0	4.514670	1.557116	-0.808724

Zero-point correction= 0.294838 (Hartree/Particle)
Thermal correction to Energy= 0.311987
Thermal correction to Enthalpy= 0.312931
Thermal correction to Gibbs Free Energy= 0.249483
Sum of electronic and zero-point Energies= -833.514891
Sum of electronic and thermal Energies= -833.497742
Sum of electronic and thermal Enthalpies= -833.496798
Sum of electronic and thermal Free Energies= -833.560246
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9878097

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.590587	-0.607482	0.059021
2	6	0	0.228276	-0.835397	0.221240
3	1	0	-0.059649	-1.440324	1.083910
4	6	0	2.716348	-1.461850	0.607126
5	1	0	2.721684	-1.562004	1.696857
6	1	0	2.651134	-2.469447	0.166267
7	8	0	3.922349	-0.825813	0.219546
8	6	0	3.661700	-0.080469	-0.959153
9	1	0	3.730305	-0.717885	-1.854464
10	1	0	4.415661	0.708521	-1.022435
11	6	0	2.238520	0.435342	-0.796106
12	6	0	2.031519	1.244239	0.443070
13	1	0	1.742610	0.763126	-1.709683
14	1	0	2.846893	1.216580	1.160389
15	6	0	0.893754	1.990868	0.738629
16	6	0	-0.210502	2.071176	-0.093883

17	1	0	0.789466	2.324657	1.769484
18	1	0	-1.101215	2.580688	0.264511
19	1	0	-0.076864	2.112873	-1.168049
20	6	0	-0.743821	-0.114374	-0.468640
21	1	0	-0.486436	0.147387	-1.492394
22	14	0	-2.569267	-0.274717	-0.071530
23	6	0	-2.835137	0.072285	1.762481
24	1	0	-2.552863	1.101225	2.010842
25	1	0	-3.883832	-0.070293	2.046824
26	1	0	-2.227992	-0.595713	2.384292
27	6	0	-3.166027	-2.022935	-0.465164
28	1	0	-4.232409	-2.143319	-0.240758
29	1	0	-3.017354	-2.259703	-1.524659
30	1	0	-2.613571	-2.766403	0.120542
31	6	0	-3.540362	0.956438	-1.119001
32	1	0	-3.359554	0.792824	-2.187772
33	1	0	-4.617590	0.850750	-0.947343
34	1	0	-3.266597	1.991952	-0.889041

Zero-point correction= 0.294430 (Hartree/Particle)
Thermal correction to Energy= 0.310356
Thermal correction to Enthalpy= 0.311300
Thermal correction to Gibbs Free Energy= 0.251963
Sum of electronic and zero-point Energies= -833.480281
Sum of electronic and thermal Energies= -833.464355
Sum of electronic and thermal Enthalpies= -833.463411
Sum of electronic and thermal Free Energies= -833.522748
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9537613

TS4a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.595746	-0.506847	0.130384
2	6	0	-0.233226	-0.571454	0.462357
3	1	0	-0.027682	-0.422036	1.526906
4	6	0	-2.460150	-1.326424	-0.805775
5	1	0	-2.239572	-1.211944	-1.871820
6	1	0	-2.357914	-2.389434	-0.542457
7	8	0	-3.794680	-0.884999	-0.587817
8	6	0	-3.883091	-0.269293	0.692661
9	1	0	-4.093839	-1.011612	1.477257
10	1	0	-4.705840	0.450342	0.649453
11	6	0	-2.514194	0.351517	0.918760
12	6	0	-2.119159	1.253553	-0.233359
13	1	0	-2.231887	0.641044	1.930894
14	1	0	-2.899397	1.298928	-0.991199
15	6	0	-0.971741	1.987920	-0.549912
16	6	0	0.321070	1.874350	-0.009209
17	1	0	-1.039627	2.497400	-1.509566
18	1	0	1.082304	2.500691	-0.473873
19	1	0	0.460971	1.778028	1.062732
20	6	0	0.762609	-0.071206	-0.394663
21	1	0	0.521445	-0.105965	-1.461293
22	14	0	2.596954	-0.267385	0.000776
23	6	0	2.887621	0.050207	1.836275
24	1	0	3.943270	-0.101554	2.088526
25	1	0	2.625797	1.077710	2.113025
26	1	0	2.297223	-0.628893	2.461068
27	6	0	3.619327	0.939033	-1.026960
28	1	0	4.690257	0.755885	-0.881927
29	1	0	3.407360	0.827646	-2.096535
30	1	0	3.422860	1.981188	-0.753318
31	6	0	3.106078	-2.030685	-0.431850
32	1	0	2.935772	-2.241611	-1.493704
33	1	0	4.168544	-2.202411	-0.223566

34	1	0	2.523635	-2.754046	0.148814

Zero-point correction= 0.294866 (Hartree/Particle)
Thermal correction to Energy= 0.310583
Thermal correction to Enthalpy= 0.311527
Thermal correction to Gibbs Free Energy= 0.252664
Sum of electronic and zero-point Energies= -833.450476
Sum of electronic and thermal Energies= -833.434759
Sum of electronic and thermal Enthalpies= -833.433815
Sum of electronic and thermal Free Energies= -833.492679
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9234757

TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.613785	-0.534229	-0.124641
2	6	0	-0.237398	-0.691739	0.014371
3	1	0	0.034859	-1.451464	0.749969
4	6	0	-2.585556	-1.463268	0.592628
5	1	0	-2.554459	-2.454942	0.111563
6	1	0	-2.376250	-1.592497	1.659071
7	8	0	-3.871227	-0.886623	0.471925
8	6	0	-3.889108	-0.126757	-0.723454
9	1	0	-4.678065	0.623566	-0.630839
10	1	0	-4.099657	-0.766165	-1.595583
11	6	0	-2.494393	0.466879	-0.833571
12	6	0	-2.002857	1.309394	0.293965
13	1	0	-2.185717	0.810110	-1.821986
14	1	0	-2.398632	1.133593	1.289221
15	6	0	-0.894105	2.120590	0.046049
16	6	0	0.310819	1.937519	0.715784
17	1	0	-0.810066	2.525084	-0.965271
18	1	0	1.165151	2.571052	0.488609
19	1	0	0.310463	1.515647	1.718800
20	6	0	0.784437	0.182045	-0.400798
21	1	0	0.617902	0.719100	-1.333563
22	14	0	2.582689	-0.274990	-0.094390
23	6	0	2.722089	-1.261120	1.508095
24	1	0	2.228144	-2.236063	1.430016
25	1	0	3.774162	-1.445202	1.753903
26	1	0	2.272434	-0.723727	2.350810
27	6	0	3.232188	-1.311465	-1.531847
28	1	0	3.143125	-0.773018	-2.482273
29	1	0	4.289797	-1.563376	-1.389827
30	1	0	2.671692	-2.247938	-1.627205
31	6	0	3.637114	1.284038	0.045839
32	1	0	3.458318	1.968794	-0.791423
33	1	0	3.428616	1.827592	0.973988
34	1	0	4.703695	1.031377	0.043558

Zero-point correction= 0.294267 (Hartree/Particle)
Thermal correction to Energy= 0.310175
Thermal correction to Enthalpy= 0.311119
Thermal correction to Gibbs Free Energy= 0.251417
Sum of electronic and zero-point Energies= -833.462217
Sum of electronic and thermal Energies= -833.446310
Sum of electronic and thermal Enthalpies= -833.445365
Sum of electronic and thermal Free Energies= -833.505067
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9356163

TS7a′

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

1	6	0	1.465842	-0.378869	-0.504746
2	6	0	0.362470	-0.352286	-1.367066
3	1	0	0.661768	-0.513058	-2.405508
4	6	0	2.830231	-0.772755	-1.068128
5	1	0	2.830672	-1.855623	-1.276629
6	1	0	3.100093	-0.245077	-1.988298
7	8	0	3.795736	-0.450692	-0.088273
8	6	0	3.163786	-0.540508	1.175498
9	1	0	3.731640	0.075535	1.877173
10	1	0	3.149356	-1.580554	1.538885
11	6	0	1.745629	-0.049438	0.944507
12	6	0	1.563633	1.300244	0.347790
13	1	0	1.010982	-0.323047	1.697216
14	1	0	2.367476	1.731711	-0.240101
15	6	0	0.295977	1.890966	0.458560
16	6	0	-0.442415	2.208387	-0.669686
17	1	0	-0.274119	1.654713	1.359329
18	1	0	-1.433809	2.645911	-0.584419
19	1	0	0.074586	2.433934	-1.599634
20	6	0	-0.930830	0.167728	-1.184953
21	1	0	-1.446960	0.275241	-2.147080
22	14	0	-2.200826	-0.366275	0.099536
23	6	0	-3.291416	-1.633814	-0.780065
24	1	0	-2.703293	-2.500048	-1.103560
25	1	0	-4.088142	-1.995370	-0.119337
26	1	0	-3.766027	-1.204079	-1.669826
27	6	0	-1.477084	-1.200141	1.629083
28	1	0	-1.058744	-0.481752	2.341684
29	1	0	-2.272799	-1.746648	2.149303
30	1	0	-0.697256	-1.921274	1.362143
31	6	0	-3.303577	1.062976	0.653373
32	1	0	-2.759440	1.800938	1.252919
33	1	0	-3.745217	1.583965	-0.203937
34	1	0	-4.128567	0.683021	1.267353

Zero-point correction= 0.294853 (Hartree/Particle)
Thermal correction to Energy= 0.310251
Thermal correction to Enthalpy= 0.311195
Thermal correction to Gibbs Free Energy= 0.254026
Sum of electronic and zero-point Energies= -833.455724
Sum of electronic and thermal Energies= -833.440326
Sum of electronic and thermal Enthalpies= -833.439382
Sum of electronic and thermal Free Energies= -833.496552
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9293972

TS8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.258636	-1.403317	-0.981390
2	6	0	-2.654509	-2.565237	-0.724344
3	6	0	-2.506567	-3.195872	0.632134
4	6	0	-1.242250	-2.758075	1.405855
5	6	0	-0.887579	-1.284106	1.451432
6	6	0	-1.772790	-0.216159	1.483460
7	6	0	-3.291237	-0.335943	1.405294
8	6	0	-3.920770	-0.465711	0.000355
9	1	0	-3.274631	-1.067983	-2.016956
10	1	0	-2.184809	-3.084958	-1.557807
11	1	0	-2.459769	-4.285664	0.520090
12	1	0	-3.399053	-3.000076	1.231812
13	1	0	-1.351138	-3.104881	2.445033
14	1	0	-0.383352	-3.306055	1.009254
15	1	0	0.102184	-1.104835	1.873972
16	1	0	-1.407611	0.699161	1.951810
17	1	0	-3.732895	0.549327	1.874933

18	1	0	-3.611227	-1.171406	2.035797
19	1	0	-4.979078	-0.739701	0.123453
20	1	0	-3.929515	0.527139	-0.463855
21	6	0	0.520248	-1.347117	-1.121960
22	6	0	0.261161	-0.386321	-1.902396
23	1	0	0.415013	0.122721	-2.839261
24	6	0	1.280608	-2.584481	-0.828183
25	1	0	1.556230	-2.597772	0.236366
26	1	0	0.647064	-3.457052	-1.018147
27	8	0	2.428227	-2.774536	-1.631714
28	6	0	3.405438	-1.759996	-1.486029
29	1	0	3.014131	-0.795130	-1.838173
30	1	0	4.219446	-2.060284	-2.153920
31	6	0	3.902335	-1.626968	-0.074847
32	6	0	3.772566	-0.517674	0.661466
33	1	0	4.366149	-2.513723	0.358543
34	1	0	3.289051	0.357923	0.225777
35	6	0	4.241093	-0.390417	2.038689
36	6	0	4.127747	0.723394	2.767565
37	1	0	4.706309	-1.273825	2.475328
38	1	0	4.487767	0.774622	3.790283
39	1	0	3.669942	1.621884	2.361485
40	28	0	-0.746315	-0.122690	-0.293038
41	6	0	-1.028502	1.634954	-0.891535
42	7	0	-2.256995	2.522071	0.042262
43	7	0	-2.737801	2.802196	1.003954
44	1	0	-1.499584	1.815838	-1.865968
45	14	0	0.444171	2.809596	-0.520143
46	6	0	-0.031504	4.632035	-0.689651
47	1	0	-0.763512	4.946923	0.062271
48	1	0	0.854469	5.266806	-0.568465
49	1	0	-0.455610	4.840682	-1.678733
50	6	0	1.017895	2.483782	1.242228
51	1	0	1.312991	1.436107	1.367234
52	1	0	1.871671	3.121335	1.501944
53	1	0	0.222454	2.691084	1.968238
54	6	0	1.825675	2.464209	-1.751364
55	1	0	2.221421	1.450699	-1.644007
56	1	0	1.484880	2.587465	-2.785744
57	1	0	2.644257	3.175144	-1.586001

Zero-point correction= 0.482867 (Hartree/Particle)
Thermal correction to Energy= 0.513719
Thermal correction to Enthalpy= 0.514663
Thermal correction to Gibbs Free Energy= 0.421337
Sum of electronic and zero-point Energies= -1423.918480
Sum of electronic and thermal Energies= -1423.887627
Sum of electronic and thermal Enthalpies= -1423.886683
Sum of electronic and thermal Free Energies= -1423.980009
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1426.3545236

INT14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.372381	-2.062078	1.121946
2	6	0	-0.612952	-2.839201	0.032458
3	6	0	0.370581	-3.782648	-0.624635
4	6	0	1.175323	-3.117174	-1.761585
5	6	0	1.636883	-1.707890	-1.475861
6	6	0	2.036437	-1.186706	-0.282602
7	6	0	2.192187	-1.942044	1.016717
8	6	0	0.919694	-1.898186	1.882510
9	1	0	-1.229086	-1.578354	1.580329
10	1	0	-1.639026	-2.880055	-0.327997
11	1	0	-0.181520	-4.629153	-1.045572

12	1	0	1.042811	-4.204710	0.126417
13	1	0	2.036907	-3.748183	-2.022046
14	1	0	0.545887	-3.074878	-2.657510
15	1	0	1.765474	-1.088311	-2.360050
16	1	0	2.407270	-0.164047	-0.279911
17	1	0	3.005967	-1.481779	1.585500
18	1	0	2.493305	-2.974445	0.821529
19	1	0	0.983108	-2.649881	2.682017
20	1	0	0.881356	-0.923799	2.382476
21	6	0	-0.067318	0.821579	-1.700054
22	6	0	-1.359988	1.122859	-1.692918
23	1	0	-1.880719	1.980047	-2.136186
24	6	0	1.083551	1.569133	-2.311619
25	1	0	2.044774	1.184060	-1.935957
26	1	0	1.087778	1.431640	-3.399268
27	8	0	1.039790	2.977137	-2.128145
28	6	0	1.011488	3.376570	-0.773536
29	1	0	0.072878	3.064221	-0.295252
30	1	0	1.033329	4.471800	-0.803027
31	6	0	2.177327	2.858108	0.021472
32	6	0	2.049819	2.164313	1.158443
33	1	0	3.169310	3.071022	-0.379842
34	1	0	1.051385	1.942862	1.536565
35	6	0	3.173181	1.666401	1.947288
36	6	0	3.041792	1.027537	3.114662
37	1	0	4.169143	1.840686	1.540018
38	1	0	3.902987	0.674613	3.673320
39	1	0	2.063213	0.855992	3.558214
40	28	0	-0.145009	-0.749054	-0.651063
41	6	0	-1.960705	0.019216	-0.857058
42	1	0	-2.541141	-0.701831	-1.454122
43	14	0	-2.901849	0.576371	0.653890
44	6	0	-3.924777	-0.845552	1.380690
45	1	0	-3.329484	-1.720412	1.666501
46	1	0	-4.475852	-0.517025	2.269971
47	1	0	-4.662859	-1.182754	0.642706
48	6	0	-1.750373	1.301416	1.971290
49	1	0	-0.966200	0.599118	2.276708
50	1	0	-1.254891	2.193295	1.569420
51	1	0	-2.303008	1.605485	2.868099
52	6	0	-4.120445	1.950221	0.190143
53	1	0	-3.595495	2.810406	-0.242051
54	1	0	-4.847598	1.600092	-0.551828
55	1	0	-4.678140	2.306277	1.064772

Zero-point correction= 0.478064 (Hartree/Particle)
Thermal correction to Energy= 0.505947
Thermal correction to Enthalpy= 0.506891
Thermal correction to Gibbs Free Energy= 0.421160
Sum of electronic and zero-point Energies= -1314.545534
Sum of electronic and thermal Energies= -1314.517651
Sum of electronic and thermal Enthalpies= -1314.516707
Sum of electronic and thermal Free Energies= -1314.602438
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.9030773

INT15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683882	-1.308325	-0.688535
2	6	0	0.426273	-1.412686	-1.418193
3	1	0	0.755058	-2.217637	-2.085531
4	6	0	-1.868170	-2.174885	-0.435678
5	1	0	-2.625587	-2.048631	-1.229892
6	1	0	-1.572927	-3.229124	-0.415076
7	8	0	-2.483479	-1.938069	0.823064

8	6	0	-3.135189	-0.694491	0.893488
9	1	0	-3.675929	-0.702092	1.845271
10	1	0	-3.874866	-0.601445	0.079434
11	6	0	-2.194047	0.484895	0.854834
12	6	0	-2.353929	1.513781	-0.060891
13	1	0	-1.535194	0.584242	1.715996
14	1	0	-3.178382	1.449180	-0.768717
15	6	0	-1.336165	2.496821	-0.354171
16	6	0	-0.095811	2.529718	0.242623
17	1	0	-1.492836	3.089347	-1.252325
18	1	0	0.677184	3.163755	-0.176585
19	1	0	0.093397	2.147709	1.241961
20	28	0	-0.592830	0.552037	-0.505264
21	6	0	1.144827	-0.126483	-1.146609
22	1	0	1.501883	0.420137	-2.031700
23	14	0	2.405324	-0.209282	0.235344
24	6	0	1.592156	-0.613388	1.892456
25	1	0	1.063508	0.254555	2.305541
26	1	0	0.857117	-1.416192	1.767568
27	1	0	2.333123	-0.933741	2.634290
28	6	0	3.345636	1.426816	0.375817
29	1	0	4.182417	1.332036	1.078047
30	1	0	3.759378	1.729145	-0.593501
31	1	0	2.706577	2.240451	0.735429
32	6	0	3.665299	-1.572447	-0.141179
33	1	0	4.173100	-1.391191	-1.095959
34	1	0	4.432441	-1.640103	0.639460
35	1	0	3.171079	-2.548888	-0.209414

Zero-point correction= 0.293424 (Hartree/Particle)
Thermal correction to Energy= 0.311843
Thermal correction to Enthalpy= 0.312787
Thermal correction to Gibbs Free Energy= 0.248283
Sum of electronic and zero-point Energies= -1002.774719
Sum of electronic and thermal Energies= -1002.756300
Sum of electronic and thermal Enthalpies= -1002.755356
Sum of electronic and thermal Free Energies= -1002.819860
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9431518

TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.042025	-1.146577	-0.462714
2	6	0	0.015161	-1.240365	-1.369577
3	1	0	0.147812	-1.808598	-2.302950
4	6	0	2.368451	-1.790409	-0.700184
5	1	0	2.223030	-2.840008	-0.971804
6	1	0	2.951005	-1.303631	-1.505218
7	8	0	3.135139	-1.782821	0.489281
8	6	0	3.237434	-0.453046	0.900354
9	1	0	3.905266	0.109561	0.224447
10	1	0	3.680391	-0.451314	1.900646
11	6	0	1.894347	0.259173	0.954062
12	6	0	1.822434	1.579545	0.421436
13	1	0	1.268562	0.013670	1.807893
14	1	0	2.594066	1.924795	-0.264750
15	6	0	0.584072	2.322566	0.565645
16	6	0	-0.035928	2.840468	-0.558534
17	1	0	0.019010	2.241524	1.494871
18	1	0	-1.033428	3.261352	-0.490516
19	1	0	0.531744	3.078685	-1.456437
20	28	0	0.347119	0.733245	-0.566014
21	6	0	-1.140379	-0.384841	-1.191159
22	1	0	-1.669920	-0.155831	-2.122612
23	14	0	-2.323127	-0.511556	0.252315

