Supplementary Information

Mechanistic differences between the Ru(II) and Zn(II)-catalyzed cross-coupling of cyclopropenes with diazo compounds: A DFT study

Tiantian Liu[a], Kang Lv[c], Xiaoguang Bao*[a,b]

[a] *Innovation Center for Chemical Sciences, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, 199 Ren-Ai Road, Suzhou Industrial Park, Suzhou, Jiangsu 215123, China.*

[b] *Jiangsu Key Laboratory of Advanced Negative Carbon Technologies, Soochow University, Suzhou, Jiangsu 215123, China.*

[c] *School of Chemistry, Chemical Engineering and Materials, Jining University, Qufu, Shandong 273155, China.*

E-mail: xgbao@suda.edu.cn

Contents

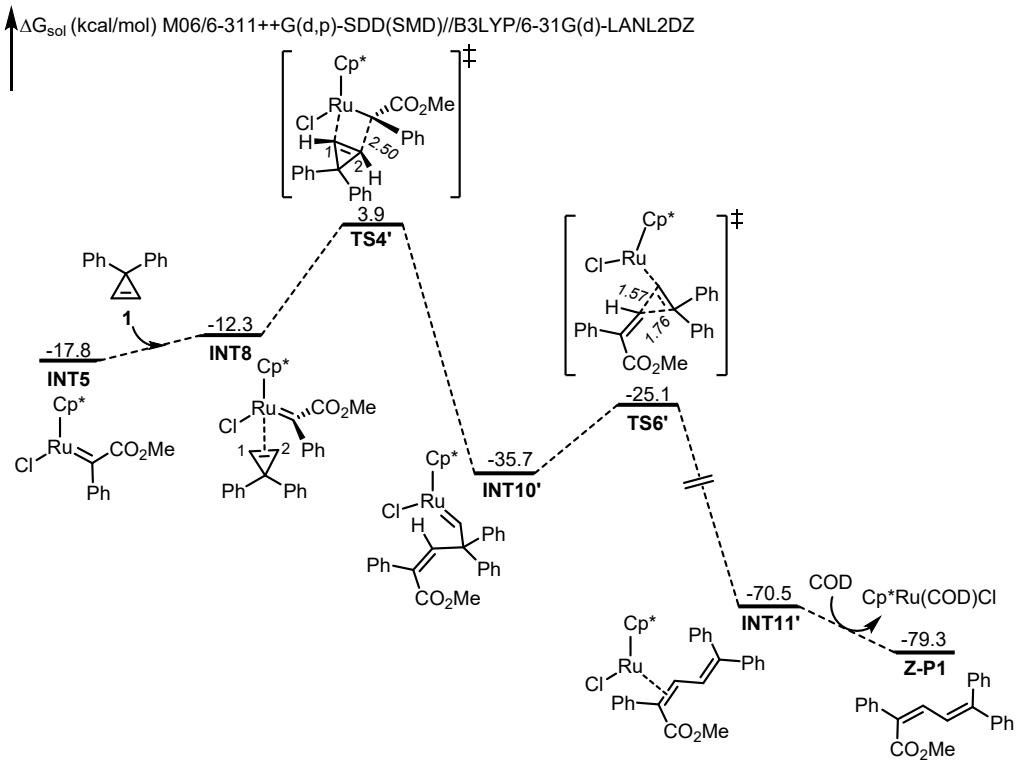

Fig. S1 Energy profiles for the Ru(II)-catalyzed cross-coupling of cyclopropenes with diazo compounds to form the product of (*Z*)-1,3-butadiene derivatives.

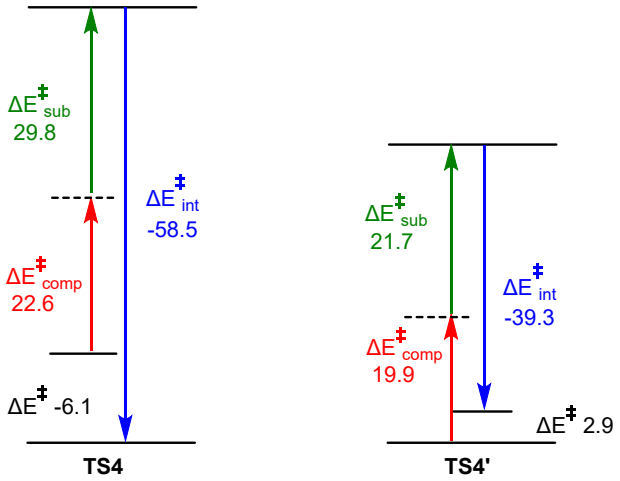

Fig. S2 Distortion, interaction and activation energies for **TS4** and **TS4′** (green arrow: distortion energy of **1**; red arrow: distortion energy of **INT5**; blue arrow: interaction energy; black: activation energy, in kcal/mol).

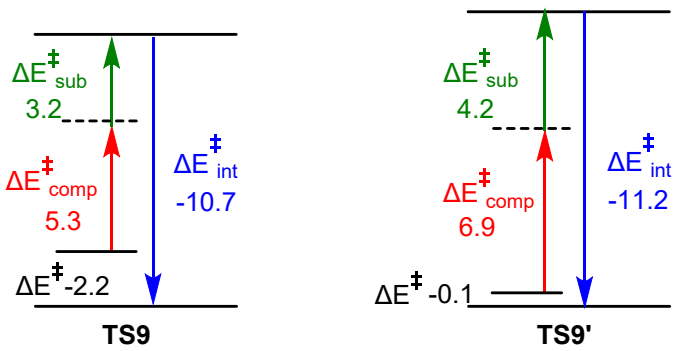

Fig. S3 Distortion, interaction and activation energies for **TS9** and **TS9′** (green arrow: distortion energy of **4**; red arrow: distortion energy of **INT15**; blue arrow: interaction energy; black: activation energy, in kcal/mol).

Cartesian Coordinates and Energies

Cp*Ru(COD)Cl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.671498	1.022080	-1.037694
2	6	0	1.305771	1.608320	0.231838
3	6	0	1.643602	0.653816	1.271531
4	6	0	2.105429	-0.525773	0.641990
5	6	0	2.105354	-0.303913	-0.803096
6	6	0	1.669212	1.729280	-2.361611
7	1	0	1.474155	1.042062	-3.190307
8	1	0	0.922321	2.527541	-2.401267
9	1	0	2.648058	2.193258	-2.545352
10	6	0	1.000441	3.061228	0.467260
11	1	0	0.539710	3.528310	-0.407450
12	1	0	0.324512	3.206865	1.315334
13	1	0	1.921883	3.619504	0.686195
14	6	0	1.638582	0.922113	2.749630
15	1	0	0.923880	1.703364	3.023906
16	1	0	1.392528	0.024931	3.325319
17	1	0	2.629036	1.264292	3.080291
18	6	0	2.664027	-1.741766	1.315988
19	1	0	3.760219	-1.745429	1.234468
20	1	0	2.408754	-1.766704	2.379010
21	1	0	2.278444	-2.655219	0.855775
22	6	0	2.631180	-1.282012	-1.810468
23	1	0	2.199929	-2.273723	-1.643227
24	1	0	2.391231	-0.976851	-2.833254
25	1	0	3.724543	-1.365126	-1.735890
26	17	0	-0.132578	-2.693325	-0.245547
27	6	0	-2.592763	1.711980	0.633808
28	6	0	-3.099177	-1.030553	-0.651041
29	6	0	-2.227403	1.981116	-0.838759
30	6	0	-1.873885	-0.518060	-1.397370
31	6	0	-1.493442	0.819867	-1.484423
32	1	0	-3.128285	2.228208	-1.423676
33	1	0	-3.908022	-0.295564	-0.744001
34	1	0	-1.464532	-1.194979	-2.139306
35	1	0	-2.663589	2.665539	1.170737
36	1	0	-3.452188	-1.934913	-1.156259
37	1	0	-1.583377	2.865417	-0.893991
38	1	0	-0.874758	1.091915	-2.336114
39	6	0	-2.846407	-1.367873	0.842692

40	6	0	-1.574452	0.816176	1.339475
41	1	0	-0.983603	1.315415	2.101746
42	6	0	-1.714059	-0.576022	1.464564
43	1	0	-1.228720	-1.061929	2.308739
44	1	0	-3.587083	1.257816	0.703359
45	44	0	-0.093810	-0.175449	-0.008000
46	1	0	-2.592746	-2.425927	0.925455
47	1	0	-3.771873	-1.211836	1.420166

Zero-point correction= 0.409322 (Hartree/Particle)
Thermal correction to Energy= 0.432134
Thermal correction to Enthalpy= 0.433078
Thermal correction to Gibbs Free Energy= 0.360079
Sum of electronic and zero-point Energies= -1255.882309
Sum of electronic and thermal Energies= -1255.859497
Sum of electronic and thermal Enthalpies= -1255.858553
Sum of electronic and thermal Free Energies= -1255.931552

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1256.959927

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001539	2.422401	0.647066
2	6	0	-0.001200	2.422580	-0.646565
3	6	0	0.000073	1.048222	0.000069
4	1	0	-0.006417	2.955630	1.586902
5	1	0	0.006966	2.956068	-1.586252
6	6	0	1.287042	0.248570	-0.038668
7	6	0	1.397869	-0.899252	-0.839124
8	6	0	2.414289	0.660225	0.684079
9	6	0	2.596734	-1.607931	-0.914431
10	1	0	0.535753	-1.239960	-1.405679
11	6	0	3.613854	-0.049319	0.616693
12	1	0	2.352847	1.552564	1.302422
13	6	0	3.710716	-1.187535	-0.184860
14	1	0	2.660223	-2.490912	-1.545495
15	1	0	4.472347	0.287552	1.192405
16	1	0	4.644158	-1.741325	-0.240905
17	6	0	-1.287022	0.248777	0.038675
18	6	0	-2.413616	0.659620	-0.685507
19	6	0	-1.398562	-0.898062	0.840454
20	6	0	-3.613305	-0.049748	-0.618209
21	1	0	-2.351575	1.551186	-1.304912
22	6	0	-2.597528	-1.606560	0.915664
23	1	0	-0.536894	-1.238116	1.408094
24	6	0	-3.710893	-1.186955	0.184671
25	1	0	-4.471310	0.286472	-1.195027
26	1	0	-2.661620	-2.488760	1.547757
27	1	0	-4.644423	-1.740604	0.240654

Zero-point correction= 0.218411 (Hartree/Particle)
Thermal correction to Energy= 0.230369
Thermal correction to Enthalpy= 0.231313
Thermal correction to Gibbs Free Energy= 0.178827
Sum of electronic and zero-point Energies= -578.507965
Sum of electronic and thermal Energies= -578.496007
Sum of electronic and thermal Enthalpies= -578.495063
Sum of electronic and thermal Free Energies= -578.547549

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -578.427961

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -578.432042

COD

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

1	6	0	1.086690	-1.107027	0.664336
2	6	0	-1.086658	1.107002	0.664437
3	6	0	1.922828	-0.010982	-0.030890
4	6	0	-0.008153	1.707200	-0.212451
5	6	0	1.214565	1.239268	-0.491884
6	1	0	2.747882	0.279461	0.639710
7	1	0	-0.674440	0.722283	1.600598
8	1	0	-0.288845	2.641527	-0.699873
9	1	0	1.777242	-1.908143	0.956289
10	1	0	-1.777177	1.908111	0.956471
11	1	0	2.415333	-0.455085	-0.908851
12	1	0	1.821948	1.849426	-1.162827
13	6	0	-1.922801	0.011048	-0.030938
14	6	0	0.008140	-1.707212	-0.212496
15	1	0	0.288651	-2.641696	-0.699712
16	6	0	-1.214585	-1.239263	-0.491832
17	1	0	-1.822120	-1.849541	-1.162533
18	1	0	0.674486	-0.722421	1.600554
19	1	0	-2.415078	0.455215	-0.908994
20	1	0	-2.748033	-0.279339	0.639475

Zero-point correction= 0.181130 (Hartree/Particle)
Thermal correction to Energy= 0.188552
Thermal correction to Enthalpy= 0.189496
Thermal correction to Gibbs Free Energy= 0.149638
Sum of electronic and zero-point Energies= -311.849277
Sum of electronic and thermal Energies= -311.841856
Sum of electronic and thermal Enthalpies= -311.840912
Sum of electronic and thermal Free Energies= -311.880770
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-311.861476

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.369600	-1.203710	1.383156
2	6	0	-1.749331	0.029252	1.799492
3	6	0	-2.210146	1.069255	0.918166
4	6	0	-3.185040	0.499818	0.015394
5	6	0	-3.275660	-0.899465	0.288348
6	6	0	-2.240735	-2.535713	2.058774
7	1	0	-2.347786	-3.358017	1.345636
8	1	0	-1.272372	-2.645594	2.555094
9	1	0	-3.019250	-2.655299	2.825317
10	6	0	-0.872988	0.230635	3.000001
11	1	0	-0.350645	-0.687235	3.282209
12	1	0	-0.120047	1.002220	2.821036
13	1	0	-1.479798	0.543849	3.860887
14	6	0	-1.846616	2.518448	1.007906
15	1	0	-0.835846	2.658712	1.396495
16	1	0	-1.894649	3.003814	0.030391
17	1	0	-2.546449	3.039711	1.677077
18	6	0	-3.963809	1.245470	-1.026063
19	1	0	-4.962212	1.501844	-0.646122
20	1	0	-3.463032	2.175074	-1.308450
21	1	0	-4.078567	0.648660	-1.934126
22	6	0	-4.172366	-1.876323	-0.409019
23	1	0	-4.274922	-1.625965	-1.467562
24	1	0	-3.779770	-2.894934	-0.345967
25	1	0	-5.171853	-1.871550	0.047707
26	17	0	-1.584953	-0.654978	-2.693826
27	44	0	-1.196499	-0.472505	-0.300849
28	6	0	0.704495	-1.126903	0.488942
29	6	0	0.791415	-1.097340	-0.888875
30	6	0	1.780210	-0.239281	-0.114966

31	1	0	0.753415	-1.874026	1.273828
32	1	0	0.922587	-1.777042	-1.720302
33	6	0	1.666727	1.267455	-0.091539
34	6	0	1.237286	1.978948	-1.219013
35	6	0	2.039604	1.988379	1.054401
36	6	0	1.174686	3.375450	-1.200905
37	1	0	0.942915	1.430242	-2.109197
38	6	0	1.976362	3.383092	1.076211
39	1	0	2.396850	1.448734	1.928660
40	6	0	1.543971	4.082245	-0.054969
41	1	0	0.842450	3.909346	-2.087657
42	1	0	2.270209	3.924033	1.972513
43	1	0	1.499480	5.168185	-0.042269
44	6	0	3.194799	-0.790629	-0.079589
45	6	0	3.423164	-2.169417	0.084249
46	6	0	4.317133	0.039272	-0.243095
47	6	0	4.715760	-2.692530	0.104599
48	1	0	2.582024	-2.847739	0.187445
49	6	0	5.610489	-0.484273	-0.228705
50	1	0	4.180404	1.105230	-0.386265
51	6	0	5.819234	-1.852206	-0.050009
52	1	0	4.858200	-3.762175	0.236729
53	1	0	6.457683	0.184091	-0.360410
54	1	0	6.826882	-2.258875	-0.037664

Zero-point correction= 0.445890 (Hartree/Particle)
Thermal correction to Energy= 0.474175
Thermal correction to Enthalpy= 0.475119
Thermal correction to Gibbs Free Energy= 0.386442
Sum of electronic and zero-point Energies= -1522.533983
Sum of electronic and thermal Energies= -1522.505698
Sum of electronic and thermal Enthalpies= -1522.504754
Sum of electronic and thermal Free Energies= -1522.593432
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1523.526172

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.384356	-0.925592	1.592811
2	6	0	-1.645250	0.296967	1.756465
3	6	0	-2.132776	1.237235	0.780324
4	6	0	-3.240296	0.624153	0.079002
5	6	0	-3.381369	-0.715161	0.554800
6	6	0	-2.262575	-2.159105	2.437607
7	1	0	-2.474499	-3.062305	1.858622
8	1	0	-1.259947	-2.262254	2.861339
9	1	0	-2.974241	-2.123744	3.274409
10	6	0	-0.623290	0.585743	2.816552
11	1	0	-0.109704	-0.322211	3.146960
12	1	0	0.135226	1.289493	2.463563
13	1	0	-1.104414	1.026324	3.700563
14	6	0	-1.695839	2.663266	0.643489
15	1	0	-0.647163	2.793338	0.918489
16	1	0	-1.815363	3.023320	-0.381394
17	1	0	-2.300934	3.308475	1.297096
18	6	0	-4.076325	1.273339	-0.983029
19	1	0	-4.982392	1.712468	-0.541905
20	1	0	-3.530514	2.074343	-1.488782
21	1	0	-4.382193	0.551310	-1.744095
22	6	0	-4.413846	-1.707123	0.109304
23	1	0	-4.607105	-1.617936	-0.962844
24	1	0	-4.088035	-2.733502	0.299011
25	1	0	-5.360429	-1.550359	0.644915
26	17	0	-1.851224	-1.228218	-2.542771
27	44	0	-1.348221	-0.530772	-0.296083

28	6	0	0.476824	-1.227261	0.220453
29	6	0	0.912292	-0.893794	-1.034944
30	6	0	2.012618	-0.130261	-0.474211
31	1	0	0.885142	-1.461521	1.192176
32	1	0	0.709932	-1.319894	-2.012269
33	6	0	1.919581	1.341817	-0.335257
34	6	0	1.358532	2.102165	-1.379051
35	6	0	2.402877	2.028663	0.796266
36	6	0	1.318864	3.494415	-1.312573
37	1	0	0.965057	1.589133	-2.251599
38	6	0	2.348549	3.421031	0.870135
39	1	0	2.824350	1.462013	1.621846
40	6	0	1.815982	4.160949	-0.189475
41	1	0	0.900423	4.060162	-2.140994
42	1	0	2.725845	3.928625	1.754264
43	1	0	1.784171	5.245933	-0.137250
44	6	0	3.280342	-0.841971	-0.191292
45	6	0	3.342684	-2.255618	-0.187338
46	6	0	4.495386	-0.146107	0.004462
47	6	0	4.540281	-2.927715	0.039332
48	1	0	2.441091	-2.831296	-0.363400
49	6	0	5.693460	-0.824750	0.217336
50	1	0	4.508226	0.936385	-0.038702
51	6	0	5.726487	-2.219752	0.247161
52	1	0	4.546900	-4.014794	0.042851
53	1	0	6.608574	-0.254431	0.355830
54	1	0	6.661523	-2.746598	0.416080

Zero-point correction= 0.443048 (Hartree/Particle)
Thermal correction to Energy= 0.471675
Thermal correction to Enthalpy= 0.472619
Thermal correction to Gibbs Free Energy= 0.382833
Sum of electronic and zero-point Energies= -1522.501984
Sum of electronic and thermal Energies= -1522.473357
Sum of electronic and thermal Enthalpies= -1522.472412
Sum of electronic and thermal Free Energies= -1522.562199
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1523.478142

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.871428	0.537308	1.583379
2	6	0	-2.282676	1.588980	0.802069
3	6	0	-2.870695	1.509062	-0.519427
4	6	0	-3.975780	0.556448	-0.470827
5	6	0	-3.947814	-0.063044	0.783927
6	6	0	-2.649197	0.273426	3.044663
7	1	0	-2.757832	-0.790024	3.280041
8	1	0	-1.647048	0.580572	3.357631
9	1	0	-3.375459	0.823578	3.660596
10	6	0	-1.335317	2.646131	1.286295
11	1	0	-0.673460	2.268684	2.071470
12	1	0	-0.708054	3.029606	0.475852
13	1	0	-1.892152	3.499076	1.699111
14	6	0	-2.593938	2.429238	-1.670636
15	1	0	-1.567799	2.806399	-1.645472
16	1	0	-2.738599	1.917957	-2.626296
17	1	0	-3.271399	3.295502	-1.644950
18	6	0	-4.850665	0.223724	-1.643513
19	1	0	-5.345237	1.123917	-2.029537
20	1	0	-4.264035	-0.218745	-2.457554
21	1	0	-5.629746	-0.493224	-1.371868
22	6	0	-4.828364	-1.172716	1.275856
23	1	0	-5.386006	-1.640474	0.461138
24	1	0	-4.239532	-1.955206	1.766529

25	1	0	-5.552169	-0.797996	2.012667
26	17	0	-1.766561	-1.757382	-2.020229
27	44	0	-1.771331	-0.321410	-0.104566
28	6	0	0.078010	-0.433100	0.317288
29	6	0	1.179164	0.436224	0.070332
30	6	0	2.515889	0.092334	0.075680
31	1	0	0.337808	-1.374961	0.827394
32	1	0	0.938028	1.459789	-0.208634
33	6	0	3.545367	1.142033	-0.107579
34	6	0	4.723247	0.884998	-0.836197
35	6	0	3.368033	2.432197	0.430580
36	6	0	5.675374	1.883324	-1.033539
37	1	0	4.877942	-0.099899	-1.265107
38	6	0	4.323527	3.427078	0.238619
39	1	0	2.484831	2.642031	1.026760
40	6	0	5.480541	3.158182	-0.497511
41	1	0	6.570057	1.665669	-1.610661
42	1	0	4.170438	4.411538	0.672822
43	1	0	6.226032	3.934452	-0.647016
44	6	0	2.959307	-1.314320	0.203385
45	6	0	2.311672	-2.349952	-0.499855
46	6	0	4.045611	-1.648676	1.037665
47	6	0	2.724471	-3.674953	-0.353552
48	1	0	1.502921	-2.110595	-1.184507
49	6	0	4.446902	-2.973078	1.188982
50	1	0	4.559199	-0.862136	1.582681
51	6	0	3.787479	-3.991594	0.493285
52	1	0	2.215945	-4.456926	-0.910465
53	1	0	5.275410	-3.212583	1.850286
54	1	0	4.107691	-5.023985	0.605646

Zero-point correction= 0.445969 (Hartree/Particle)
Thermal correction to Energy= 0.474759
Thermal correction to Enthalpy= 0.475703
Thermal correction to Gibbs Free Energy= 0.383980
Sum of electronic and zero-point Energies= -1522.563770
Sum of electronic and thermal Energies= -1522.534981
Sum of electronic and thermal Enthalpies= -1522.534036
Sum of electronic and thermal Free Energies= -1522.625759
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1523.525989

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.562636	0.679734	-0.084066
2	7	0	-0.705160	1.987532	-0.187300
3	7	0	-0.821506	3.114937	-0.273660
4	6	0	0.817234	0.145413	-0.033957
5	6	0	1.116468	-1.158196	-0.467123
6	6	0	1.870551	0.956430	0.426681
7	6	0	2.427152	-1.630333	-0.426871
8	1	0	0.322296	-1.798272	-0.829037
9	6	0	3.179513	0.481604	0.451394
10	1	0	1.665804	1.964611	0.777514
11	6	0	3.466030	-0.816938	0.027761
12	1	0	2.635849	-2.642298	-0.763907
13	1	0	3.974899	1.127795	0.812851
14	1	0	4.486015	-1.189946	0.051953
15	6	0	-1.865488	-0.001619	0.006510
16	8	0	-1.736696	-1.336133	0.179568
17	8	0	-2.937176	0.573341	-0.055246
18	6	0	-2.978791	-2.050462	0.298585
19	1	0	-3.544909	-1.692692	1.162203
20	1	0	-3.584485	-1.922082	-0.602103
21	1	0	-2.698025	-3.095856	0.429188