24	6	0	-3.561341	-1.902733	-0.084816
25	1	0	-3.051296	-2.871216	-0.144149
26	1	0	-4.318563	-1.968244	0.705853
27	1	0	-4.082872	-1.744379	-1.036092
28	6	0	-1.461769	-0.874028	1.891710
29	1	0	-0.973262	0.020061	2.297447
30	1	0	-2.184918	-1.221732	2.638818
31	1	0	-0.696218	-1.646853	1.762401
32	6	0	-3.285861	1.108510	0.397471
33	1	0	-2.637196	1.922589	0.740684
34	1	0	-3.708334	1.405381	-0.569767
35	1	0	-4.113418	1.018081	1.110793

Zero-point correction= 0.293008 (Hartree/Particle)
Thermal correction to Energy= 0.310604
Thermal correction to Enthalpy= 0.311548
Thermal correction to Gibbs Free Energy= 0.248873
Sum of electronic and zero-point Energies= -1002.752854
Sum of electronic and thermal Energies= -1002.735258
Sum of electronic and thermal Enthalpies= -1002.734314
Sum of electronic and thermal Free Energies= -1002.796989
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.879763

INT20a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.393791	-0.894735	0.032159
2	6	0	0.012135	-1.078692	0.093806
3	1	0	0.329474	-1.723151	0.916398
4	6	0	-2.347175	-1.684767	0.906963
5	1	0	-1.909384	-2.616807	1.273830
6	1	0	-2.707166	-1.104883	1.772900
7	8	0	-3.424306	-2.010722	0.049419
8	6	0	-3.656359	-0.902290	-0.800826
9	1	0	-4.448173	-0.257304	-0.391042
10	1	0	-3.991249	-1.291083	-1.766053
11	6	0	-2.328725	-0.120257	-0.901996
12	6	0	-2.256147	1.197623	-0.141867
13	1	0	-1.964193	-0.019820	-1.929475
14	1	0	-2.906673	1.338989	0.719106
15	6	0	-1.346949	2.206301	-0.587641
16	6	0	-0.513645	2.895259	0.303907
17	1	0	-1.065232	2.207442	-1.642975
18	1	0	0.241895	3.574168	-0.079398
19	1	0	-0.831298	3.068727	1.333881
20	28	0	-0.390904	0.844885	0.454520
21	6	0	1.012671	-0.312542	-0.554226
22	1	0	0.756479	0.134207	-1.520349
23	14	0	2.826943	-0.436937	-0.148475
24	6	0	3.027323	-1.068862	1.619700
25	1	0	4.085576	-1.101013	1.903466
26	1	0	2.507960	-0.414917	2.329898
27	1	0	2.626154	-2.082275	1.739948
28	6	0	3.584137	1.283456	-0.301141
29	1	0	4.665441	1.267857	-0.121329
30	1	0	3.418382	1.697893	-1.302785
31	1	0	3.124473	1.967896	0.420723
32	6	0	3.723849	-1.609338	-1.329567
33	1	0	3.618130	-1.278541	-2.369417
34	1	0	4.795697	-1.665185	-1.104737
35	1	0	3.312320	-2.622997	-1.261486

Zero-point correction= 0.294103 (Hartree/Particle)
Thermal correction to Energy= 0.312376
Thermal correction to Enthalpy= 0.313320

Thermal correction to Gibbs Free Energy= 0.247727
Sum of electronic and zero-point Energies= -1002.800276
Sum of electronic and thermal Energies= -1002.782002
Sum of electronic and thermal Enthalpies= -1002.781058
Sum of electronic and thermal Free Energies= -1002.846652
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.9259262

INT21a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001745	-1.592238	-0.947103
2	6	0	-0.933611	-0.535331	-1.123372
3	1	0	-0.603671	0.269665	-1.777294
4	6	0	1.217340	-1.816345	-1.817402
5	1	0	1.176278	-1.258716	-2.757699
6	1	0	2.161165	-1.567302	-1.307225
7	8	0	1.185135	-3.200516	-2.119358
8	6	0	0.761857	-3.860292	-0.941521
9	1	0	1.621115	-4.054018	-0.278522
10	1	0	0.327285	-4.818423	-1.233746
11	6	0	-0.245066	-2.919149	-0.250685
12	6	0	0.123902	-2.426143	1.123459
13	1	0	-1.280504	-3.271320	-0.318118
14	1	0	1.166201	-2.489374	1.428932
15	6	0	-0.858147	-1.859782	1.969569
16	6	0	-0.585058	-0.781392	2.829076
17	1	0	-1.899246	-2.098619	1.768660
18	1	0	-1.412791	-0.319739	3.360535
19	1	0	0.381874	-0.703061	3.317590
20	28	0	-0.122458	-0.381125	0.816598
21	6	0	-2.103668	-0.358929	-0.394125
22	1	0	-2.521791	-1.246024	0.079355
23	14	0	-3.225325	1.123991	-0.368611
24	6	0	-2.408027	2.649466	-1.121633
25	1	0	-3.147219	3.450538	-1.239590
26	1	0	-1.608697	3.029915	-0.476082
27	1	0	-1.983033	2.447826	-2.111937
28	6	0	-3.658085	1.478815	1.434199
29	1	0	-4.380647	2.297492	1.532173
30	1	0	-4.093289	0.591709	1.910545
31	1	0	-2.753905	1.743961	1.994358
32	6	0	-4.821725	0.755720	-1.312057
33	1	0	-5.314972	-0.139409	-0.915132
34	1	0	-5.532338	1.587597	-1.236332
35	1	0	-4.621568	0.578739	-2.375000
36	6	0	3.484115	3.041079	-0.273577
37	6	0	4.212474	1.965060	0.031255
38	6	0	3.862660	0.515690	-0.193521
39	6	0	3.007150	-0.088280	0.937468
40	6	0	1.715303	0.623211	1.302618
41	6	0	0.927799	1.465391	0.548549
42	6	0	1.202693	1.906887	-0.868451
43	6	0	2.128714	3.135836	-0.927884
44	1	0	3.920057	4.009810	-0.029655
45	1	0	5.168795	2.140589	0.522883
46	1	0	4.789907	-0.067155	-0.244847
47	1	0	3.375569	0.376225	-1.160880
48	1	0	2.815959	-1.142825	0.703174
49	1	0	3.622744	-0.101153	1.845971
50	1	0	1.560506	0.696796	2.374553
51	1	0	0.251028	2.116008	1.103722
52	1	0	0.262159	2.196230	-1.344661
53	1	0	1.601942	1.086307	-1.467716
54	1	0	2.261119	3.422706	-1.981691
55	1	0	1.598064	3.979138	-0.464813

Zero-point correction= 0.480996 (Hartree/Particle)
Thermal correction to Energy= 0.507497
Thermal correction to Enthalpy= 0.508441
Thermal correction to Gibbs Free Energy= 0.425481
Sum of electronic and zero-point Energies= -1314.580000
Sum of electronic and thermal Energies= -1314.553499
Sum of electronic and thermal Enthalpies= -1314.552555
Sum of electronic and thermal Free Energies= -1314.635515
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.978113

TS10a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.778617	1.621289	-0.401017
2	6	0	-0.932793	0.472775	-1.252771
3	1	0	-0.371242	0.572137	-2.183715
4	6	0	-0.198437	2.904305	-0.989295
5	1	0	0.866777	2.846037	-1.232341
6	1	0	-0.754794	3.151298	-1.907687
7	8	0	-0.367258	3.912645	-0.013146
8	6	0	-1.470823	3.549283	0.798743
9	1	0	-2.422637	3.856158	0.338052
10	1	0	-1.355666	4.055373	1.760811
11	6	0	-1.402067	2.033598	0.889377
12	6	0	-0.081484	1.517248	1.354661
13	1	0	-2.287788	1.521235	1.248820
14	1	0	0.718011	2.249938	1.404826
15	6	0	0.130116	0.259561	2.023292
16	6	0	-0.802788	-0.769688	2.060145
17	1	0	1.095947	0.132886	2.502561
18	1	0	-0.556681	-1.688769	2.583558
19	1	0	-1.858679	-0.581009	1.919120
20	28	0	0.129388	-0.473535	0.164369
21	6	0	-1.600660	-0.744067	-1.042606
22	1	0	-1.377989	-1.435979	-1.864386
23	14	0	-3.271032	-1.264529	-0.376808
24	6	0	-4.231606	-0.025042	0.682481
25	1	0	-3.854319	0.097565	1.702991
26	1	0	-4.272795	0.960958	0.205501
27	1	0	-5.263872	-0.386913	0.766873
28	6	0	-3.127165	-2.917142	0.518964
29	1	0	-4.116017	-3.359889	0.687741
30	1	0	-2.544435	-3.621121	-0.086646
31	1	0	-2.623695	-2.821503	1.485458
32	6	0	-4.335102	-1.543453	-1.917918
33	1	0	-3.871175	-2.267085	-2.598464
34	1	0	-5.327030	-1.927901	-1.651132
35	1	0	-4.475161	-0.608655	-2.473237
36	6	0	5.135737	-0.994450	-0.110656
37	6	0	4.844485	0.073542	-0.858035
38	6	0	3.574772	0.891141	-0.951871
39	6	0	2.478911	0.182375	-1.761388
40	6	0	1.746872	-0.965752	-1.100461
41	6	0	1.924974	-1.542760	0.144289
42	6	0	2.924527	-1.199676	1.229926
43	6	0	4.344457	-1.705394	0.953021
44	1	0	6.120642	-1.434956	-0.271289
45	1	0	5.617116	0.380338	-1.562869
46	1	0	3.817425	1.827526	-1.467417
47	1	0	3.182360	1.186262	0.024970
48	1	0	1.748669	0.930730	-2.096885
49	1	0	2.937671	-0.203020	-2.682988
50	1	0	1.204243	-1.581758	-1.818476
51	1	0	1.509893	-2.545940	0.251904

52	1	0	2.574688	-1.670988	2.156694
53	1	0	2.964510	-0.128650	1.438544
54	1	0	4.923164	-1.655273	1.887639
55	1	0	4.302647	-2.773962	0.696339

Zero-point correction= 0.481430 (Hartree/Particle)
Thermal correction to Energy= 0.506911
Thermal correction to Enthalpy= 0.507855
Thermal correction to Gibbs Free Energy= 0.427432
Sum of electronic and zero-point Energies= -1314.566474
Sum of electronic and thermal Energies= -1314.540993
Sum of electronic and thermal Enthalpies= -1314.540049
Sum of electronic and thermal Free Energies= -1314.620472
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9617545

TS11a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.405213	-0.327794	-0.604508
2	6	0	-0.307339	-0.183474	-1.461224
3	1	0	-0.569126	-0.238221	-2.520737
4	6	0	-2.675324	-1.071306	-0.981117
5	1	0	-3.164532	-0.695730	-1.885275
6	1	0	-2.439905	-2.137105	-1.131141
7	8	0	-3.572215	-0.908319	0.102723
8	6	0	-2.799174	-0.714886	1.275598
9	1	0	-2.482907	-1.677984	1.706676
10	1	0	-3.425250	-0.187224	2.000009
11	6	0	-1.581172	0.075781	0.824645
12	6	0	-1.911199	1.344174	0.113219
13	1	0	-0.737997	0.079727	1.506510
14	1	0	-2.957092	1.493270	-0.138579
15	6	0	-0.981751	2.354203	-0.169944
16	6	0	0.358859	2.228756	0.113854
17	1	0	-1.303753	3.137006	-0.853654
18	1	0	1.066132	2.981843	-0.220178
19	1	0	0.668564	1.671202	0.990196
20	6	0	0.939905	0.334719	-1.130665
21	1	0	1.488896	0.678440	-2.016596
22	14	0	2.199954	-0.349542	0.080341
23	6	0	3.057607	-1.767272	-0.826630
24	1	0	3.860783	-2.199396	-0.217825
25	1	0	2.344755	-2.564625	-1.064286
26	1	0	3.500454	-1.426914	-1.769594
27	6	0	1.532826	-1.048071	1.702263
28	1	0	2.344348	-1.594139	2.198477
29	1	0	1.191614	-0.278245	2.402847
30	1	0	0.713982	-1.756407	1.536387
31	6	0	3.496570	0.967941	0.462942
32	1	0	4.355025	0.520582	0.977331
33	1	0	3.869620	1.429324	-0.458787
34	1	0	3.107182	1.768116	1.101069

Zero-point correction= 0.294876 (Hartree/Particle)
Thermal correction to Energy= 0.310483
Thermal correction to Enthalpy= 0.311427
Thermal correction to Gibbs Free Energy= 0.253242
Sum of electronic and zero-point Energies= -833.473033
Sum of electronic and thermal Energies= -833.457426
Sum of electronic and thermal Enthalpies= -833.456482
Sum of electronic and thermal Free Energies= -833.514667
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9469545

TS11a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.309858	-0.171663	-0.670040
2	6	0	0.319074	0.316161	-1.532475
3	1	0	0.713103	0.973120	-2.315256
4	6	0	1.567652	-1.516140	-0.020775
5	1	0	0.849331	-1.829177	0.742930
6	1	0	1.588762	-2.285477	-0.807548
7	8	0	2.838579	-1.407730	0.606139
8	6	0	3.577561	-0.361108	-0.013438
9	1	0	4.127374	-0.729661	-0.892570
10	1	0	4.292193	0.011524	0.726201
11	6	0	2.527844	0.649368	-0.444606
12	6	0	1.657907	1.079250	0.714791
13	1	0	2.802107	1.393648	-1.192489
14	1	0	1.962087	0.598009	1.643687
15	6	0	0.530525	1.895914	0.843446
16	6	0	-0.354659	2.363754	-0.143038
17	1	0	0.154276	1.934020	1.863458
18	1	0	-1.233975	2.895616	0.221927
19	1	0	0.017891	2.772162	-1.075911
20	6	0	-0.978574	0.643334	-1.112708
21	1	0	-1.581383	1.143750	-1.877511
22	14	0	-2.077509	-0.367964	0.052041
23	6	0	-3.804631	0.383000	-0.056833
24	1	0	-4.506157	-0.145751	0.598300
25	1	0	-3.797183	1.436539	0.246483
26	1	0	-4.199793	0.331822	-1.077754
27	6	0	-1.561443	-0.374852	1.865854
28	1	0	-2.140421	-1.134618	2.404410
29	1	0	-0.499271	-0.590355	2.011848
30	1	0	-1.769359	0.593300	2.333540
31	6	0	-2.124320	-2.142403	-0.589156
32	1	0	-2.798570	-2.762380	0.013256
33	1	0	-2.473448	-2.174855	-1.627133
34	1	0	-1.131840	-2.605610	-0.563679

Zero-point correction= 0.295118 (Hartree/Particle)
Thermal correction to Energy= 0.310642
Thermal correction to Enthalpy= 0.311586
Thermal correction to Gibbs Free Energy= 0.253921
Sum of electronic and zero-point Energies= -833.448683
Sum of electronic and thermal Energies= -833.433158
Sum of electronic and thermal Enthalpies= -833.432214
Sum of electronic and thermal Free Energies= -833.489879
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9216384

TS13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.093323	1.711699	-0.870953
2	6	0	0.940537	0.564053	-1.023255
3	1	0	0.569374	-0.193216	-1.707992
4	6	0	-1.143370	1.989949	-1.696913
5	1	0	-1.184599	1.380620	-2.604612
6	1	0	-2.074466	1.829472	-1.129811
7	8	0	-1.030358	3.349222	-2.076171
8	6	0	-0.426229	4.045024	-0.999558
9	1	0	-1.192894	4.452976	-0.322523
10	1	0	0.142733	4.877735	-1.419249
11	6	0	0.466093	3.031914	-0.263835
12	6	0	-0.066963	2.432171	0.989555
13	1	0	1.531437	3.272541	-0.245286
14	1	0	-1.124877	2.572475	1.200844

15	6	0	0.788489	1.804122	1.950496
16	6	0	0.328704	0.845979	2.859668
17	1	0	1.855830	1.993406	1.883879
18	1	0	1.042231	0.381502	3.534858
19	1	0	-0.698794	0.871404	3.211826
20	28	0	0.132689	0.243346	0.862710
21	6	0	2.110058	0.321908	-0.312816
22	1	0	2.580207	1.175224	0.174230
23	14	0	3.144830	-1.222610	-0.337362
24	6	0	2.309515	-2.626386	-1.283875
25	1	0	3.024924	-3.440922	-1.447534
26	1	0	1.461017	-3.039471	-0.728074
27	1	0	1.950595	-2.303598	-2.268372
28	6	0	3.436049	-1.763804	1.447401
29	1	0	4.065901	-2.659021	1.511072
30	1	0	3.927457	-0.966645	2.018550
31	1	0	2.477859	-1.975201	1.936029
32	6	0	4.819299	-0.866531	-1.141081
33	1	0	5.325837	-0.029472	-0.646026
34	1	0	5.483084	-1.737649	-1.083425
35	1	0	4.700204	-0.603143	-2.198343
36	6	0	-3.570061	-2.909706	-0.468978
37	6	0	-4.244204	-1.848679	-0.020843
38	6	0	-3.836937	-0.398180	-0.077567
39	6	0	-2.929620	0.026111	1.093487
40	6	0	-1.648696	-0.764578	1.315132
41	6	0	-0.910974	-1.516023	0.417503
42	6	0	-1.266366	-1.798363	-1.024196
43	6	0	-2.235821	-2.985238	-1.166838
44	1	0	-4.042298	-3.881971	-0.327351
45	1	0	-5.196241	-2.042931	0.472206
46	1	0	-4.739132	0.223596	-0.033043
47	1	0	-3.363870	-0.160365	-1.032608
48	1	0	-2.713132	1.096573	0.984654
49	1	0	-3.517656	-0.057867	2.016172
50	1	0	-1.471898	-1.006370	2.359036
51	1	0	-0.245451	-2.259626	0.859607
52	1	0	-0.358407	-2.067313	-1.572003
53	1	0	-1.663438	-0.910772	-1.520181
54	1	0	-2.406160	-3.171705	-2.237782
55	1	0	-1.722364	-3.883861	-0.797407

Zero-point correction= 0.481047 (Hartree/Particle)
Thermal correction to Energy= 0.506829
Thermal correction to Enthalpy= 0.507773
Thermal correction to Gibbs Free Energy= 0.426835
Sum of electronic and zero-point Energies= -1314.578567
Sum of electronic and thermal Energies= -1314.552786
Sum of electronic and thermal Enthalpies= -1314.551841
Sum of electronic and thermal Free Energies= -1314.632780
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9750966

TS14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.405145	-0.327825	-0.604432
2	6	0	0.307260	-0.183457	-1.461138
3	1	0	0.569056	-0.238239	-2.520648
4	6	0	2.675168	-1.071480	-0.981062
5	1	0	2.439660	-2.137289	-1.130875
6	1	0	3.164293	-0.696091	-1.885343
7	8	0	3.572193	-0.908376	0.102646
8	6	0	2.799283	-0.714797	1.275580
9	1	0	3.425453	-0.187085	1.999874
10	1	0	2.483020	-1.677838	1.706788

11	6	0	1.581266	0.075878	0.824673
12	6	0	1.911276	1.344173	0.113070
13	1	0	0.738190	0.079944	1.506658
14	1	0	2.957145	1.493248	-0.138839
15	6	0	0.981819	2.354215	-0.170053
16	6	0	-0.358778	2.228792	0.113840
17	1	0	1.303765	3.136970	-0.853845
18	1	0	-1.066074	2.981879	-0.220144
19	1	0	-0.668429	1.671239	0.990202
20	6	0	-0.939954	0.334834	-1.130603
21	1	0	-1.488922	0.678549	-2.016547
22	14	0	-2.199976	-0.349522	0.080379
23	6	0	-1.532608	-1.048824	1.701863
24	1	0	-1.191560	-0.279308	2.402864
25	1	0	-2.343962	-1.595376	2.197817
26	1	0	-0.713588	-1.756850	1.535539
27	6	0	-3.496304	0.968031	0.463732
28	1	0	-3.869512	1.429759	-0.457762
29	1	0	-4.354702	0.520604	0.978158
30	1	0	-3.106689	1.767950	1.102042
31	6	0	-3.058109	-1.766694	-0.827014
32	1	0	-3.500834	-1.425882	-1.769873
33	1	0	-2.345536	-2.564221	-1.064924
34	1	0	-3.861442	-2.198726	-0.218350

Zero-point correction= 0.294890 (Hartree/Particle)
Thermal correction to Energy= 0.310492
Thermal correction to Enthalpy= 0.311436
Thermal correction to Gibbs Free Energy= 0.253263
Sum of electronic and zero-point Energies= -833.473020
Sum of electronic and thermal Energies= -833.457417
Sum of electronic and thermal Enthalpies= -833.456473
Sum of electronic and thermal Free Energies= -833.514646

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9469532

TS14a′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.309936	-0.171689	-0.670074
2	6	0	-0.319138	0.316141	-1.532465
3	1	0	-0.713137	0.973138	-2.315229
4	6	0	-1.567666	-1.516122	-0.020708
5	1	0	-1.588645	-2.285554	-0.807390
6	1	0	-0.849358	-1.828999	0.743079
7	8	0	-2.838655	-1.407763	0.606096
8	6	0	-3.577619	-0.361083	-0.013409
9	1	0	-4.292169	0.011572	0.726300
10	1	0	-4.127531	-0.729574	-0.892503
11	6	0	-2.527895	0.649372	-0.444607
12	6	0	-1.657973	1.079274	0.714796
13	1	0	-2.802171	1.393630	-1.192508
14	1	0	-1.962169	0.598026	1.643684
15	6	0	-0.530545	1.895870	0.843473
16	6	0	0.354640	2.363721	-0.142998
17	1	0	-0.154262	1.933872	1.863476
18	1	0	1.233984	2.895536	0.221962
19	1	0	-0.017911	2.772169	-1.075853
20	6	0	0.978525	0.643261	-1.112722
21	1	0	1.581310	1.143656	-1.877560
22	14	0	2.077546	-0.367960	0.052002
23	6	0	1.561686	-0.374861	1.865877
24	1	0	0.499609	-0.590645	2.012103
25	1	0	2.140947	-1.134449	2.404384
26	1	0	1.769439	0.593375	2.333458
27	6	0	2.124399	-2.142412	-0.589146

28	1	0	2.473177	-2.174878	-1.627240
29	1	0	2.798930	-2.762267	0.013077
30	1	0	1.131982	-2.605740	-0.563303
31	6	0	3.804611	0.383128	-0.056933
32	1	0	4.199510	0.332594	-1.077987
33	1	0	3.797207	1.436478	0.247038
34	1	0	4.506325	-0.145991	0.597703

Zero-point correction= 0.295109 (Hartree/Particle)
Thermal correction to Energy= 0.310638
Thermal correction to Enthalpy= 0.311582
Thermal correction to Gibbs Free Energy= 0.253903
Sum of electronic and zero-point Energies= -833.448691
Sum of electronic and thermal Energies= -833.433162
Sum of electronic and thermal Enthalpies= -833.432218
Sum of electronic and thermal Free Energies= -833.489898

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9216392

INT22a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.854163	1.242835	-0.657729
2	6	0	1.242667	-0.108266	-0.758374
3	1	0	0.591258	-0.257221	-1.617095
4	6	0	1.712775	2.238194	-1.795364
5	1	0	1.923219	1.739572	-2.756015
6	1	0	0.725326	2.708114	-1.854305
7	8	0	2.654725	3.261331	-1.530767
8	6	0	3.761360	2.680590	-0.857732
9	1	0	4.238272	3.475515	-0.276898
10	1	0	4.493187	2.274277	-1.573535
11	6	0	3.183075	1.558446	-0.018094
12	6	0	1.939581	1.889954	0.746592
13	1	0	3.836805	0.764539	0.333916
14	1	0	1.647870	2.939011	0.792979
15	6	0	1.505342	1.027447	1.887314
16	6	0	0.327785	1.249861	2.574292
17	1	0	2.230256	0.331415	2.303546
18	1	0	0.137078	0.723288	3.505949
19	1	0	-0.254338	2.153429	2.415448
20	28	0	-0.002413	0.036505	0.908258
21	6	0	1.576152	-1.177124	0.047985
22	1	0	2.442019	-1.051096	0.699504
23	14	0	1.038825	-2.963198	-0.125414
24	6	0	-0.122603	-3.240900	-1.584771
25	1	0	-0.187290	-4.313568	-1.802598
26	1	0	-1.137487	-2.884227	-1.386504
27	1	0	0.242749	-2.743188	-2.490581
28	6	0	0.237109	-3.538895	1.481930
29	1	0	-0.037238	-4.599393	1.435466
30	1	0	0.930623	-3.409309	2.321375
31	1	0	-0.664652	-2.959882	1.708206
32	6	0	2.606261	-3.980772	-0.406404
33	1	0	3.325771	-3.836854	0.408320
34	1	0	2.378875	-5.051977	-0.462381
35	1	0	3.100942	-3.693738	-1.341405
36	6	0	-4.603319	-0.054706	-0.806538
37	6	0	-4.649513	1.047675	-0.055653
38	6	0	-3.601072	2.126829	-0.028391
39	6	0	-2.401509	1.864573	0.928769
40	6	0	-1.992301	0.408210	1.114826
41	6	0	-1.774791	-0.494319	0.074691
42	6	0	-2.050835	-0.159756	-1.372187
43	6	0	-3.513069	-0.481165	-1.765457
44	1	0	-5.441389	-0.746792	-0.732623

45	1	0	-5.506897	1.180560	0.602652
46	1	0	-4.062941	3.077811	0.260883
47	1	0	-3.222637	2.279984	-1.043751
48	1	0	-1.561163	2.466136	0.559358
49	1	0	-2.643214	2.267727	1.918360
50	1	0	-2.250630	-0.015534	2.083995
51	1	0	-1.889972	-1.552562	0.318393
52	1	0	-1.406791	-0.745625	-2.037702
53	1	0	-1.812175	0.889450	-1.570177
54	1	0	-3.710833	-0.060839	-2.762832
55	1	0	-3.591946	-1.569297	-1.887461

Zero-point correction= 0.481385 (Hartree/Particle)
Thermal correction to Energy= 0.507458
Thermal correction to Enthalpy= 0.508402
Thermal correction to Gibbs Free Energy= 0.426828
Sum of electronic and zero-point Energies= -1314.600226
Sum of electronic and thermal Energies= -1314.574153
Sum of electronic and thermal Enthalpies= -1314.573209
Sum of electronic and thermal Free Energies= -1314.654783
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1316.9918295

INT23a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.082660	-0.150381	0.600913
2	6	0	-0.261397	0.925552	1.222364
3	1	0	-0.809519	1.548981	1.932128
4	6	0	-1.059485	-1.544274	1.224288
5	1	0	-0.029286	-1.799931	1.509304
6	1	0	-1.702265	-1.641077	2.105120
7	8	0	-1.561999	-2.427970	0.235943
8	6	0	-1.262565	-1.900418	-1.047517
9	1	0	-2.032609	-2.264956	-1.734409
10	1	0	-0.281200	-2.248807	-1.407261
11	6	0	-1.250443	-0.398301	-0.873300
12	6	0	-2.403622	0.173831	-0.076788
13	1	0	-0.765330	0.228790	-1.613257
14	1	0	-3.228753	-0.506099	0.132414
15	6	0	-2.781194	1.587402	-0.284597
16	6	0	-4.020117	2.062745	-0.174856
17	1	0	-1.968988	2.268039	-0.541841
18	1	0	-4.241261	3.112298	-0.341557
19	1	0	-4.857005	1.417833	0.082990
20	6	0	1.040825	1.166475	1.022766
21	1	0	1.447048	1.993279	1.612046
22	14	0	2.322259	0.321118	-0.075280
23	6	0	2.470155	-1.528939	0.261101
24	1	0	1.587405	-2.087079	-0.066049
25	1	0	3.335705	-1.936050	-0.275166
26	1	0	2.616244	-1.728939	1.328319
27	6	0	2.005854	0.585423	-1.920216
28	1	0	1.608200	1.584835	-2.126781
29	1	0	2.945665	0.478332	-2.474488
30	1	0	1.303284	-0.150442	-2.324536
31	6	0	3.961195	1.141007	0.373268
32	1	0	3.938044	2.217546	0.167866
33	1	0	4.190088	1.010456	1.437246
34	1	0	4.789630	0.710368	-0.200293

Zero-point correction= 0.295064 (Hartree/Particle)
Thermal correction to Energy= 0.311980
Thermal correction to Enthalpy= 0.312925
Thermal correction to Gibbs Free Energy= 0.250562
Sum of electronic and zero-point Energies= -833.511357

Sum of electronic and thermal Energies= -833.494440
Sum of electronic and thermal Enthalpies= -833.493496
Sum of electronic and thermal Free Energies= -833.555859
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9841362

TS9a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.920691	-1.101215	-0.608528
2	6	0	0.155293	-1.134082	-1.445041
3	1	0	0.168670	-1.760439	-2.348044
4	6	0	-2.128501	-1.971735	-0.637946
5	1	0	-2.895891	-1.595484	-1.338728
6	1	0	-1.858246	-2.989073	-0.934481
7	8	0	-2.681814	-2.063915	0.659967
8	6	0	-2.996106	-0.765166	1.083611
9	1	0	-3.242224	-0.831070	2.147038
10	1	0	-3.887089	-0.402104	0.542922
11	6	0	-1.862653	0.231817	0.887704
12	6	0	-2.190885	1.458554	0.211010
13	1	0	-1.127911	0.243901	1.688017
14	1	0	-3.148941	1.496918	-0.302919
15	6	0	-1.292482	2.537411	-0.019418
16	6	0	0.059912	2.479106	0.345324
17	1	0	-1.630458	3.316664	-0.698561
18	1	0	0.740405	3.231858	-0.039025
19	1	0	0.376505	1.999215	1.268503
20	28	0	-0.496423	0.772423	-0.654746
21	6	0	1.168504	-0.117573	-1.178133
22	1	0	1.683201	0.250485	-2.074453
23	14	0	2.367943	-0.360188	0.238747
24	6	0	1.517065	-0.776556	1.871272
25	1	0	1.054433	0.102982	2.333883
26	1	0	0.736656	-1.531235	1.722386
27	1	0	2.244880	-1.175892	2.587547
28	6	0	3.429931	1.188250	0.437308
29	1	0	4.219436	1.026970	1.180878
30	1	0	3.915471	1.450075	-0.510232
31	1	0	2.839164	2.052633	0.757679
32	6	0	3.518293	-1.802520	-0.186802
33	1	0	4.032421	-1.631689	-1.140055
34	1	0	4.283944	-1.948958	0.584801
35	1	0	2.952658	-2.737394	-0.278616

Zero-point correction= 0.293912 (Hartree/Particle)
Thermal correction to Energy= 0.311169
Thermal correction to Enthalpy= 0.312113
Thermal correction to Gibbs Free Energy= 0.250642
Sum of electronic and zero-point Energies= -1002.762337
Sum of electronic and thermal Energies= -1002.745080
Sum of electronic and thermal Enthalpies= -1002.744136
Sum of electronic and thermal Free Energies= -1002.805607
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.8902979

INT19a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.278544	0.147281	-0.669214
2	6	0	0.228709	-0.462276	-1.525863
3	1	0	0.633759	-0.906317	-2.438019
4	6	0	1.829307	1.512902	-1.072483
5	1	0	2.500354	1.486320	-1.936961
6	1	0	0.988146	2.188267	-1.295965

7	8	0	2.580775	1.971819	0.034984
8	6	0	1.976854	1.469090	1.217779
9	1	0	1.194326	2.152557	1.579057
10	1	0	2.761234	1.400881	1.977532
11	6	0	1.384190	0.128348	0.826905
12	6	0	2.317606	-0.741978	0.021135
13	1	0	0.636508	-0.334754	1.462679
14	1	0	3.340940	-0.376463	-0.046816
15	6	0	2.194412	-2.221315	-0.001362
16	6	0	1.147734	-2.949399	0.385322
17	1	0	3.065924	-2.739006	-0.399270
18	1	0	1.161196	-4.031925	0.305386
19	1	0	0.238871	-2.503682	0.779449
20	6	0	-1.093631	-0.516322	-1.328159
21	1	0	-1.647456	-1.019094	-2.126535
22	14	0	-2.205949	0.120624	0.049316
23	6	0	-3.910621	0.314019	-0.735892
24	1	0	-4.649681	0.639803	0.004900
25	1	0	-3.893832	1.059366	-1.539125
26	1	0	-4.264549	-0.630344	-1.165235
27	6	0	-1.679742	1.788449	0.754738
28	1	0	-2.540286	2.282042	1.221342
29	1	0	-0.907515	1.681990	1.521450
30	1	0	-1.293154	2.456151	-0.022587
31	6	0	-2.335839	-1.143164	1.447272
32	1	0	-3.098098	-0.833649	2.171982
33	1	0	-2.621589	-2.128413	1.062473
34	1	0	-1.393144	-1.260826	1.992914

Zero-point correction= 0.295502 (Hartree/Particle)
Thermal correction to Energy= 0.312202
Thermal correction to Enthalpy= 0.313146
Thermal correction to Gibbs Free Energy= 0.251904
Sum of electronic and zero-point Energies= -833.509082
Sum of electronic and thermal Energies= -833.492382
Sum of electronic and thermal Enthalpies= -833.491438
Sum of electronic and thermal Free Energies= -833.552680
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9825423

TS12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269200	-1.242680	-0.324589
2	6	0	0.076237	-1.477899	-0.133929
3	1	0	0.410409	-2.247418	0.579922
4	6	0	-2.314465	-2.019369	0.406440
5	1	0	-2.152340	-3.089097	0.245289
6	1	0	-2.325080	-1.834624	1.497819
7	8	0	-3.595500	-1.724048	-0.120710
8	6	0	-3.784269	-0.346437	-0.002873
9	1	0	-3.946590	-0.071553	1.054314
10	1	0	-4.686350	-0.089882	-0.566554
11	6	0	-2.619066	0.474403	-0.536742
12	6	0	-2.142319	1.548142	0.264968
13	1	0	-2.561712	0.574126	-1.617057
14	1	0	-2.398616	1.587854	1.322250
15	6	0	-1.097820	2.403139	-0.271390
16	6	0	0.067670	2.601148	0.447394
17	1	0	-1.120131	2.667089	-1.328960
18	1	0	0.910140	3.112011	-0.006845
19	1	0	0.088756	2.498675	1.530888
20	28	0	-0.454705	0.563810	0.008140
21	6	0	1.029694	-0.543450	-0.682238
22	1	0	0.850978	-0.263573	-1.724538
23	14	0	2.770053	-0.368678	-0.041544

24	6	0	2.723989	-0.076266	1.824511
25	1	0	3.730245	-0.009964	2.254326
26	1	0	2.194388	0.855675	2.054679
27	1	0	2.196848	-0.891812	2.334683
28	6	0	3.589566	1.097646	-0.901860
29	1	0	4.624403	1.230800	-0.566134
30	1	0	3.608230	0.954690	-1.988698
31	1	0	3.048334	2.028203	-0.696953
32	6	0	3.783526	-1.929940	-0.376490
33	1	0	3.873918	-2.119782	-1.452002
34	1	0	4.795596	-1.844653	0.037171
35	1	0	3.312302	-2.810203	0.076567

Zero-point correction= 0.291776 (Hartree/Particle)
Thermal correction to Energy= 0.309976
Thermal correction to Enthalpy= 0.310920
Thermal correction to Gibbs Free Energy= 0.245986
Sum of electronic and zero-point Energies= -1002.748354
Sum of electronic and thermal Energies= -1002.730155
Sum of electronic and thermal Enthalpies= -1002.729211
Sum of electronic and thermal Free Energies= -1002.794145
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -1004.8753022

INT13a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.434457	-0.407150	0.312928
2	6	0	0.027836	-0.289237	0.541734
3	1	0	0.307214	-0.160867	1.589714
4	6	0	-2.183789	-1.541121	1.007512
5	1	0	-1.593215	-2.467933	0.927730
6	1	0	-2.403201	-1.351355	2.062975
7	8	0	-3.420988	-1.662728	0.329601
8	6	0	-3.210709	-1.309728	-1.029263
9	1	0	-4.170699	-0.968791	-1.427975
10	1	0	-2.869620	-2.177086	-1.616517
11	6	0	-2.133740	-0.244772	-1.003073
12	6	0	-2.306877	0.821162	0.059202
13	1	0	-1.598720	-0.003823	-1.916516
14	1	0	-3.267061	0.830906	0.573674
15	6	0	-1.684566	2.147261	-0.132992
16	6	0	-2.235465	3.294813	0.257725
17	1	0	-0.713464	2.159303	-0.626494
18	1	0	-1.741229	4.246964	0.091594
19	1	0	-3.201483	3.323935	0.756484
20	6	0	0.981613	-0.315236	-0.396424
21	1	0	0.657153	-0.451491	-1.431853
22	14	0	2.814295	-0.113343	-0.056298
23	6	0	3.096502	0.085217	1.795993
24	1	0	2.746853	-0.790910	2.353444
25	1	0	4.164483	0.208835	2.008339
26	1	0	2.577028	0.965660	2.190290
27	6	0	3.738152	-1.630845	-0.688522
28	1	0	3.568496	-1.782726	-1.760519
29	1	0	4.818240	-1.523640	-0.535352
30	1	0	3.413145	-2.538107	-0.167648
31	6	0	3.439085	1.416274	-0.966292
32	1	0	3.270082	1.332974	-2.045939
33	1	0	2.927593	2.319845	-0.616511
34	1	0	4.514670	1.557116	-0.808724

Zero-point correction= 0.294838 (Hartree/Particle)
Thermal correction to Energy= 0.311987
Thermal correction to Enthalpy= 0.312931
Thermal correction to Gibbs Free Energy= 0.249483

Sum of electronic and zero-point Energies= -833.514891
Sum of electronic and thermal Energies= -833.497742
Sum of electronic and thermal Enthalpies= -833.496798
Sum of electronic and thermal Free Energies= -833.560246
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -833.9878097

(1R, 5R)-3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.414872	-0.593022	0.559287
2	6	0	0.370537	-0.648707	1.379907
3	1	0	0.437711	-1.297422	2.253498
4	6	0	2.738019	-1.302021	0.727510
5	1	0	3.067609	-1.380280	1.766554
6	1	0	2.700835	-2.317903	0.294340
7	8	0	3.665756	-0.501014	0.022444
8	6	0	2.987803	-0.042732	-1.129735
9	1	0	3.008702	-0.816384	-1.914108
10	1	0	3.514489	0.840740	-1.499443
11	6	0	1.525986	0.241926	-0.702295
12	6	0	1.214125	1.710141	-0.532817
13	1	0	0.852414	-0.163490	-1.472228
14	1	0	1.784214	2.371802	-1.184830
15	6	0	0.312845	2.280505	0.267142
16	6	0	-0.633527	1.672258	1.271860
17	1	0	0.246662	3.367703	0.219249
18	1	0	-0.251924	1.927463	2.272239
19	1	0	-1.592782	2.203971	1.188183
20	6	0	-0.897509	0.151463	1.218705
21	1	0	-1.521446	-0.063821	2.097237
22	14	0	-2.036012	-0.392564	-0.232533
23	6	0	-1.581416	-2.133115	-0.793842
24	1	0	-0.568988	-2.169718	-1.210314
25	1	0	-1.616219	-2.840290	0.042471
26	1	0	-2.277402	-2.488029	-1.562531
27	6	0	-2.000201	0.788204	-1.704410
28	1	0	-2.752616	0.477023	-2.439118
29	1	0	-2.238880	1.812764	-1.398646
30	1	0	-1.029097	0.817923	-2.206425
31	6	0	-3.798147	-0.392535	0.447897
32	1	0	-4.527131	-0.638330	-0.332521
33	1	0	-3.913310	-1.125255	1.255007
34	1	0	-4.065054	0.591353	0.852048

Zero-point correction= 0.298324 (Hartree/Particle)
Thermal correction to Energy= 0.313970
Thermal correction to Enthalpy= 0.314915
Thermal correction to Gibbs Free Energy= 0.256432
Sum of electronic and zero-point Energies= -833.539899
Sum of electronic and thermal Energies= -833.524253
Sum of electronic and thermal Enthalpies= -833.523309
Sum of electronic and thermal Free Energies= -833.581791
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -834.0174712

(1S, 5R)-3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.468673	-0.593569	-0.254232
2	6	0	0.226378	-0.592993	-0.736877
3	1	0	-0.092343	-1.500983	-1.254220
4	6	0	2.430019	-1.766097	-0.361771
5	1	0	2.032321	-2.695448	0.057137
6	1	0	2.703693	-1.950900	-1.414122