Zero-point correction=	0.158452 (Hartree/Particle)
Thermal correction to Energy=	0.170224
Thermal correction to Enthalpy=	0.171168
Thermal correction to Gibbs Free Energy=	0.119336
Sum of electronic and zero-point Energies=	-607.520801
Sum of electronic and thermal Energies=	-607.509028
Sum of electronic and thermal Enthalpies=	-607.508084
Sum of electronic and thermal Free Energies=	-607.559916

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -607.447819

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.941935	-1.952373	-0.000544
2	6	0	-2.526670	-1.338822	1.162007
3	6	0	-3.543727	-0.398306	0.713424
4	6	0	-3.542790	-0.397631	-0.715172
5	6	0	-2.525153	-1.337721	-1.163304
6	6	0	-0.924664	-3.056138	-0.000397
7	1	0	-0.281361	-3.012939	-0.884322
8	1	0	-0.282547	-3.013783	0.884431
9	1	0	-1.419191	-4.037170	-0.001196
10	6	0	-2.242342	-1.695312	2.590271
11	1	0	-1.222918	-2.070604	2.716422
12	1	0	-2.363477	-0.830785	3.248791
13	1	0	-2.932073	-2.477973	2.936718
14	6	0	-4.442238	0.409933	1.600856
15	1	0	-3.969497	0.616670	2.564908
16	1	0	-4.687278	1.371798	1.144230
17	1	0	-5.379980	-0.129370	1.794041
18	6	0	-4.440144	0.411421	-1.603039
19	1	0	-3.966135	0.619038	-2.566276
20	1	0	-5.377631	-0.127707	-1.797935
21	1	0	-4.685752	1.372884	-1.145877
22	6	0	-2.238963	-1.692866	-2.591531
23	1	0	-2.358981	-0.827651	-3.249350
24	1	0	-1.219470	-2.068307	-2.716669
25	1	0	-2.928427	-2.475002	-2.939690
26	17	0	-1.856938	2.617788	-0.000281
27	44	0	-1.575574	0.237578	0.000642
28	6	0	2.844576	0.610056	0.000793
29	7	0	1.541881	0.469693	0.001602
30	7	0	0.389427	0.386813	0.002447
31	6	0	3.695338	-0.597475	0.000292
32	6	0	5.100535	-0.511702	-0.000407
33	6	0	3.103690	-1.876337	0.000516
34	6	0	5.874796	-1.671646	-0.000869
35	1	0	5.572178	0.461514	-0.000602
36	6	0	3.885908	-3.027237	0.000052
37	1	0	2.021616	-1.973201	0.001056
38	6	0	5.279648	-2.933569	-0.000648
39	1	0	6.957926	-1.581429	-0.001407
40	1	0	3.403145	-4.001142	0.000232
41	1	0	5.890849	-3.831746	-0.001015
42	6	0	3.325408	2.013099	0.000316
43	8	0	2.289617	2.876073	0.000933
44	8	0	4.493346	2.356918	-0.000531
45	6	0	2.631256	4.269872	0.000352
46	1	0	3.214159	4.521394	0.890595
47	1	0	3.212960	4.520933	-0.890805
48	1	0	1.677037	4.795797	0.000849

Zero-point correction=	0.384404 (Hartree/Particle)
Thermal correction to Energy=	0.413351

Thermal correction to Enthalpy= 0.414295
Thermal correction to Gibbs Free Energy= 0.320326
Sum of electronic and zero-point Energies= -1551.548321
Sum of electronic and thermal Energies= -1551.519374
Sum of electronic and thermal Enthalpies= -1551.518430
Sum of electronic and thermal Free Energies= -1551.612398
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1552.531178

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.051628	0.301886	-1.890326
2	6	0	0.683428	1.612840	-1.424407
3	6	0	1.608072	2.010684	-0.386367
4	6	0	2.549213	0.925826	-0.199058
5	6	0	2.188592	-0.130320	-1.118528
6	6	0	0.439937	-0.426598	-3.050260
7	1	0	0.587475	-1.506826	-2.965539
8	1	0	-0.635569	-0.244259	-3.116961
9	1	0	0.900944	-0.102581	-3.994259
10	6	0	-0.398519	2.474267	-2.005187
11	1	0	-1.222697	1.872836	-2.396546
12	1	0	-0.800941	3.167629	-1.260278
13	1	0	0.000436	3.076366	-2.833945
14	6	0	1.657941	3.340075	0.305375
15	1	0	0.686201	3.841432	0.278120
16	1	0	1.936407	3.224021	1.355865
17	1	0	2.390820	4.001675	-0.177807
18	6	0	3.732866	0.945597	0.721662
19	1	0	4.043265	-0.066163	0.997756
20	1	0	4.588867	1.439249	0.239548
21	1	0	3.501875	1.480691	1.645850
22	6	0	2.930722	-1.419766	-1.306910
23	1	0	3.490549	-1.693923	-0.408700
24	1	0	2.252012	-2.245314	-1.539819
25	1	0	3.649254	-1.330723	-2.134023
26	17	0	0.649487	0.823579	2.684381
27	44	0	0.566672	0.249588	0.295210
28	6	0	-1.821882	-0.447177	0.544773
29	7	0	-2.176302	-0.175674	1.814589
30	7	0	-2.387423	0.078651	2.893042
31	6	0	-1.020741	-1.685288	0.321960
32	6	0	-1.222635	-2.498729	-0.824493
33	6	0	-0.105423	-2.122317	1.313377
34	6	0	-0.500007	-3.668591	-0.982827
35	1	0	-1.937731	-2.187303	-1.574175
36	6	0	0.619146	-3.312829	1.123306
37	1	0	-0.012327	-1.594267	2.255867
38	6	0	0.436755	-4.080774	-0.016118
39	1	0	-0.670599	-4.280204	-1.865186
40	1	0	1.310945	-3.630468	1.898457
41	1	0	0.991068	-5.005072	-0.152734
42	6	0	-2.694890	0.199305	-0.457140
43	8	0	-3.506690	1.115297	0.117821
44	8	0	-2.696918	-0.041469	-1.651204
45	6	0	-4.398393	1.805532	-0.772945
46	1	0	-3.833776	2.405504	-1.491093
47	1	0	-5.028074	1.094349	-1.313294
48	1	0	-5.003183	2.447445	-0.132495

Zero-point correction= 0.384412 (Hartree/Particle)
Thermal correction to Energy= 0.412994
Thermal correction to Enthalpy= 0.413939
Thermal correction to Gibbs Free Energy= 0.326177
Sum of electronic and zero-point Energies= -1551.528004

Sum of electronic and thermal Energies= -1551.499421
Sum of electronic and thermal Enthalpies= -1551.498477
Sum of electronic and thermal Free Energies= -1551.586239
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1552.519619

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.830355	-0.743121	-1.795279
2	6	0	1.782542	0.306030	-1.574123
3	6	0	2.769777	-0.173225	-0.613424
4	6	0	2.409100	-1.499951	-0.230631
5	6	0	1.174488	-1.833720	-0.917771
6	6	0	-0.259812	-0.750829	-2.825404
7	1	0	-1.070197	-1.430948	-2.549554
8	1	0	-0.693257	0.242439	-2.957742
9	1	0	0.140167	-1.085703	-3.793024
10	6	0	1.868045	1.597517	-2.332154
11	1	0	0.877670	1.962902	-2.613396
12	1	0	2.364041	2.374280	-1.741487
13	1	0	2.453919	1.461927	-3.252744
14	6	0	3.981099	0.588213	-0.163978
15	1	0	3.772102	1.659413	-0.085875
16	1	0	4.326360	0.247917	0.815447
17	1	0	4.806653	0.460797	-0.878572
18	6	0	3.160203	-2.398993	0.706593
19	1	0	2.481578	-3.047288	1.268143
20	1	0	3.857494	-3.042513	0.151990
21	1	0	3.735755	-1.824358	1.436419
22	6	0	0.468711	-3.154328	-0.843904
23	1	0	0.615947	-3.631575	0.129066
24	1	0	-0.606941	-3.044179	-1.003454
25	1	0	0.855915	-3.839093	-1.612152
26	17	0	1.177826	0.005645	2.685421
27	44	0	0.802255	-0.096800	0.348932
28	6	0	-1.172164	0.762231	0.414717
29	7	0	-1.498768	1.292249	1.925971
30	7	0	-1.231868	1.295999	3.017090
31	6	0	-2.273132	-0.237872	0.157737
32	6	0	-3.235870	-0.080062	-0.852756
33	6	0	-2.339132	-1.383410	0.974793
34	6	0	-4.215976	-1.054698	-1.053551
35	1	0	-3.203177	0.790865	-1.494977
36	6	0	-3.331051	-2.342115	0.783401
37	1	0	-1.604660	-1.515615	1.764873
38	6	0	-4.271827	-2.185541	-0.238624
39	1	0	-4.945424	-0.919330	-1.847876
40	1	0	-3.365753	-3.214566	1.430360
41	1	0	-5.041704	-2.936453	-0.394317
42	6	0	-1.145806	2.030686	-0.386727
43	8	0	-0.800283	3.107427	0.353807
44	8	0	-1.351125	2.100176	-1.587820
45	6	0	-0.673018	4.344939	-0.363280
46	1	0	0.149946	4.288325	-1.080746
47	1	0	-1.598277	4.579342	-0.895629
48	1	0	-0.463865	5.097596	0.396975

Zero-point correction= 0.382234 (Hartree/Particle)
Thermal correction to Energy= 0.410657
Thermal correction to Enthalpy= 0.411602
Thermal correction to Gibbs Free Energy= 0.323106
Sum of electronic and zero-point Energies= -1551.522213
Sum of electronic and thermal Energies= -1551.493789
Sum of electronic and thermal Enthalpies= -1551.492845
Sum of electronic and thermal Free Energies= -1551.581341

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1552.509048

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.099953	-0.230892	1.793855
2	6	0	-1.962307	0.775062	1.242310
3	6	0	-2.895648	0.115909	0.327083
4	6	0	-2.542012	-1.244749	0.244360
5	6	0	-1.378004	-1.461063	1.104579
6	6	0	-0.114665	-0.036480	2.909089
7	1	0	0.683632	-0.783572	2.874177
8	1	0	0.348537	0.951380	2.860648
9	1	0	-0.621702	-0.138131	3.878622
10	6	0	-2.049441	2.202544	1.691029
11	1	0	-1.060146	2.604416	1.921605
12	1	0	-2.501141	2.832896	0.919603
13	1	0	-2.675112	2.282541	2.591779
14	6	0	-4.001033	0.811382	-0.409546
15	1	0	-3.689724	1.803894	-0.749098
16	1	0	-4.311946	0.246822	-1.291706
17	1	0	-4.878610	0.940942	0.238893
18	6	0	-3.195256	-2.302000	-0.595161
19	1	0	-2.459299	-3.009129	-0.989190
20	1	0	-3.924436	-2.873302	-0.004255
21	1	0	-3.717383	-1.867450	-1.450878
22	6	0	-0.750162	-2.793246	1.385803
23	1	0	-0.779383	-3.441530	0.505512
24	1	0	0.294404	-2.690693	1.691063
25	1	0	-1.288578	-3.308023	2.194554
26	17	0	-1.010029	-0.084884	-2.758271
27	44	0	-0.725990	-0.008678	-0.411705
28	6	0	1.125556	0.472333	-0.197494
29	6	0	2.258724	-0.447313	-0.126611
30	6	0	3.424244	-0.132712	0.611535
31	6	0	2.207954	-1.694031	-0.792811
32	6	0	4.480245	-1.034585	0.697399
33	1	0	3.481714	0.815381	1.138847
34	6	0	3.272168	-2.587023	-0.715554
35	1	0	1.333532	-1.924937	-1.393217
36	6	0	4.408083	-2.263184	0.033407
37	1	0	5.362530	-0.780638	1.278655
38	1	0	3.222110	-3.533990	-1.245978
39	1	0	5.237978	-2.962332	0.092943
40	6	0	1.420250	1.904211	0.098389
41	8	0	1.932698	2.526031	-0.981225
42	8	0	1.228642	2.467929	1.166172
43	6	0	2.210973	3.927777	-0.824493
44	1	0	1.295966	4.474363	-0.581072
45	1	0	2.946273	4.089866	-0.031462
46	1	0	2.605814	4.252774	-1.787014

Zero-point correction= 0.374515 (Hartree/Particle)
Thermal correction to Energy= 0.401338
Thermal correction to Enthalpy= 0.402282
Thermal correction to Gibbs Free Energy= 0.315537
Sum of electronic and zero-point Energies= -1442.057136
Sum of electronic and thermal Energies= -1442.030313
Sum of electronic and thermal Enthalpies= -1442.029369
Sum of electronic and thermal Free Energies= -1442.116114
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1443.064257

N_2

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

1	7	0	0.000000	0.000000	0.552749
2	7	0	0.000000	0.000000	-0.552749

Zero-point correction= 0.005598 (Hartree/Particle)
Thermal correction to Energy= 0.007959
Thermal correction to Enthalpy= 0.008903
Thermal correction to Gibbs Free Energy= -0.012851
Sum of electronic and zero-point Energies= -109.518530
Sum of electronic and thermal Energies= -109.516170
Sum of electronic and thermal Enthalpies= -109.515226
Sum of electronic and thermal Free Energies= -109.536980
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -109.484865

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.480490	-0.951124	-2.021111
2	6	0	2.816860	-2.161986	-1.323874
3	6	0	1.579038	-2.905122	-1.086408
4	6	0	0.502470	-2.113052	-1.530365
5	6	0	1.047479	-0.862038	-2.061079
6	6	0	3.454031	0.018434	-2.624937
7	1	0	3.018222	1.016919	-2.722035
8	1	0	4.356841	0.104589	-2.016135
9	1	0	3.742094	-0.317361	-3.630724
10	6	0	4.201466	-2.683963	-1.085755
11	1	0	4.892416	-1.873617	-0.842376
12	1	0	4.216995	-3.403148	-0.261730
13	1	0	4.573848	-3.199907	-1.982587
14	6	0	1.506197	-4.254770	-0.437125
15	1	0	2.222011	-4.339424	0.386189
16	1	0	0.512484	-4.448547	-0.026607
17	1	0	1.735741	-5.048019	-1.161924
18	6	0	-0.958444	-2.443523	-1.462581
19	1	0	-1.317553	-2.813755	-2.432782
20	1	0	-1.163539	-3.210406	-0.712316
21	1	0	-1.556867	-1.566111	-1.200799
22	6	0	0.244211	0.204953	-2.742016
23	1	0	-0.737660	0.331512	-2.277285
24	1	0	0.752285	1.172173	-2.713818
25	1	0	0.080333	-0.057934	-3.797190
26	17	0	0.396516	-1.468907	2.008539
27	44	0	1.640051	-0.913373	0.057271
28	6	0	2.586670	0.688646	0.560425
29	6	0	2.173684	2.070584	0.337478
30	6	0	3.118657	3.119981	0.237246
31	6	0	0.803893	2.395355	0.195689
32	6	0	2.711360	4.426811	-0.010923
33	1	0	4.177569	2.896072	0.329059
34	6	0	0.398422	3.703819	-0.045381
35	1	0	0.067454	1.604903	0.298975
36	6	0	1.351756	4.721969	-0.152476
37	1	0	3.452276	5.217291	-0.094487
38	1	0	-0.659564	3.927600	-0.146805
39	1	0	1.035603	5.744733	-0.340375
40	6	0	3.975656	0.489851	1.069012
41	8	0	4.029326	0.639364	2.406563
42	8	0	4.952063	0.219171	0.385415
43	6	0	5.314496	0.417233	3.011798
44	1	0	5.653882	-0.604834	2.823631
45	1	0	6.054624	1.118763	2.617007
46	1	0	5.162424	0.578919	4.078877
47	6	0	-3.812542	1.049139	2.614298
48	6	0	-2.706418	0.536090	2.182468

49	6	0	-3.845014	0.582003	1.172649
50	1	0	-4.398545	1.486078	3.410208
51	6	0	-4.590093	-0.698779	0.855486
52	6	0	-4.037566	-1.947379	1.172285
53	6	0	-5.870290	-0.664861	0.279772
54	6	0	-4.740162	-3.128009	0.920845
55	1	0	-3.050236	-1.993510	1.625830
56	6	0	-6.576128	-1.842150	0.030760
57	1	0	-6.315446	0.293661	0.025074
58	6	0	-6.012866	-3.080395	0.349456
59	1	0	-4.291386	-4.085275	1.174545
60	1	0	-7.569079	-1.792185	-0.409442
61	1	0	-6.562319	-3.998110	0.156153
62	6	0	-3.768687	1.608257	0.059578
63	6	0	-3.698719	2.979626	0.348816
64	6	0	-3.726699	1.221595	-1.290853
65	6	0	-3.595718	3.930979	-0.667813
66	1	0	-3.724895	3.303779	1.385845
67	6	0	-3.614043	2.169200	-2.310270
68	1	0	-3.798408	0.168178	-1.545305
69	6	0	-3.549368	3.530251	-2.005220
70	1	0	-3.561770	4.987887	-0.413643
71	1	0	-3.585047	1.841511	-3.346661
72	1	0	-3.471140	4.268848	-2.798566
73	1	0	-1.682236	0.214518	2.322031

Zero-point correction= 0.593675 (Hartree/Particle)
Thermal correction to Energy= 0.634754
Thermal correction to Enthalpy= 0.635698
Thermal correction to Gibbs Free Energy= 0.511342
Sum of electronic and zero-point Energies= -2020.559584
Sum of electronic and thermal Energies= -2020.518505
Sum of electronic and thermal Enthalpies= -2020.517561
Sum of electronic and thermal Free Energies= -2020.641917
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.500318

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.805381	-0.428592	-0.497687
2	6	0	3.957858	0.918981	-0.017644
3	6	0	4.055035	0.864540	1.443354
4	6	0	3.890547	-0.466173	1.848801
5	6	0	3.629445	-1.276316	0.657794
6	6	0	3.958313	-0.880615	-1.918880
7	1	0	3.405352	-1.800624	-2.119383
8	1	0	3.606158	-0.127245	-2.628827
9	1	0	5.019163	-1.073009	-2.133088
10	6	0	4.262860	2.132534	-0.849531
11	1	0	3.835386	2.049497	-1.852891
12	1	0	3.862057	3.043621	-0.393369
13	1	0	5.347927	2.272523	-0.960208
14	6	0	4.288021	2.062175	2.317734
15	1	0	5.345122	2.361500	2.298422
16	1	0	3.702318	2.923049	1.978152
17	1	0	4.014240	1.864662	3.357228
18	6	0	3.896650	-1.007785	3.246528
19	1	0	4.027127	-0.214792	3.987426
20	1	0	2.956310	-1.521484	3.471708
21	1	0	4.718101	-1.725298	3.374580
22	6	0	3.519272	-2.772717	0.664796
23	1	0	2.873046	-3.113694	1.478936
24	1	0	3.103019	-3.147659	-0.274098
25	1	0	4.506948	-3.237269	0.800659
26	17	0	0.529853	-0.673324	2.346471

27	44	0	1.979544	0.162951	0.576406
28	6	0	0.728025	0.260586	-0.938499
29	6	0	0.608473	-0.517501	-2.177649
30	6	0	0.392138	0.057524	-3.449749
31	6	0	0.710445	-1.924464	-2.095973
32	6	0	0.316694	-0.746363	-4.588718
33	1	0	0.290896	1.132830	-3.532882
34	6	0	0.615883	-2.721969	-3.231937
35	1	0	0.844120	-2.370983	-1.115251
36	6	0	0.427061	-2.134458	-4.487842
37	1	0	0.164337	-0.282849	-5.560202
38	1	0	0.686739	-3.802886	-3.140843
39	1	0	0.359075	-2.755049	-5.377521
40	6	0	0.309867	1.690078	-0.883875
41	8	0	0.433448	2.060732	0.443486
42	8	0	0.003704	2.492738	-1.744467
43	6	0	0.264416	3.449594	0.759389
44	1	0	0.956866	4.066988	0.179884
45	1	0	-0.762666	3.755040	0.543509
46	1	0	0.466995	3.531998	1.826988
47	6	0	-2.382199	-0.348994	-1.194269
48	6	0	-1.499611	-0.225418	-0.240964
49	6	0	-3.459789	-0.204737	-0.225807
50	6	0	-4.142110	1.100325	-0.124484
51	6	0	-3.528972	2.278881	-0.607273
52	6	0	-5.463906	1.207209	0.363629
53	6	0	-4.196026	3.501078	-0.577378
54	1	0	-2.521847	2.238625	-1.007059
55	6	0	-6.126465	2.431987	0.387334
56	1	0	-5.983428	0.317625	0.701182
57	6	0	-5.496683	3.589369	-0.075639
58	1	0	-3.694976	4.389444	-0.953584
59	1	0	-7.144965	2.479129	0.764230
60	1	0	-6.014670	4.544247	-0.052762
61	6	0	-3.914481	-1.393542	0.527699
62	6	0	-3.888539	-2.664756	-0.079700
63	6	0	-4.352928	-1.309132	1.864847
64	6	0	-4.301243	-3.800560	0.612385
65	1	0	-3.543117	-2.753074	-1.105832
66	6	0	-4.762249	-2.446547	2.556914
67	1	0	-4.345861	-0.347294	2.368131
68	6	0	-4.743250	-3.696986	1.933679
69	1	0	-4.279511	-4.768822	0.119116
70	1	0	-5.084042	-2.358304	3.591184
71	1	0	-5.061730	-4.583337	2.475585
72	1	0	-1.211872	-0.323674	0.797713
73	1	0	-2.314866	-0.277961	-2.279160

Zero-point correction= 0.592402 (Hartree/Particle)
Thermal correction to Energy= 0.632582
Thermal correction to Enthalpy= 0.633526
Thermal correction to Gibbs Free Energy= 0.516268
Sum of electronic and zero-point Energies= -2020.519746
Sum of electronic and thermal Energies= -2020.479566
Sum of electronic and thermal Enthalpies= -2020.478622
Sum of electronic and thermal Free Energies= -2020.595880
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.449675

TS3′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.489509	-0.925556	0.016933
2	6	0	-3.466325	-0.060204	1.165062
3	6	0	-3.657165	1.290084	0.694006
4	6	0	-3.937127	1.233845	-0.734612