7	8	0	3.571546	-1.402221	0.391908
8	6	0	3.681257	0.001139	0.299446
9	1	0	4.117334	0.296477	-0.670982
10	1	0	4.344046	0.342736	1.097961
11	6	0	2.244113	0.534828	0.410912
12	6	0	2.029715	1.880075	-0.233751
13	1	0	1.977332	0.580769	1.477691
14	1	0	2.904761	2.398189	-0.623935
15	6	0	0.819896	2.420742	-0.360838
16	6	0	-0.423650	1.737971	0.150430
17	1	0	0.708574	3.382245	-0.857788
18	1	0	-0.268795	1.454429	1.201611
19	1	0	-1.258105	2.447195	0.144350
20	6	0	-0.829604	0.479601	-0.648913
21	1	0	-1.082910	0.787177	-1.677406
22	14	0	-2.424909	-0.285619	0.075831
23	6	0	-2.069360	-0.920133	1.813929
24	1	0	-1.789522	-0.104303	2.489890
25	1	0	-2.946590	-1.418138	2.241938
26	1	0	-1.243380	-1.639769	1.801999
27	6	0	-2.991641	-1.711177	-1.022959
28	1	0	-3.943579	-2.119031	-0.663923
29	1	0	-3.140735	-1.383437	-2.058163
30	1	0	-2.266207	-2.531860	-1.032007
31	6	0	-3.780714	1.025944	0.130415
32	1	0	-3.923706	1.494799	-0.850036
33	1	0	-4.736968	0.580326	0.427445
34	1	0	-3.549349	1.817978	0.850908

Zero-point correction= 0.297681 (Hartree/Particle)
Thermal correction to Energy= 0.313598
Thermal correction to Enthalpy= 0.314542
Thermal correction to Gibbs Free Energy= 0.254940
Sum of electronic and zero-point Energies= -833.544514
Sum of electronic and thermal Energies= -833.528597
Sum of electronic and thermal Enthalpies= -833.527653
Sum of electronic and thermal Free Energies= -833.587256
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -834.0213737

(1S, 5S)-3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.540171	0.579856	-0.508854
2	6	0	0.311284	0.893571	-0.919886
3	1	0	0.112519	1.952785	-1.099375
4	6	0	2.637982	1.604994	-0.265906
5	1	0	2.928958	2.152756	-1.168607
6	1	0	2.323227	2.338439	0.493454
7	8	0	3.769573	0.879444	0.183687
8	6	0	3.293318	-0.315250	0.763077
9	1	0	2.919074	-0.140285	1.787014
10	1	0	4.122869	-1.025353	0.808923
11	6	0	2.139978	-0.767267	-0.142238
12	6	0	1.221110	-1.782704	0.482200
13	1	0	2.589673	-1.199405	-1.050870
14	1	0	1.567120	-2.265485	1.395506
15	6	0	0.044235	-2.126101	-0.037015
16	6	0	-0.515741	-1.501796	-1.291042
17	1	0	-0.558367	-2.877806	0.470166
18	1	0	0.218238	-1.600852	-2.104175
19	1	0	-1.408130	-2.050054	-1.610825
20	6	0	-0.872214	-0.008821	-1.135444
21	1	0	-1.355535	0.309862	-2.072841
22	14	0	-2.184443	0.342703	0.216210
23	6	0	-2.848842	2.085359	-0.075335

24	1	0	-2.058629	2.837379	0.030354
25	1	0	-3.280179	2.190947	-1.077438
26	1	0	-3.632511	2.329722	0.650886
27	6	0	-1.449300	0.246616	1.947720
28	1	0	-2.136373	0.675370	2.686574
29	1	0	-1.237059	-0.786842	2.236976
30	1	0	-0.505129	0.800302	1.995163
31	6	0	-3.589634	-0.904624	0.036947
32	1	0	-4.391429	-0.695516	0.754256
33	1	0	-4.026220	-0.875276	-0.968039
34	1	0	-3.240568	-1.927082	0.221119

Zero-point correction= 0.297834 (Hartree/Particle)
Thermal correction to Energy= 0.313682
Thermal correction to Enthalpy= 0.314627
Thermal correction to Gibbs Free Energy= 0.254972
Sum of electronic and zero-point Energies= -833.546521
Sum of electronic and thermal Energies= -833.530673
Sum of electronic and thermal Enthalpies= -833.529729
Sum of electronic and thermal Free Energies= -833.589383
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in tetrahydrohuran solvent = -834.0213737

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.500194	0.396019	-0.000002
2	7	0	0.848155	1.662358	-0.000045
3	7	0	1.120891	2.760093	-0.000112
4	6	0	-0.942959	0.077722	0.000001
5	6	0	-1.386436	-1.251494	-0.000117
6	6	0	-1.897589	1.104599	0.000116
7	6	0	-2.748055	-1.532580	-0.000120
8	1	0	-0.662530	-2.055434	-0.000196
9	6	0	-3.255275	0.811926	0.000107
10	1	0	-1.589396	2.146656	0.000222
11	6	0	-3.690456	-0.509668	-0.000012
12	1	0	-3.070977	-2.569570	-0.000214
13	1	0	-3.974983	1.625039	0.000195
14	1	0	-4.751866	-0.737545	-0.000019
15	6	0	1.620351	-0.551569	0.000058
16	8	0	1.520414	-1.758543	0.000154
17	8	0	2.803543	0.094151	-0.000039
18	6	0	3.955232	-0.747847	-0.000002
19	1	0	4.808614	-0.070610	-0.000114
20	1	0	3.968098	-1.381505	0.890051
21	1	0	3.968016	-1.381700	-0.889915

Zero-point correction= 0.160592 (Hartree/Particle)
Thermal correction to Energy= 0.172220
Thermal correction to Enthalpy= 0.173164
Thermal correction to Gibbs Free Energy= 0.120577
Sum of electronic and zero-point Energies= -607.314533
Sum of electronic and thermal Energies= -607.302905
Sum of electronic and thermal Enthalpies= -607.301961
Sum of electronic and thermal Free Energies= -607.354548
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -607.6401776

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.057784	3.169762	0.905780
2	6	0	2.329417	2.716323	1.033807
3	6	0	1.101891	1.046784	0.193600

4	7	0	0.317092	2.124650	0.385744
5	1	0	0.612762	4.125960	1.130246
6	1	0	3.226361	3.193653	1.395040
7	7	0	2.334276	1.405990	0.587973
8	79	0	0.420465	-0.697152	-0.551211
9	6	0	-1.085057	2.120172	0.061166
10	6	0	-1.992772	1.689792	1.033329
11	6	0	-1.466822	2.456088	-1.241493
12	6	0	-3.334584	1.611125	0.667911
13	6	0	-2.820377	2.352132	-1.559267
14	6	0	-3.765068	1.933528	-0.620546
15	1	0	-4.056270	1.275589	1.407002
16	1	0	-3.144069	2.603198	-2.566428
17	6	0	3.477233	0.534251	0.529529
18	6	0	3.773446	-0.250953	1.646079
19	6	0	4.216008	0.485803	-0.656298
20	6	0	4.873434	-1.101632	1.556079
21	6	0	5.306145	-0.380077	-0.694748
22	6	0	5.652925	-1.174600	0.400393
23	1	0	5.129067	-1.722588	2.410935
24	1	0	5.900489	-0.436484	-1.603432
25	6	0	-0.448840	2.888133	-2.265106
26	1	0	0.096228	3.780285	-1.938330
27	1	0	0.295331	2.102718	-2.444436
28	1	0	-0.930349	3.119335	-3.217837
29	6	0	-5.225144	1.838373	-0.978926
30	1	0	-5.706253	1.008047	-0.452683
31	1	0	-5.752477	2.756747	-0.696707
32	1	0	-5.368053	1.691778	-2.053143
33	6	0	-1.536578	1.293598	2.413368
34	1	0	-2.386496	0.967686	3.017432
35	1	0	-0.814600	0.469202	2.371069
36	1	0	-1.047377	2.125744	2.931460
37	6	0	3.826775	1.313979	-1.853900
38	1	0	2.888627	0.951742	-2.292432
39	1	0	3.677522	2.367036	-1.592975
40	1	0	4.596809	1.263901	-2.626921
41	6	0	6.860315	-2.074132	0.341030
42	1	0	6.798911	-2.876420	1.081346
43	1	0	6.972256	-2.527819	-0.648252
44	1	0	7.773918	-1.504127	0.545704
45	6	0	2.923341	-0.190056	2.888927
46	1	0	2.938024	0.808218	3.340312
47	1	0	1.876666	-0.429562	2.666527
48	1	0	3.279845	-0.900869	3.637751
49	6	0	-1.156839	-2.069932	-1.461944
50	6	0	-0.134612	-2.743845	-1.348847
51	1	0	0.622368	-3.503303	-1.373847
52	6	0	-2.503184	-1.453726	-1.665198
53	1	0	-2.718390	-0.770298	-0.830646
54	1	0	-2.478252	-0.866601	-2.587085
55	8	0	-3.472014	-2.441813	-1.813145
56	6	0	-3.862003	-3.060354	-0.584995
57	1	0	-2.982740	-3.474309	-0.069268
58	1	0	-4.494117	-3.896145	-0.895758
59	6	0	-4.616688	-2.126571	0.310668
60	6	0	-4.250868	-1.831143	1.563862
61	1	0	-5.529112	-1.701543	-0.106833
62	1	0	-3.337490	-2.266873	1.972779
63	6	0	-5.022449	-0.973224	2.458771
64	6	0	-4.668744	-0.701777	3.718994
65	1	0	-5.942197	-0.551025	2.054612
66	1	0	-5.277368	-0.070362	4.357921
67	1	0	-3.768288	-1.124390	4.159573

Zero-point correction= 0.567230 (Hartree/Particle)
Thermal correction to Energy= 0.603379

Thermal correction to Enthalpy= 0.604323
Thermal correction to Gibbs Free Energy= 0.495595
Sum of electronic and zero-point Energies= -1444.509900
Sum of electronic and thermal Energies= -1444.473751
Sum of electronic and thermal Enthalpies= -1444.472807
Sum of electronic and thermal Free Energies= -1444.581535
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1445.8266075

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.109468	-3.875945	-0.686846
2	6	0	-1.443390	-3.635345	-0.746319
3	6	0	-0.437418	-1.728285	-0.144143
4	7	0	0.491631	-2.686459	-0.316214
5	1	0	0.463110	-4.770207	-0.874865
6	1	0	-2.273553	-4.276329	-0.997264
7	7	0	-1.623083	-2.305404	-0.409311
8	79	0	-0.073580	0.195482	0.310822
9	6	0	1.899683	-2.427318	-0.172029
10	6	0	2.486260	-2.612825	1.084478
11	6	0	2.596616	-1.912449	-1.267439
12	6	0	3.831333	-2.280946	1.219920
13	6	0	3.943610	-1.600958	-1.081323
14	6	0	4.576116	-1.779820	0.148110
15	1	0	4.312490	-2.416564	2.185467
16	1	0	4.507630	-1.200174	-1.919767
17	6	0	-2.861067	-1.572741	-0.382198
18	6	0	-3.592751	-1.542125	0.808317
19	6	0	-3.229535	-0.852793	-1.521572
20	6	0	-4.746929	-0.763184	0.831457
21	6	0	-4.393362	-0.088357	-1.447456
22	6	0	-5.162844	-0.033056	-0.284382
23	1	0	-5.334952	-0.721951	1.745149
24	1	0	-4.705360	0.477554	-2.321878
25	6	0	1.913176	-1.638892	-2.581964
26	1	0	1.214420	-2.433675	-2.860041
27	1	0	1.342498	-0.702861	-2.528836
28	1	0	2.646633	-1.533769	-3.384816
29	6	0	6.038446	-1.458839	0.322407
30	1	0	6.636465	-2.377212	0.325140
31	1	0	6.411491	-0.826691	-0.488765
32	1	0	6.223115	-0.946667	1.271951
33	6	0	1.675105	-3.111092	2.252187
34	1	0	2.303761	-3.239230	3.136256
35	1	0	0.876800	-2.402513	2.504420
36	1	0	1.197724	-4.072676	2.035828
37	6	0	-2.381293	-0.865866	-2.767062
38	1	0	-1.453563	-0.300735	-2.614540
39	1	0	-2.100225	-1.883405	-3.058050
40	1	0	-2.913394	-0.408698	-3.604293
41	6	0	-6.430558	0.781037	-0.237897
42	1	0	-7.302862	0.146206	-0.431132
43	1	0	-6.573757	1.242064	0.744232
44	1	0	-6.427124	1.572137	-0.993199
45	6	0	-3.122944	-2.291028	2.028206
46	1	0	-2.963179	-3.353843	1.818213
47	1	0	-2.171219	-1.885745	2.393236
48	1	0	-3.854098	-2.214363	2.836179
49	6	0	0.395067	2.299524	0.560800
50	7	0	0.406064	2.553707	1.936719
51	7	0	0.462626	2.716081	3.033665
52	6	0	1.750501	2.638941	-0.031205
53	6	0	1.955001	3.872331	-0.654621
54	6	0	2.806930	1.727043	0.067035

55	6	0	3.200866	4.179493	-1.190035
56	1	0	1.140782	4.582944	-0.746539
57	6	0	4.053067	2.045290	-0.460583
58	1	0	2.664981	0.761342	0.546821
59	6	0	4.250716	3.269441	-1.092616
60	1	0	3.350745	5.134454	-1.682777
61	1	0	4.862964	1.327174	-0.382282
62	1	0	5.221021	3.514385	-1.512638
63	6	0	-0.860180	2.893433	-0.062388
64	8	0	-0.959156	3.114804	-1.239882
65	8	0	-1.820768	3.047998	0.848752
66	6	0	-3.118924	3.386485	0.331540
67	1	0	-3.752044	3.512923	1.207462
68	1	0	-3.066258	4.309239	-0.248203
69	1	0	-3.484458	2.569007	-0.294677

Zero-point correction= 0.567836 (Hartree/Particle)
Thermal correction to Energy= 0.606041
Thermal correction to Enthalpy= 0.606986
Thermal correction to Gibbs Free Energy= 0.493037
Sum of electronic and zero-point Energies= -1666.149528
Sum of electronic and thermal Energies= -1666.111323
Sum of electronic and thermal Enthalpies= -1666.110379
Sum of electronic and thermal Free Energies= -1666.224327
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1667.5163632

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505351	-3.913660	-0.423369
2	6	0	-1.820216	-3.581475	-0.443055
3	6	0	-0.653168	-1.696548	-0.108018
4	7	0	0.194588	-2.739152	-0.217154
5	1	0	-0.006635	-4.862830	-0.538228
6	1	0	-2.707346	-4.179601	-0.577939
7	7	0	-1.887410	-2.213487	-0.247209
8	79	0	-0.077382	0.231635	0.146387
9	6	0	1.622148	-2.588148	-0.127289
10	6	0	2.223030	-2.699249	1.131519
11	6	0	2.335118	-2.259639	-1.282256
12	6	0	3.596287	-2.485356	1.209184
13	6	0	3.709948	-2.058970	-1.152333
14	6	0	4.355893	-2.172571	0.078065
15	1	0	4.088501	-2.569572	2.175023
16	1	0	4.287372	-1.804884	-2.037729
17	6	0	-3.082158	-1.413784	-0.209543
18	6	0	-3.706089	-1.207588	1.023070
19	6	0	-3.529730	-0.829983	-1.397416
20	6	0	-4.838442	-0.396094	1.040627
21	6	0	-4.665145	-0.025548	-1.326915
22	6	0	-5.333869	0.197377	-0.121776
23	1	0	-5.345065	-0.221509	1.986620
24	1	0	-5.038193	0.437913	-2.236949
25	6	0	1.643020	-2.075938	-2.607697
26	1	0	0.920091	-2.872961	-2.807930
27	1	0	1.095018	-1.125615	-2.629195
28	1	0	2.368074	-2.060544	-3.424564
29	6	0	5.847194	-1.984456	0.193025
30	1	0	6.348500	-2.951052	0.316020
31	1	0	6.263439	-1.509851	-0.700330
32	1	0	6.106436	-1.372304	1.063283
33	6	0	1.402777	-3.011606	2.356134
34	1	0	2.034341	-3.058811	3.246252
35	1	0	0.636765	-2.244634	2.522416
36	1	0	0.883627	-3.971252	2.259827

37	6	0	-2.789185	-1.033971	-2.693777
38	1	0	-1.805919	-0.548801	-2.662041
39	1	0	-2.621396	-2.095603	-2.904062
40	1	0	-3.345341	-0.606884	-3.531251
41	6	0	-6.581340	1.042406	-0.083197
42	1	0	-7.468813	0.426441	-0.268986
43	1	0	-6.711898	1.520599	0.891920
44	1	0	-6.559169	1.822973	-0.849264
45	6	0	-3.147073	-1.808146	2.286961
46	1	0	-3.013449	-2.891578	2.199430
47	1	0	-2.165120	-1.378269	2.519777
48	1	0	-3.808897	-1.616594	3.134720
49	6	0	0.650316	2.188772	0.241140
50	7	0	0.552504	2.560214	1.948910
51	7	0	0.637110	2.586337	3.047233
52	6	0	2.075382	2.445267	-0.071811
53	6	0	2.511190	3.722366	-0.459401
54	6	0	3.008762	1.400200	0.017935
55	6	0	3.846839	3.944182	-0.760535
56	1	0	1.799955	4.537402	-0.547658
57	6	0	4.345714	1.628545	-0.277230
58	1	0	2.689583	0.404039	0.314185
59	6	0	4.764917	2.898642	-0.666664
60	1	0	4.174415	4.931259	-1.069304
61	1	0	5.057579	0.812613	-0.209615
62	1	0	5.810048	3.075962	-0.900379
63	6	0	-0.382716	3.122836	-0.337519
64	8	0	-0.398653	3.344464	-1.522507
65	8	0	-1.279939	3.552066	0.546399
66	6	0	-2.389957	4.281547	-0.002432
67	1	0	-2.969866	4.611375	0.857269
68	1	0	-2.033398	5.134499	-0.582063
69	1	0	-2.983478	3.622851	-0.639964

Zero-point correction= 0.566022 (Hartree/Particle)
Thermal correction to Energy= 0.604235
Thermal correction to Enthalpy= 0.605179
Thermal correction to Gibbs Free Energy= 0.491238
Sum of electronic and zero-point Energies= -1666.141860
Sum of electronic and thermal Energies= -1666.103647
Sum of electronic and thermal Enthalpies= -1666.102703
Sum of electronic and thermal Free Energies= -1666.216644
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1667.5073356

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.699501	-3.810103	-0.003465
2	6	0	2.000224	-3.427249	0.034485
3	6	0	0.751659	-1.563270	0.007516
4	7	0	-0.050457	-2.649353	-0.019108
5	1	0	0.241117	-4.786058	-0.021613
6	1	0	2.914164	-3.999300	0.057478
7	7	0	2.007856	-2.044746	0.040139
8	79	0	0.047658	0.356773	0.023709
9	6	0	-1.484699	-2.556892	-0.067894
10	6	0	-2.102989	-2.452909	-1.317951
11	6	0	-2.192806	-2.505193	1.135982
12	6	0	-3.489070	-2.310845	-1.339602
13	6	0	-3.578367	-2.364029	1.060994
14	6	0	-4.242074	-2.274453	-0.163778
15	1	0	-3.993671	-2.230085	-2.299221
16	1	0	-4.151972	-2.326726	1.983866
17	6	0	3.178733	-1.209685	0.064233
18	6	0	3.748895	-0.832560	-1.153351

19	6	0	3.667311	-0.779152	1.300845
20	6	0	4.870877	-0.007203	-1.107200
21	6	0	4.789127	0.045803	1.292979
22	6	0	5.406265	0.436543	0.102568
23	1	0	5.337167	0.298188	-2.040550
24	1	0	5.191513	0.395816	2.240477
25	6	0	-1.478224	-2.557566	2.461019
26	1	0	-0.817844	-3.427980	2.532242
27	1	0	-0.855643	-1.665833	2.603367
28	1	0	-2.192333	-2.605282	3.286159
29	6	0	-5.744967	-2.167728	-0.221427
30	1	0	-6.196249	-3.158664	-0.346250
31	1	0	-6.154373	-1.738040	0.698063
32	1	0	-6.071167	-1.555259	-1.068192
33	6	0	-1.293510	-2.451529	-2.588527
34	1	0	-1.944540	-2.496757	-3.464596
35	1	0	-0.689478	-1.539029	-2.663607
36	1	0	-0.603948	-3.300747	-2.632787
37	6	0	2.982473	-1.164572	2.586499
38	1	0	1.997544	-0.687902	2.662883
39	1	0	2.827531	-2.246396	2.659128
40	1	0	3.572834	-0.849659	3.450071
41	6	0	6.638829	1.303329	0.130249
42	1	0	7.528487	0.701484	0.348942
43	1	0	6.802293	1.798334	-0.831012
44	1	0	6.566631	2.072954	0.904751
45	6	0	3.150395	-1.274490	-2.463811
46	1	0	3.034686	-2.362456	-2.515649
47	1	0	2.155635	-0.834629	-2.606251
48	1	0	3.778101	-0.962743	-3.301850
49	6	0	-0.821490	2.181183	0.062905
50	6	0	-2.213724	2.414023	0.120569
51	6	0	-2.749648	3.730352	0.201113
52	6	0	-3.115098	1.312277	0.093361
53	6	0	-4.113916	3.928747	0.252060
54	1	0	-2.077401	4.581472	0.241376
55	6	0	-4.478944	1.520481	0.136952
56	1	0	-2.720961	0.301909	0.032665
57	6	0	-4.974259	2.824878	0.218605
58	1	0	-4.520805	4.931435	0.321447
59	1	0	-5.159904	0.676862	0.114014
60	1	0	-6.047316	2.987137	0.260277
61	6	0	0.088962	3.355250	0.129988
62	8	0	0.405442	3.817415	1.201214
63	8	0	0.512185	3.751331	-1.059927
64	6	0	1.482678	4.814354	-1.057015
65	1	0	1.702915	5.002548	-2.105585
66	1	0	1.066780	5.705050	-0.582482
67	1	0	2.379554	4.497259	-0.521463

Zero-point correction= 0.558209 (Hartree/Particle)
Thermal correction to Energy= 0.594527
Thermal correction to Enthalpy= 0.595472
Thermal correction to Gibbs Free Energy= 0.484348
Sum of electronic and zero-point Energies= -1556.692195
Sum of electronic and thermal Energies= -1556.655877
Sum of electronic and thermal Enthalpies= -1556.654933
Sum of electronic and thermal Free Energies= -1556.766057
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1558.0211242

TS1b′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.653012	-3.404486	0.294717
2	6	0	2.838441	-2.750276	0.241872

3	6	0	1.214269	-1.210331	0.078831
4	7	0	0.666842	-2.440010	0.192754
5	1	0	1.418927	-4.452385	0.394936
6	1	0	3.854963	-3.107699	0.285544
7	7	0	2.545562	-1.403744	0.109409
8	79	0	0.124132	0.492865	-0.098736
9	6	0	-0.753641	-2.660685	0.193304
10	6	0	-1.400319	-2.842110	-1.032332
11	6	0	-1.436591	-2.617336	1.412329
12	6	0	-2.787392	-2.982142	-1.013687
13	6	0	-2.823056	-2.761045	1.377696
14	6	0	-3.515089	-2.933336	0.176582
15	1	0	-3.312917	-3.126311	-1.954644
16	1	0	-3.377944	-2.730098	2.312258
17	6	0	3.512399	-0.343861	0.015555
18	6	0	3.936578	0.061059	-1.251841
19	6	0	3.964263	0.250882	1.196450
20	6	0	4.869123	1.094421	-1.315073
21	6	0	4.896758	1.278581	1.079861
22	6	0	5.364562	1.708228	-0.163775
23	1	0	5.219103	1.428079	-2.288846
24	1	0	5.268916	1.756305	1.982837
25	6	0	-0.700988	-2.389354	2.707070
26	1	0	0.077194	-3.143215	2.867385
27	1	0	-0.208644	-1.409621	2.710653
28	1	0	-1.387658	-2.426806	3.555825
29	6	0	-5.020147	-3.002705	0.162704
30	1	0	-5.442642	-1.991476	0.112842
31	1	0	-5.388295	-3.561128	-0.702480
32	1	0	-5.408460	-3.478238	1.067740
33	6	0	-0.625323	-2.850003	-2.324255
34	1	0	-1.282515	-3.061624	-3.170913
35	1	0	-0.146105	-1.879211	-2.498887
36	1	0	0.167727	-3.605023	-2.315616
37	6	0	3.440603	-0.192736	2.537901
38	1	0	2.363342	-0.004925	2.620769
39	1	0	3.596300	-1.264851	2.700403
40	1	0	3.939320	0.345306	3.347447
41	6	0	6.405037	2.794197	-0.258732
42	1	0	6.368019	3.300298	-1.227393
43	1	0	6.272453	3.545184	0.525813
44	1	0	7.410154	2.372093	-0.143324
45	6	0	3.385472	-0.580485	-2.498861
46	1	0	3.520111	-1.667704	-2.489146
47	1	0	2.310539	-0.386972	-2.597624
48	1	0	3.880921	-0.187207	-3.389453
49	6	0	-2.315071	1.694397	-0.312568
50	6	0	-1.141441	2.173598	-0.271736
51	1	0	-0.763796	3.187051	-0.305556
52	6	0	-3.255564	0.518714	-0.275748
53	1	0	-3.154132	-0.025135	-1.227392
54	1	0	-2.947810	-0.146267	0.535073
55	8	0	-4.581655	0.883533	-0.039447
56	6	0	-4.998586	1.827145	-1.009037
57	1	0	-6.036254	2.073214	-0.769633
58	1	0	-4.970595	1.385895	-2.015110
59	6	0	-4.106988	3.041730	-0.941985
60	6	0	-3.781357	3.626714	0.239142
61	1	0	-3.785318	3.500895	-1.874559
62	1	0	-4.147495	3.186199	1.166013
63	6	0	-2.954365	4.816223	0.338393
64	6	0	-2.550234	5.319447	1.510671
65	1	0	-2.665012	5.299022	-0.593376
66	1	0	-1.938481	6.214055	1.564156
67	1	0	-2.830134	4.857326	2.454124

Zero-point correction= 0.566800 (Hartree/Particle)

Thermal correction to Energy= 0.601987
Thermal correction to Enthalpy= 0.602931
Thermal correction to Gibbs Free Energy= 0.495835
Sum of electronic and zero-point Energies= -1444.494172
Sum of electronic and thermal Energies= -1444.458985
Sum of electronic and thermal Enthalpies= -1444.458041
Sum of electronic and thermal Free Energies= -1444.565136
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1445.8009841

INT2b′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.519143	-3.401054	0.537506
2	6	0	2.726908	-2.786921	0.485555
3	6	0	1.159070	-1.215960	0.143451
4	7	0	0.570639	-2.419005	0.325236
5	1	0	1.248748	-4.431841	0.703000
6	1	0	3.728531	-3.170700	0.597539
7	7	0	2.482010	-1.447831	0.242542
8	79	0	0.100182	0.513377	-0.184399
9	6	0	-0.855583	-2.597443	0.282827
10	6	0	-1.461129	-2.831216	-0.954821
11	6	0	-1.582684	-2.458684	1.468434
12	6	0	-2.851900	-2.922363	-0.983653
13	6	0	-2.970244	-2.560306	1.387296
14	6	0	-3.622036	-2.778096	0.171932
15	1	0	-3.347042	-3.101148	-1.934961
16	1	0	-3.558580	-2.455892	2.295835
17	6	0	3.486069	-0.429479	0.094973
18	6	0	4.016353	-0.199791	-1.177054
19	6	0	3.866416	0.302531	1.221802
20	6	0	4.982696	0.795680	-1.298278
21	6	0	4.835189	1.289107	1.048045
22	6	0	5.407929	1.544062	-0.198824
23	1	0	5.415333	0.992533	-2.276087
24	1	0	5.151444	1.872580	1.909208
25	6	0	-0.889301	-2.170351	2.774439
26	1	0	-0.136613	-2.929728	3.011067
27	1	0	-0.372590	-1.203610	2.737197
28	1	0	-1.607489	-2.140112	3.597076
29	6	0	-5.126869	-2.795786	0.100902
30	1	0	-5.508227	-1.776103	-0.033877
31	1	0	-5.481736	-3.398412	-0.739910
32	1	0	-5.566986	-3.196497	1.018500
33	6	0	-0.640190	-2.936812	-2.213710
34	1	0	-1.267728	-3.207938	-3.065931
35	1	0	-0.151565	-1.981808	-2.441875
36	1	0	0.149319	-3.690086	-2.121588
37	6	0	3.232223	0.048609	2.564891
38	1	0	2.163036	0.292246	2.546083
39	1	0	3.320201	-1.002172	2.861999
40	1	0	3.703625	0.658524	3.338975
41	6	0	6.482639	2.589107	-0.354470
42	1	0	6.431458	3.070976	-1.335158
43	1	0	6.401952	3.364046	0.413044
44	1	0	7.475783	2.134356	-0.261700
45	6	0	3.538417	-0.984985	-2.371118
46	1	0	3.681547	-2.062255	-2.232693
47	1	0	2.468607	-0.819261	-2.545852
48	1	0	4.077717	-0.687549	-3.273375
49	6	0	-2.489851	1.997732	-0.359991
50	6	0	-1.120039	2.089108	-0.480223
51	1	0	-0.743748	3.086806	-0.715901
52	6	0	-3.260360	0.720077	-0.048023
53	1	0	-2.908328	-0.084351	-0.709716

54	1	0	-3.156040	0.389532	0.987882
55	8	0	-4.623539	1.021008	-0.278604
56	6	0	-4.681315	1.930568	-1.354333
57	1	0	-5.657638	2.419467	-1.332201
58	1	0	-4.545901	1.428768	-2.322604
59	6	0	-3.533375	2.909580	-1.128552
60	6	0	-3.289611	3.365900	0.213031
61	1	0	-3.155600	3.486484	-1.967444
62	1	0	-3.957747	2.997130	0.989435
63	6	0	-2.548891	4.599731	0.519584
64	6	0	-2.564895	5.155478	1.731055
65	1	0	-2.023401	5.086194	-0.299790
66	1	0	-2.056569	6.093560	1.926751
67	1	0	-3.097045	4.701103	2.562976

Zero-point correction= 0.570260 (Hartree/Particle)
Thermal correction to Energy= 0.604681
Thermal correction to Enthalpy= 0.605625
Thermal correction to Gibbs Free Energy= 0.500412
Sum of electronic and zero-point Energies= -1444.526414
Sum of electronic and thermal Energies= -1444.491993
Sum of electronic and thermal Enthalpies= -1444.491048
Sum of electronic and thermal Free Energies= -1444.596262
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1445.8343602

INT2b″

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.228310	2.402951	0.516175
2	6	0	1.969973	1.112106	0.290893
3	1	0	2.724501	0.333170	0.261237
4	6	0	3.519126	3.170354	0.576858
5	1	0	3.742738	3.522310	1.597457
6	1	0	4.381980	2.628398	0.186794
7	8	0	3.244206	4.260135	-0.292484
8	6	0	1.903702	4.677869	-0.067065
9	1	0	1.526571	5.099087	-1.002757
10	1	0	1.871722	5.458737	0.704665
11	6	0	1.128191	3.422960	0.403523
12	6	0	0.103349	2.797354	-0.535621
13	1	0	0.660310	3.600738	1.380102
14	1	0	0.374245	2.837874	-1.593868
15	6	0	-1.306963	2.697436	-0.232000
16	6	0	-2.147007	1.933098	-1.006066
17	1	0	-1.642268	3.005968	0.758186
18	1	0	-3.148886	1.692348	-0.668051
19	1	0	-1.897436	1.688639	-2.037084
20	6	0	-0.207169	-3.560564	0.307210
21	6	0	-1.529469	-3.276545	0.365449
22	6	0	-0.428855	-1.336710	0.070378
23	7	0	0.449358	-2.358228	0.126581
24	1	0	0.328774	-4.493839	0.375946
25	1	0	-2.393430	-3.908107	0.498442
26	7	0	-1.645662	-1.906508	0.217466
27	79	0	-0.007254	0.696547	-0.151821
28	6	0	1.876984	-2.221938	0.029573
29	6	0	2.615959	-2.165444	1.213824
30	6	0	2.455776	-2.112328	-1.236568
31	6	0	3.995732	-2.006812	1.100828
32	6	0	3.838013	-1.947034	-1.295955
33	6	0	4.623334	-1.898513	-0.142083
34	1	0	4.594547	-1.957330	2.006743
35	1	0	4.314942	-1.854200	-2.268402
36	6	0	-2.895063	-1.198545	0.200776
37	6	0	-3.327535	-0.566512	1.368562

38	6	0	-3.615254	-1.159241	-0.997424
39	6	0	-4.542293	0.117078	1.315316
40	6	0	-4.826289	-0.471388	-0.997190
41	6	0	-5.309253	0.165884	0.149423
42	1	0	-4.905585	0.613048	2.211971
43	1	0	-5.407223	-0.427935	-1.915201
44	6	0	1.615595	-2.126035	-2.487446
45	1	0	0.857801	-2.915776	-2.462751
46	1	0	1.090204	-1.171069	-2.614042
47	1	0	2.238166	-2.280793	-3.371650
48	6	0	6.119959	-1.755138	-0.240061
49	1	0	6.406843	-1.138692	-1.097045
50	1	0	6.539924	-1.304453	0.663484
51	1	0	6.590755	-2.736615	-0.368830
52	6	0	1.936603	-2.219584	2.557200
53	1	0	2.664215	-2.106643	3.363924
54	1	0	1.196391	-1.416043	2.652471
55	1	0	1.411065	-3.168523	2.710529
56	6	0	-3.074710	-1.803592	-2.247659
57	1	0	-2.079316	-1.412706	-2.491263
58	1	0	-2.974562	-2.888529	-2.135367
59	1	0	-3.732623	-1.614707	-3.098845
60	6	0	-6.641231	0.870255	0.129627
61	1	0	-6.701897	1.637457	0.906338
62	1	0	-6.827976	1.344731	-0.838209
63	1	0	-7.452541	0.154966	0.306713
64	6	0	-2.499792	-0.591233	2.628003
65	1	0	-2.096185	-1.588074	2.831355
66	1	0	-1.645254	0.093233	2.551055
67	1	0	-3.095324	-0.282963	3.490527

Zero-point correction= 0.571187 (Hartree/Particle)
Thermal correction to Energy= 0.604922
Thermal correction to Enthalpy= 0.605866
Thermal correction to Gibbs Free Energy= 0.504479
Sum of electronic and zero-point Energies= -1444.505321
Sum of electronic and thermal Energies= -1444.471585
Sum of electronic and thermal Enthalpies= -1444.470641
Sum of electronic and thermal Free Energies= -1444.572029

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1445.8261238

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.987412	-1.790038	-2.620238
2	6	0	1.854744	-2.459053	-2.947811
3	6	0	1.421142	-1.245783	-1.106043
4	7	0	2.697210	-1.050072	-1.486699
5	1	0	3.962793	-1.768533	-3.079576
6	1	0	1.636280	-3.144872	-3.750831
7	7	0	0.904494	-2.108647	-2.005112
8	79	0	0.380181	-0.454556	0.455003
9	6	0	3.563701	-0.108281	-0.834076
10	6	0	4.287003	-0.519232	0.287093
11	6	0	3.594585	1.202087	-1.320875
12	6	0	5.080526	0.433420	0.923342
13	6	0	4.401882	2.117476	-0.648457
14	6	0	5.149601	1.752594	0.473051
15	1	0	5.658554	0.137814	1.795536
16	1	0	4.453653	3.140684	-1.013210
17	6	0	-0.484495	-2.479586	-1.991206
18	6	0	-0.894431	-3.540187	-1.178073
19	6	0	-1.379110	-1.692942	-2.720942
20	6	0	-2.258882	-3.810762	-1.117042
21	6	0	-2.735153	-2.008320	-2.631447

22	6	0	-3.191196	-3.059837	-1.836172
23	1	0	-2.604843	-4.627614	-0.488304
24	1	0	-3.450252	-1.416482	-3.198311
25	6	0	2.767799	1.610174	-2.514153
26	1	0	3.024436	1.026068	-3.404851
27	1	0	1.696979	1.463686	-2.327598
28	1	0	2.928034	2.665220	-2.750401
29	6	0	5.993930	2.768135	1.199225
30	1	0	6.312366	3.573773	0.531677
31	1	0	5.429794	3.221877	2.022475
32	1	0	6.888384	2.308146	1.629067
33	6	0	4.181489	-1.929390	0.806796
34	1	0	4.929966	-2.114713	1.580952
35	1	0	3.190841	-2.108066	1.242862
36	1	0	4.324059	-2.669113	0.012068
37	6	0	-0.895637	-0.518554	-3.531296
38	1	0	-0.435029	0.234925	-2.880684
39	1	0	-0.144848	-0.814592	-4.271501
40	1	0	-1.725253	-0.050144	-4.067512
41	6	0	-4.658553	-3.393837	-1.751564
42	1	0	-5.272607	-2.644291	-2.259505
43	1	0	-4.864011	-4.362863	-2.219341
44	1	0	-4.986926	-3.458872	-0.708572
45	6	0	0.100107	-4.325505	-0.364164
46	1	0	0.957166	-4.643746	-0.966550
47	1	0	0.489606	-3.717420	0.461451
48	1	0	-0.365180	-5.216300	0.064185
49	6	0	-0.824667	0.184226	2.010289
50	6	0	-0.483871	2.545836	1.155776
51	6	0	-0.992943	2.361526	2.247812
52	1	0	-1.432291	2.481642	3.213895
53	6	0	0.097613	2.786852	-0.172804
54	1	0	0.031128	3.872238	-0.348879
55	1	0	1.154546	2.503755	-0.174240
56	8	0	-0.527910	2.060658	-1.197714
57	6	0	-1.893915	2.423151	-1.429154
58	1	0	-2.470746	2.314417	-0.500139
59	1	0	-2.250100	1.669594	-2.137735
60	6	0	-2.026574	3.804802	-1.986285
61	6	0	-2.667898	4.798820	-1.358839
62	1	0	-1.559073	3.980932	-2.954420
63	1	0	-3.128138	4.606171	-0.387892
64	6	0	-2.817596	6.148882	-1.892532
65	6	0	-3.471553	7.123648	-1.255543
66	1	0	-2.364639	6.343806	-2.863310
67	1	0	-3.567602	8.116671	-1.681964
68	1	0	-3.937932	6.958936	-0.286964
69	6	0	-0.165520	0.033350	3.364771
70	8	0	0.290763	0.891482	4.080603
71	8	0	-0.130791	-1.274601	3.638273
72	6	0	0.544426	-1.635700	4.851174
73	1	0	0.090877	-1.130644	5.706233
74	1	0	0.427606	-2.714552	4.934584
75	1	0	1.600417	-1.364540	4.786599
76	6	0	-2.267735	-0.051487	1.941607
77	6	0	-3.066055	-0.046548	3.102278
78	6	0	-2.880408	-0.324563	0.704285
79	6	0	-4.422779	-0.318837	3.029391
80	1	0	-2.613596	0.165245	4.067904
81	6	0	-4.240850	-0.583445	0.631050
82	1	0	-2.279818	-0.340201	-0.200934
83	6	0	-5.012517	-0.582263	1.791852
84	1	0	-5.024882	-0.322656	3.932009
85	1	0	-4.697003	-0.792783	-0.330969
86	1	0	-6.077172	-0.786948	1.734372

Zero-point correction= 0.718486 (Hartree/Particle)

Thermal correction to Energy= 0.765305
Thermal correction to Enthalpy= 0.766249
Thermal correction to Gibbs Free Energy= 0.629711
Sum of electronic and zero-point Energies= -1942.364810
Sum of electronic and thermal Energies= -1942.317992
Sum of electronic and thermal Enthalpies= -1942.317047
Sum of electronic and thermal Free Energies= -1942.453586
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1943.9642749