5	6	0	-3.792916	-0.109965	-1.149805
6	6	0	-3.433140	-2.425270	0.034274
7	1	0	-3.064537	-2.820798	-0.916459
8	1	0	-2.770023	-2.792913	0.821832
9	1	0	-4.433957	-2.847411	0.204505
10	6	0	-3.422295	-0.488020	2.601207
11	1	0	-2.927885	-1.455833	2.715219
12	1	0	-2.895591	0.241905	3.221853
13	1	0	-4.443409	-0.588210	2.995328
14	6	0	-3.782434	2.518124	1.545560
15	1	0	-3.279389	2.387173	2.507631
16	1	0	-3.332644	3.383599	1.051589
17	1	0	-4.839190	2.746318	1.745267
18	6	0	-4.291278	2.418544	-1.583323
19	1	0	-5.333664	2.718655	-1.406337
20	1	0	-3.648224	3.273299	-1.355829
21	1	0	-4.185241	2.199170	-2.649215
22	6	0	-3.952221	-0.649193	-2.541018
23	1	0	-3.922946	0.148173	-3.287936
24	1	0	-3.159056	-1.363360	-2.785073
25	1	0	-4.913070	-1.171922	-2.644468
26	17	0	-0.907773	2.769971	-0.607488
27	44	0	-1.796685	0.519993	-0.183049
28	6	0	-0.167082	-0.363085	0.631483
29	6	0	0.037072	-1.017709	-0.672001
30	6	0	-0.048870	-2.422582	-0.909780
31	6	0	0.117288	-0.156670	-1.804911
32	6	0	-0.112009	-2.911764	-2.199493
33	1	0	-0.072299	-3.092450	-0.061556
34	6	0	0.028771	-0.680014	-3.110331
35	1	0	0.375610	0.886938	-1.679486
36	6	0	-0.098318	-2.043273	-3.312358
37	1	0	-0.168558	-3.985982	-2.358508
38	1	0	0.095270	0.000345	-3.955074
39	1	0	-0.150276	-2.449309	-4.319196
40	6	0	-0.268770	-1.144977	1.897069
41	8	0	-0.134543	-0.380211	3.008943
42	8	0	-0.543931	-2.334170	1.980396
43	6	0	-0.203420	-1.086338	4.254861
44	1	0	-1.186810	-1.540885	4.397199
45	1	0	0.556558	-1.872154	4.297761
46	1	0	-0.019326	-0.334656	5.023759
47	6	0	2.187502	0.694902	1.908151
48	6	0	1.396732	0.909528	0.849079
49	6	0	2.856258	0.400098	0.619423
50	1	0	2.360377	0.912861	2.953220
51	6	0	3.910129	1.411498	0.198985
52	6	0	3.557720	2.697435	-0.237168
53	6	0	5.274620	1.087311	0.287660
54	6	0	4.539105	3.626089	-0.589621
55	1	0	2.511500	2.977670	-0.313937
56	6	0	6.254666	2.017935	-0.053909
57	1	0	5.566375	0.095748	0.621644
58	6	0	5.890779	3.292187	-0.496974
59	1	0	4.242304	4.612434	-0.936451
60	1	0	7.304501	1.746899	0.024799
61	1	0	6.654293	4.017077	-0.766680
62	6	0	3.132579	-1.025049	0.195533
63	6	0	3.086578	-2.076765	1.118738
64	6	0	3.477337	-1.318827	-1.133436
65	6	0	3.357306	-3.390335	0.727771
66	1	0	2.841552	-1.861534	2.156027
67	6	0	3.750366	-2.627462	-1.526915
68	1	0	3.530995	-0.513210	-1.860023
69	6	0	3.690388	-3.670069	-0.597467
70	1	0	3.315680	-4.190704	1.462075
71	1	0	4.008863	-2.834759	-2.562134

72	1	0	3.906761	-4.690009	-0.904375
73	1	0	0.855603	1.776969	0.473707

Zero-point correction= 0.594020 (Hartree/Particle)
Thermal correction to Energy= 0.633112
Thermal correction to Enthalpy= 0.634057
Thermal correction to Gibbs Free Energy= 0.521872
Sum of electronic and zero-point Energies= -2020.515656
Sum of electronic and thermal Energies= -2020.476563
Sum of electronic and thermal Enthalpies= -2020.475619
Sum of electronic and thermal Free Energies= -2020.587803
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.466694

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.454829	1.212437	0.652245
2	6	0	-4.346897	0.334364	-0.051766
3	6	0	-4.501277	-0.883030	0.727481
4	6	0	-3.680164	-0.762206	1.908530
5	6	0	-3.013922	0.524574	1.840371
6	6	0	-3.119464	2.620850	0.257247
7	1	0	-2.183635	2.958624	0.709074
8	1	0	-3.014520	2.727710	-0.826151
9	1	0	-3.912864	3.307597	0.585202
10	6	0	-5.069168	0.663122	-1.325311
11	1	0	-4.467146	1.312196	-1.968588
12	1	0	-5.317206	-0.239815	-1.891786
13	1	0	-6.012079	1.187179	-1.113383
14	6	0	-5.409536	-2.030448	0.400430
15	1	0	-6.406406	-1.869131	0.835235
16	1	0	-5.533491	-2.148776	-0.680161
17	1	0	-5.016524	-2.971701	0.792941
18	6	0	-3.592070	-1.751826	3.032105
19	1	0	-3.690710	-2.776952	2.665591
20	1	0	-2.630190	-1.683494	3.548324
21	1	0	-4.384477	-1.574377	3.773070
22	6	0	-2.095693	1.081370	2.887162
23	1	0	-1.520919	0.289531	3.376510
24	1	0	-1.388518	1.798313	2.461164
25	1	0	-2.670972	1.603326	3.665382
26	17	0	-1.502099	-2.912954	0.062028
27	44	0	-2.457273	-0.713214	0.156484
28	6	0	0.367028	1.320056	-1.091760
29	6	0	0.507095	2.725737	-0.624412
30	6	0	0.329614	3.822809	-1.486788
31	6	0	0.818583	2.983424	0.724394
32	6	0	0.470833	5.127569	-1.013877
33	1	0	0.076269	3.646926	-2.524856
34	6	0	0.958692	4.289709	1.194180
35	1	0	0.939359	2.148459	1.408653
36	6	0	0.785874	5.368571	0.325076
37	1	0	0.335130	5.960655	-1.698674
38	1	0	1.197694	4.462095	2.240332
39	1	0	0.893052	6.387131	0.688336
40	6	0	-0.799991	0.985796	-1.945225
41	8	0	-1.158219	-0.350260	-1.852593
42	8	0	-1.391375	1.742607	-2.688488
43	6	0	-1.872314	-0.886483	-2.994394
44	1	0	-2.829915	-0.379921	-3.121502
45	1	0	-1.261247	-0.755383	-3.891677
46	1	0	-2.007807	-1.942088	-2.764358
47	6	0	2.601433	0.540807	-0.286138
48	6	0	1.304968	0.342420	-0.877163
49	6	0	3.571112	-0.408367	-0.098005

50	6	0	4.909223	0.027220	0.383312
51	6	0	5.477891	1.244608	-0.037134
52	6	0	5.635014	-0.762974	1.295216
53	6	0	6.715679	1.663200	0.447748
54	1	0	4.955394	1.851496	-0.770648
55	6	0	6.868779	-0.339570	1.785748
56	1	0	5.216156	-1.706616	1.630390
57	6	0	7.414980	0.875161	1.364688
58	1	0	7.139420	2.601702	0.100197
59	1	0	7.404464	-0.959925	2.499407
60	1	0	8.380693	1.201012	1.741608
61	6	0	3.373368	-1.858104	-0.352689
62	6	0	2.220866	-2.542584	0.072074
63	6	0	4.363078	-2.583807	-1.046974
64	6	0	2.052808	-3.900138	-0.204434
65	1	0	1.450574	-2.022219	0.631293
66	6	0	4.192086	-3.937093	-1.325738
67	1	0	5.261674	-2.073177	-1.380354
68	6	0	3.035512	-4.600494	-0.904596
69	1	0	1.144333	-4.393929	0.125067
70	1	0	4.961544	-4.474650	-1.873879
71	1	0	2.903808	-5.657575	-1.120053
72	1	0	1.075494	-0.649839	-1.249611
73	1	0	2.850883	1.558393	-0.002809

Zero-point correction= 0.599824 (Hartree/Particle)
Thermal correction to Energy= 0.639220
Thermal correction to Enthalpy= 0.640165
Thermal correction to Gibbs Free Energy= 0.523957
Sum of electronic and zero-point Energies= -2020.661929
Sum of electronic and thermal Energies= -2020.622533
Sum of electronic and thermal Enthalpies= -2020.621588
Sum of electronic and thermal Free Energies= -2020.737796
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.593816

INT7′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.963144	1.736565	-0.011282
2	6	0	-1.679254	2.336363	-0.272866
3	6	0	-1.326191	2.049449	-1.643527
4	6	0	-2.440974	1.332753	-2.243038
5	6	0	-3.419912	1.118079	-1.235500
6	6	0	-3.806496	1.912032	1.216763
7	1	0	-4.470076	1.055288	1.366998
8	1	0	-3.196794	2.018939	2.113926
9	1	0	-4.438736	2.805568	1.112136
10	6	0	-0.928907	3.248078	0.653074
11	1	0	-1.096193	2.986907	1.700017
12	1	0	0.147269	3.225490	0.458104
13	1	0	-1.263882	4.284987	0.508604
14	6	0	-0.136169	2.560459	-2.398956
15	1	0	0.667616	2.862764	-1.722606
16	1	0	0.260636	1.788362	-3.063873
17	1	0	-0.407217	3.435227	-3.007035
18	6	0	-2.551823	0.970952	-3.692049
19	1	0	-2.880050	1.848784	-4.266720
20	1	0	-1.593825	0.630189	-4.089119
21	1	0	-3.277088	0.170110	-3.856226
22	6	0	-4.731166	0.408161	-1.396811
23	1	0	-4.746901	-0.204459	-2.301439
24	1	0	-4.936788	-0.247842	-0.544746
25	1	0	-5.554920	1.132045	-1.465504
26	17	0	-0.366185	-1.137469	-2.411701
27	44	0	-1.456765	0.156518	-0.571413

28	6	0	-0.675583	-0.521236	1.434112
29	6	0	-1.849386	-1.416059	1.319976
30	6	0	-2.948628	-1.359338	2.226857
31	6	0	-1.952355	-2.315783	0.223591
32	6	0	-4.080043	-2.125091	2.020887
33	1	0	-2.897982	-0.698481	3.082426
34	6	0	-3.128256	-3.063606	0.018079
35	1	0	-1.109487	-2.522233	-0.421269
36	6	0	-4.191671	-2.970728	0.898615
37	1	0	-4.894964	-2.070738	2.738513
38	1	0	-3.170614	-3.737043	-0.833244
39	1	0	-5.090555	-3.561741	0.746536
40	6	0	-0.564545	0.326845	2.674157
41	8	0	0.639807	0.161895	3.259073
42	8	0	-1.427436	1.029070	3.172483
43	6	0	0.850905	0.900462	4.473451
44	1	0	0.756436	1.974535	4.292408
45	1	0	0.124213	0.602893	5.233932
46	1	0	1.864239	0.652389	4.789104
47	6	0	1.608819	0.193600	0.585640
48	6	0	0.436264	-0.662947	0.568312
49	6	0	2.852469	-0.147144	0.145173
50	1	0	1.476070	1.199181	0.974462
51	6	0	3.931868	0.872444	0.100868
52	6	0	3.659294	2.220843	-0.199402
53	6	0	5.267289	0.520753	0.377885
54	6	0	4.670650	3.179661	-0.199979
55	1	0	2.646665	2.509598	-0.464558
56	6	0	6.279023	1.479424	0.378490
57	1	0	5.506328	-0.513161	0.606441
58	6	0	5.986910	2.814864	0.092061
59	1	0	4.432886	4.211793	-0.445114
60	1	0	7.299631	1.181738	0.605246
61	1	0	6.777118	3.560835	0.086196
62	6	0	3.202694	-1.540755	-0.248897
63	6	0	2.952927	-2.619314	0.617000
64	6	0	3.818469	-1.805748	-1.484673
65	6	0	3.288860	-3.923916	0.251365
66	1	0	2.506947	-2.424262	1.588325
67	6	0	4.146341	-3.108738	-1.853082
68	1	0	4.021314	-0.982654	-2.163477
69	6	0	3.882667	-4.173366	-0.986586
70	1	0	3.090498	-4.743572	0.937241
71	1	0	4.605040	-3.295092	-2.820546
72	1	0	4.141975	-5.188839	-1.274187
73	1	0	0.559337	-1.593115	0.029453

Zero-point correction= 0.599903 (Hartree/Particle)
Thermal correction to Energy= 0.638950
Thermal correction to Enthalpy= 0.639894
Thermal correction to Gibbs Free Energy= 0.526816
Sum of electronic and zero-point Energies= -2020.660919
Sum of electronic and thermal Energies= -2020.621873
Sum of electronic and thermal Enthalpies= -2020.620929
Sum of electronic and thermal Free Energies= -2020.734007
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.606463

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.636627	1.516307	-0.522776
2	6	0	3.000100	0.551282	-1.520612
3	6	0	2.080089	0.704472	-2.635445
4	6	0	1.153615	1.722772	-2.295484
5	6	0	1.473067	2.222372	-0.979265

6	6	0	3.438008	1.818381	0.710335
7	1	0	2.824297	2.234698	1.512418
8	1	0	3.928369	0.921651	1.098529
9	1	0	4.222107	2.551603	0.475349
10	6	0	4.220586	-0.322826	-1.518247
11	1	0	4.522838	-0.586182	-0.501158
12	1	0	4.030285	-1.257091	-2.051294
13	1	0	5.062807	0.190947	-2.003889
14	6	0	2.186894	-0.008307	-3.951026
15	1	0	2.380409	-1.074254	-3.805047
16	1	0	1.265471	0.086438	-4.533031
17	1	0	3.005846	0.413704	-4.550539
18	6	0	0.124665	2.301700	-3.223447
19	1	0	-0.621223	2.886237	-2.683093
20	1	0	0.610129	2.970704	-3.947854
21	1	0	-0.395934	1.526561	-3.793498
22	6	0	0.890475	3.462480	-0.362311
23	1	0	-0.201210	3.480856	-0.417435
24	1	0	1.178673	3.564274	0.686954
25	1	0	1.260425	4.356337	-0.885299
26	17	0	1.427228	-2.457876	-1.621792
27	44	0	1.031765	-0.135443	-0.761636
28	6	0	1.054794	-0.821799	1.113783
29	6	0	1.022148	-0.045800	2.373329
30	6	0	1.518007	-0.573727	3.588831
31	6	0	0.502607	1.263089	2.399570
32	6	0	1.503671	0.180348	4.759226
33	1	0	1.946178	-1.568569	3.613924
34	6	0	0.475389	2.011951	3.572295
35	1	0	0.101266	1.674300	1.484569
36	6	0	0.980498	1.475351	4.759512
37	1	0	1.900924	-0.247546	5.675498
38	1	0	0.054468	3.013851	3.558863
39	1	0	0.963215	2.058619	5.676267
40	6	0	1.571962	-2.226368	1.320081
41	8	0	0.650263	-3.196333	1.417562
42	8	0	2.766154	-2.400281	1.468381
43	6	0	1.173233	-4.539580	1.437307
44	1	0	1.699944	-4.734373	0.500688
45	1	0	1.851579	-4.674172	2.283128
46	1	0	0.301303	-5.186493	1.534453
47	6	0	-0.952998	-0.689305	-1.237541
48	6	0	-0.839741	-1.005593	0.149651
49	6	0	-2.054585	-0.198089	-0.303207
50	6	0	-2.325380	1.251265	0.000197
51	6	0	-2.472815	1.704319	1.318331
52	6	0	-2.629357	2.133924	-1.044919
53	6	0	-2.866334	3.018285	1.584597
54	1	0	-2.287535	1.017210	2.138134
55	6	0	-3.030565	3.446290	-0.784934
56	1	0	-2.568375	1.774451	-2.067485
57	6	0	-3.142889	3.895455	0.533535
58	1	0	-2.970295	3.351183	2.614246
59	1	0	-3.264753	4.114049	-1.610244
60	1	0	-3.456200	4.915482	0.739520
61	6	0	-3.322927	-1.047751	-0.353951
62	6	0	-4.589293	-0.507909	-0.067223
63	6	0	-3.261387	-2.413726	-0.695106
64	6	0	-5.739805	-1.295477	-0.116059
65	1	0	-4.683629	0.538667	0.196588
66	6	0	-4.412798	-3.199735	-0.743529
67	1	0	-2.309704	-2.877306	-0.931231
68	6	0	-5.660135	-2.646581	-0.453924
69	1	0	-6.702791	-0.845406	0.111622
70	1	0	-4.329238	-4.249682	-1.011972
71	1	0	-6.557008	-3.258983	-0.492525
72	1	0	-1.093614	-1.387587	-2.055537

73	1	0	-0.893432	-2.002697	0.565840

Zero-point correction= 0.597329 (Hartree/Particle)
Thermal correction to Energy= 0.635428
Thermal correction to Enthalpy= 0.636372
Thermal correction to Gibbs Free Energy= 0.527719
Sum of electronic and zero-point Energies= -2020.542536
Sum of electronic and thermal Energies= -2020.504437
Sum of electronic and thermal Enthalpies= -2020.503493
Sum of electronic and thermal Free Energies= -2020.612146
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.501971

TS4′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.171653	0.419470	-1.099388
2	6	0	2.817002	-0.816649	-1.747183
3	6	0	1.901198	-0.496567	-2.831298
4	6	0	1.650043	0.896015	-2.786379
5	6	0	2.417059	1.475392	-1.702722
6	6	0	4.247098	0.561550	-0.061373
7	1	0	4.114347	1.453768	0.555502
8	1	0	4.275477	-0.304767	0.605060
9	1	0	5.228039	0.637755	-0.550452
10	6	0	3.454216	-2.156553	-1.522117
11	1	0	3.774322	-2.277692	-0.484092
12	1	0	2.743866	-2.958861	-1.734436
13	1	0	4.331601	-2.284181	-2.172621
14	6	0	1.402077	-1.479032	-3.848206
15	1	0	1.003010	-2.371894	-3.358276
16	1	0	0.606830	-1.051610	-4.465674
17	1	0	2.218159	-1.784587	-4.517383
18	6	0	0.833956	1.689846	-3.764666
19	1	0	0.340107	2.544193	-3.288566
20	1	0	1.477021	2.096715	-4.557389
21	1	0	0.064114	1.079866	-4.244569
22	6	0	2.591031	2.953245	-1.485367
23	1	0	1.632066	3.484044	-1.459333
24	1	0	3.120065	3.168523	-0.553498
25	1	0	3.178722	3.397821	-2.301065
26	17	0	0.030737	-2.433209	-0.853445
27	44	0	0.946032	-0.134387	-0.746290
28	6	0	1.148003	-0.309806	1.218390
29	6	0	1.659383	0.676668	2.184690
30	6	0	2.050570	0.296893	3.492165
31	6	0	1.764225	2.046887	1.850813
32	6	0	2.525405	1.233920	4.404798
33	1	0	2.006657	-0.745474	3.785748
34	6	0	2.229397	2.984895	2.766114
35	1	0	1.471575	2.361159	0.857298
36	6	0	2.613231	2.581762	4.048716
37	1	0	2.826125	0.911780	5.397690
38	1	0	2.291007	4.032086	2.482678
39	1	0	2.975553	3.313585	4.765575
40	6	0	1.055969	-1.689940	1.798215
41	8	0	-0.120757	-2.019013	2.327706
42	8	0	2.059848	-2.380599	1.828005
43	6	0	-0.256756	-3.403561	2.707330
44	1	0	-0.106194	-4.032803	1.828070
45	1	0	0.467330	-3.661897	3.484521
46	1	0	-1.276758	-3.500731	3.075729
47	6	0	-0.996444	0.803250	-1.061053
48	6	0	-0.816158	0.941103	0.310061
49	6	0	-2.172713	0.443706	-0.173511
50	1	0	-0.994530	1.530059	-1.866050

51	1	0	-0.590389	1.756525	0.983777
52	6	0	-3.230138	1.548053	-0.133179
53	6	0	-4.596297	1.256269	0.032356
54	6	0	-2.873190	2.904055	-0.273225
55	6	0	-5.555335	2.268528	0.056170
56	1	0	-4.914077	0.226678	0.140847
57	6	0	-3.832387	3.917153	-0.245817
58	1	0	-1.833187	3.182282	-0.406796
59	6	0	-5.181611	3.606157	-0.080872
60	1	0	-6.602455	2.005515	0.183151
61	1	0	-3.519416	4.952660	-0.355043
62	1	0	-5.930512	4.393372	-0.060471
63	6	0	-2.744464	-0.933574	0.037946
64	6	0	-3.016029	-1.394372	1.330475
65	6	0	-3.182367	-1.690542	-1.054231
66	6	0	-3.698389	-2.596646	1.528625
67	1	0	-2.690482	-0.806125	2.183489
68	6	0	-3.861506	-2.892968	-0.861402
69	1	0	-2.974237	-1.337293	-2.060041
70	6	0	-4.122374	-3.350546	0.432315
71	1	0	-3.908484	-2.939040	2.539482
72	1	0	-4.183521	-3.475104	-1.720982
73	1	0	-4.654575	-4.286193	0.584608

Zero-point correction= 0.595830 (Hartree/Particle)
Thermal correction to Energy= 0.634260
Thermal correction to Enthalpy= 0.635204
Thermal correction to Gibbs Free Energy= 0.525332
Sum of electronic and zero-point Energies= -2020.531579
Sum of electronic and thermal Energies= -2020.493150
Sum of electronic and thermal Enthalpies= -2020.492205
Sum of electronic and thermal Free Energies= -2020.602078
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.488559

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.967485	-1.043746	-0.461928
2	6	0	-3.490491	0.265201	-0.526866
3	6	0	-3.008315	0.875170	-1.758675
4	6	0	-2.190163	-0.086810	-2.432243
5	6	0	-2.125463	-1.271662	-1.622580
6	6	0	-3.292882	-2.045640	0.605862
7	1	0	-2.614820	-2.901110	0.586968
8	1	0	-3.232216	-1.591244	1.598056
9	1	0	-4.315135	-2.422324	0.462372
10	6	0	-4.433877	0.905799	0.448065
11	1	0	-4.308769	0.487450	1.449937
12	1	0	-4.252119	1.982113	0.514427
13	1	0	-5.479135	0.754995	0.141390
14	6	0	-3.481337	2.183950	-2.318430
15	1	0	-3.579210	2.939680	-1.536929
16	1	0	-2.789418	2.575862	-3.069110
17	1	0	-4.460395	2.049029	-2.800456
18	6	0	-1.610283	0.053660	-3.811144
19	1	0	-0.687877	-0.523406	-3.920852
20	1	0	-2.323737	-0.317712	-4.560986
21	1	0	-1.388233	1.095782	-4.055141
22	6	0	-1.658664	-2.606440	-2.136729
23	1	0	-0.659725	-2.557142	-2.582538
24	1	0	-1.638477	-3.364901	-1.351708
25	1	0	-2.344481	-2.967361	-2.917085
26	17	0	-1.429063	2.993779	0.198424
27	44	0	-1.138632	0.623137	-0.560159
28	6	0	-0.171281	-0.150746	1.317210

29	6	0	0.040652	-1.614678	1.608619
30	6	0	0.151914	-2.015268	2.955383
31	6	0	0.164115	-2.606459	0.629177
32	6	0	0.366719	-3.348339	3.300586
33	1	0	0.070269	-1.280264	3.749474
34	6	0	0.370040	-3.943540	0.969967
35	1	0	0.100146	-2.322459	-0.408861
36	6	0	0.469316	-4.324372	2.308089
37	1	0	0.446843	-3.622079	4.349210
38	1	0	0.460247	-4.685202	0.180778
39	1	0	0.625349	-5.366228	2.574960
40	6	0	-0.969242	0.517014	2.435516
41	8	0	-0.340809	1.569634	2.991229
42	8	0	-2.047825	0.111063	2.824991
43	6	0	-1.130981	2.362382	3.895148
44	1	0	-1.931473	2.854107	3.337727
45	1	0	-1.552397	1.737198	4.685563
46	1	0	-0.443630	3.100996	4.308183
47	6	0	0.710833	1.171922	-0.980440
48	6	0	0.792086	0.746591	0.685409
49	6	0	1.924684	0.536661	-0.394313
50	6	0	2.335404	-0.859224	-0.794423
51	6	0	3.067355	-1.674808	0.080100
52	6	0	2.112415	-1.304548	-2.103235
53	6	0	3.551839	-2.912598	-0.339572
54	1	0	3.256848	-1.335516	1.094550
55	6	0	2.590412	-2.548128	-2.524674
56	1	0	1.569569	-0.664677	-2.792669
57	6	0	3.311526	-3.355561	-1.643001
58	1	0	4.111288	-3.534630	0.353635
59	1	0	2.412389	-2.877518	-3.545139
60	1	0	3.690669	-4.319832	-1.970855
61	6	0	3.116112	1.491947	-0.210087
62	6	0	4.419024	1.113266	-0.572824
63	6	0	2.930445	2.805488	0.263390
64	6	0	5.491976	1.998359	-0.450587
65	1	0	4.606221	0.120144	-0.961725
66	6	0	4.003164	3.687358	0.389097
67	1	0	1.943029	3.169195	0.529821
68	6	0	5.293048	3.288752	0.036740
69	1	0	6.486409	1.670793	-0.742447
70	1	0	3.823057	4.691921	0.762264
71	1	0	6.128462	3.976529	0.135446
72	1	0	0.829050	2.247314	-1.132442
73	1	0	0.848676	1.696906	1.198563

Zero-point correction= 0.599068 (Hartree/Particle)
Thermal correction to Energy= 0.637561
Thermal correction to Enthalpy= 0.638505
Thermal correction to Gibbs Free Energy= 0.528942
Sum of electronic and zero-point Energies= -2020.563692
Sum of electronic and thermal Energies= -2020.525198
Sum of electronic and thermal Enthalpies= -2020.524254
Sum of electronic and thermal Free Energies= -2020.633817
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.970889	1.042333	-0.528332
2	6	0	3.510728	-0.259567	-0.467823
3	6	0	3.068042	-0.980149	-1.655977
4	6	0	2.247120	-0.102116	-2.423561
5	6	0	2.140275	1.149653	-1.713853
6	6	0	3.256260	2.141345	0.451326

7	1	0	2.559316	2.975097	0.345154
8	1	0	3.186920	1.777064	1.479387
9	1	0	4.272068	2.527905	0.289693
10	6	0	4.436805	-0.801835	0.580614
11	1	0	4.286178	-0.296202	1.538017
12	1	0	4.261262	-1.869859	0.738492
13	1	0	5.488308	-0.670456	0.286737
14	6	0	3.571433	-2.324814	-2.086043
15	1	0	3.641849	-3.013995	-1.242527
16	1	0	2.916360	-2.782563	-2.832211
17	1	0	4.569559	-2.216918	-2.534610
18	6	0	1.697567	-0.369205	-3.796242
19	1	0	0.764404	0.174713	-3.968242
20	1	0	2.415523	-0.044819	-4.563270
21	1	0	1.501970	-1.432862	-3.955848
22	6	0	1.653871	2.424521	-2.347816
23	1	0	0.668173	2.310138	-2.811282
24	1	0	1.593262	3.243819	-1.628921
25	1	0	2.350090	2.738782	-3.139102
26	17	0	1.436863	-2.937924	0.377130
27	44	0	1.142221	-0.607502	-0.525452
28	6	0	0.100701	0.305031	1.338561
29	6	0	-0.120174	1.789316	1.463460
30	6	0	-0.251839	2.331011	2.757256
31	6	0	-0.236363	2.667662	0.380419
32	6	0	-0.485003	3.691290	2.952928
33	1	0	-0.170245	1.686088	3.626307
34	6	0	-0.464712	4.030536	0.571243
35	1	0	-0.152547	2.272469	-0.619712
36	6	0	-0.587283	4.552315	1.859198
37	1	0	-0.580602	4.076570	3.964603
38	1	0	-0.552018	4.681658	-0.294513
39	1	0	-0.759439	5.614742	2.009715
40	6	0	0.946766	-0.238950	2.484155
41	8	0	0.400439	-1.310467	3.088955
42	8	0	1.990608	0.265708	2.854601
43	6	0	1.244946	-1.998582	4.027375
44	1	0	2.076192	-2.463984	3.492684
45	1	0	1.624019	-1.305902	4.782159
46	1	0	0.611370	-2.760708	4.481562
47	6	0	-0.663417	-1.169324	-0.982705
48	6	0	-0.799889	-0.662003	0.782249
49	6	0	-1.888195	-0.589606	-0.333711
50	6	0	-2.407066	0.759363	-0.780351
51	6	0	-3.152437	1.566049	0.090490
52	6	0	-2.263711	1.160340	-2.114060
53	6	0	-3.726925	2.754273	-0.357679
54	1	0	-3.279736	1.260560	1.125291
55	6	0	-2.832469	2.354384	-2.564643
56	1	0	-1.707064	0.528596	-2.800679
57	6	0	-3.565568	3.154731	-1.686796
58	1	0	-4.294626	3.371559	0.333043
59	1	0	-2.712931	2.650898	-3.603517
60	1	0	-4.013738	4.080967	-2.036397
61	6	0	-3.013953	-1.622904	-0.124448
62	6	0	-4.348905	-1.336327	-0.450039
63	6	0	-2.720144	-2.919220	0.342022
64	6	0	-5.352159	-2.296058	-0.299307
65	1	0	-4.616979	-0.358300	-0.829977
66	6	0	-3.723382	-3.875765	0.494265
67	1	0	-1.700812	-3.208474	0.581253
68	6	0	-5.047579	-3.569423	0.178344
69	1	0	-6.375600	-2.040274	-0.561171
70	1	0	-3.462132	-4.865207	0.859802
71	1	0	-5.828948	-4.314971	0.298398
72	1	0	-0.768119	-2.237327	-1.202264
73	1	0	-0.789427	-1.605747	1.309060

Zero-point correction=	0.598211 (Hartree/Particle)
Thermal correction to Energy=	0.636301
Thermal correction to Enthalpy=	0.637245
Thermal correction to Gibbs Free Energy=	0.528505
Sum of electronic and zero-point Energies=	-2020.564138
Sum of electronic and thermal Energies=	-2020.526049
Sum of electronic and thermal Enthalpies=	-2020.525105
Sum of electronic and thermal Free Energies=	-2020.633845

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.521764

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.625039	-1.213719	0.908025
2	6	0	-3.648060	-0.248801	0.556431
3	6	0	-4.290092	-0.691837	-0.676542
4	6	0	-3.563910	-1.785264	-1.163535
5	6	0	-2.496395	-2.108105	-0.209029
6	6	0	-1.974162	-1.336228	2.253862
7	1	0	-1.074071	-1.954756	2.212149
8	1	0	-1.699167	-0.361428	2.665432
9	1	0	-2.669619	-1.811644	2.960469
10	6	0	-4.160703	0.847868	1.439338
11	1	0	-3.368116	1.255811	2.071110
12	1	0	-4.575351	1.667969	0.846864
13	1	0	-4.958197	0.467622	2.094764
14	6	0	-5.432464	0.022296	-1.335409
15	1	0	-5.140915	1.037217	-1.630659
16	1	0	-5.768649	-0.501226	-2.234144
17	1	0	-6.287993	0.097319	-0.652649
18	6	0	-3.781547	-2.525268	-2.449103
19	1	0	-2.834396	-2.690770	-2.973745
20	1	0	-4.224886	-3.512091	-2.258186
21	1	0	-4.445034	-1.980466	-3.124649
22	6	0	-1.631126	-3.333679	-0.283270
23	1	0	-1.316212	-3.538204	-1.311576
24	1	0	-0.729028	-3.227351	0.325374
25	1	0	-2.177048	-4.218931	0.074154
26	17	0	-2.478925	1.874719	-2.154933
27	44	0	-1.969998	-0.064136	-0.823228
28	6	0	2.401608	-1.327126	0.580031
29	6	0	3.359037	-1.147906	-0.550926
30	6	0	4.734454	-1.008088	-0.303577
31	6	0	2.918380	-1.187801	-1.881063
32	6	0	5.634571	-0.869830	-1.357641
33	1	0	5.095308	-1.007595	0.719415
34	6	0	3.820751	-1.054448	-2.937755
35	1	0	1.866096	-1.349788	-2.092819
36	6	0	5.180911	-0.888624	-2.678927
37	1	0	6.694194	-0.752194	-1.146928
38	1	0	3.457691	-1.085235	-3.961462
39	1	0	5.884838	-0.783073	-3.500056
40	6	0	2.625363	-2.580954	1.381959
41	8	0	1.546895	-2.947452	2.127424
42	8	0	3.655479	-3.222968	1.380448
43	6	0	1.745723	-4.110902	2.946534
44	1	0	1.992574	-4.977795	2.328361
45	1	0	2.555778	-3.944620	3.661701
46	1	0	0.800131	-4.265728	3.467206
47	6	0	-0.157308	0.292112	-0.533247
48	6	0	1.405056	-0.502679	0.981371
49	6	0	0.867359	0.828886	0.454887
50	6	0	1.881858	1.754591	-0.248082
51	6	0	3.137002	2.002828	0.321731

52	6	0	1.514230	2.457979	-1.403038
53	6	0	4.015816	2.913062	-0.262682
54	1	0	3.429761	1.481321	1.228292
55	6	0	2.395660	3.369910	-1.988526
56	1	0	0.529330	2.315076	-1.841974
57	6	0	3.649999	3.598357	-1.423667
58	1	0	4.988636	3.086441	0.189984
59	1	0	2.092535	3.905262	-2.884352
60	1	0	4.335368	4.308581	-1.878512
61	6	0	0.250455	1.647081	1.611131
62	6	0	0.735609	1.538881	2.921518
63	6	0	-0.746851	2.596970	1.345129
64	6	0	0.224015	2.339711	3.946565
65	1	0	1.526132	0.829949	3.152746
66	6	0	-1.254638	3.399773	2.367363
67	1	0	-1.129634	2.708787	0.335746
68	6	0	-0.776180	3.272249	3.674177
69	1	0	0.614730	2.234157	4.955421
70	1	0	-2.025705	4.130616	2.137489
71	1	0	-1.173487	3.898818	4.468299
72	1	0	0.368857	-0.047781	-1.445181
73	1	0	0.811885	-0.866933	1.810622

Zero-point correction= 0.597698 (Hartree/Particle)
Thermal correction to Energy= 0.637003
Thermal correction to Enthalpy= 0.637948
Thermal correction to Gibbs Free Energy= 0.522950
Sum of electronic and zero-point Energies= -2020.599656
Sum of electronic and thermal Energies= -2020.560351
Sum of electronic and thermal Enthalpies= -2020.559406
Sum of electronic and thermal Free Energies= -2020.674404
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.546827

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.908462	-0.680535	1.189681
2	6	0	-3.814461	-0.005486	0.271378
3	6	0	-4.041053	-0.855551	-0.860149
4	6	0	-3.207680	-2.016214	-0.696708
5	6	0	-2.541281	-1.933554	0.591670
6	6	0	-2.560015	-0.202781	2.569087
7	1	0	-1.644706	-0.673906	2.939081
8	1	0	-2.411585	0.881091	2.595600
9	1	0	-3.365847	-0.444495	3.277540
10	6	0	-4.465236	1.321224	0.524432
11	1	0	-3.794905	1.997427	1.063126
12	1	0	-4.751300	1.808120	-0.411518
13	1	0	-5.373954	1.195219	1.130536
14	6	0	-4.931990	-0.555933	-2.028988
15	1	0	-4.923439	0.510200	-2.271901
16	1	0	-4.603796	-1.087712	-2.925958
17	1	0	-5.969249	-0.852676	-1.820460
18	6	0	-3.121203	-3.173901	-1.645716
19	1	0	-2.152481	-3.677339	-1.575597
20	1	0	-3.899221	-3.917240	-1.419966
21	1	0	-3.256460	-2.851831	-2.681695
22	6	0	-1.701305	-3.010938	1.211655
23	1	0	-1.148604	-3.575697	0.453964
24	1	0	-0.971267	-2.601712	1.915156
25	1	0	-2.329466	-3.727628	1.760447
26	17	0	-1.750807	0.960380	-2.790879
27	44	0	-1.867826	-0.286961	-0.684625
28	6	0	1.912442	-1.140674	0.972077
29	6	0	2.840306	-1.598808	-0.087573

30	6	0	4.233802	-1.497037	0.083219
31	6	0	2.351044	-2.199080	-1.261566
32	6	0	5.103265	-1.938944	-0.909641
33	1	0	4.629031	-1.059850	0.992784
34	6	0	3.226192	-2.655193	-2.248042
35	1	0	1.283098	-2.347891	-1.384293
36	6	0	4.603816	-2.517616	-2.079883
37	1	0	6.175573	-1.835601	-0.767893
38	1	0	2.827302	-3.122001	-3.144464
39	1	0	5.285974	-2.866666	-2.850369
40	6	0	2.112571	-1.763865	2.314317
41	8	0	1.119898	-1.471421	3.200607
42	8	0	3.069161	-2.450116	2.620881
43	6	0	1.302571	-2.019883	4.515605
44	1	0	1.362778	-3.110413	4.472356
45	1	0	2.219011	-1.633164	4.969256
46	1	0	0.428681	-1.704528	5.086479
47	6	0	0.148535	0.139178	-0.620849
48	6	0	0.890385	-0.216746	0.828209
49	6	0	0.932309	1.200291	-0.043597
50	6	0	2.219205	1.642716	-0.698210
51	6	0	3.326333	2.064631	0.052895
52	6	0	2.283997	1.708448	-2.097629
53	6	0	4.482409	2.515805	-0.580721
54	1	0	3.286607	2.035666	1.137709
55	6	0	3.437780	2.174062	-2.730553
56	1	0	1.418032	1.419475	-2.687470
57	6	0	4.541525	2.572332	-1.975855
58	1	0	5.336467	2.827812	0.014656
59	1	0	3.469319	2.227232	-3.815380
60	1	0	5.440908	2.930994	-2.469328
61	6	0	0.260676	2.282535	0.783099
62	6	0	0.623266	2.563884	2.107710
63	6	0	-0.709477	3.079906	0.157288
64	6	0	0.023779	3.617934	2.798816
65	1	0	1.361392	1.945020	2.610986
66	6	0	-1.299118	4.140864	0.848178
67	1	0	-0.997902	2.861651	-0.866646
68	6	0	-0.937541	4.412087	2.169433
69	1	0	0.309172	3.818004	3.828266
70	1	0	-2.045613	4.753275	0.349336
71	1	0	-1.400978	5.235835	2.705863
72	1	0	0.683546	-0.341646	-1.438183
73	1	0	0.255156	-0.061867	1.686110

Zero-point correction= 0.596853 (Hartree/Particle)
Thermal correction to Energy= 0.636062
Thermal correction to Enthalpy= 0.637006
Thermal correction to Gibbs Free Energy= 0.521623
Sum of electronic and zero-point Energies= -2020.581613
Sum of electronic and thermal Energies= -2020.542403
Sum of electronic and thermal Enthalpies= -2020.541459
Sum of electronic and thermal Free Energies= -2020.656842
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.532993

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.831582	2.659809	0.731292
2	6	0	1.972495	2.538066	-0.134018
3	6	0	1.576106	2.915422	-1.478046
4	6	0	0.176654	3.261607	-1.442906
5	6	0	-0.285331	3.076057	-0.079900
6	6	0	0.824401	2.487101	2.222397
7	1	0	-0.161742	2.186492	2.587226

8	1	0	1.543045	1.730146	2.548314
9	1	0	1.087204	3.431024	2.721350
10	6	0	3.377448	2.223658	0.283803
11	1	0	3.405343	1.686659	1.233810
12	1	0	3.895992	1.617583	-0.466015
13	1	0	3.951016	3.153347	0.408494
14	6	0	2.480125	3.010702	-2.670232
15	1	0	3.314103	2.306613	-2.596003
16	1	0	1.940274	2.786514	-3.593464
17	1	0	2.902077	4.022395	-2.755168
18	6	0	-0.633782	3.783803	-2.590988
19	1	0	-1.694854	3.548279	-2.470647
20	1	0	-0.537599	4.876313	-2.664431
21	1	0	-0.307665	3.344624	-3.536753
22	6	0	-1.666458	3.388964	0.412179
23	1	0	-2.418410	3.201744	-0.359932
24	1	0	-1.926954	2.788119	1.285844
25	1	0	-1.738194	4.449229	0.694632
26	17	0	-0.061895	0.243310	-3.083132
27	44	0	0.420148	1.203211	-0.909155
28	6	0	-2.471949	-0.571983	0.741265
29	6	0	-3.229614	-1.400999	-0.236325
30	6	0	-4.181883	-2.331545	0.219518
31	6	0	-3.007113	-1.294285	-1.617808
32	6	0	-4.872048	-3.142332	-0.678553
33	1	0	-4.381346	-2.417586	1.282252
34	6	0	-3.703475	-2.105475	-2.515729
35	1	0	-2.290814	-0.575140	-2.000950
36	6	0	-4.635562	-3.033541	-2.051438
37	1	0	-5.598946	-3.858923	-0.304789
38	1	0	-3.512611	-2.003118	-3.580616
39	1	0	-5.177237	-3.664623	-2.751334
40	6	0	-3.296310	0.139286	1.760409
41	8	0	-2.556246	0.815764	2.692143
42	8	0	-4.511670	0.132993	1.803570
43	6	0	-3.327892	1.471682	3.708354
44	1	0	-3.992337	2.220875	3.269493
45	1	0	-3.932773	0.747036	4.260128
46	1	0	-2.599621	1.944480	4.368861
47	6	0	-0.133008	-1.229581	0.041083
48	6	0	-1.104968	-0.493880	0.831763
49	6	0	1.133555	-1.587852	0.471422
50	6	0	1.981675	-2.475878	-0.370806
51	6	0	2.801651	-3.450438	0.235389
52	6	0	1.948615	-2.420110	-1.778078
53	6	0	3.553763	-4.335846	-0.534324
54	1	0	2.831523	-3.531553	1.316685
55	6	0	2.710136	-3.301292	-2.542500
56	1	0	1.343752	-1.669833	-2.276843
57	6	0	3.515299	-4.263386	-1.927811
58	1	0	4.167493	-5.085597	-0.042013
59	1	0	2.675013	-3.229034	-3.626158
60	1	0	4.106794	-4.949166	-2.528604
61	6	0	1.641475	-1.290249	1.841744
62	6	0	0.843530	-1.492092	2.982508
63	6	0	2.975533	-0.881071	2.033083
64	6	0	1.348349	-1.256151	4.262600
65	1	0	-0.169346	-1.863161	2.868388
66	6	0	3.476629	-0.635762	3.309916
67	1	0	3.618196	-0.757846	1.167425
68	6	0	2.662108	-0.818273	4.431771
69	1	0	0.713807	-1.426505	5.128059
70	1	0	4.506762	-0.311121	3.430768
71	1	0	3.054571	-0.634966	5.428268
72	1	0	-0.483151	-1.681469	-0.879739
73	1	0	-0.714729	0.085775	1.657640

Zero-point correction= 0.599985 (Hartree/Particle)
Thermal correction to Energy= 0.639477
Thermal correction to Enthalpy= 0.640421
Thermal correction to Gibbs Free Energy= 0.524946
Sum of electronic and zero-point Energies= -2020.654125
Sum of electronic and thermal Energies= -2020.614634
Sum of electronic and thermal Enthalpies= -2020.613689
Sum of electronic and thermal Free Energies= -2020.729165
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.59743

E-P

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.175313	0.447678	-0.112141
2	6	0	2.793685	-0.873215	0.171650
3	6	0	3.830117	-1.385360	-0.629568
4	6	0	2.351790	-1.645839	1.259976
5	6	0	4.384634	-2.634975	-0.362374
6	1	0	4.200276	-0.797235	-1.461289
7	6	0	2.911004	-2.895004	1.529297
8	1	0	1.576146	-1.251454	1.910059
9	6	0	3.927927	-3.396084	0.716364
10	1	0	5.180071	-3.014956	-0.998186
11	1	0	2.556025	-3.471172	2.379802
12	1	0	4.366679	-4.368307	0.924916
13	6	0	3.108535	1.589158	-0.340278
14	8	0	2.466747	2.773117	-0.523477
15	8	0	4.322485	1.502573	-0.366062
16	6	0	3.323362	3.900758	-0.743293
17	1	0	3.990381	4.052997	0.109836
18	1	0	3.929756	3.756857	-1.641899
19	1	0	2.655638	4.754705	-0.864909
20	6	0	-0.196386	-0.348465	-0.121669
21	6	0	0.828266	0.664233	-0.169072
22	6	0	-1.544294	-0.126902	-0.070442
23	6	0	-2.482882	-1.268285	-0.219966
24	6	0	-2.184503	-2.350877	-1.069345
25	6	0	-3.692242	-1.307477	0.499867
26	6	0	-3.050699	-3.436350	-1.179616
27	1	0	-1.277622	-2.325144	-1.666123
28	6	0	-4.556014	-2.395482	0.391999
29	1	0	-3.944705	-0.483994	1.160664
30	6	0	-4.239424	-3.465612	-0.447219
31	1	0	-2.801941	-4.256017	-1.848515
32	1	0	-5.478014	-2.408143	0.967326
33	1	0	-4.916253	-4.311112	-0.535775
34	6	0	-2.125850	1.224756	0.148507
35	6	0	-1.661203	2.064189	1.176270
36	6	0	-3.171255	1.691680	-0.670186
37	6	0	-2.209831	3.332400	1.368366
38	1	0	-0.878163	1.707584	1.838650
39	6	0	-3.712007	2.961732	-0.484046
40	1	0	-3.549046	1.053710	-1.463839
41	6	0	-3.233599	3.787467	0.536709
42	1	0	-1.839940	3.961542	2.173592
43	1	0	-4.509434	3.307916	-1.136287
44	1	0	-3.660946	4.775413	0.685791
45	1	0	0.500466	1.686481	-0.322371
46	1	0	0.140089	-1.379941	-0.173888