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.187231	-3.073652	1.767338
2	6	0	0.890694	-3.328920	2.084688
3	6	0	0.932815	-1.467019	0.835426
4	7	0	2.187201	-1.925641	1.001055
5	1	0	3.098256	-3.597388	2.010026
6	1	0	0.441167	-4.120816	2.662465
7	7	0	0.139229	-2.330267	1.501653
8	79	0	0.356726	0.212091	-0.261614
9	6	0	3.327426	-1.274918	0.413512
10	6	0	4.024722	-0.338987	1.180749
11	6	0	3.638102	-1.553255	-0.920908
12	6	0	5.090354	0.322125	0.573628
13	6	0	4.710583	-0.862552	-1.481470
14	6	0	5.445116	0.075858	-0.753974
15	1	0	5.660866	1.044190	1.152999
16	1	0	4.980006	-1.063600	-2.515485
17	6	0	-1.289833	-2.175919	1.504644
18	6	0	-1.853301	-1.248260	2.384659
19	6	0	-2.031951	-2.867634	0.544551
20	6	0	-3.212417	-0.981057	2.245117
21	6	0	-3.388773	-2.564431	0.445671
22	6	0	-3.989104	-1.613974	1.273211
23	1	0	-3.673066	-0.249674	2.903163
24	1	0	-3.987769	-3.070565	-0.307404
25	6	0	2.826100	-2.527225	-1.736042
26	1	0	2.572755	-3.427223	-1.165949
27	1	0	1.885902	-2.073355	-2.076217
28	1	0	3.379458	-2.838080	-2.625662
29	6	0	6.585282	0.819169	-1.401395
30	1	0	7.177725	0.157817	-2.040638
31	1	0	6.208413	1.632668	-2.032110
32	1	0	7.253708	1.257772	-0.655420
33	6	0	3.613651	-0.039035	2.598904
34	1	0	4.308903	0.664987	3.063241
35	1	0	2.609029	0.400944	2.626455
36	1	0	3.591008	-0.941029	3.219620
37	6	0	-1.386200	-3.894666	-0.349551
38	1	0	-0.462179	-3.517730	-0.801862
39	1	0	-1.128975	-4.800315	0.211534
40	1	0	-2.064515	-4.187724	-1.154422
41	6	0	-5.454944	-1.293701	1.137801
42	1	0	-5.804784	-1.450485	0.112940
43	1	0	-6.056437	-1.933297	1.793903
44	1	0	-5.657877	-0.254643	1.416559
45	6	0	-1.017657	-0.568656	3.437957
46	1	0	-0.507248	-1.301425	4.072497
47	1	0	-0.247372	0.069381	2.991231
48	1	0	-1.640964	0.060117	4.077209
49	6	0	-0.239129	2.335933	-0.386586
50	6	0	-0.139611	1.126289	-2.085707
51	6	0	-0.503462	2.366002	-1.849986
52	1	0	-0.829476	3.192427	-2.472256
53	6	0	0.079869	0.335093	-3.351323

54	1	0	-0.585154	0.793502	-4.100886
55	1	0	1.114583	0.478478	-3.675609
56	8	0	-0.098862	-1.049812	-3.284406
57	6	0	-1.357729	-1.506043	-2.800711
58	1	0	-1.373610	-1.457477	-1.701559
59	1	0	-1.385400	-2.561765	-3.088061
60	6	0	-2.554885	-0.776322	-3.326728
61	6	0	-3.460106	-0.229510	-2.506553
62	1	0	-2.689022	-0.736838	-4.407381
63	1	0	-3.301030	-0.298635	-1.427998
64	6	0	-4.675176	0.452130	-2.939420
65	6	0	-5.595099	0.915763	-2.087953
66	1	0	-4.819993	0.573159	-4.011749
67	1	0	-6.494502	1.416062	-2.430980
68	1	0	-5.478346	0.786831	-1.014297
69	6	0	1.023852	3.111691	-0.038591
70	8	0	1.379389	4.057893	-0.691944
71	8	0	1.679575	2.636857	1.025938
72	6	0	2.902449	3.317258	1.346811
73	1	0	2.718170	4.383114	1.490232
74	1	0	3.255430	2.857681	2.268081
75	1	0	3.627390	3.171655	0.543297
76	6	0	-1.393738	2.386776	0.554732
77	6	0	-1.214964	2.568007	1.935193
78	6	0	-2.699914	2.308563	0.044097
79	6	0	-2.314480	2.692008	2.775705
80	1	0	-0.214069	2.624430	2.346972
81	6	0	-3.792638	2.432614	0.889816
82	1	0	-2.859990	2.159949	-1.018960
83	6	0	-3.604889	2.627911	2.256967
84	1	0	-2.160618	2.850284	3.838460
85	1	0	-4.795151	2.399617	0.475817
86	1	0	-4.461866	2.738964	2.914340

Zero-point correction= 0.722551 (Hartree/Particle)
Thermal correction to Energy= 0.766318
Thermal correction to Enthalpy= 0.767262
Thermal correction to Gibbs Free Energy= 0.644558
Sum of electronic and zero-point Energies= -1942.416505
Sum of electronic and thermal Energies= -1942.372737
Sum of electronic and thermal Enthalpies= -1942.371793
Sum of electronic and thermal Free Energies= -1942.494497
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0213212

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.883811	-0.389351	3.539778
2	6	0	-0.556557	-0.506794	3.795218
3	6	0	-0.792602	-0.108364	1.599536
4	7	0	-2.005424	-0.145154	2.185053
5	1	0	-2.744056	-0.452922	4.187025
6	1	0	-0.019897	-0.698612	4.710647
7	7	0	0.093292	-0.328308	2.589183
8	79	0	-0.406785	0.383130	-0.382791
9	6	0	-3.237439	-0.002207	1.456612
10	6	0	-3.922760	-1.170672	1.099225
11	6	0	-3.676226	1.273463	1.095872
12	6	0	-5.103959	-1.026166	0.378081
13	6	0	-4.863174	1.361192	0.365730
14	6	0	-5.588914	0.229935	0.000733
15	1	0	-5.663600	-1.917714	0.103648
16	1	0	-5.228135	2.344562	0.079419
17	6	0	1.508494	-0.419784	2.361624
18	6	0	2.029707	-1.664598	1.988344

19	6	0	2.290016	0.729865	2.477286
20	6	0	3.397679	-1.739284	1.754098
21	6	0	3.656787	0.602996	2.220763
22	6	0	4.225595	-0.619067	1.867186
23	1	0	3.831464	-2.694521	1.471687
24	1	0	4.287355	1.485668	2.293933
25	6	0	-2.898392	2.522497	1.427542
26	1	0	-2.258911	2.396573	2.305687
27	1	0	-2.261841	2.810561	0.580673
28	1	0	-3.578045	3.357278	1.619264
29	6	0	-6.858339	0.347269	-0.802982
30	1	0	-7.307218	1.338968	-0.700671
31	1	0	-6.658751	0.182394	-1.868323
32	1	0	-7.597408	-0.395402	-0.488240
33	6	0	-3.378223	-2.532267	1.445019
34	1	0	-3.227302	-2.655516	2.522603
35	1	0	-4.064184	-3.315473	1.113401
36	1	0	-2.414349	-2.698755	0.950761
37	6	0	1.695534	2.057503	2.871153
38	1	0	0.708128	2.211146	2.423959
39	1	0	1.573965	2.129515	3.958215
40	1	0	2.342481	2.878776	2.552114
41	6	0	5.704573	-0.746667	1.608214
42	1	0	6.170954	-1.418276	2.337048
43	1	0	5.890625	-1.167387	0.613276
44	1	0	6.210889	0.220399	1.670720
45	6	0	1.132195	-2.864549	1.835758
46	1	0	0.575963	-3.070950	2.757006
47	1	0	0.398241	-2.711847	1.035532
48	1	0	1.716671	-3.754064	1.588674
49	6	0	0.319604	-1.030902	-2.124954
50	6	0	1.631244	-1.609478	-1.821978
51	6	0	1.804225	-2.971170	-1.504091
52	6	0	2.774925	-0.796540	-1.965823
53	6	0	3.080431	-3.502314	-1.383537
54	1	0	0.942511	-3.612587	-1.378402
55	6	0	4.044049	-1.334820	-1.835335
56	1	0	2.657940	0.264019	-2.164414
57	6	0	4.200686	-2.691523	-1.553257
58	1	0	3.201225	-4.558715	-1.166444
59	1	0	4.912303	-0.696325	-1.960547
60	1	0	5.195775	-3.116644	-1.462216
61	6	0	-0.936594	-1.882266	-1.945456
62	8	0	-1.070212	-2.739158	-1.096980
63	8	0	-1.851418	-1.574266	-2.850002
64	6	0	-3.113519	-2.242071	-2.710375
65	1	0	-3.706277	-1.914904	-3.562259
66	1	0	-2.974122	-3.324531	-2.724511
67	1	0	-3.584694	-1.938632	-1.771611
68	6	0	-0.119626	1.115843	-2.277601
69	6	0	0.259034	0.112192	-3.062170
70	1	0	0.605080	0.087401	-4.092659
71	6	0	-0.131791	2.593662	-2.614013
72	1	0	0.854320	2.871629	-3.008411
73	1	0	-0.871419	2.727711	-3.410513
74	8	0	-0.525939	3.467427	-1.591031
75	6	0	0.375071	3.606147	-0.502810
76	1	0	0.285818	2.735145	0.173896
77	1	0	0.011685	4.479244	0.046725
78	6	0	1.813478	3.768461	-0.892883
79	6	0	2.746977	2.840686	-0.647108
80	1	0	2.079772	4.685865	-1.417073
81	1	0	2.466677	1.921504	-0.126556
82	6	0	4.149809	2.962656	-1.032052
83	6	0	5.058402	2.010264	-0.801262
84	1	0	4.442922	3.883136	-1.534584
85	1	0	6.095557	2.126140	-1.099344

86	1	0	4.783800	1.088398	-0.294681

Zero-point correction= 0.722968 (Hartree/Particle)
Thermal correction to Energy= 0.767362
Thermal correction to Enthalpy= 0.768306
Thermal correction to Gibbs Free Energy= 0.644758
Sum of electronic and zero-point Energies= -1942.419240
Sum of electronic and thermal Energies= -1942.374846
Sum of electronic and thermal Enthalpies= -1942.373901
Sum of electronic and thermal Free Energies= -1942.497449
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0196474

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.339385	-3.848516	1.348391
2	6	0	-2.460416	-3.121654	1.570078
3	6	0	-0.983287	-1.788778	0.519362
4	7	0	-0.445323	-3.011977	0.704754
5	1	0	-1.092364	-4.872239	1.579903
6	1	0	-3.398538	-3.374970	2.037791
7	7	0	-2.222680	-1.859980	1.051804
8	79	0	-0.108844	-0.189064	-0.429977
9	6	0	0.827907	-3.418460	0.170083
10	6	0	1.948936	-3.447099	0.999384
11	6	0	0.883939	-3.760004	-1.188789
12	6	0	3.161526	-3.835039	0.429101
13	6	0	2.117728	-4.137499	-1.707856
14	6	0	3.267133	-4.181980	-0.914892
15	1	0	4.048851	-3.857685	1.057637
16	1	0	2.185542	-4.405789	-2.759302
17	6	0	-3.211619	-0.820928	0.947423
18	6	0	-3.301972	0.148593	1.949230
19	6	0	-4.051219	-0.829577	-0.170807
20	6	0	-4.289086	1.122665	1.817142
21	6	0	-5.013791	0.173981	-0.263823
22	6	0	-5.150413	1.154676	0.718473
23	1	0	-4.386094	1.882118	2.589577
24	1	0	-5.674098	0.190124	-1.127166
25	6	0	-0.337318	-3.700249	-2.071527
26	1	0	-1.223862	-4.110360	-1.576578
27	1	0	-0.567071	-2.664794	-2.352544
28	1	0	-0.173328	-4.262819	-2.993734
29	6	0	4.584403	-4.629975	-1.493539
30	1	0	4.642706	-4.421801	-2.565737
31	1	0	5.425642	-4.132211	-1.002270
32	1	0	4.716655	-5.709916	-1.359239
33	6	0	1.905557	-3.052023	2.452318
34	1	0	2.340918	-3.835458	3.080645
35	1	0	2.494160	-2.140723	2.595251
36	1	0	0.889281	-2.863031	2.807990
37	6	0	-3.893667	-1.867276	-1.251826
38	1	0	-2.905053	-1.796752	-1.721411
39	1	0	-3.993252	-2.884105	-0.856677
40	1	0	-4.647666	-1.734008	-2.031174
41	6	0	-6.173608	2.251275	0.587167
42	1	0	-5.682784	3.195263	0.323343
43	1	0	-6.911000	2.023333	-0.186811
44	1	0	-6.705258	2.410083	1.530661
45	6	0	-2.333239	0.171059	3.101237
46	1	0	-2.185252	-0.821601	3.538496
47	1	0	-1.355692	0.528551	2.757438
48	1	0	-2.680212	0.843520	3.889773
49	6	0	2.689166	1.960592	-0.093254
50	6	0	3.881044	2.776224	0.113757

51	6	0	4.944858	2.289893	0.897745
52	6	0	3.990651	4.056803	-0.462382
53	6	0	6.091715	3.049494	1.071873
54	1	0	4.888172	1.299342	1.335674
55	6	0	5.132374	4.817542	-0.267594
56	1	0	3.163509	4.477048	-1.024365
57	6	0	6.187920	4.312695	0.491684
58	1	0	6.913461	2.655938	1.660546
59	1	0	5.200435	5.808357	-0.703955
60	1	0	7.083870	4.907933	0.636160
61	6	0	2.428533	0.935178	0.983016
62	8	0	2.948493	-0.154164	0.995556
63	8	0	1.657118	1.443567	1.935006
64	6	0	1.423712	0.591045	3.064525
65	1	0	0.823034	1.182705	3.752580
66	1	0	0.885637	-0.305242	2.747342
67	1	0	2.372186	0.307822	3.526086
68	6	0	0.701339	1.357568	-1.462028
69	6	0	1.871571	2.097889	-1.190678
70	1	0	2.186745	2.833588	-1.931733
71	6	0	0.052075	1.809509	-2.737454
72	1	0	-0.179130	2.882343	-2.602506
73	1	0	0.814243	1.760191	-3.529566
74	8	0	-1.042783	1.104393	-3.227701
75	6	0	-2.286503	1.258842	-2.539199
76	1	0	-2.307718	0.607563	-1.655941
77	1	0	-3.030684	0.883323	-3.247428
78	6	0	-2.602768	2.660212	-2.113656
79	6	0	-2.675136	3.004021	-0.821831
80	1	0	-2.780548	3.400092	-2.893813
81	1	0	-2.490387	2.239734	-0.064822
82	6	0	-3.005051	4.335642	-0.325206
83	6	0	-3.072239	4.629852	0.976944
84	1	0	-3.203820	5.106948	-1.068046
85	1	0	-3.317527	5.626997	1.327629
86	1	0	-2.879816	3.872801	1.734149

Zero-point correction= 0.723118 (Hartree/Particle)
Thermal correction to Energy= 0.768774
Thermal correction to Enthalpy= 0.769719
Thermal correction to Gibbs Free Energy= 0.637439
Sum of electronic and zero-point Energies= -1942.443327
Sum of electronic and thermal Energies= -1942.397670
Sum of electronic and thermal Enthalpies= -1942.396726
Sum of electronic and thermal Free Energies= -1942.529006
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0450894

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.165403	3.028903	1.000509
2	6	0	3.919336	1.910419	1.131634
3	6	0	1.910257	1.291899	0.326728
4	7	0	1.937302	2.625327	0.506498
5	1	0	3.379597	4.065020	1.208692
6	1	0	4.929532	1.765620	1.479755
7	7	0	3.130533	0.854486	0.710266
8	79	0	0.451657	0.122055	-0.482232
9	6	0	0.820554	3.481829	0.212105
10	6	0	-0.134390	3.696357	1.209270
11	6	0	0.713282	4.014348	-1.074220
12	6	0	-1.226531	4.496927	0.885145
13	6	0	-0.397272	4.810328	-1.347876
14	6	0	-1.372769	5.063132	-0.382503
15	1	0	-1.987600	4.676641	1.640443

16	1	0	-0.504498	5.241597	-2.340141
17	6	0	3.479520	-0.537773	0.709262
18	6	0	3.371528	-1.248726	1.908538
19	6	0	3.834542	-1.144556	-0.499965
20	6	0	3.607735	-2.621816	1.870155
21	6	0	4.069480	-2.519321	-0.482769
22	6	0	3.955778	-3.273889	0.686160
23	1	0	3.527934	-3.194751	2.791213
24	1	0	4.361333	-3.012742	-1.407586
25	6	0	1.745029	3.709619	-2.129585
26	1	0	2.752249	3.998110	-1.808848
27	1	0	1.772101	2.635970	-2.353394
28	1	0	1.522190	4.242237	-3.057145
29	6	0	-2.555790	5.945223	-0.689714
30	1	0	-2.691272	6.076212	-1.766818
31	1	0	-3.478697	5.526315	-0.276643
32	1	0	-2.420947	6.939248	-0.247808
33	6	0	-0.010274	3.048521	2.563149
34	1	0	-0.713607	3.494886	3.270210
35	1	0	-0.249191	1.981190	2.495018
36	1	0	0.998854	3.150453	2.976799
37	6	0	3.930011	-0.360035	-1.783715
38	1	0	2.938903	-0.209612	-2.230533
39	1	0	4.369039	0.629277	-1.623722
40	1	0	4.547523	-0.891868	-2.512411
41	6	0	4.247075	-4.752720	0.678649
42	1	0	4.003199	-5.205771	-0.286830
43	1	0	5.311699	-4.934287	0.865591
44	1	0	3.683957	-5.276693	1.456612
45	6	0	3.035135	-0.554670	3.203392
46	1	0	3.923977	-0.077893	3.632516
47	1	0	2.285039	0.230766	3.066881
48	1	0	2.659722	-1.268183	3.941833
49	6	0	-2.899019	-0.895532	0.079312
50	6	0	-4.358115	-0.909089	0.321126
51	6	0	-4.859409	-1.448922	1.512026
52	6	0	-5.256233	-0.411004	-0.629773
53	6	0	-6.229235	-1.511572	1.736547
54	1	0	-4.173589	-1.835118	2.261915
55	6	0	-6.625846	-0.469649	-0.400986
56	1	0	-4.879501	0.052801	-1.536672
57	6	0	-7.115841	-1.023978	0.779318
58	1	0	-6.606035	-1.938659	2.660494
59	1	0	-7.312867	-0.071245	-1.140880
60	1	0	-8.185697	-1.067449	0.956765
61	6	0	-2.058057	-0.583682	1.286846
62	8	0	-2.087129	0.481102	1.852593
63	8	0	-1.315314	-1.625698	1.687629
64	6	0	-0.473316	-1.374827	2.818026
65	1	0	0.066837	-2.304757	2.992575
66	1	0	0.225222	-0.568116	2.587579
67	1	0	-1.072419	-1.102419	3.689611
68	6	0	-0.941091	-1.074678	-1.514868
69	6	0	-2.362512	-1.090712	-1.142199
70	1	0	-3.071380	-1.299096	-1.946558
71	6	0	-0.713311	-0.974034	-3.015729
72	1	0	-1.389468	-1.620942	-3.603905
73	1	0	-0.888157	0.061945	-3.323646
74	8	0	0.628255	-1.278285	-3.283330
75	6	0	0.915286	-2.527447	-2.688603
76	1	0	1.988696	-2.563976	-2.495207
77	1	0	0.652334	-3.336872	-3.384332
78	6	0	0.139808	-2.717565	-1.382554
79	6	0	-1.024646	-3.463693	-1.373810
80	1	0	0.699387	-2.651082	-0.453365
81	1	0	-1.528995	-3.632538	-2.326018
82	6	0	-1.681145	-3.964917	-0.201328

83	6	0	-2.946018	-4.412002	-0.260767
84	1	0	-1.155401	-3.907000	0.744951
85	1	0	-3.470261	-4.758822	0.623545
86	1	0	-3.495687	-4.440559	-1.198330

Zero-point correction= 0.723679 (Hartree/Particle)
Thermal correction to Energy= 0.768369
Thermal correction to Enthalpy= 0.769313
Thermal correction to Gibbs Free Energy= 0.641518
Sum of electronic and zero-point Energies= -1942.432786
Sum of electronic and thermal Energies= -1942.388096
Sum of electronic and thermal Enthalpies= -1942.387152
Sum of electronic and thermal Free Energies= -1942.514947
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0351096

INT6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777700	0.131759	-0.080693
2	6	0	-2.235478	-0.151205	-0.153476
3	6	0	-3.088174	0.112941	0.924963
4	6	0	-2.776157	-0.698435	-1.322910
5	6	0	-4.444211	-0.182171	0.835839
6	1	0	-2.679611	0.540866	1.833719
7	6	0	-4.131607	-0.995258	-1.406942
8	1	0	-2.130962	-0.870754	-2.179617
9	6	0	-4.970780	-0.738439	-0.326482
10	1	0	-5.092474	0.023110	1.682653
11	1	0	-4.534694	-1.416314	-2.323213
12	1	0	-6.031076	-0.963028	-0.393710
13	6	0	-0.360076	1.388114	0.624290
14	8	0	-0.583829	1.632897	1.788433
15	8	0	0.290032	2.229494	-0.190851
16	6	0	0.732772	3.444525	0.416405
17	1	0	1.261567	3.985503	-0.367553
18	1	0	-0.120376	4.023544	0.777379
19	1	0	1.400066	3.233316	1.255893
20	6	0	1.613935	-0.505895	-0.572585
21	6	0	0.142629	-0.705501	-0.576947
22	1	0	-0.205673	-1.640589	-1.014601
23	6	0	2.270369	0.107745	-1.808347
24	1	0	2.397722	-0.594212	-2.638172
25	1	0	1.666936	0.963754	-2.143047
26	8	0	3.562677	0.514602	-1.395296
27	6	0	3.486374	0.903721	-0.033413
28	1	0	3.191402	1.960218	0.061931
29	1	0	4.483887	0.776652	0.397489
30	6	0	2.429739	0.009415	0.579849
31	6	0	2.521992	-1.453022	0.196212
32	1	0	1.975677	0.282496	1.527944
33	1	0	3.434108	-1.758096	-0.314976
34	6	0	1.926191	-2.468603	1.090181
35	6	0	2.418032	-3.693290	1.265382
36	1	0	1.026137	-2.169804	1.627963
37	1	0	1.946327	-4.402933	1.937783
38	1	0	3.312910	-4.028086	0.745898

Zero-point correction= 0.317985 (Hartree/Particle)
Thermal correction to Energy= 0.336289
Thermal correction to Enthalpy= 0.337233
Thermal correction to Gibbs Free Energy= 0.269967
Sum of electronic and zero-point Energies= -883.650400
Sum of electronic and thermal Energies= -883.632096
Sum of electronic and thermal Enthalpies= -883.631152
Sum of electronic and thermal Free Energies= -883.698418

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.2128507

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.898558	-0.605952	-0.604965
2	6	0	0.533404	-0.689858	-0.801597
3	1	0	0.181580	-1.608882	-1.270589
4	6	0	2.908103	-1.471203	-1.336384
5	1	0	2.710809	-2.545834	-1.273517
6	1	0	2.922077	-1.181053	-2.399121
7	8	0	4.162337	-1.215982	-0.733136
8	6	0	4.119853	0.102713	-0.210367
9	1	0	4.328789	0.846807	-0.993206
10	1	0	4.883448	0.173928	0.568406
11	6	0	2.696510	0.280560	0.302442
12	6	0	2.310951	-0.723200	1.336127
13	1	0	2.364580	1.308126	0.429864
14	1	0	2.981435	-1.571696	1.444984
15	6	0	1.152954	-0.665302	2.104329
16	6	0	0.234349	0.360059	1.981248
17	1	0	0.873007	-1.563285	2.651843
18	1	0	-0.720017	0.314594	2.495930
19	1	0	0.585381	1.358200	1.748641
20	6	0	-0.463919	0.144456	-0.259400
21	6	0	-1.835477	-0.447383	-0.205379
22	6	0	-1.991894	-1.695703	0.409503
23	6	0	-2.957284	0.137650	-0.804299
24	6	0	-3.223725	-2.340251	0.431441
25	1	0	-1.130401	-2.153888	0.888984
26	6	0	-4.189816	-0.504971	-0.782987
27	1	0	-2.866700	1.099898	-1.294684
28	6	0	-4.330648	-1.744812	-0.165235
29	1	0	-3.319378	-3.305536	0.920136
30	1	0	-5.045947	-0.035065	-1.258516
31	1	0	-5.296112	-2.241619	-0.148406
32	6	0	-0.289032	1.616871	-0.329253
33	8	0	0.675309	2.199741	-0.784252
34	8	0	-1.333844	2.287010	0.202839
35	6	0	-1.219189	3.705167	0.178927
36	1	0	-2.146156	4.081256	0.611742
37	1	0	-0.361629	4.033818	0.772698
38	1	0	-1.097361	4.071042	-0.843691

Zero-point correction= 0.318050 (Hartree/Particle)
Thermal correction to Energy= 0.334959
Thermal correction to Enthalpy= 0.335903
Thermal correction to Gibbs Free Energy= 0.273942
Sum of electronic and zero-point Energies= -883.615990
Sum of electronic and thermal Energies= -883.599081
Sum of electronic and thermal Enthalpies= -883.598137
Sum of electronic and thermal Free Energies= -883.660098

ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.1780019

TS5b′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.893931	-0.770657	-0.332918
2	6	0	-0.521033	-1.017834	-0.319146
3	1	0	-0.255310	-1.969753	0.147703
4	6	0	-2.859070	-0.155130	-1.327949
5	1	0	-2.745273	0.915928	-1.490395
6	1	0	-2.734244	-0.669010	-2.291732

7	8	0	-4.161017	-0.390270	-0.798183
8	6	0	-4.111935	-1.458317	0.136000
9	1	0	-4.237849	-2.433020	-0.359783
10	1	0	-4.931018	-1.310487	0.846255
11	6	0	-2.724530	-1.366658	0.748630
12	6	0	-2.458397	0.003770	1.334093
13	1	0	-2.335236	-2.234028	1.282872
14	1	0	-3.302333	0.677416	1.195594
15	6	0	-1.335579	0.591202	1.909499
16	6	0	-0.008092	0.122836	1.920926
17	1	0	-1.467137	1.645921	2.144706
18	1	0	0.725644	0.786315	2.372417
19	1	0	0.208315	-0.926137	2.092293
20	6	0	0.474802	-0.044945	-0.086649
21	6	0	0.233029	1.350952	-0.605947
22	8	0	-0.475932	1.620332	-1.547354
23	8	0	0.907407	2.287318	0.080449
24	6	0	0.747759	3.622561	-0.394224
25	1	0	1.070616	3.703950	-1.434775
26	1	0	-0.298044	3.931305	-0.321139
27	1	0	1.373916	4.239263	0.249986
28	6	0	1.913883	-0.489458	-0.080853
29	6	0	2.275150	-1.614204	-0.830956
30	6	0	2.913758	0.175058	0.639573
31	6	0	3.587409	-2.076733	-0.843197
32	1	0	1.518744	-2.117282	-1.425327
33	6	0	4.225289	-0.284288	0.623718
34	1	0	2.664467	1.060848	1.211475
35	6	0	4.568366	-1.414947	-0.113276
36	1	0	3.842276	-2.951883	-1.433787
37	1	0	4.983696	0.244689	1.193588
38	1	0	5.593834	-1.772320	-0.123182

Zero-point correction= 0.317522 (Hartree/Particle)
Thermal correction to Energy= 0.334643
Thermal correction to Enthalpy= 0.335587
Thermal correction to Gibbs Free Energy= 0.272187
Sum of electronic and zero-point Energies= -883.585149
Sum of electronic and thermal Energies= -883.568028
Sum of electronic and thermal Enthalpies= -883.567084
Sum of electronic and thermal Free Energies= -883.630485
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.145402

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.058199	0.348134	-0.568118
2	6	0	0.767558	0.416076	-0.882137
3	1	0	0.496454	0.411003	-1.935879
4	6	0	3.173607	0.203049	-1.577372
5	1	0	2.876650	-0.319423	-2.489563
6	1	0	3.586517	1.189330	-1.854541
7	8	0	4.150624	-0.572872	-0.911771
8	6	0	4.178355	-0.106019	0.423149
9	1	0	4.831304	0.777185	0.501997
10	1	0	4.595776	-0.900350	1.047673
11	6	0	2.724566	0.266731	0.798950
12	6	0	2.021697	-0.699204	1.722303
13	1	0	2.718948	1.261426	1.267130
14	1	0	2.580974	-1.555832	2.093079
15	6	0	0.745644	-0.524075	2.057062
16	6	0	-0.064052	0.638352	1.541698
17	1	0	0.248192	-1.244096	2.701116
18	1	0	-0.986847	0.740394	2.115856
19	1	0	0.491271	1.576281	1.672389

20	6	0	-0.435097	0.489565	0.042550
21	6	0	-1.315647	-0.764498	-0.122897
22	6	0	-0.768908	-1.971391	-0.558253
23	6	0	-2.665966	-0.731999	0.236647
24	6	0	-1.555570	-3.116867	-0.642994
25	1	0	0.282930	-2.015923	-0.821266
26	6	0	-3.453750	-1.874455	0.149209
27	1	0	-3.108983	0.193065	0.596056
28	6	0	-2.901131	-3.072765	-0.293907
29	1	0	-1.110981	-4.046976	-0.984827
30	1	0	-4.502730	-1.826131	0.426738
31	1	0	-3.514781	-3.965995	-0.363751
32	6	0	-1.257867	1.691328	-0.458046
33	8	0	-1.402713	1.977128	-1.621996
34	8	0	-1.831024	2.387797	0.537451
35	6	0	-2.636367	3.490576	0.118737
36	1	0	-3.024926	3.934592	1.034655
37	1	0	-2.033707	4.213747	-0.435407
38	1	0	-3.452781	3.146065	-0.520409

Zero-point correction= 0.320293 (Hartree/Particle)
Thermal correction to Energy= 0.337544
Thermal correction to Enthalpy= 0.338488
Thermal correction to Gibbs Free Energy= 0.274099
Sum of electronic and zero-point Energies= -883.673850
Sum of electronic and thermal Energies= -883.656598
Sum of electronic and thermal Enthalpies= -883.655654
Sum of electronic and thermal Free Energies= -883.720043
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.2392756

TS8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.246467	-4.057992	0.830712
2	6	0	0.028470	-4.291519	0.434366
3	6	0	-0.368089	-2.097828	0.165670
4	7	0	-1.469029	-2.703865	0.656540
5	1	0	-2.007670	-4.718888	1.213696
6	1	0	0.610253	-5.198881	0.399537
7	7	0	0.549358	-3.073876	0.030985
8	79	0	-0.271505	-0.116434	-0.298650
9	6	0	-2.664919	-1.974319	0.975450
10	6	0	-3.641327	-1.821319	-0.009947
11	6	0	-2.756015	-1.373321	2.236064
12	6	0	-4.761163	-1.052257	0.308183
13	6	0	-3.888547	-0.608352	2.502605
14	6	0	-4.903606	-0.444519	1.555168
15	1	0	-5.537277	-0.922012	-0.441937
16	1	0	-3.987819	-0.133401	3.475862
17	6	0	1.894463	-2.833268	-0.413277
18	6	0	2.146108	-2.725630	-1.781420
19	6	0	2.887190	-2.665997	0.558592
20	6	0	3.456760	-2.446967	-2.172810
21	6	0	4.178631	-2.395514	0.116160
22	6	0	4.481842	-2.280747	-1.243521
23	1	0	3.679555	-2.362593	-3.233699
24	1	0	4.970136	-2.264929	0.850805
25	6	0	-1.652508	-1.533532	3.250349
26	1	0	-1.475168	-2.588513	3.486115
27	1	0	-0.704605	-1.128039	2.875026
28	1	0	-1.901808	-1.019509	4.182010
29	6	0	-6.133089	0.360878	1.891115
30	1	0	-5.871585	1.299515	2.390565
31	1	0	-6.715656	0.597591	0.995734
32	1	0	-6.786684	-0.198462	2.569782

33	6	0	-3.463370	-2.425325	-1.378001
34	1	0	-4.350170	-2.260991	-1.994269
35	1	0	-2.604446	-1.974726	-1.889891
36	1	0	-3.281547	-3.503884	-1.324549
37	6	0	2.555394	-2.727274	2.027499
38	1	0	1.845674	-1.936003	2.297360
39	1	0	2.103698	-3.685168	2.306539
40	1	0	3.456536	-2.594872	2.631498
41	6	0	5.894419	-1.991193	-1.681536
42	1	0	6.279117	-1.088178	-1.195936
43	1	0	6.562505	-2.816311	-1.411320
44	1	0	5.959669	-1.847817	-2.763362
45	6	0	1.044365	-2.870441	-2.799688
46	1	0	0.383103	-3.711694	-2.568733
47	1	0	0.422088	-1.967101	-2.832081
48	1	0	1.460001	-3.028578	-3.797983
49	6	0	-0.391607	1.841794	-0.950996
50	6	0	-1.699411	2.445957	-1.190351
51	6	0	-1.863940	3.501073	-2.108954
52	6	0	-2.833133	1.954774	-0.515583
53	6	0	-3.120314	4.028277	-2.360756
54	1	0	-1.001946	3.897947	-2.638372
55	6	0	-4.086969	2.495065	-0.757385
56	1	0	-2.723215	1.146284	0.202153
57	6	0	-4.232708	3.527978	-1.682070
58	1	0	-3.237553	4.829971	-3.082330
59	1	0	-4.951258	2.103539	-0.231024
60	1	0	-5.214954	3.948048	-1.875024
61	6	0	0.743484	2.135422	-1.903732
62	8	0	1.795025	2.680770	-1.662866
63	8	0	0.430459	1.590931	-3.083572
64	6	0	1.485599	1.568280	-4.055459
65	1	0	1.042310	1.132952	-4.949064
66	1	0	1.846142	2.579229	-4.253509
67	1	0	2.310467	0.950489	-3.692464
68	6	0	0.386453	2.613274	1.316056
69	6	0	0.291070	3.444369	0.431682
70	1	0	0.300478	4.326304	-0.170506
71	6	0	0.579577	1.659740	2.419064
72	1	0	0.983404	2.255821	3.252576
73	1	0	-0.383227	1.243271	2.729290
74	8	0	1.407229	0.571898	2.113715
75	6	0	2.678473	0.917811	1.538721
76	1	0	2.523515	1.394998	0.562001
77	1	0	3.157673	-0.049121	1.369055
78	6	0	3.498442	1.795056	2.430068
79	6	0	3.873880	3.033419	2.085432
80	1	0	3.789601	1.380491	3.394996
81	1	0	3.566319	3.426393	1.114757
82	6	0	4.690741	3.909865	2.918501
83	6	0	5.057345	5.140489	2.551082
84	1	0	5.006370	3.515609	3.883386
85	1	0	5.667253	5.768655	3.191979
86	1	0	4.762446	5.558968	1.591500

Zero-point correction= 0.718645 (Hartree/Particle)
Thermal correction to Energy= 0.765224
Thermal correction to Enthalpy= 0.766169
Thermal correction to Gibbs Free Energy= 0.633921
Sum of electronic and zero-point Energies= -1942.366226
Sum of electronic and thermal Energies= -1942.319647
Sum of electronic and thermal Enthalpies= -1942.318703
Sum of electronic and thermal Free Energies= -1942.450950
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1943.9652076

INT7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.664887	-0.210785	-0.236208
2	6	0	-2.094126	-0.552233	-0.030883
3	6	0	-3.065379	-0.111467	-0.936921
4	6	0	-2.495972	-1.339446	1.052342
5	6	0	-4.399147	-0.463533	-0.773052
6	1	0	-2.771420	0.504434	-1.782593
7	6	0	-3.831319	-1.692584	1.217122
8	1	0	-1.757871	-1.657869	1.782938
9	6	0	-4.786668	-1.257141	0.304101
10	1	0	-5.138604	-0.118698	-1.489590
11	1	0	-4.126551	-2.300151	2.067527
12	1	0	-5.830265	-1.526810	0.435370
13	6	0	-0.325791	1.172650	-0.706783
14	8	0	0.492921	1.438897	-1.556834
15	8	0	-1.051086	2.096384	-0.062008
16	6	0	-0.739896	3.447255	-0.392616
17	1	0	-1.408275	4.059045	0.212404
18	1	0	0.304293	3.660432	-0.148374
19	1	0	-0.905099	3.632938	-1.456859
20	6	0	1.776006	-0.824957	-0.147978
21	6	0	0.322597	-1.089863	-0.011335
22	1	0	0.044790	-2.103269	0.278551
23	6	0	2.442216	-1.189831	-1.471737
24	1	0	2.017409	-2.134396	-1.849004
25	1	0	2.322326	-0.412772	-2.229365
26	8	0	3.824042	-1.326266	-1.188914
27	6	0	3.960495	-1.797372	0.140804
28	1	0	4.941042	-1.473276	0.502393
29	1	0	3.913171	-2.897669	0.183558
30	6	0	2.791153	-1.199378	0.895742
31	6	0	2.507907	0.263363	0.615860
32	1	0	2.495263	-1.621702	1.852092
33	1	0	3.263065	0.802099	0.046283
34	6	0	1.800086	1.067393	1.633607
35	6	0	2.010444	2.366550	1.840825
36	1	0	1.060011	0.545087	2.239517
37	1	0	1.466969	2.913465	2.605112
38	1	0	2.736428	2.925275	1.254746

Zero-point correction= 0.318008 (Hartree/Particle)
Thermal correction to Energy= 0.336138
Thermal correction to Enthalpy= 0.337083
Thermal correction to Gibbs Free Energy= 0.271170
Sum of electronic and zero-point Energies= -883.651119
Sum of electronic and thermal Energies= -883.632989
Sum of electronic and thermal Enthalpies= -883.632045
Sum of electronic and thermal Free Energies= -883.697957
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.2140565

TS7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.396642	0.074776	-0.017414
2	6	0	-1.818065	-0.433414	-0.163512
3	6	0	-2.783505	0.309780	-0.848375
4	6	0	-2.177472	-1.694084	0.320454
5	6	0	-4.069556	-0.186725	-1.033155
6	1	0	-2.529265	1.283728	-1.257797
7	6	0	-3.461244	-2.195474	0.134879
8	1	0	-1.446091	-2.294591	0.853775
9	6	0	-4.415396	-1.441123	-0.540643
10	1	0	-4.801482	0.409437	-1.570169

11	1	0	-3.715549	-3.176683	0.524783
12	1	0	-5.419210	-1.829276	-0.684333
13	6	0	-0.320068	1.580668	-0.081087
14	8	0	0.295656	2.225541	-0.899859
15	8	0	-1.052456	2.152133	0.888644
16	6	0	-1.085896	3.576924	0.874733
17	1	0	-1.724268	3.862652	1.710103
18	1	0	-0.081669	3.989425	1.000723
19	1	0	-1.502478	3.943019	-0.067264
20	6	0	1.943104	-0.509027	-0.769960
21	6	0	0.590612	-0.688616	-0.757983
22	1	0	0.320164	-1.746475	-0.717692
23	6	0	2.822780	0.701398	-0.999089
24	1	0	2.816788	0.932986	-2.073982
25	1	0	2.527273	1.605073	-0.464909
26	8	0	4.129371	0.344053	-0.563486
27	6	0	4.243037	-1.068523	-0.510211
28	1	0	5.019542	-1.308818	0.220541
29	1	0	4.528813	-1.484245	-1.488899
30	6	0	2.856482	-1.555463	-0.126087
31	6	0	2.330216	-1.009775	1.189900
32	1	0	2.628579	-2.604220	-0.323974
33	1	0	2.721096	-0.019717	1.424449
34	6	0	1.125503	-1.350203	1.743131
35	6	0	0.147628	-0.302658	1.836563
36	1	0	0.749470	-2.360393	1.568762
37	1	0	-0.808132	-0.500715	2.319625
38	1	0	0.546746	0.674229	2.111001

Zero-point correction= 0.317188 (Hartree/Particle)
Thermal correction to Energy= 0.334135
Thermal correction to Enthalpy= 0.335079
Thermal correction to Gibbs Free Energy= 0.272592
Sum of electronic and zero-point Energies= -883.565638
Sum of electronic and thermal Energies= -883.548692
Sum of electronic and thermal Enthalpies= -883.547748
Sum of electronic and thermal Free Energies= -883.610234
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.1277975