Zero-point correction= 0.373635 (Hartree/Particle)
Thermal correction to Energy= 0.396044
Thermal correction to Enthalpy= 0.396988
Thermal correction to Gibbs Free Energy= 0.318923
Sum of electronic and zero-point Energies= -1076.666807

Sum of electronic and thermal Energies= -1076.644399
Sum of electronic and thermal Enthalpies= -1076.643455
Sum of electronic and thermal Free Energies= -1076.721519
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1076.530716

INT10′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.263480	0.221524	-0.407103
2	6	0	-3.940487	1.548415	-0.678877
3	6	0	-2.841580	1.554093	-1.658024
4	6	0	-2.636364	0.191858	-2.101109
5	6	0	-3.414628	-0.648916	-1.232517
6	6	0	-5.269494	-0.295254	0.578946
7	1	0	-4.825818	-1.046002	1.242481
8	1	0	-5.670622	0.504132	1.206560
9	1	0	-6.112314	-0.775310	0.063189
10	6	0	-4.499775	2.787555	-0.048066
11	1	0	-3.720513	3.324637	0.505493
12	1	0	-4.900483	3.465809	-0.812356
13	1	0	-5.308123	2.556624	0.650779
14	6	0	-2.296555	2.794933	-2.302503
15	1	0	-2.120875	3.575878	-1.557754
16	1	0	-1.347765	2.598946	-2.809239
17	1	0	-3.003256	3.187316	-3.048421
18	6	0	-1.853701	-0.233146	-3.308236
19	1	0	-1.472656	-1.254208	-3.208292
20	1	0	-2.487826	-0.202306	-4.204728
21	1	0	-0.998333	0.425073	-3.488154
22	6	0	-3.619694	-2.131518	-1.370748
23	1	0	-2.751202	-2.619149	-1.823355
24	1	0	-3.798795	-2.606298	-0.400473
25	1	0	-4.490179	-2.351677	-2.005595
26	17	0	-1.239180	2.251073	1.368115
27	44	0	-1.832252	0.438038	-0.103075
28	6	0	2.815567	0.607630	-0.041447
29	6	0	3.451346	1.935499	0.196202
30	6	0	4.848238	2.103472	0.169878
31	6	0	2.642742	3.060584	0.452163
32	6	0	5.415772	3.353939	0.412309
33	1	0	5.483345	1.246807	-0.023990
34	6	0	3.218133	4.306432	0.695537
35	1	0	1.560764	2.962362	0.446254
36	6	0	4.606193	4.459970	0.677722
37	1	0	6.497395	3.461167	0.397213
38	1	0	2.575547	5.161258	0.889031
39	1	0	5.052165	5.433613	0.863321
40	6	0	3.504190	-0.277133	-1.043454
41	8	0	2.739520	-0.495751	-2.134757
42	8	0	4.633557	-0.707829	-0.927912
43	6	0	3.330563	-1.346626	-3.134890
44	1	0	4.283407	-0.931957	-3.472630
45	1	0	3.492487	-2.348241	-2.729950
46	1	0	2.610638	-1.374906	-3.953226
47	6	0	-0.166436	-0.320909	-0.521748
48	6	0	1.700754	0.256711	0.638672
49	6	0	0.773004	-0.948819	0.503649
50	1	0	0.264782	-0.338847	-1.527916
51	1	0	1.316810	0.990599	1.339174
52	6	0	0.028340	-1.216772	1.830526
53	6	0	0.545676	-0.836900	3.075430
54	6	0	-1.194492	-1.908261	1.802523
55	6	0	-0.151622	-1.107736	4.252945
56	1	0	1.496578	-0.316415	3.132009
57	6	0	-1.896550	-2.175180	2.982169

58	1	0	-1.575012	-2.284230	0.858334
59	6	0	-1.380882	-1.769289	4.211885
60	1	0	0.266845	-0.795324	5.205928
61	1	0	-2.840031	-2.713481	2.935805
62	1	0	-1.923843	-1.974629	5.130323
63	6	0	1.428683	-2.267353	0.060963
64	6	0	2.584106	-2.734879	0.703498
65	6	0	0.837380	-3.078711	-0.916362
66	6	0	3.138158	-3.970521	0.369351
67	1	0	3.058093	-2.124111	1.466059
68	6	0	1.386964	-4.318495	-1.250477
69	1	0	-0.063341	-2.740111	-1.421463
70	6	0	2.541790	-4.769224	-0.609077
71	1	0	4.039176	-4.307625	0.874500
72	1	0	0.910216	-4.931349	-2.011499
73	1	0	2.972122	-5.733128	-0.867098

Zero-point correction= 0.598034 (Hartree/Particle)
Thermal correction to Energy= 0.637285
Thermal correction to Enthalpy= 0.638230
Thermal correction to Gibbs Free Energy= 0.524130
Sum of electronic and zero-point Energies= -2020.605527
Sum of electronic and thermal Energies= -2020.566275
Sum of electronic and thermal Enthalpies= -2020.565331
Sum of electronic and thermal Free Energies= -2020.679431
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.550576

TS6′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.048656	0.341574	-0.120100
2	6	0	4.088799	-1.002438	-0.597183
3	6	0	3.172415	-1.090067	-1.709024
4	6	0	2.681126	0.245535	-2.005706
5	6	0	3.202452	1.130744	-1.005884
6	6	0	4.827621	0.891526	1.039169
7	1	0	4.310098	1.735187	1.505812
8	1	0	4.993021	0.133137	1.809028
9	1	0	5.810834	1.253409	0.706936
10	6	0	4.853562	-2.151339	-0.011098
11	1	0	4.208838	-3.024122	0.130884
12	1	0	5.684847	-2.440730	-0.668801
13	1	0	5.273803	-1.897020	0.965244
14	6	0	2.913010	-2.319575	-2.527800
15	1	0	2.948475	-3.220928	-1.910183
16	1	0	1.930227	-2.280086	-3.006237
17	1	0	3.667828	-2.422104	-3.321025
18	6	0	1.865124	0.620781	-3.207239
19	1	0	1.370911	1.587530	-3.073018
20	1	0	2.502882	0.697721	-4.098597
21	1	0	1.086897	-0.120113	-3.414904
22	6	0	3.055709	2.624475	-0.964497
23	1	0	2.130833	2.950272	-1.449726
24	1	0	3.040880	3.001882	0.062943
25	1	0	3.890689	3.117144	-1.482901
26	17	0	1.542809	-2.249336	1.457031
27	44	0	1.951816	-0.408893	-0.055852
28	6	0	-2.185075	-0.918923	-0.624599
29	6	0	-2.912446	-2.122635	-0.166054
30	6	0	-3.555138	-2.985264	-1.079587
31	6	0	-2.971022	-2.460248	1.203081
32	6	0	-4.209968	-4.133911	-0.644575
33	1	0	-3.539926	-2.752476	-2.137670
34	6	0	-3.632747	-3.605357	1.635589
35	1	0	-2.511202	-1.810373	1.941025

36	6	0	-4.253254	-4.452638	0.714391
37	1	0	-4.688026	-4.784066	-1.372517
38	1	0	-3.666080	-3.834152	2.697338
39	1	0	-4.766655	-5.348698	1.052358
40	6	0	-2.728444	-0.254561	-1.838647
41	8	0	-1.802923	0.425769	-2.565608
42	8	0	-3.898278	-0.302163	-2.177929
43	6	0	-2.334676	1.167583	-3.674645
44	1	0	-2.843994	0.500799	-4.374974
45	1	0	-3.040945	1.924176	-3.322989
46	1	0	-1.472791	1.638298	-4.149200
47	6	0	0.074456	0.500655	-0.305689
48	6	0	-1.079930	-0.479740	0.111706
49	6	0	-0.797885	1.178324	0.641844
50	1	0	-0.101042	0.874255	-1.307852
51	1	0	-0.806653	-1.100992	0.953035
52	6	0	-0.562430	1.154514	2.117854
53	6	0	-1.628116	1.243223	3.035153
54	6	0	0.745710	1.078507	2.623981
55	6	0	-1.390948	1.216489	4.405422
56	1	0	-2.646749	1.325467	2.671045
57	6	0	0.983384	1.052153	3.998991
58	1	0	1.582611	1.061215	1.929064
59	6	0	-0.082856	1.117183	4.893523
60	1	0	-2.227180	1.274300	5.096903
61	1	0	2.003610	0.983490	4.365717
62	1	0	0.099723	1.100758	5.964542
63	6	0	-1.708179	2.273592	0.148684
64	6	0	-3.107992	2.190648	0.166037
65	6	0	-1.111507	3.458388	-0.312525
66	6	0	-3.888370	3.261393	-0.277932
67	1	0	-3.593654	1.279741	0.500071
68	6	0	-1.890991	4.530988	-0.743808
69	1	0	-0.027595	3.538031	-0.322210
70	6	0	-3.284745	4.435229	-0.730204
71	1	0	-4.971032	3.170566	-0.271348
72	1	0	-1.409323	5.440815	-1.092582
73	1	0	-3.894049	5.267967	-1.070750

Zero-point correction= 0.596993 (Hartree/Particle)
Thermal correction to Energy= 0.636093
Thermal correction to Enthalpy= 0.637037
Thermal correction to Gibbs Free Energy= 0.522131
Sum of electronic and zero-point Energies= -2020.583958
Sum of electronic and thermal Energies= -2020.544857
Sum of electronic and thermal Enthalpies= -2020.543913
Sum of electronic and thermal Free Energies= -2020.658819
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.531723

INT11′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.747499	-0.538329	2.835171
2	6	0	-2.948443	-0.841863	2.136122
3	6	0	-2.646928	-1.864115	1.140127
4	6	0	-1.252876	-2.174448	1.234675
5	6	0	-0.672996	-1.304063	2.237781
6	6	0	-1.606126	0.413015	3.983855
7	1	0	-0.609346	0.858436	4.014569
8	1	0	-2.324741	1.232424	3.918074
9	1	0	-1.771618	-0.120298	4.930727
10	6	0	-4.305785	-0.268261	2.416977
11	1	0	-4.910073	-0.208999	1.507137
12	1	0	-4.851491	-0.892327	3.138748
13	1	0	-4.231633	0.740724	2.830460

14	6	0	-3.665689	-2.602198	0.321937
15	1	0	-4.551029	-1.986329	0.137141
16	1	0	-3.258400	-2.906640	-0.644239
17	1	0	-4.001757	-3.502776	0.855605
18	6	0	-0.554885	-3.322569	0.565662
19	1	0	0.510598	-3.123346	0.418209
20	1	0	-0.630195	-4.220769	1.195010
21	1	0	-1.001566	-3.559312	-0.402530
22	6	0	0.738583	-1.359200	2.742191
23	1	0	1.443479	-1.620163	1.949560
24	1	0	1.052324	-0.397370	3.156920
25	1	0	0.831743	-2.112604	3.537571
26	17	0	-1.378223	2.341864	1.207464
27	44	0	-1.480733	-0.028579	0.658652
28	6	0	-0.848569	-0.097089	-1.490335
29	6	0	-1.956957	0.827449	-1.905573
30	6	0	-3.297949	0.388024	-1.943948
31	6	0	-1.687479	2.164417	-2.268289
32	6	0	-4.326407	1.263166	-2.299515
33	1	0	-3.520016	-0.646843	-1.721857
34	6	0	-2.714842	3.028824	-2.623575
35	1	0	-0.664149	2.522404	-2.280636
36	6	0	-4.042100	2.585719	-2.632973
37	1	0	-5.351382	0.902257	-2.320120
38	1	0	-2.480444	4.053013	-2.900037
39	1	0	-4.842724	3.265713	-2.911225
40	6	0	-0.852484	-1.417708	-2.217411
41	8	0	0.335043	-1.678161	-2.811391
42	8	0	-1.809017	-2.158931	-2.358365
43	6	0	0.378353	-2.874761	-3.606783
44	1	0	0.202825	-3.758925	-2.987751
45	1	0	-0.377866	-2.837646	-4.394751
46	1	0	1.380441	-2.900554	-4.035864
47	6	0	1.529342	-0.280767	-0.606035
48	6	0	0.297065	0.439416	-0.855373
49	6	0	2.754746	0.228396	-0.283777
50	1	0	1.476393	-1.357349	-0.718693
51	1	0	0.324192	1.513015	-0.718844
52	6	0	3.037469	1.672702	-0.059114
53	6	0	4.159612	2.266324	-0.670061
54	6	0	2.221091	2.475773	0.755200
55	6	0	4.441975	3.618495	-0.489688
56	1	0	4.806210	1.659709	-1.297749
57	6	0	2.508288	3.829824	0.937982
58	1	0	1.353545	2.049849	1.247501
59	6	0	3.616337	4.407049	0.316918
60	1	0	5.307368	4.057535	-0.979707
61	1	0	1.856363	4.428753	1.567788
62	1	0	3.837633	5.461561	0.459935
63	6	0	3.901619	-0.715492	-0.165313
64	6	0	4.034549	-1.821195	-1.026950
65	6	0	4.879667	-0.537102	0.831990
66	6	0	5.087076	-2.724160	-0.882262
67	1	0	3.317844	-1.951877	-1.832686
68	6	0	5.929223	-1.442543	0.979056
69	1	0	4.803996	0.314031	1.501805
70	6	0	6.037964	-2.542044	0.124226
71	1	0	5.172831	-3.564400	-1.566794
72	1	0	6.664323	-1.288900	1.764920
73	1	0	6.860480	-3.243572	0.234930

Zero-point correction= 0.599958 (Hartree/Particle)
Thermal correction to Energy= 0.639116
Thermal correction to Enthalpy= 0.640061
Thermal correction to Gibbs Free Energy= 0.525788
Sum of electronic and zero-point Energies= -2020.661868
Sum of electronic and thermal Energies= -2020.622709

Sum of electronic and thermal Enthalpies= -2020.621765
Sum of electronic and thermal Free Energies= -2020.736038
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -2021.607627

Z-P1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.009461	-0.752146	-0.032237
2	6	0	3.255880	0.034167	-0.238874
3	6	0	4.414033	-0.202292	0.524550
4	6	0	3.293324	1.072035	-1.187327
5	6	0	5.551355	0.584700	0.360674
6	1	0	4.421183	-1.006840	1.250927
7	6	0	4.432598	1.858247	-1.352449
8	1	0	2.427599	1.246688	-1.819887
9	6	0	5.567154	1.620473	-0.576065
10	1	0	6.430572	0.386835	0.968323
11	1	0	4.435993	2.648767	-2.098451
12	1	0	6.458201	2.228975	-0.705856
13	6	0	2.193318	-2.214442	0.204858
14	8	0	1.098521	-2.828998	0.724208
15	8	0	3.222829	-2.823330	-0.019373
16	6	0	1.246406	-4.238396	0.954169
17	1	0	1.470098	-4.762861	0.021249
18	1	0	2.053683	-4.428258	1.666470
19	1	0	0.289847	-4.567818	1.361611
20	6	0	-0.536423	-0.654036	-0.070315
21	6	0	0.799987	-0.114500	-0.092985
22	6	0	-1.684160	0.088648	-0.027046
23	1	0	-0.636884	-1.730366	-0.119808
24	6	0	-2.997755	-0.585123	-0.190637
25	6	0	-3.147208	-1.693609	-1.045958
26	6	0	-4.130040	-0.142183	0.519246
27	6	0	-4.372820	-2.343916	-1.171160
28	1	0	-2.299190	-2.027798	-1.636273
29	6	0	-5.354442	-0.795973	0.396956
30	1	0	-4.040266	0.711292	1.184063
31	6	0	-5.482087	-1.900411	-0.447792
32	1	0	-4.464924	-3.191518	-1.845258
33	1	0	-6.210867	-0.442521	0.965163
34	1	0	-6.438818	-2.405823	-0.548014
35	6	0	-1.687450	1.559717	0.196468
36	6	0	-0.957855	2.142051	1.248088
37	6	0	-2.439615	2.405738	-0.639937
38	6	0	-0.964980	3.523251	1.445667
39	1	0	-0.399268	1.501198	1.923680
40	6	0	-2.438622	3.785362	-0.447966
41	1	0	-3.017326	1.972616	-1.451392
42	6	0	-1.701081	4.349850	0.596165
43	1	0	-0.398502	3.951248	2.268382
44	1	0	-3.015485	4.421824	-1.113790
45	1	0	-1.706035	5.425675	0.749235
46	1	0	0.855722	0.964025	-0.215610

Zero-point correction= 0.373676 (Hartree/Particle)
Thermal correction to Energy= 0.396045
Thermal correction to Enthalpy= 0.396989
Thermal correction to Gibbs Free Energy= 0.318907
Sum of electronic and zero-point Energies= -1076.663146
Sum of electronic and thermal Energies= -1076.640777
Sum of electronic and thermal Enthalpies= -1076.639833
Sum of electronic and thermal Free Energies= -1076.717915
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1076.526851

$ZnCl_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.000000	0.000000	0.000000
2	17	0	0.000000	0.000000	2.158093
3	17	0	0.000000	0.000000	-2.158093

Zero-point correction= 0.002149 (Hartree/Particle)
Thermal correction to Energy= 0.006704
Thermal correction to Enthalpy= 0.007648
Thermal correction to Gibbs Free Energy= -0.024433
Sum of electronic and zero-point Energies= -986.073236
Sum of electronic and thermal Energies= -986.068681
Sum of electronic and thermal Enthalpies= -986.067737
Sum of electronic and thermal Free Energies= -986.099818
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1147.703746

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.184857	2.373714	1.144418
2	6	0	0.524986	2.974727	0.045405
3	6	0	-0.005541	1.567913	-0.123187
4	1	0	0.081192	2.402535	2.220315
5	1	0	0.905681	3.858104	-0.448666
6	6	0	-1.426224	1.369397	-0.671762
7	1	0	-1.952724	2.332640	-0.638354
8	1	0	-1.369790	1.083291	-1.733558
9	6	0	0.948752	0.414498	-0.472285
10	1	0	0.526689	-0.528359	-0.093848
11	1	0	0.973767	0.306551	-1.568197
12	6	0	2.382104	0.556864	0.048776
13	1	0	2.366847	0.659757	1.143461
14	1	0	2.820398	1.491384	-0.330215
15	6	0	3.283353	-0.622090	-0.339364
16	1	0	3.299420	-0.723245	-1.434939
17	1	0	2.845928	-1.556546	0.043078
18	6	0	4.721875	-0.489392	0.176892
19	1	0	4.707359	-0.389126	1.272626
20	1	0	5.161091	0.444086	-0.205982
21	6	0	5.624890	-1.667702	-0.209968
22	1	0	5.640213	-1.767589	-1.304740
23	1	0	5.186625	-2.600386	0.173130
24	6	0	7.059418	-1.527221	0.309502
25	1	0	7.079761	-1.460539	1.404383
26	1	0	7.677971	-2.383481	0.016802
27	1	0	7.536766	-0.621424	-0.084571
28	6	0	-2.263506	0.325003	0.085499
29	1	0	-2.314690	0.608466	1.147140
30	1	0	-1.761317	-0.651990	0.055517
31	6	0	-3.686452	0.172766	-0.468149
32	1	0	-3.634377	-0.107236	-1.531018
33	1	0	-4.194056	1.148565	-0.437540
34	6	0	-4.532036	-0.861311	0.286175
35	1	0	-4.584971	-0.582219	1.349297
36	1	0	-4.025714	-1.837849	0.255047
37	6	0	-5.954974	-1.013212	-0.266865
38	1	0	-5.902375	-1.292696	-1.328854
39	1	0	-6.461472	-0.037943	-0.235029
40	6	0	-6.792281	-2.047855	0.492012
41	1	0	-7.801759	-2.132345	0.073352
42	1	0	-6.329417	-3.041567	0.448220
43	1	0	-6.892371	-1.777443	1.550546

Zero-point correction=	0.398438 (Hartree/Particle)
Thermal correction to Energy=	0.417890
Thermal correction to Enthalpy=	0.418834
Thermal correction to Gibbs Free Energy=	0.347686
Sum of electronic and zero-point Energies=	-587.989541
Sum of electronic and thermal Energies=	-587.970089
Sum of electronic and thermal Enthalpies=	-587.969145
Sum of electronic and thermal Free Energies=	-588.040293

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -588.070642

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -588.067119

4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.683074	0.628721	-0.000103
2	6	0	0.262161	0.962278	-0.000048
3	8	0	-0.155574	2.103444	-0.000033
4	7	0	2.086594	-0.613793	-0.000047
5	7	0	2.425260	-1.700589	0.000177
6	8	0	-0.518435	-0.146179	0.000083
7	6	0	-1.944695	0.094218	0.000143
8	1	0	-2.202442	0.686797	0.883757
9	1	0	-2.202461	0.687263	-0.883148
10	1	0	2.441506	1.397979	-0.000102
11	6	0	-2.632443	-1.257820	-0.000171
12	1	0	-3.719185	-1.120137	-0.000121
13	1	0	-2.358464	-1.836655	-0.888012
14	1	0	-2.358443	-1.837074	0.887393

Zero-point correction=	0.105490 (Hartree/Particle)
Thermal correction to Energy=	0.114001
Thermal correction to Enthalpy=	0.114946
Thermal correction to Gibbs Free Energy=	0.071416
Sum of electronic and zero-point Energies=	-415.837969
Sum of electronic and thermal Energies=	-415.829458
Sum of electronic and thermal Enthalpies=	-415.828514
Sum of electronic and thermal Free Energies=	-415.872044

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -415.815035

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.450469	1.515753	0.000436
2	6	0	1.328360	0.087187	0.000954
3	8	0	0.232595	-0.511227	0.001821
4	7	0	2.644060	2.067425	-0.001278
5	7	0	3.665916	2.555958	-0.002689
6	8	0	2.480166	-0.573887	0.000481
7	6	0	2.420622	-2.033405	0.000932
8	1	0	1.865557	-2.351863	0.887226
9	1	0	1.864183	-2.352413	-0.884302
10	1	0	0.583746	2.169681	0.000849
11	6	0	3.849598	-2.537339	0.000008
12	1	0	3.845860	-3.632318	0.000357
13	1	0	4.387528	-2.195367	-0.889544
14	1	0	4.388890	-2.194791	0.888512
15	30	0	-1.764871	-0.033387	0.000342
16	17	0	-2.994355	-1.859526	-0.001831
17	17	0	-1.955988	2.193805	0.000772

Zero-point correction=	0.109215 (Hartree/Particle)
Thermal correction to Energy=	0.123510

Thermal correction to Enthalpy= 0.124455
Thermal correction to Gibbs Free Energy= 0.063545
Sum of electronic and zero-point Energies= -1401.943252
Sum of electronic and thermal Energies= -1401.928956
Sum of electronic and thermal Enthalpies= -1401.928012
Sum of electronic and thermal Free Energies= -1401.988921
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1563.531373

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.070414	0.934106	0.856232
2	6	0	1.367317	0.320861	1.071327
3	8	0	1.245730	-0.361299	2.084488
4	7	0	0.349348	2.255993	-0.751332
5	7	0	0.380333	2.680369	-1.770990
6	8	0	2.385152	0.422693	0.257108
7	6	0	3.518805	-0.479408	0.515468
8	1	0	3.945098	-0.209266	1.485324
9	1	0	3.121155	-1.495369	0.571582
10	1	0	-0.141051	1.764164	1.532761
11	6	0	4.499079	-0.300246	-0.623853
12	1	0	5.359137	-0.959117	-0.464635
13	1	0	4.036565	-0.562728	-1.579784
14	1	0	4.861203	0.731240	-0.676199
15	30	0	-1.491846	-0.359353	0.000201
16	17	0	-0.415546	-1.916246	-1.188014
17	17	0	-3.544174	0.364135	0.431154

Zero-point correction= 0.104706 (Hartree/Particle)
Thermal correction to Energy= 0.120104
Thermal correction to Enthalpy= 0.121048
Thermal correction to Gibbs Free Energy= 0.055532
Sum of electronic and zero-point Energies= -1401.884108
Sum of electronic and thermal Energies= -1401.868710
Sum of electronic and thermal Enthalpies= -1401.867766
Sum of electronic and thermal Free Energies= -1401.933282
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1563.485958

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.022055	-1.510061	-0.119902
2	6	0	-1.368083	-1.126687	0.077403
3	8	0	-1.180234	-1.325709	1.300880
4	8	0	-2.360346	-0.658515	-0.579786
5	6	0	-3.471097	-0.064782	0.213682
6	1	0	-3.901082	-0.866570	0.818700
7	1	0	-3.015909	0.688991	0.859542
8	1	0	0.131611	-2.585904	-0.223906
9	6	0	-4.450768	0.521398	-0.776263
10	1	0	-5.280701	0.975566	-0.224708
11	1	0	-3.973403	1.297387	-1.381029
12	1	0	-4.856862	-0.249468	-1.437970
13	30	0	1.426208	0.116812	-0.014314
14	17	0	0.105085	1.905687	0.359757
15	17	0	3.560018	-0.365085	-0.366785

Zero-point correction= 0.097827 (Hartree/Particle)
Thermal correction to Energy= 0.110398
Thermal correction to Enthalpy= 0.111342
Thermal correction to Gibbs Free Energy= 0.054454
Sum of electronic and zero-point Energies= -1292.370544
Sum of electronic and thermal Energies= -1292.357974

Sum of electronic and thermal Enthalpies= -1292.357030
Sum of electronic and thermal Free Energies= -1292.413917
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1453.995487

INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554709	-1.028920	0.747022
2	6	0	-0.798512	-1.599924	-0.411078
3	6	0	-0.630338	-0.094670	-0.444609
4	1	0	-0.495455	-1.116879	1.824062
5	1	0	-1.074053	-2.492276	-0.958030
6	30	0	1.626232	-2.370674	0.225437
7	17	0	2.657680	-1.552782	1.996846
8	17	0	1.665793	-3.888184	-1.373918
9	6	0	0.649929	0.524767	-1.015138
10	1	0	1.416027	-0.263397	-1.127582
11	1	0	0.455026	0.876862	-2.038175
12	6	0	-1.876074	0.784807	-0.626364
13	1	0	-1.683949	1.762374	-0.163222
14	1	0	-1.996364	0.981359	-1.701987
15	6	0	-3.185146	0.215318	-0.067242
16	1	0	-3.075036	0.020925	1.009747
17	1	0	-3.393320	-0.760803	-0.529365
18	6	0	-4.382974	1.147053	-0.293294
19	1	0	-4.493964	1.340270	-1.370499
20	1	0	-4.176003	2.123009	0.170094
21	6	0	-5.701171	0.591153	0.261153
22	1	0	-5.590449	0.398620	1.338777
23	1	0	-5.907876	-0.385315	-0.201846
24	6	0	-6.900316	1.521460	0.034795
25	1	0	-7.011036	1.713230	-1.041988
26	1	0	-6.693622	2.497007	0.497500
27	6	0	-8.212943	0.959896	0.591293
28	1	0	-8.144857	0.790547	1.673039
29	1	0	-9.048497	1.646468	0.413889
30	1	0	-8.464522	0.000748	0.122005
31	6	0	1.243728	1.666756	-0.175726
32	1	0	1.438146	1.300313	0.841330
33	1	0	0.506406	2.475774	-0.082240
34	6	0	2.541157	2.232183	-0.769339
35	1	0	2.351897	2.583072	-1.794840
36	1	0	3.281761	1.423347	-0.853960
37	6	0	3.138390	3.377512	0.058591
38	1	0	3.325429	3.024226	1.083064
39	1	0	2.399419	4.188398	0.145093
40	6	0	4.439782	3.940357	-0.527996
41	1	0	4.253434	4.291261	-1.553175
42	1	0	5.177487	3.130047	-0.612921
43	6	0	5.030831	5.083554	0.303831
44	1	0	5.958414	5.462855	-0.139912
45	1	0	4.329289	5.923824	0.378605
46	1	0	5.260475	4.752957	1.324248

Zero-point correction= 0.401623 (Hartree/Particle)
Thermal correction to Energy= 0.427245
Thermal correction to Enthalpy= 0.428189
Thermal correction to Gibbs Free Energy= 0.338946
Sum of electronic and zero-point Energies= -1574.068457
Sum of electronic and thermal Energies= -1574.042836
Sum of electronic and thermal Enthalpies= -1574.041892
Sum of electronic and thermal Free Energies= -1574.131134
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1735.783348

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.229483	0.342332	-2.352969
2	6	0	-0.505806	1.442935	-1.640328
3	6	0	-0.033575	-0.264762	-1.074725
4	1	0	-0.607017	-0.055996	-3.292250
5	1	0	-1.370954	2.045752	-1.942280
6	30	0	0.205243	2.518248	0.126099
7	17	0	1.972959	3.814011	-0.280799
8	17	0	-1.097904	2.087720	1.900163
9	6	0	1.276506	-0.184229	-0.313296
10	1	0	1.867585	0.670473	-0.660913
11	1	0	1.076166	-0.064412	0.759857
12	6	0	-1.025261	-1.316261	-0.605479
13	1	0	-0.906228	-2.196638	-1.257465
14	1	0	-0.751305	-1.634478	0.406816
15	6	0	-2.497293	-0.866689	-0.615741
16	1	0	-2.796578	-0.600093	-1.638667
17	1	0	-2.588541	0.043191	-0.008358
18	6	0	-3.441335	-1.946632	-0.072356
19	1	0	-3.141205	-2.205572	0.953038
20	1	0	-3.330016	-2.865941	-0.666881
21	6	0	-4.913063	-1.512447	-0.074783
22	1	0	-5.215158	-1.253062	-1.100628
23	1	0	-5.019705	-0.592090	0.517128
24	6	0	-5.864117	-2.583124	0.476512
25	1	0	-5.563055	-2.839725	1.501955
26	1	0	-5.754034	-3.504558	-0.113182
27	6	0	-7.332202	-2.144230	0.470014
28	1	0	-7.672964	-1.913454	-0.546958
29	1	0	-7.984943	-2.928421	0.869876
30	1	0	-7.479269	-1.244766	1.080197
31	6	0	2.112743	-1.468769	-0.524213
32	1	0	2.289694	-1.610444	-1.599169
33	1	0	1.551101	-2.345532	-0.177115
34	6	0	3.456696	-1.398514	0.216066
35	1	0	3.271517	-1.244344	1.288612
36	1	0	4.014962	-0.516916	-0.128482
37	6	0	4.314005	-2.656122	0.020970
38	1	0	4.495933	-2.810330	-1.053034
39	1	0	3.752957	-3.537800	0.365134
40	6	0	5.658809	-2.592764	0.757831
41	1	0	5.476336	-2.438282	1.830542
42	1	0	6.217846	-1.711224	0.414278
43	6	0	6.512487	-3.849669	0.559705
44	1	0	7.464298	-3.773367	1.097203
45	1	0	5.993640	-4.744038	0.926399
46	1	0	6.741038	-4.011129	-0.501045

Zero-point correction= 0.401332 (Hartree/Particle)
Thermal correction to Energy= 0.426472
Thermal correction to Enthalpy= 0.427417
Thermal correction to Gibbs Free Energy= 0.339232
Sum of electronic and zero-point Energies= -1574.055795
Sum of electronic and thermal Energies= -1574.030654
Sum of electronic and thermal Enthalpies= -1574.029710
Sum of electronic and thermal Free Energies= -1574.117895
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1735.764641

INT15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.714957	1.606070	1.367737
2	6	0	-0.432406	2.326753	1.065754

3	6	0	1.041512	0.356821	0.814829
4	1	0	1.435765	1.994805	2.091683
5	1	0	-0.464357	3.269091	1.626753
6	30	0	-2.155313	1.952088	-0.096486
7	17	0	-3.918715	1.332719	1.166523
8	17	0	-1.929387	2.009150	-2.342575
9	6	0	0.205480	-0.378294	-0.171010
10	1	0	-0.305551	0.300491	-0.861264
11	1	0	0.849089	-1.032865	-0.771007
12	6	0	2.322276	-0.289647	1.229104
13	1	0	2.610921	0.027572	2.237349
14	1	0	2.210043	-1.380612	1.225076
15	6	0	3.464322	0.092880	0.237799
16	1	0	3.588795	1.182813	0.240661
17	1	0	3.171505	-0.187775	-0.781714
18	6	0	4.789737	-0.588097	0.605361
19	1	0	4.650501	-1.678548	0.604598
20	1	0	5.067973	-0.313103	1.632687
21	6	0	5.931185	-0.216624	-0.351118
22	1	0	6.066688	0.874747	-0.350564
23	1	0	5.649006	-0.488764	-1.378599
24	6	0	7.262282	-0.893055	0.005296
25	1	0	7.125393	-1.983637	0.005000
26	1	0	7.542768	-0.621005	1.032664
27	6	0	8.399156	-0.519629	-0.951736
28	1	0	8.582747	0.561726	-0.947135
29	1	0	9.334125	-1.017393	-0.671534
30	1	0	8.162172	-0.810949	-1.982254
31	6	0	-0.849331	-1.274892	0.557067
32	1	0	-1.527007	-0.635989	1.135750
33	1	0	-0.341687	-1.931132	1.276661
34	6	0	-1.653091	-2.116367	-0.443617
35	1	0	-0.972171	-2.786624	-0.988192
36	1	0	-2.103405	-1.453499	-1.194607
37	6	0	-2.755763	-2.936607	0.239921
38	1	0	-3.433628	-2.253189	0.769226
39	1	0	-2.308411	-3.588384	1.005708
40	6	0	-3.563747	-3.792256	-0.745596
41	1	0	-2.884489	-4.471587	-1.280668
42	1	0	-4.007569	-3.138481	-1.508734
43	6	0	-4.669249	-4.605047	-0.063539
44	1	0	-5.229674	-5.203276	-0.790960
45	1	0	-4.253888	-5.292292	0.684256
46	1	0	-5.382460	-3.948602	0.449109

Zero-point correction= 0.403545 (Hartree/Particle)
Thermal correction to Energy= 0.428892
Thermal correction to Enthalpy= 0.429837
Thermal correction to Gibbs Free Energy= 0.341316
Sum of electronic and zero-point Energies= -1574.079651
Sum of electronic and thermal Energies= -1574.054303
Sum of electronic and thermal Enthalpies= -1574.053359
Sum of electronic and thermal Free Energies= -1574.141880
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1735.791994

TS8′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.414440	-1.221549	0.733175
2	6	0	0.077433	-1.589964	-0.447091
3	6	0	-0.998859	-0.229455	-0.110442
4	1	0	-0.097156	-1.390260	1.759599
5	1	0	-0.048084	-1.799426	-1.494259
6	30	0	2.243389	-2.052752	-0.062712
7	17	0	2.552557	-2.597515	2.075819

8	17	0	3.343899	-1.728548	-1.968611
9	6	0	-2.370322	-0.468029	-0.730592
10	1	0	-2.549863	-1.546291	-0.812836
11	1	0	-2.386470	-0.055447	-1.749085
12	6	0	-3.513339	0.167238	0.088554
13	1	0	-3.481946	-0.222680	1.115599
14	1	0	-3.360550	1.252046	0.162964
15	6	0	-4.893956	-0.107676	-0.523796
16	1	0	-4.915627	0.272433	-1.555734
17	1	0	-5.049403	-1.194091	-0.595404
18	6	0	-6.045705	0.519338	0.273051
19	1	0	-5.890315	1.606195	0.343469
20	1	0	-6.021823	0.141208	1.305829
21	6	0	-7.427895	0.244347	-0.334387
22	1	0	-7.451134	0.621988	-1.366499
23	1	0	-7.582620	-0.841698	-0.404261
24	6	0	-8.573237	0.873296	0.465989
25	1	0	-8.465053	1.963426	0.523662
26	1	0	-9.545165	0.659098	0.007429
27	1	0	-8.597401	0.488647	1.493029
28	6	0	-0.479731	1.202571	-0.138438
29	1	0	-1.011301	1.766405	0.643925
30	1	0	-0.776072	1.662870	-1.091560
31	6	0	1.032482	1.370406	0.061569
32	1	0	1.330486	0.942830	1.030075
33	1	0	1.569239	0.801564	-0.711932
34	6	0	1.481807	2.836478	0.000601
35	1	0	0.944104	3.413986	0.767171
36	1	0	1.186869	3.265215	-0.968327
37	6	0	2.993719	3.010377	0.195428
38	1	0	3.286454	2.584849	1.166675
39	1	0	3.527798	2.424942	-0.566882
40	6	0	3.452581	4.473057	0.125421
41	1	0	2.916632	5.058247	0.886522
42	1	0	3.161371	4.897442	-0.846052
43	6	0	4.963055	4.638561	0.323005
44	1	0	5.259945	5.692036	0.266706
45	1	0	5.279209	4.254475	1.300597
46	1	0	5.524891	4.091655	-0.443877

Zero-point correction= 0.400337 (Hartree/Particle)
Thermal correction to Energy= 0.425748
Thermal correction to Enthalpy= 0.426693
Thermal correction to Gibbs Free Energy= 0.338145
Sum of electronic and zero-point Energies= -1574.049216
Sum of electronic and thermal Energies= -1574.023804
Sum of electronic and thermal Enthalpies= -1574.022860
Sum of electronic and thermal Free Energies= -1574.111407
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1735.758875

INT15′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.210038	-0.706966	0.151475
2	6	0	-1.461509	-0.876908	-0.425618
3	6	0	0.593969	0.437875	0.049159
4	1	0	0.173190	-1.520629	0.769259
5	1	0	-1.804087	-0.052319	-1.059942
6	30	0	-2.600626	-2.636174	-0.060635
7	17	0	-1.287478	-4.061536	1.116755
8	17	0	-4.710714	-2.745412	-0.805666
9	6	0	0.212114	1.668422	-0.703249
10	1	0	-0.464616	1.443420	-1.531806
11	1	0	1.117496	2.128061	-1.119372
12	6	0	-0.475233	2.702174	0.239282

13	1	0	-1.395251	2.255619	0.635913
14	1	0	0.173276	2.905788	1.101258
15	6	0	-0.796728	4.013862	-0.489029
16	1	0	0.132617	4.448692	-0.884086
17	1	0	-1.432088	3.799403	-1.359910
18	6	0	-1.497487	5.037162	0.415264
19	1	0	-0.862049	5.248689	1.287852
20	1	0	-2.424667	4.598319	0.811208
21	6	0	-1.826187	6.353054	-0.303577
22	1	0	-0.899059	6.790090	-0.700776
23	1	0	-2.461175	6.139981	-1.174875
24	6	0	-2.525612	7.371721	0.602451
25	1	0	-1.900225	7.630813	1.465571
26	1	0	-2.746927	8.298329	0.061371
27	1	0	-3.473402	6.975696	0.986731
28	6	0	1.917263	0.445080	0.739358
29	1	0	1.878341	-0.165254	1.648153
30	1	0	2.207100	1.466026	1.013998
31	6	0	3.010096	-0.146933	-0.205781
32	1	0	2.728941	-1.171900	-0.475473
33	1	0	3.038947	0.431169	-1.138719
34	6	0	4.395506	-0.139030	0.454964
35	1	0	4.351716	-0.708553	1.393702
36	1	0	4.663189	0.891389	0.729397
37	6	0	5.485166	-0.728496	-0.451139
38	1	0	5.212469	-1.757575	-0.725867
39	1	0	5.524875	-0.160316	-1.392187
40	6	0	6.875438	-0.728919	0.199871
41	1	0	6.833892	-1.296731	1.139840
42	1	0	7.146423	0.299979	0.476071
43	6	0	7.960790	-1.318702	-0.706756
44	1	0	8.939616	-1.305485	-0.214685
45	1	0	7.734622	-2.358803	-0.971033
46	1	0	8.049585	-0.750955	-1.641118

Zero-point correction= 0.403256 (Hartree/Particle)
Thermal correction to Energy= 0.428853
Thermal correction to Enthalpy= 0.429797
Thermal correction to Gibbs Free Energy= 0.339338
Sum of electronic and zero-point Energies= -1574.075728
Sum of electronic and thermal Energies= -1574.050131
Sum of electronic and thermal Enthalpies= -1574.049187
Sum of electronic and thermal Free Energies= -1574.139646
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1735.785887

INT16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.484403	-1.125994	-1.462339
2	6	0	0.117233	-1.198404	-1.221050
3	6	0	2.362246	-0.217492	-0.851848
4	1	0	1.953410	-1.803392	-2.181795
5	1	0	-0.335923	-1.990747	-1.833033
6	30	0	-1.370628	-0.134831	-0.135206
7	17	0	-2.121516	1.668648	-1.352597
8	17	0	-1.050764	0.005493	2.173392
9	6	0	1.963784	0.828286	0.122941
10	1	0	1.108759	0.520471	0.730245
11	1	0	2.804882	1.027151	0.799456
12	6	0	3.816087	-0.299034	-1.196461
13	1	0	3.953740	-0.693021	-2.209877
14	1	0	4.268498	0.698734	-1.147954
15	6	0	4.559421	-1.229535	-0.192956
16	1	0	4.119773	-2.233532	-0.244377
17	1	0	4.395328	-0.867287	0.829798

18	6	0	6.064553	-1.301088	-0.483815
19	1	0	6.492817	-0.289832	-0.432684
20	1	0	6.220262	-1.649668	-1.514868
21	6	0	6.814432	-2.223845	0.486528
22	1	0	6.383425	-3.234442	0.434944
23	1	0	6.653888	-1.876203	1.517505
24	6	0	8.321648	-2.300869	0.206579
25	1	0	8.751341	-1.290511	0.258671
26	1	0	8.481078	-2.647101	-0.824449
27	6	0	9.065906	-3.223908	1.177154
28	1	0	8.681599	-4.249850	1.122538
29	1	0	10.137773	-3.257332	0.952042
30	1	0	8.953389	-2.883190	2.213668
31	6	0	1.612656	2.161706	-0.615970
32	1	0	0.748213	1.989169	-1.265576
33	1	0	2.452732	2.463937	-1.256702
34	6	0	1.286559	3.277642	0.385241
35	1	0	2.161986	3.468376	1.023998
36	1	0	0.480789	2.936985	1.047831
37	6	0	0.857844	4.575247	-0.312871
38	1	0	-0.024870	4.368489	-0.932538
39	1	0	1.653077	4.906402	-0.998594
40	6	0	0.534907	5.707595	0.671625
41	1	0	1.415347	5.908554	1.299367
42	1	0	-0.258282	5.373545	1.354289
43	6	0	0.097750	7.000333	-0.025562
44	1	0	-0.128714	7.789403	0.700976
45	1	0	0.883116	7.377194	-0.693051
46	1	0	-0.801262	6.836319	-0.631794
47	6	0	-4.221491	-1.245493	1.678252
48	6	0	-4.071369	-1.628757	0.299789
49	8	0	-3.010185	-1.509343	-0.330954
50	7	0	-5.383656	-1.373155	2.271140
51	7	0	-6.382355	-1.482670	2.799403
52	8	0	-5.175053	-2.142581	-0.252571
53	6	0	-5.110073	-2.478278	-1.664725
54	1	0	-4.776226	-1.594596	-2.215313
55	1	0	-4.363679	-3.267377	-1.798347
56	1	0	-3.395207	-0.821457	2.244092
57	6	0	-6.497092	-2.927852	-2.081733
58	1	0	-6.490586	-3.194999	-3.143897
59	1	0	-6.816624	-3.803358	-1.507578
60	1	0	-7.228677	-2.127704	-1.932603

Zero-point correction= 0.510383 (Hartree/Particle)
Thermal correction to Energy= 0.545983
Thermal correction to Enthalpy= 0.546927
Thermal correction to Gibbs Free Energy= 0.432518
Sum of electronic and zero-point Energies= -1989.937971
Sum of electronic and thermal Energies= -1989.902371
Sum of electronic and thermal Enthalpies= -1989.901427
Sum of electronic and thermal Free Energies= -1990.015836
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2151.616909

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.433028	-0.745549	1.531762
2	6	0	0.699713	-1.589262	1.333189
3	6	0	-0.656769	0.454242	0.891555
4	1	0	-1.154126	-1.008750	2.309832
5	1	0	0.754072	-2.342495	2.125420
6	30	0	2.621824	-1.041055	0.629335
7	17	0	3.259214	-1.134094	-1.537044
8	17	0	3.857376	-0.418344	2.419157

9	6	0	0.179827	0.993575	-0.232687
10	1	0	0.694805	0.193820	-0.772626
11	1	0	-0.486604	1.478961	-0.958808
12	6	0	-1.809658	1.315143	1.339690
13	1	0	-2.054128	1.103644	2.387230
14	1	0	-1.519923	2.371692	1.277632
15	6	0	-3.080268	1.104009	0.479242
16	1	0	-3.401629	0.058889	0.576305
17	1	0	-2.838601	1.262096	-0.580522
18	6	0	-4.225842	2.039642	0.888510
19	1	0	-3.892841	3.082891	0.790735
20	1	0	-4.454411	1.890130	1.953660
21	6	0	-5.500405	1.832339	0.059554
22	1	0	-5.834351	0.788469	0.158887
23	1	0	-5.269906	1.978769	-1.006159
24	6	0	-6.647485	2.769311	0.461943
25	1	0	-6.313846	3.811732	0.362000
26	1	0	-6.876565	2.623781	1.527085
27	6	0	-7.917694	2.557205	-0.368357
28	1	0	-8.295983	1.533028	-0.260815
29	1	0	-8.715753	3.240628	-0.057507
30	1	0	-7.728088	2.729882	-1.434913
31	6	0	1.209503	2.053391	0.249039
32	1	0	1.905396	1.594280	0.965393
33	1	0	0.691685	2.846054	0.805817
34	6	0	1.994399	2.667537	-0.918167
35	1	0	1.289933	3.144348	-1.616121
36	1	0	2.494095	1.865779	-1.477464
37	6	0	3.035037	3.695869	-0.455225
38	1	0	3.734546	3.213173	0.241878
39	1	0	2.535803	4.494835	0.114202
40	6	0	3.825190	4.317614	-1.614711
41	1	0	3.126039	4.797457	-2.314946
42	1	0	4.322982	3.517693	-2.179560
43	6	0	4.867019	5.340862	-1.150338
44	1	0	5.415190	5.765853	-1.999075
45	1	0	4.395588	6.170603	-0.608576
46	1	0	5.599986	4.880258	-0.476971
47	6	0	-0.091840	-3.356703	0.047224
48	6	0	-1.076298	-2.817969	-0.925670
49	8	0	-0.812743	-2.415183	-2.036595
50	7	0	1.037931	-3.822211	-0.497800
51	7	0	2.032058	-4.136654	-0.923952
52	8	0	-2.302948	-2.850128	-0.371788
53	6	0	-3.389874	-2.430154	-1.239543
54	1	0	-3.258966	-1.369942	-1.473901
55	1	0	-3.320189	-2.990935	-2.176002
56	1	0	-0.440511	-3.956375	0.879714
57	6	0	-4.688164	-2.701978	-0.504721
58	1	0	-5.534228	-2.397334	-1.129995
59	1	0	-4.794257	-3.767430	-0.277512
60	1	0	-4.736526	-2.142583	0.435290