TS7b′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.463855	0.144340	-0.259480
2	6	0	1.835451	-0.447398	-0.205367
3	6	0	2.957117	0.137731	-0.804456
4	6	0	1.992077	-1.695645	0.409599
5	6	0	4.189735	-0.504721	-0.783224
6	1	0	2.866317	1.099925	-1.294934
7	6	0	3.224001	-2.340022	0.431469
8	1	0	1.130706	-2.153898	0.889230
9	6	0	4.330785	-1.744493	-0.165376
10	1	0	5.045751	-0.034762	-1.258908
11	1	0	3.319836	-3.305237	0.920266
12	1	0	5.296315	-2.241173	-0.148599
13	6	0	0.289079	1.616790	-0.329501
14	8	0	-0.675112	2.199745	-0.784691
15	8	0	1.333805	2.286838	0.202875
16	6	0	1.219011	3.704989	0.179503
17	1	0	0.362208	4.033349	0.774553
18	1	0	2.146491	4.081026	0.611264
19	1	0	1.095803	4.071217	-0.842814
20	6	0	-1.898612	-0.606028	-0.604906
21	6	0	-0.533435	-0.690070	-0.801508
22	1	0	-0.181648	-1.609197	-1.270318
23	6	0	-2.908219	-1.471321	-1.336191

24	1	0	-2.921955	-1.181617	-2.399048
25	1	0	-2.711134	-2.545966	-1.272848
26	8	0	-4.162511	-1.215654	-0.733243
27	6	0	-4.119796	0.103018	-0.210432
28	1	0	-4.883421	0.174358	0.568303
29	1	0	-4.328547	0.847173	-0.993261
30	6	0	-2.696459	0.280596	0.302454
31	6	0	-2.311020	-0.723253	1.336066
32	1	0	-2.364394	1.308112	0.429941
33	1	0	-2.981490	-1.571763	1.444890
34	6	0	-1.153010	-0.665470	2.104326
35	6	0	-0.234242	0.359713	1.981370
36	1	0	-0.873274	-1.563498	2.651876
37	1	0	0.720072	0.314045	2.496133
38	1	0	-0.584999	1.357934	1.748679

Zero-point correction= 0.318048 (Hartree/Particle)
Thermal correction to Energy= 0.334957
Thermal correction to Enthalpy= 0.335902
Thermal correction to Gibbs Free Energy= 0.273940
Sum of electronic and zero-point Energies= -883.615992
Sum of electronic and thermal Energies= -883.599083
Sum of electronic and thermal Enthalpies= -883.598138
Sum of electronic and thermal Free Energies= -883.660100
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.1780026

INT8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.679795	-3.873875	-0.369576
2	6	0	0.388935	-4.177139	-0.070096
3	6	0	0.553871	-1.948016	-0.176165
4	7	0	1.756572	-2.497570	-0.428603
5	1	0	2.538300	-4.503104	-0.543281
6	1	0	-0.106813	-5.124551	0.070497
7	7	0	-0.283587	-2.976769	0.044408
8	79	0	0.143239	0.080200	-0.142964
9	6	0	2.916649	-1.681500	-0.670666
10	6	0	3.677336	-1.276101	0.428936
11	6	0	3.153593	-1.228806	-1.971383
12	6	0	4.727868	-0.394521	0.189420
13	6	0	4.209516	-0.338829	-2.155203
14	6	0	5.002756	0.089737	-1.089191
15	1	0	5.332579	-0.059378	1.027397
16	1	0	4.412789	0.036204	-3.155345
17	6	0	-1.669342	-2.786231	0.379680
18	6	0	-1.997932	-2.537744	1.714026
19	6	0	-2.613257	-2.784579	-0.651844
20	6	0	-3.338745	-2.291430	2.008970
21	6	0	-3.938444	-2.538316	-0.302780
22	6	0	-4.319494	-2.285280	1.017364
23	1	0	-3.623101	-2.106934	3.042241
24	1	0	-4.695780	-2.537249	-1.083193
25	6	0	2.271818	-1.653110	-3.117972
26	1	0	2.222856	-2.743382	-3.210956
27	1	0	1.243163	-1.296254	-2.982607
28	1	0	2.646452	-1.252245	-4.062734
29	6	0	6.140890	1.050211	-1.316331
30	1	0	5.899024	1.776371	-2.098201
31	1	0	6.384439	1.598484	-0.401493
32	1	0	7.044058	0.515441	-1.631999
33	6	0	3.338517	-1.731114	1.824364
34	1	0	4.078750	-1.366163	2.540081
35	1	0	2.358487	-1.346612	2.132110
36	1	0	3.300792	-2.822901	1.903378

37	6	0	-2.202048	-2.975677	-2.087960
38	1	0	-1.704008	-2.072878	-2.463356
39	1	0	-1.511373	-3.815696	-2.212141
40	1	0	-3.075019	-3.162202	-2.718381
41	6	0	-5.763145	-2.007912	1.348302
42	1	0	-6.116235	-1.110189	0.829160
43	1	0	-6.403408	-2.839036	1.034553
44	1	0	-5.909278	-1.856742	2.421091
45	6	0	-0.941554	-2.492533	2.788005
46	1	0	-0.224011	-3.314163	2.697473
47	1	0	-0.374631	-1.554699	2.730852
48	1	0	-1.396930	-2.552608	3.779896
49	6	0	0.093285	2.105571	0.685835
50	6	0	1.506874	2.261792	1.142555
51	6	0	1.982108	1.708625	2.343158
52	6	0	2.401567	2.974347	0.328634
53	6	0	3.306426	1.890800	2.723561
54	1	0	1.312048	1.144706	2.980144
55	6	0	3.721812	3.153932	0.714455
56	1	0	2.058497	3.384906	-0.615320
57	6	0	4.178201	2.615971	1.916030
58	1	0	3.656067	1.467336	3.659948
59	1	0	4.395173	3.718703	0.077749
60	1	0	5.209867	2.762781	2.220967
61	6	0	-1.047837	2.010366	1.688343
62	8	0	-2.011023	2.735127	1.632418
63	8	0	-0.897075	1.045591	2.601503
64	6	0	-1.987356	0.894009	3.522901
65	1	0	-1.666037	0.126753	4.225212
66	1	0	-2.182276	1.835604	4.038392
67	1	0	-2.881709	0.573704	2.983899
68	6	0	-0.489414	1.754423	-1.277066
69	6	0	-0.358850	2.828226	-0.538400
70	1	0	-0.548486	3.884449	-0.695901
71	6	0	-0.921604	1.417454	-2.679385
72	1	0	-1.339571	2.352812	-3.084939
73	1	0	-0.055501	1.128658	-3.281321
74	8	0	-1.831311	0.359987	-2.773636
75	6	0	-3.032728	0.533694	-2.012700
76	1	0	-2.803644	0.453459	-0.938795
77	1	0	-3.644117	-0.330286	-2.286296
78	6	0	-3.741020	1.823150	-2.292301
79	6	0	-3.847564	2.794444	-1.376761
80	1	0	-4.158052	1.953642	-3.290363
81	1	0	-3.404942	2.643808	-0.390955
82	6	0	-4.501197	4.080695	-1.591773
83	6	0	-4.528790	5.038402	-0.660482
84	1	0	-4.970473	4.245726	-2.560533
85	1	0	-5.012291	5.993653	-0.837480
86	1	0	-4.066139	4.890229	0.312807

Zero-point correction= 0.723456 (Hartree/Particle)
Thermal correction to Energy= 0.768863
Thermal correction to Enthalpy= 0.769807
Thermal correction to Gibbs Free Energy= 0.642005
Sum of electronic and zero-point Energies= -1942.416436
Sum of electronic and thermal Energies= -1942.371028
Sum of electronic and thermal Enthalpies= -1942.370084
Sum of electronic and thermal Free Energies= -1942.497887
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0223284

TS9b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.329803	-3.936708	0.235149

2	6	0	0.003838	-4.143141	0.433240
3	6	0	0.293516	-1.958700	-0.002392
4	7	0	1.483320	-2.588694	-0.031587
5	1	0	2.168791	-4.614070	0.255224
6	1	0	-0.552454	-5.038361	0.661271
7	7	0	-0.613110	-2.915872	0.280944
8	79	0	-0.105751	0.018720	-0.474596
9	6	0	2.720722	-1.910967	-0.302895
10	6	0	3.410685	-1.335698	0.766077
11	6	0	3.152275	-1.813639	-1.628669
12	6	0	4.602600	-0.675439	0.477914
13	6	0	4.343412	-1.131587	-1.865821
14	6	0	5.085032	-0.567353	-0.826060
15	1	0	5.163628	-0.227379	1.293290
16	1	0	4.704952	-1.042797	-2.887517
17	6	0	-2.011980	-2.629581	0.444663
18	6	0	-2.498039	-2.462165	1.745361
19	6	0	-2.810654	-2.463298	-0.690373
20	6	0	-3.834768	-2.101466	1.894649
21	6	0	-4.144629	-2.113830	-0.485009
22	6	0	-4.670760	-1.916041	0.791431
23	1	0	-4.236370	-1.964818	2.895853
24	1	0	-4.790266	-1.985369	-1.350686
25	6	0	2.341905	-2.403003	-2.754204
26	1	0	2.162818	-3.473491	-2.606803
27	1	0	1.360850	-1.918184	-2.829970
28	1	0	2.853982	-2.275987	-3.710729
29	6	0	6.394487	0.122132	-1.109091
30	1	0	6.348700	0.701824	-2.036526
31	1	0	6.676426	0.795909	-0.294815
32	1	0	7.199807	-0.612510	-1.223071
33	6	0	2.864146	-1.398571	2.168413
34	1	0	3.580945	-0.983810	2.881696
35	1	0	1.933929	-0.822710	2.246190
36	1	0	2.641210	-2.427257	2.472165
37	6	0	-2.261309	-2.606555	-2.086866
38	1	0	-1.880933	-1.645591	-2.458834
39	1	0	-1.443931	-3.331758	-2.136435
40	1	0	-3.045684	-2.931568	-2.775570
41	6	0	-6.105212	-1.489672	0.966537
42	1	0	-6.219901	-0.423616	0.738472
43	1	0	-6.767311	-2.042807	0.293529
44	1	0	-6.450550	-1.650522	1.991344
45	6	0	-1.601970	-2.671068	2.939276
46	1	0	-1.391129	-3.734579	3.099261
47	1	0	-0.638370	-2.165751	2.808694
48	1	0	-2.072515	-2.290305	3.849380
49	6	0	0.644826	2.214193	0.551155
50	6	0	2.077280	2.298642	0.755824
51	6	0	2.677025	2.175041	2.027061
52	6	0	2.889966	2.619789	-0.352577
53	6	0	4.030754	2.425308	2.184056
54	1	0	2.076400	1.911599	2.887851
55	6	0	4.243786	2.853659	-0.189370
56	1	0	2.443219	2.662220	-1.340205
57	6	0	4.812758	2.770202	1.081603
58	1	0	4.480239	2.356156	3.169100
59	1	0	4.859744	3.098651	-1.048005
60	1	0	5.872902	2.964876	1.212998
61	6	0	-0.319300	1.950974	1.703240
62	8	0	-1.301153	2.631072	1.862514
63	8	0	0.049152	0.959725	2.518428
64	6	0	-0.866452	0.688105	3.590973
65	1	0	-0.380009	-0.072001	4.199381
66	1	0	-1.053158	1.593404	4.170766
67	1	0	-1.806491	0.312106	3.179362
68	6	0	-0.540482	1.855902	-1.287210

69	6	0	0.018272	2.857899	-0.608307
70	1	0	0.126526	3.911803	-0.855814
71	6	0	-1.102921	1.930893	-2.681443
72	1	0	-1.501978	2.949440	-2.815295
73	1	0	-0.302072	1.779006	-3.412876
74	8	0	-2.070390	0.958916	-2.981070
75	6	0	-3.201776	0.942972	-2.108551
76	1	0	-2.912354	0.529737	-1.129934
77	1	0	-3.888898	0.232058	-2.576684
78	6	0	-3.844869	2.282633	-1.915760
79	6	0	-3.789832	2.942203	-0.751962
80	1	0	-4.342599	2.724950	-2.778118
81	1	0	-3.260871	2.490524	0.088595
82	6	0	-4.370491	4.258770	-0.510784
83	6	0	-4.230097	4.911294	0.646563
84	1	0	-4.929117	4.711552	-1.328766
85	1	0	-4.664886	5.893284	0.803117
86	1	0	-3.670547	4.478764	1.472670

Zero-point correction= 0.722816 (Hartree/Particle)
Thermal correction to Energy= 0.767521
Thermal correction to Enthalpy= 0.768465
Thermal correction to Gibbs Free Energy= 0.641969
Sum of electronic and zero-point Energies= -1942.412796
Sum of electronic and thermal Energies= -1942.368090
Sum of electronic and thermal Enthalpies= -1942.367146
Sum of electronic and thermal Free Energies= -1942.493642
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0165805

TS6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.864398	1.525958	1.467541
2	6	0	4.066511	0.191701	1.584305
3	6	0	2.080739	0.499233	0.562735
4	7	0	2.641581	1.691954	0.839662
5	1	0	4.467598	2.369020	1.764697
6	1	0	4.883661	-0.373374	2.003519
7	7	0	2.960208	-0.421589	1.020406
8	79	0	0.360572	0.070579	-0.453661
9	6	0	2.102422	2.949853	0.393354
10	6	0	1.241864	3.668148	1.224354
11	6	0	2.453059	3.381984	-0.890928
12	6	0	0.742945	4.876174	0.739005
13	6	0	1.926084	4.593250	-1.329333
14	6	0	1.074461	5.355527	-0.527373
15	1	0	0.069834	5.453953	1.368074
16	1	0	2.185136	4.951257	-2.322644
17	6	0	2.764232	-1.831855	0.842554
18	6	0	2.262718	-2.582741	1.911863
19	6	0	3.029860	-2.392370	-0.410621
20	6	0	2.015217	-3.936037	1.694024
21	6	0	2.762110	-3.753320	-0.578896
22	6	0	2.252007	-4.538083	0.454411
23	1	0	1.632926	-4.540839	2.513868
24	1	0	2.965930	-4.210904	-1.544218
25	6	0	3.338353	2.547577	-1.781030
26	1	0	4.277066	2.274998	-1.286023
27	1	0	2.836513	1.615052	-2.066930
28	1	0	3.586297	3.088367	-2.697411
29	6	0	0.533148	6.676902	-1.009409
30	1	0	0.676715	6.800789	-2.086211
31	1	0	-0.536254	6.768672	-0.795159
32	1	0	1.040118	7.509460	-0.508102
33	6	0	0.798742	3.148139	2.566116

34	1	0	0.670536	3.968038	3.278459
35	1	0	-0.168784	2.646782	2.451741
36	1	0	1.509783	2.434770	2.993517
37	6	0	3.548811	-1.565252	-1.559061
38	1	0	2.728314	-1.044390	-2.069416
39	1	0	4.258387	-0.802762	-1.224872
40	1	0	4.051098	-2.199940	-2.293680
41	6	0	1.959672	-6.002484	0.252248
42	1	0	2.151175	-6.311526	-0.778672
43	1	0	2.581421	-6.620107	0.909031
44	1	0	0.913295	-6.228947	0.485530
45	6	0	2.002384	-1.944875	3.251219
46	1	0	2.939407	-1.742336	3.782054
47	1	0	1.481334	-0.989040	3.141341
48	1	0	1.399014	-2.599245	3.886061
49	6	0	-3.188718	0.093216	-0.138928
50	6	0	-4.646759	0.161403	0.101136
51	6	0	-5.194254	1.177728	0.895891
52	6	0	-5.502166	-0.798274	-0.457133
53	6	0	-6.566294	1.241653	1.106527
54	1	0	-4.546620	1.935888	1.324967
55	6	0	-6.872622	-0.734605	-0.239041
56	1	0	-5.089672	-1.612313	-1.046689
57	6	0	-7.408555	0.287461	0.541239
58	1	0	-6.979116	2.041841	1.712417
59	1	0	-7.523418	-1.488021	-0.671412
60	1	0	-8.479303	0.337676	0.711264
61	6	0	-2.345581	0.572694	1.011413
62	8	0	-2.023589	1.728026	1.166553
63	8	0	-2.090360	-0.403272	1.886054
64	6	0	-1.350026	-0.011795	3.044667
65	1	0	-1.251526	-0.913964	3.647357
66	1	0	-0.366835	0.364437	2.750990
67	1	0	-1.885101	0.763366	3.597877
68	6	0	-1.254145	-0.437991	-1.665113
69	6	0	-2.668815	-0.304098	-1.319880
70	1	0	-3.389764	-0.517004	-2.112864
71	6	0	-0.955670	-0.131786	-3.141185
72	1	0	-1.820061	-0.358707	-3.789635
73	1	0	-0.734224	0.936082	-3.231264
74	8	0	0.182903	-0.836320	-3.550739
75	6	0	0.022648	-2.203215	-3.206353
76	1	0	0.973273	-2.564437	-2.800094
77	1	0	-0.219506	-2.788940	-4.102255
78	6	0	-1.096169	-2.359034	-2.193524
79	6	0	-0.864076	-2.797475	-0.905496
80	1	0	-2.095003	-2.521293	-2.596818
81	1	0	0.159780	-2.813318	-0.531567
82	6	0	-1.904417	-3.166598	0.010200
83	6	0	-1.632895	-3.344411	1.312444
84	1	0	-2.921474	-3.246510	-0.363401
85	1	0	-2.411846	-3.579371	2.030108
86	1	0	-0.616768	-3.242750	1.686610

Zero-point correction= 0.723990 (Hartree/Particle)
Thermal correction to Energy= 0.768415
Thermal correction to Enthalpy= 0.769359
Thermal correction to Gibbs Free Energy= 0.643818
Sum of electronic and zero-point Energies= -1942.434589
Sum of electronic and thermal Energies= -1942.390164
Sum of electronic and thermal Enthalpies= -1942.389220
Sum of electronic and thermal Free Energies= -1942.514761
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -1944.0348418

(1S,5R)-3b

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.933808	-0.838213	-0.388818
2	6	0	0.652674	-0.605601	-0.657495
3	1	0	0.245233	-1.045565	-1.565634
4	6	0	2.834350	-1.678250	-1.281544
5	1	0	2.473158	-2.701410	-1.421726
6	1	0	2.937649	-1.207107	-2.272051
7	8	0	4.088536	-1.741130	-0.626853
8	6	0	4.210467	-0.554503	0.124875
9	1	0	4.488188	0.296658	-0.520808
10	1	0	4.996214	-0.701775	0.869684
11	6	0	2.818980	-0.319834	0.731547
12	6	0	2.547775	1.096917	1.160710
13	1	0	2.715353	-0.993325	1.596965
14	1	0	3.382855	1.795584	1.156856
15	6	0	1.337401	1.504631	1.532880
16	6	0	0.148994	0.577672	1.550098
17	1	0	1.174225	2.539594	1.821139
18	1	0	0.420342	-0.355040	2.060173
19	1	0	-0.669794	1.032384	2.111512
20	6	0	-0.355337	0.211821	0.136780
21	6	0	-1.676298	-0.586963	0.180126
22	6	0	-2.390080	-0.790154	-1.007046
23	6	0	-2.174033	-1.151578	1.354693
24	6	0	-3.565600	-1.530910	-1.017749
25	1	0	-2.024340	-0.356837	-1.934020
26	6	0	-3.351568	-1.896496	1.344989
27	1	0	-1.651586	-1.020300	2.295596
28	6	0	-4.052805	-2.089152	0.160778
29	1	0	-4.101373	-1.671253	-1.951978
30	1	0	-3.719224	-2.326559	2.272095
31	1	0	-4.971570	-2.667953	0.155140
32	6	0	-0.652469	1.495316	-0.655093
33	8	0	-0.445017	1.647469	-1.835412
34	8	0	-1.227346	2.431630	0.114822
35	6	0	-1.592930	3.633900	-0.560242
36	1	0	-2.015749	4.284285	0.204971
37	1	0	-0.716304	4.097966	-1.018282
38	1	0	-2.332648	3.425288	-1.337025

Zero-point correction= 0.321146 (Hartree/Particle)
Thermal correction to Energy= 0.338198
Thermal correction to Enthalpy= 0.339142
Thermal correction to Gibbs Free Energy= 0.275960
Sum of electronic and zero-point Energies= -883.674150
Sum of electronic and thermal Energies= -883.657098
Sum of electronic and thermal Enthalpies= -883.656154
Sum of electronic and thermal Free Energies= -883.719335
ωB97XD /6-311++G(d,p)-SDD/SMD//ωB97XD /6-31G(d)-LANL2DZ energy in chloroform solvent = -884.2409625