Zero-point correction= 0.510210 (Hartree/Particle)
Thermal correction to Energy= 0.545048
Thermal correction to Enthalpy= 0.545992
Thermal correction to Gibbs Free Energy= 0.434276
Sum of electronic and zero-point Energies= -1989.904569
Sum of electronic and thermal Energies= -1989.869731
Sum of electronic and thermal Enthalpies= -1989.868787
Sum of electronic and thermal Free Energies= -1989.980503
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2151.610504

INT17

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

1	6	0	0.108152	0.702552	-1.792743
2	6	0	0.859639	1.972516	-1.910098
3	6	0	-0.148445	-0.044141	-0.673297
4	1	0	-0.397372	0.403007	-2.716475
5	1	0	1.643624	1.986846	-2.667197
6	30	0	1.828861	-1.024147	-2.133994
7	17	0	3.756604	-0.200159	-1.414027
8	17	0	0.996631	-2.627421	-3.413671
9	6	0	0.469054	0.263347	0.670919
10	1	0	1.270106	0.998326	0.543195
11	1	0	-0.306117	0.756904	1.272518
12	6	0	-1.158342	-1.170279	-0.758748
13	1	0	-1.390266	-1.381343	-1.808191
14	1	0	-0.748534	-2.096749	-0.338289
15	6	0	-2.464017	-0.816763	-0.006913
16	1	0	-2.831268	0.153663	-0.363416
17	1	0	-2.252544	-0.690098	1.062958
18	6	0	-3.543315	-1.891972	-0.189519
19	1	0	-3.155235	-2.861817	0.154875
20	1	0	-3.758026	-2.013558	-1.261050
21	6	0	-4.844726	-1.569773	0.556999
22	1	0	-5.229107	-0.597617	0.214557
23	1	0	-4.629805	-1.450448	1.629440
24	6	0	-5.932242	-2.637117	0.374951
25	1	0	-5.547276	-3.608235	0.717131
26	1	0	-6.146660	-2.755886	-0.696564
27	6	0	-7.229150	-2.309276	1.122406
28	1	0	-7.656784	-1.359933	0.776841
29	1	0	-7.984732	-3.088858	0.972631
30	1	0	-7.053085	-2.218848	2.201498
31	6	0	1.016995	-0.956515	1.437339
32	1	0	1.730631	-1.504932	0.803974
33	1	0	0.204714	-1.656322	1.672184
34	6	0	1.726848	-0.550066	2.735453
35	1	0	1.027760	0.019177	3.366318
36	1	0	2.552430	0.133983	2.494106
37	6	0	2.271819	-1.745612	3.527219
38	1	0	2.967337	-2.313866	2.892473
39	1	0	1.446202	-2.432475	3.766955
40	6	0	2.986426	-1.342218	4.823933
41	1	0	2.292285	-0.771999	5.457930
42	1	0	3.811668	-0.657432	4.583031
43	6	0	3.529625	-2.540249	5.609859
44	1	0	4.033929	-2.220019	6.528714
45	1	0	2.722716	-3.226955	5.894476
46	1	0	4.253197	-3.109612	5.013675
47	6	0	0.644578	3.140210	-1.276648
48	6	0	-0.442214	3.437262	-0.312011
49	8	0	-1.309278	2.675239	0.077828
50	8	0	-0.359427	4.727606	0.078400
51	6	0	-1.373377	5.178219	1.005716
52	1	0	-2.356901	5.034143	0.546745
53	1	0	-1.332254	4.550819	1.902108
54	1	0	1.277026	3.987853	-1.522204
55	6	0	-1.093491	6.636975	1.314621
56	1	0	-1.843064	7.016779	2.017276
57	1	0	-0.104100	6.758678	1.766897
58	1	0	-1.134585	7.244751	0.405119

Zero-point correction= 0.504061 (Hartree/Particle)
Thermal correction to Energy= 0.536782
Thermal correction to Enthalpy= 0.537726
Thermal correction to Gibbs Free Energy= 0.430933
Sum of electronic and zero-point Energies= -1880.529314
Sum of electronic and thermal Energies= -1880.496593
Sum of electronic and thermal Enthalpies= -1880.495649

Sum of electronic and thermal Free Energies= -1880.602443
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2042.246407

Z-P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.039771	0.098994	-0.015590
2	6	0	-1.924312	-0.811930	-0.709485
3	6	0	0.314822	0.034219	-0.023297
4	1	0	-1.522731	0.886894	0.553682
5	1	0	-1.455747	-1.600887	-1.295362
6	6	0	1.118293	-1.034202	-0.734229
7	1	0	0.599283	-1.394019	-1.629960
8	1	0	2.063218	-0.598397	-1.086453
9	6	0	1.116002	1.073461	0.730111
10	1	0	0.490884	1.534935	1.504027
11	1	0	1.956596	0.588366	1.248405
12	6	0	1.677475	2.185161	-0.183949
13	1	0	0.837622	2.692852	-0.676896
14	1	0	2.279935	1.737455	-0.986925
15	6	0	2.528228	3.210643	0.576403
16	1	0	3.366471	2.694990	1.068441
17	1	0	1.927022	3.652545	1.384581
18	6	0	3.075769	4.330057	-0.318304
19	1	0	2.237227	4.844677	-0.810513
20	1	0	3.677133	3.888663	-1.127243
21	6	0	3.925612	5.359111	0.438521
22	1	0	4.763722	4.844983	0.930397
23	1	0	3.324509	5.800595	1.246099
24	6	0	4.468142	6.473744	-0.461797
25	1	0	3.652093	7.028912	-0.940626
26	1	0	5.069728	7.191541	0.107524
27	1	0	5.102061	6.066285	-1.259105
28	6	0	1.442639	-2.240671	0.174929
29	1	0	0.501210	-2.704563	0.498722
30	1	0	1.937863	-1.886997	1.089996
31	6	0	2.328386	-3.287488	-0.512365
32	1	0	3.269001	-2.814632	-0.831862
33	1	0	1.835101	-3.633217	-1.433110
34	6	0	2.645043	-4.496581	0.377260
35	1	0	1.704435	-4.968874	0.697488
36	1	0	3.139179	-4.151526	1.297758
37	6	0	3.529750	-5.546158	-0.307991
38	1	0	4.469732	-5.074101	-0.627703
39	1	0	3.035570	-5.891217	-1.227394
40	6	0	3.841665	-6.750257	0.586531
41	1	0	4.474047	-7.480576	0.068928
42	1	0	4.367624	-6.441180	1.498284
43	1	0	2.922627	-7.264209	0.894167
44	6	0	-3.280032	-0.804226	-0.716659
45	6	0	-4.139386	0.154071	-0.001072
46	8	0	-3.789806	1.084432	0.706610
47	8	0	-5.448669	-0.133932	-0.234348
48	6	0	-6.404757	0.731848	0.408619
49	1	0	-6.244004	0.698436	1.491588
50	1	0	-6.226491	1.762797	0.084354
51	1	0	-3.811777	-1.556382	-1.290718
52	6	0	-7.790712	0.246934	0.024511
53	1	0	-8.551282	0.880393	0.494191
54	1	0	-7.931752	0.285848	-1.060522
55	1	0	-7.949448	-0.784778	0.354771

Zero-point correction= 0.501188 (Hartree/Particle)
Thermal correction to Energy= 0.527721
Thermal correction to Enthalpy= 0.528665

Thermal correction to Gibbs Free Energy= 0.438696
Sum of electronic and zero-point Energies= -894.463234
Sum of electronic and thermal Energies= -894.436701
Sum of electronic and thermal Enthalpies= -894.435757
Sum of electronic and thermal Free Energies= -894.525726
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -894.539735

TS9′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.626801	-0.718779	1.255692
2	6	0	0.761350	-0.825327	0.943482
3	6	0	-1.492980	0.242945	0.780695
4	1	0	-1.052655	-1.407454	1.991500
5	1	0	1.238412	-1.505482	1.661785
6	30	0	2.271383	0.322840	-0.093530
7	17	0	3.475522	1.773909	1.146525
8	17	0	1.755192	0.457379	-2.366552
9	6	0	-1.114496	1.336766	-0.169871
10	1	0	-0.346462	1.010781	-0.876445
11	1	0	-1.997538	1.622065	-0.756750
12	6	0	-2.919012	0.238612	1.262637
13	1	0	-2.993984	-0.255742	2.238359
14	1	0	-3.267715	1.272278	1.386068
15	6	0	-3.857528	-0.484363	0.261987
16	1	0	-3.526689	-1.526269	0.155511
17	1	0	-3.761861	-0.024077	-0.730350
18	6	0	-5.326101	-0.448392	0.705457
19	1	0	-5.647208	0.598001	0.810494
20	1	0	-5.415385	-0.897794	1.705182
21	6	0	-6.265965	-1.175030	-0.265857
22	1	0	-5.943014	-2.221428	-0.371153
23	1	0	-6.174205	-0.726105	-1.265895
24	6	0	-7.736906	-1.141241	0.170798
25	1	0	-8.059025	-0.095551	0.275547
26	1	0	-7.827942	-1.589322	1.170468
27	6	0	-8.670421	-1.868564	-0.802617
28	1	0	-8.394636	-2.925707	-0.901817
29	1	0	-9.711585	-1.826586	-0.463436
30	1	0	-8.627540	-1.420400	-1.802911
31	6	0	-0.603133	2.597138	0.584340
32	1	0	0.305349	2.335023	1.140590
33	1	0	-1.346634	2.913144	1.329755
34	6	0	-0.303410	3.755919	-0.375530
35	1	0	-1.226311	4.043194	-0.901533
36	1	0	0.398700	3.411182	-1.146430
37	6	0	0.286033	4.978301	0.340717
38	1	0	1.212546	4.680839	0.851002
39	1	0	-0.407788	5.314418	1.126682
40	6	0	0.582333	6.148501	-0.606891
41	1	0	-0.343153	6.443317	-1.122834
42	1	0	1.274525	5.809815	-1.390000
43	6	0	1.178371	7.364797	0.109753
44	1	0	1.381457	8.182398	-0.591681
45	1	0	0.495170	7.747192	0.878753
46	1	0	2.122549	7.107084	0.604516
47	6	0	1.076551	-2.332981	-0.662423
48	6	0	2.482639	-2.640439	-0.327041
49	8	0	3.319177	-1.746941	-0.272364
50	7	0	0.160026	-3.285928	-0.524448
51	7	0	-0.701598	-3.990530	-0.318587
52	8	0	2.716609	-3.919268	-0.048939
53	6	0	4.076996	-4.256304	0.369585
54	1	0	4.755756	-3.980973	-0.441713
55	1	0	4.324207	-3.647848	1.243751

56	1	0	0.895080	-1.620307	-1.474407
57	6	0	4.099658	-5.741710	0.667035
58	1	0	5.107851	-6.032050	0.980621
59	1	0	3.403519	-5.993843	1.473142
60	1	0	3.834246	-6.325086	-0.220046

Zero-point correction= 0.510670 (Hartree/Particle)
Thermal correction to Energy= 0.545056
Thermal correction to Enthalpy= 0.546000
Thermal correction to Gibbs Free Energy= 0.436760
Sum of electronic and zero-point Energies= -1989.921667
Sum of electronic and thermal Energies= -1989.887282
Sum of electronic and thermal Enthalpies= -1989.886337
Sum of electronic and thermal Free Energies= -1989.995578
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2151.607069

INT17′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.979760	-0.919967	-0.582087
2	6	0	-0.375231	-0.694345	-0.124790
3	6	0	2.104809	-0.176360	-0.411371
4	1	0	1.104503	-1.873788	-1.093356
5	1	0	-0.988015	-1.595717	-0.107128
6	30	0	-4.115477	-2.032171	-0.237756
7	17	0	-2.751013	-3.720920	-0.702770
8	17	0	-6.192821	-1.333445	-0.570710
9	6	0	2.173060	1.142626	0.317949
10	1	0	1.400768	1.199039	1.093159
11	1	0	3.139997	1.213558	0.833859
12	6	0	3.418596	-0.705021	-0.943442
13	1	0	3.234285	-1.408576	-1.764234
14	1	0	4.003304	0.127126	-1.361266
15	6	0	4.268065	-1.411725	0.138067
16	1	0	3.698497	-2.263400	0.533194
17	1	0	4.432005	-0.731170	0.985068
18	6	0	5.623049	-1.895878	-0.394849
19	1	0	6.186777	-1.037251	-0.788872
20	1	0	5.457746	-2.569370	-1.248524
21	6	0	6.468173	-2.616426	0.663966
22	1	0	5.903718	-3.474773	1.057231
23	1	0	6.632331	-1.943500	1.518887
24	6	0	7.824528	-3.102482	0.135639
25	1	0	8.388502	-2.244465	-0.257270
26	1	0	7.659957	-3.774851	-0.718274
27	6	0	8.662561	-3.821671	1.197979
28	1	0	8.139269	-4.704880	1.584565
29	1	0	9.623307	-4.155973	0.790230
30	1	0	8.873102	-3.163232	2.049860
31	6	0	2.044455	2.359037	-0.629828
32	1	0	1.085344	2.309367	-1.162657
33	1	0	2.822086	2.298685	-1.403436
34	6	0	2.159587	3.700092	0.106962
35	1	0	3.120739	3.739478	0.640351
36	1	0	1.380376	3.758853	0.881514
37	6	0	2.043601	4.914755	-0.823487
38	1	0	1.083145	4.873569	-1.358406
39	1	0	2.824095	4.856332	-1.596609
40	6	0	2.157120	6.258510	-0.091001
41	1	0	3.116820	6.299168	0.443596
42	1	0	1.376528	6.316878	0.680872
43	6	0	2.041844	7.466438	-1.026799
44	1	0	2.126600	8.409186	-0.474530
45	1	0	2.831001	7.454506	-1.788688
46	1	0	1.077686	7.472253	-1.550029

47	6	0	-0.995868	0.457401	0.244466
48	6	0	-2.383374	0.445064	0.677247
49	8	0	-3.117779	-0.561738	0.746947
50	8	0	-2.832419	1.644158	1.028870
51	6	0	-4.221837	1.747133	1.462202
52	1	0	-4.861790	1.306702	0.693102
53	1	0	-4.335131	1.156680	2.376377
54	1	0	-0.525117	1.430948	0.214244
55	6	0	-4.512332	3.217380	1.688411
56	1	0	-5.548714	3.334160	2.022056
57	1	0	-3.853223	3.637677	2.454662
58	1	0	-4.382834	3.789391	0.764343

Zero-point correction= 0.504816 (Hartree/Particle)
Thermal correction to Energy= 0.537423
Thermal correction to Enthalpy= 0.538367
Thermal correction to Gibbs Free Energy= 0.430022
Sum of electronic and zero-point Energies= -1880.556917
Sum of electronic and thermal Energies= -1880.524310
Sum of electronic and thermal Enthalpies= -1880.523366
Sum of electronic and thermal Free Energies= -1880.631711
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2042.253091

E-P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.408102	-1.102052	-0.584086
2	6	0	-1.745779	-0.943353	-0.059999
3	6	0	0.650262	-0.289998	-0.347478
4	1	0	-0.254517	-1.962427	-1.236600
5	1	0	-1.956610	-0.109244	0.605698
6	6	0	0.575702	0.964164	0.496662
7	1	0	-0.184535	0.868778	1.279629
8	1	0	1.533284	1.106821	1.015832
9	6	0	1.998126	-0.607881	-0.956315
10	1	0	1.870181	-1.270074	-1.821843
11	1	0	2.459107	0.317137	-1.333013
12	6	0	2.974138	-1.273466	0.039080
13	1	0	2.531749	-2.215000	0.391682
14	1	0	3.088751	-0.637312	0.927707
15	6	0	4.355118	-1.546072	-0.570919
16	1	0	4.790701	-0.598749	-0.922054
17	1	0	4.239441	-2.176541	-1.465003
18	6	0	5.328584	-2.221879	0.403291
19	1	0	4.892914	-3.169177	0.754240
20	1	0	5.444182	-1.591975	1.297984
21	6	0	6.710879	-2.495668	-0.203552
22	1	0	7.146312	-1.548896	-0.553736
23	1	0	6.595258	-3.125302	-1.097272
24	6	0	7.677144	-3.170889	0.775058
25	1	0	7.285225	-4.137086	1.116057
26	1	0	8.653842	-3.352604	0.312237
27	1	0	7.840312	-2.548944	1.663889
28	6	0	0.275952	2.228206	-0.340020
29	1	0	-0.699615	2.106269	-0.829183
30	1	0	1.014882	2.317384	-1.148794
31	6	0	0.278861	3.513221	0.497513
32	1	0	1.258558	3.627700	0.985062
33	1	0	-0.456092	3.418118	1.310307
34	6	0	-0.030968	4.773090	-0.321176
35	1	0	-1.010363	4.657854	-0.808603
36	1	0	0.703551	4.868463	-1.134948
37	6	0	-0.030423	6.060652	0.513137
38	1	0	0.948102	6.175545	1.001008
39	1	0	-0.765207	5.965450	1.325114

40	6	0	-0.340217	7.314350	-0.311221
41	1	0	-0.332517	8.215651	0.312325
42	1	0	0.397846	7.455922	-1.110479
43	1	0	-1.328066	7.244237	-0.783014
44	6	0	-2.777236	-1.767435	-0.342460
45	6	0	-4.109726	-1.529057	0.237644
46	8	0	-4.411683	-0.617171	0.987937
47	8	0	-4.992857	-2.475123	-0.174667
48	6	0	-6.335556	-2.341131	0.333520
49	1	0	-6.305771	-2.365980	1.428114
50	1	0	-6.731045	-1.362817	0.040057
51	1	0	-2.665396	-2.625160	-0.999866
52	6	0	-7.156965	-3.481643	-0.239052
53	1	0	-8.188773	-3.417356	0.123670
54	1	0	-7.173005	-3.441176	-1.333048
55	1	0	-6.745142	-4.450116	0.062909

Zero-point correction= 0.500899 (Hartree/Particle)
Thermal correction to Energy= 0.527548
Thermal correction to Enthalpy= 0.528492
Thermal correction to Gibbs Free Energy= 0.438274
Sum of electronic and zero-point Energies= -894.466518
Sum of electronic and thermal Energies= -894.439870
Sum of electronic and thermal Enthalpies= -894.438926
Sum of electronic and thermal Free Energies= -894.529144
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -894.543558

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.605319	-0.967723	1.986477
2	6	0	1.904887	-1.363787	1.928698
3	6	0	-0.162960	-0.337603	0.910514
4	1	0	0.027108	-1.107331	2.905780
5	1	0	2.254961	-1.761026	2.888030
6	30	0	3.283962	-1.437263	0.370542
7	17	0	5.227043	-0.311280	0.314249
8	17	0	2.480773	-2.725386	-1.393411
9	6	0	0.547620	0.463990	-0.157893
10	1	0	1.375357	-0.113701	-0.578792
11	1	0	-0.133825	0.668515	-0.989427
12	6	0	-1.524142	0.170026	1.387080
13	1	0	-2.110838	-0.683744	1.754427
14	1	0	-1.299935	0.754353	2.293492
15	6	0	-2.384048	1.041797	0.461307
16	1	0	-2.575534	0.542971	-0.493696
17	1	0	-1.840705	1.961853	0.213449
18	6	0	-3.722144	1.413550	1.118239
19	1	0	-3.531208	1.909641	2.081244
20	1	0	-4.278743	0.494444	1.356478
21	6	0	-4.594063	2.323994	0.243717
22	1	0	-4.782783	1.831405	-0.722198
23	1	0	-4.037987	3.243434	0.009265
24	6	0	-5.933870	2.694473	0.893679
25	1	0	-5.743578	3.188115	1.857158
26	1	0	-6.489673	1.775197	1.128147
27	6	0	-6.798340	3.604719	0.015014
28	1	0	-7.034208	3.124819	-0.942853
29	1	0	-7.746240	3.850497	0.506666
30	1	0	-6.283354	4.547549	-0.206043
31	6	0	1.112619	1.797324	0.397186
32	1	0	1.795168	1.577208	1.225650
33	1	0	0.300450	2.409819	0.810796
34	6	0	1.854379	2.589331	-0.688852
35	1	0	1.174168	2.785968	-1.530320

36	1	0	2.673396	1.974241	-1.085891
37	6	0	2.426170	3.915259	-0.169123
38	1	0	3.105897	3.710540	0.670225
39	1	0	1.610764	4.533254	0.237117
40	6	0	3.178003	4.710936	-1.244723
41	1	0	2.501012	4.911067	-2.087657
42	1	0	3.992033	4.092069	-1.645722
43	6	0	3.750152	6.033103	-0.722720
44	1	0	4.280849	6.577056	-1.512374
45	1	0	2.955932	6.688056	-0.342565
46	1	0	4.458577	5.861047	0.096738
47	6	0	-0.652200	-2.016655	-0.326035
48	6	0	-1.838291	-1.774797	-1.204435
49	8	0	-1.770807	-1.132321	-2.226795
50	7	0	-0.804663	-3.015161	0.569059
51	7	0	-0.848420	-3.741651	1.424468
52	8	0	-2.957315	-2.318254	-0.689870
53	6	0	-4.170314	-2.149484	-1.477426
54	1	0	-4.390722	-1.079667	-1.543513
55	1	0	-3.976002	-2.517327	-2.488670
56	1	0	0.321880	-2.120605	-0.833126
57	6	0	-5.273809	-2.921844	-0.781973
58	1	0	-6.205654	-2.815564	-1.347278
59	1	0	-5.029401	-3.986846	-0.720188
60	1	0	-5.442135	-2.543455	0.231391

Zero-point correction= 0.510167 (Hartree/Particle)
Thermal correction to Energy= 0.544588
Thermal correction to Enthalpy= 0.545532
Thermal correction to Gibbs Free Energy= 0.436065
Sum of electronic and zero-point Energies= -1989.900793
Sum of electronic and thermal Energies= -1989.866372
Sum of electronic and thermal Enthalpies= -1989.865428
Sum of electronic and thermal Free Energies= -1989.974895
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2151.608136

TS10′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.344721	-0.504833	-1.735014
2	6	0	-1.576768	0.069351	-1.719963
3	6	0	0.670599	-0.458800	-0.684145
4	1	0	-0.028570	-1.086810	-2.606015
5	1	0	-2.088731	-0.064318	-2.680439
6	30	0	-2.954789	0.775115	-0.319254
7	17	0	-2.454136	1.842463	1.642113
8	17	0	-5.069839	0.127935	-0.854252
9	6	0	0.772208	0.769210	0.185303
10	1	0	-0.210784	1.061708	0.564495
11	1	0	1.421885	0.575948	1.047413
12	6	0	1.969551	-1.150510	-1.087449
13	1	0	1.728129	-2.168217	-1.422260
14	1	0	2.292284	-0.624431	-1.999937
15	6	0	3.146920	-1.167121	-0.104891
16	1	0	2.859005	-1.637891	0.846962
17	1	0	3.440587	-0.140295	0.146619
18	6	0	4.362749	-1.913036	-0.675761
19	1	0	4.661762	-1.442745	-1.623735
20	1	0	4.072785	-2.943837	-0.926112
21	6	0	5.562967	-1.937968	0.279422
22	1	0	5.264589	-2.408536	1.228346
23	1	0	5.851089	-0.906132	0.529428
24	6	0	6.779670	-2.679092	-0.290942
25	1	0	7.077848	-2.208318	-1.238363
26	1	0	6.490874	-3.709774	-0.540964

27	6	0	7.974868	-2.700879	0.667589
28	1	0	7.717791	-3.197217	1.611489
29	1	0	8.825664	-3.236015	0.231353
30	1	0	8.308877	-1.684208	0.908604
31	6	0	1.346198	1.979608	-0.597494
32	1	0	0.689092	2.187416	-1.449526
33	1	0	2.334758	1.735363	-1.010499
34	6	0	1.452449	3.223338	0.295879
35	1	0	2.117032	3.007625	1.145644
36	1	0	0.465229	3.441982	0.724100
37	6	0	1.973824	4.454660	-0.457271
38	1	0	1.306059	4.671653	-1.303889
39	1	0	2.958253	4.229210	-0.895058
40	6	0	2.087750	5.702786	0.428538
41	1	0	2.756050	5.486640	1.274298
42	1	0	1.104814	5.924769	0.866238
43	6	0	2.601466	6.932396	-0.327861
44	1	0	2.671756	7.805303	0.330975
45	1	0	3.598178	6.752063	-0.749775
46	1	0	1.933602	7.194684	-1.157582
47	6	0	-0.000807	-1.931633	0.739670
48	6	0	-1.035836	-2.750878	0.023919
49	8	0	-0.702071	-3.579350	-0.793215
50	7	0	-0.421849	-1.294150	1.861450
51	7	0	-0.758484	-0.657676	2.724022
52	8	0	-2.271777	-2.415929	0.390451
53	6	0	-3.396739	-3.132081	-0.233762
54	1	0	-3.719594	-2.520478	-1.078530
55	1	0	-3.020363	-4.092278	-0.590423
56	1	0	0.935855	-2.447145	0.920854
57	6	0	-4.492445	-3.265848	0.803109
58	1	0	-5.340128	-3.795286	0.354514
59	1	0	-4.150414	-3.836199	1.673277
60	1	0	-4.844283	-2.281487	1.123038

Zero-point correction= 0.510548 (Hartree/Particle)
Thermal correction to Energy= 0.544836
Thermal correction to Enthalpy= 0.545781
Thermal correction to Gibbs Free Energy= 0.438503
Sum of electronic and zero-point Energies= -1989.896260
Sum of electronic and thermal Energies= -1989.861972
Sum of electronic and thermal Enthalpies= -1989.861028
Sum of electronic and thermal Free Energies= -1989.968306
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -2151.603324

Entry 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501248	-0.647485	-0.000047
2	6	0	0.501346	0.647419	0.000047
3	6	0	-0.861521	0.000099	-0.000000
4	1	0	1.042734	-1.581656	0.000101
5	1	0	1.043060	1.581466	-0.000101
6	1	0	-1.466117	0.000019	-0.912847
7	1	0	-1.466117	-0.000029	0.912847

Zero-point correction= 0.056277 (Hartree/Particle)
Thermal correction to Energy= 0.059594
Thermal correction to Enthalpy= 0.060538
Thermal correction to Gibbs Free Energy= 0.032331
Sum of electronic and zero-point Energies= -116.562764
Sum of electronic and thermal Energies= -116.559447
Sum of electronic and thermal Enthalpies= -116.558503
Sum of electronic and thermal Free Energies= -116.586710
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -116.564456

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent =-116.565862

Entry 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.268632	-0.000215	-0.648963
2	6	0	1.268820	-0.000059	0.648870
3	6	0	-0.097562	-0.000046	0.000105
4	1	0	1.822540	-0.000762	-1.577739
5	1	0	1.822429	-0.000138	1.577807
6	6	0	-0.940873	1.273507	-0.000067
7	1	0	-1.592576	1.317176	-0.883559
8	1	0	-1.592336	1.317459	0.883592
9	1	0	-0.309560	2.168005	-0.000305
10	6	0	-0.941370	-1.273223	0.000059
11	1	0	-1.592903	-1.316795	0.883684
12	1	0	-1.593037	-1.316738	-0.883473
13	1	0	-0.310441	-2.168000	-0.000031

Zero-point correction= 0.112207 (Hartree/Particle)
Thermal correction to Energy= 0.118166
Thermal correction to Enthalpy= 0.119110
Thermal correction to Gibbs Free Energy= 0.083895
Sum of electronic and zero-point Energies= -195.140861
Sum of electronic and thermal Energies= -195.134901
Sum of electronic and thermal Enthalpies= -195.133957
Sum of electronic and thermal Free Energies= -195.169172
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -195.152582

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent =-195.154290

Entry 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.900611	-1.048515	-0.599581
2	6	0	2.592536	-1.048003	0.660659
3	6	0	2.128877	0.163724	-0.118228
4	1	0	3.389349	-1.529243	-1.435570
5	1	0	2.652299	-1.527640	1.627888
6	6	0	2.891948	1.479426	0.065723
7	1	0	2.765683	2.140243	-0.802932
8	1	0	2.551441	2.034968	0.948590
9	1	0	3.962414	1.287061	0.191253
10	6	0	0.668528	0.370403	-0.583502
11	1	0	0.762639	0.910092	-1.541669
12	6	0	-0.198873	1.273506	0.339566
13	6	0	-0.137370	-0.921481	-0.883149
14	1	0	0.352443	2.187780	0.589570
15	6	0	-0.577973	0.530384	1.638308
16	6	0	-1.488426	1.663760	-0.416340
17	1	0	0.469716	-1.590104	-1.508407
18	6	0	-0.545572	-1.660325	0.410501
19	6	0	-1.424633	-0.533452	-1.645600
20	1	0	-1.163194	1.195999	2.288450
21	1	0	0.325222	0.254689	2.198555
22	6	0	-1.397353	-0.732440	1.298760
23	1	0	-1.234172	2.219818	-1.329545
24	1	0	-2.099097	2.334397	0.204770
25	6	0	-2.292598	0.396698	-0.770209
26	1	0	0.338381	-2.002142	0.960474
27	1	0	-1.119049	-2.561073	0.148574
28	1	0	-1.170179	-0.032808	-2.590143
29	1	0	-1.991074	-1.438525	-1.906882
30	1	0	-1.670495	-1.255749	2.225211

31	6	0	-2.676835	-0.332806	0.534084
32	1	0	-3.201993	0.676021	-1.319290
33	1	0	-3.273037	-1.227733	0.306718
34	1	0	-3.304509	0.318673	1.158446

Zero-point correction= 0.309417 (Hartree/Particle)
Thermal correction to Energy= 0.320842
Thermal correction to Enthalpy= 0.321786
Thermal correction to Gibbs Free Energy= 0.273031
Sum of electronic and zero-point Energies= -545.145944
Sum of electronic and thermal Energies= -545.134520
Sum of electronic and thermal Enthalpies= -545.133575
Sum of electronic and thermal Free Energies= -545.182330
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -545.182695

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent =-545.185209

Entry 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.299681	0.770949	-0.131893
2	6	0	2.592234	-0.448441	-0.480316
3	6	0	1.591431	-0.318791	0.652027
4	6	0	2.081087	-0.610024	2.078134
5	1	0	1.847098	-1.639480	2.383609
6	1	0	1.624684	0.056566	2.821016
7	6	0	0.117206	-0.745038	0.438500
8	1	0	0.105579	-1.814443	0.711791
9	6	0	-0.422396	-0.665761	-1.015093
10	6	0	-0.919854	-0.054206	1.370627
11	1	0	0.307292	-1.118567	-1.699266
12	6	0	-0.699081	0.788411	-1.455107
13	6	0	-1.751022	-1.453040	-1.089460
14	1	0	-0.557099	-0.069799	2.405442
15	6	0	-1.167451	1.405877	0.936536
16	6	0	-2.251800	-0.834103	1.299825
17	1	0	-1.090901	0.788949	-2.482552
18	1	0	0.227685	1.369989	-1.474454
19	6	0	-1.722958	1.438337	-0.503116
20	1	0	-1.585769	-2.504064	-0.814386
21	1	0	-2.130317	-1.449433	-2.121316
22	6	0	-2.792746	-0.816203	-0.144020
23	1	0	-0.237164	1.985380	0.996984
24	1	0	-1.880448	1.881104	1.625235
25	1	0	-2.098659	-1.869420	1.635129
26	1	0	-2.987886	-0.384510	1.981561
27	1	0	-1.902601	2.478769	-0.806963
28	6	0	-3.045927	0.646311	-0.566052
29	1	0	-3.732065	-1.383472	-0.195201
30	1	0	-3.794765	1.104308	0.095610
31	1	0	-3.456419	0.681359	-1.585097
32	1	0	3.167069	-0.478596	2.146079
33	6	0	2.579737	2.227404	-0.212684
34	1	0	2.992811	2.591294	0.737692
35	1	0	3.302454	2.451989	-1.005176
36	1	0	1.669504	2.808458	-0.404937
37	6	0	3.403837	-1.409352	-1.267612
38	1	0	2.767406	-2.097172	-1.838602
39	1	0	4.068721	-0.895147	-1.970710
40	1	0	4.021910	-2.028040	-0.603257

Zero-point correction= 0.366171 (Hartree/Particle)
Thermal correction to Energy= 0.381159
Thermal correction to Enthalpy= 0.382103
Thermal correction to Gibbs Free Energy= 0.325287
Sum of electronic and zero-point Energies= -623.736171

Sum of electronic and thermal Energies= -623.721183
Sum of electronic and thermal Enthalpies= -623.720239
Sum of electronic and thermal Free Energies= -623.777056
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -623.780245

M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent =-623.783077

TS(Ru)-Entry 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.916745	-1.876624	1.775769
2	6	0	-2.849535	-0.949829	1.174902
3	6	0	-3.441667	-1.576344	0.007015
4	6	0	-2.804881	-2.843560	-0.167157
5	6	0	-1.847973	-3.028151	0.920202
6	6	0	-1.200221	-1.704897	3.083284
7	1	0	-0.192759	-2.133740	3.053239
8	1	0	-1.105090	-0.649588	3.359086
9	1	0	-1.744134	-2.201520	3.899047
10	6	0	-3.258310	0.377875	1.742324
11	1	0	-2.450008	0.836768	2.319662
12	1	0	-3.542396	1.079325	0.952555
13	1	0	-4.121990	0.265049	2.413287
14	6	0	-4.510089	-0.993009	-0.868198
15	1	0	-4.504508	0.100191	-0.830412
16	1	0	-4.365542	-1.282331	-1.912572
17	1	0	-5.506807	-1.332987	-0.553024
18	6	0	-3.097515	-3.838010	-1.251053
19	1	0	-3.387421	-3.338381	-2.178805
20	1	0	-2.222677	-4.456561	-1.471631
21	1	0	-3.915048	-4.509150	-0.951852
22	6	0	-1.042423	-4.268699	1.169848
23	1	0	-0.735727	-4.742274	0.232534
24	1	0	-0.137275	-4.049333	1.743810
25	1	0	-1.628035	-5.006128	1.737948
26	17	0	-1.120551	-0.820391	-2.627074
27	44	0	-1.256249	-1.315554	-0.251460
28	6	0	0.909330	0.091803	0.748807
29	6	0	0.821337	-0.800350	-0.256936
30	6	0	1.390211	0.908665	-0.319295
31	1	0	0.433616	0.199569	1.717818
32	1	0	1.378926	-1.284377	-1.040810
33	6	0	0.534474	2.014554	-0.911426
34	1	0	-0.410074	1.581200	-1.262327
35	1	0	1.032890	2.423295	-1.800712
36	6	0	2.875104	0.980515	-0.668448
37	1	0	2.989267	0.928760	-1.761067
38	1	0	3.195684	1.999613	-0.393418
39	6	0	0.249510	3.156873	0.083626
40	1	0	-0.277794	2.752545	0.960067
41	1	0	1.198825	3.566789	0.459516
42	6	0	-0.585553	4.288811	-0.529648
43	1	0	-1.531075	3.874253	-0.908666
44	1	0	-0.059141	4.692830	-1.406801
45	6	0	-0.884799	5.428964	0.452479
46	1	0	-1.412471	5.025254	1.329905
47	1	0	0.062383	5.841139	0.832053
48	6	0	-1.718730	6.562465	-0.159692
49	1	0	-2.665089	6.151090	-0.538577
50	1	0	-1.191588	6.966472	-1.035630
51	6	0	-2.013390	7.697099	0.827255
52	1	0	-2.609455	8.489598	0.360304
53	1	0	-2.570938	7.330426	1.698197
54	1	0	-1.085933	8.151922	1.197034
55	6	0	3.822410	-0.020719	0.000508
56	1	0	3.552386	-1.046315	-0.284101

57	1	0	3.701562	0.030003	1.092005
58	6	0	5.292042	0.228118	-0.366679
59	1	0	5.406433	0.184162	-1.459883
60	1	0	5.573518	1.250314	-0.073042
61	6	0	6.258730	-0.770042	0.283904
62	1	0	5.978633	-1.792372	-0.011028
63	1	0	6.144136	-0.727886	1.377484
64	6	0	7.729090	-0.524508	-0.079813
65	1	0	7.843298	-0.567208	-1.172325
66	1	0	8.009107	0.496920	0.215057
67	6	0	8.688063	-1.525529	0.573303
68	1	0	9.728596	-1.323643	0.294332
69	1	0	8.622025	-1.481881	1.667579
70	1	0	8.455202	-2.553618	0.269369

Zero-point correction= 0.622266 (Hartree/Particle)
Thermal correction to Energy= 0.658762
Thermal correction to Enthalpy= 0.659706
Thermal correction to Gibbs Free Energy= 0.547578
Sum of electronic and zero-point Energies= -1531.977940
Sum of electronic and thermal Energies= -1531.941444
Sum of electronic and thermal Enthalpies= -1531.940500
Sum of electronic and thermal Free Energies= -1532.052628
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1533.112907

TS(Ru)-Entry 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.038338	1.531986	0.230413
2	6	0	1.065623	0.582861	1.322805
3	6	0	1.580695	-0.681880	0.827450
4	6	0	1.772647	-0.540882	-0.580761
5	6	0	1.433104	0.829619	-0.955860
6	6	0	0.707493	2.992481	0.331237
7	1	0	0.260252	3.368856	-0.594014
8	1	0	0.001765	3.193576	1.143924
9	1	0	1.608865	3.589226	0.530188
10	6	0	0.765905	0.888020	2.760998
11	1	0	0.042521	1.703330	2.858597
12	1	0	0.357198	0.015041	3.278041
13	1	0	1.679151	1.193052	3.291929
14	6	0	1.845756	-1.907449	1.649212
15	1	0	1.162917	-1.971324	2.501204
16	1	0	1.713098	-2.818031	1.059403
17	1	0	2.872694	-1.901852	2.041521
18	6	0	2.290323	-1.593323	-1.516050
19	1	0	2.035061	-2.597101	-1.166871
20	1	0	1.869857	-1.477082	-2.519554
21	1	0	3.384262	-1.531657	-1.604703
22	6	0	1.599465	1.419450	-2.325351
23	1	0	1.374078	0.687595	-3.107213
24	1	0	0.940436	2.279826	-2.474763
25	1	0	2.633036	1.760919	-2.481310
26	17	0	-1.569072	-2.214164	-0.136968
27	44	0	-0.329580	-0.143427	-0.155400
28	6	0	-2.727815	1.341327	0.267848
29	6	0	-2.191993	0.704437	-0.791062
30	6	0	-3.774000	0.421829	-0.010212
31	1	0	-2.317418	1.852493	1.131603
32	1	0	-2.401885	0.471486	-1.823690
33	1	0	-4.513873	0.658016	-0.767750
34	1	0	-3.959500	-0.455639	0.605512

Zero-point correction= 0.279867 (Hartree/Particle)
Thermal correction to Energy= 0.299733

Thermal correction to Enthalpy= 0.300677
Thermal correction to Gibbs Free Energy= 0.230494
Sum of electronic and zero-point Energies= -1060.556617
Sum of electronic and thermal Energies= -1060.536751
Sum of electronic and thermal Enthalpies= -1060.535807
Sum of electronic and thermal Free Energies= -1060.605989
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent = -1061.604004

TS(Ru)-Entry 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327772	1.618112	0.040476
2	6	0	1.253429	0.883174	1.281114
3	6	0	1.835387	-0.432174	1.078565
4	6	0	2.183103	-0.538897	-0.300457
5	6	0	1.849461	0.721595	-0.956063
6	6	0	0.992806	3.066287	-0.167624
7	1	0	0.542665	3.240947	-1.150641
8	1	0	0.293425	3.435770	0.589344
9	1	0	1.894411	3.691399	-0.103129
10	6	0	0.805135	1.430158	2.604932
11	1	0	0.071438	2.232776	2.485027
12	1	0	0.350520	0.652662	3.226187
13	1	0	1.657789	1.842541	3.163054
14	6	0	2.021237	-1.490179	2.124500
15	1	0	1.294420	-1.383394	2.935175
16	1	0	1.892735	-2.489719	1.700529
17	1	0	3.025440	-1.433867	2.568223
18	6	0	2.808678	-1.729211	-0.964357
19	1	0	2.459974	-2.661886	-0.514176
20	1	0	2.559901	-1.768265	-2.028502
21	1	0	3.903489	-1.690100	-0.876142
22	6	0	2.146968	1.066135	-2.385132
23	1	0	2.034069	0.195920	-3.038029
24	1	0	1.478422	1.848879	-2.755047
25	1	0	3.179515	1.429867	-2.490384
26	17	0	-0.796626	-2.432934	-0.399696
27	44	0	0.029503	-0.148115	-0.197262
28	6	0	-2.190792	1.325993	-0.246220
29	6	0	-1.810980	0.331426	-1.085557
30	6	0	-3.221554	0.401476	0.101474
31	1	0	-1.700255	2.191397	0.186908
32	1	0	-2.214293	-0.294173	-1.865226
33	6	0	-4.506120	0.329255	-0.699109
34	1	0	-4.819313	-0.709388	-0.862608
35	1	0	-5.313749	0.827333	-0.142196
36	1	0	-4.413468	0.828770	-1.667522
37	6	0	-3.210782	-0.375871	1.396150
38	1	0	-4.140328	-0.201263	1.955431
39	1	0	-3.132774	-1.452496	1.193047
40	1	0	-2.362007	-0.100441	2.028862

Zero-point correction= 0.336202 (Hartree/Particle)
Thermal correction to Energy= 0.358961
Thermal correction to Enthalpy= 0.359905
Thermal correction to Gibbs Free Energy= 0.283291
Sum of electronic and zero-point Energies= -1139.136681
Sum of electronic and thermal Energies= -1139.113922
Sum of electronic and thermal Enthalpies= -1139.112978
Sum of electronic and thermal Free Energies= -1139.189592
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1140.199257

TS(Ru)-Entry 5

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

1	6	0	-2.664658	1.723014	-0.524575
2	6	0	-3.163311	0.642550	-1.347156
3	6	0	-3.962318	-0.241799	-0.519999
4	6	0	-3.872779	0.235445	0.824815
5	6	0	-3.061223	1.449255	0.827632
6	6	0	-1.927017	2.940978	-0.998939
7	1	0	-1.172451	3.266147	-0.274535
8	1	0	-1.418825	2.762151	-1.952153
9	1	0	-2.615567	3.783219	-1.155603
10	6	0	-3.010240	0.528402	-2.835586
11	1	0	-2.086464	1.000039	-3.183953
12	1	0	-2.990583	-0.517342	-3.155719
13	1	0	-3.847943	1.018936	-3.351816
14	6	0	-4.722968	-1.447341	-0.984629
15	1	0	-4.294579	-1.860202	-1.902449
16	1	0	-4.702413	-2.240560	-0.232465
17	1	0	-5.773216	-1.195682	-1.189510
18	6	0	-4.539390	-0.370559	2.023798
19	1	0	-5.546914	0.047271	2.160888
20	1	0	-4.630721	-1.454650	1.920197
21	1	0	-3.970709	-0.174673	2.937602
22	6	0	-2.810226	2.325783	2.018990
23	1	0	-2.718411	1.737519	2.936927
24	1	0	-1.890419	2.906592	1.902466
25	1	0	-3.637558	3.036051	2.162163
26	17	0	-1.531989	-2.539544	0.764504
27	44	0	-1.854241	-0.210751	0.155160
28	6	0	0.744739	0.517836	-0.591180
29	6	0	0.258060	-0.057962	0.522991
30	6	0	1.521546	-0.679969	-0.596458
31	1	0	0.369836	1.252969	-1.296477
32	1	0	0.524229	-0.479543	1.477088
33	6	0	1.189875	-1.796672	-1.565485
34	1	0	1.650395	-2.743694	-1.262519
35	1	0	1.542079	-1.559762	-2.580412
36	6	0	2.880293	-0.801942	0.115823
37	1	0	2.848124	-1.755399	0.665889
38	6	0	3.263936	0.311081	1.126898
39	6	0	4.049031	-0.929072	-0.915688
40	1	0	2.458694	0.446673	1.858838
41	6	0	3.544145	1.656196	0.421669
42	6	0	4.543285	-0.127103	1.876939
43	1	0	3.800197	-1.694758	-1.658811
44	6	0	4.304495	0.416971	-1.625171
45	6	0	5.327282	-1.362107	-0.164334
46	1	0	3.808037	2.411408	1.175159
47	1	0	2.644868	2.024372	-0.088184
48	6	0	4.696741	1.489974	-0.588440
49	1	0	4.364302	-1.069598	2.412213
50	1	0	4.800415	0.625865	2.634579
51	6	0	5.708339	-0.294976	0.879804
52	1	0	3.410809	0.735727	-2.179002
53	1	0	5.106962	0.294818	-2.365727
54	1	0	5.165452	-2.332755	0.324103
55	1	0	6.147771	-1.499501	-0.882345
56	1	0	4.882698	2.445166	-1.097396
57	6	0	5.970695	1.045526	0.161489
58	1	0	6.612015	-0.609445	1.418488
59	1	0	6.806666	0.937670	-0.543682
60	1	0	6.264819	1.813981	0.889917
61	1	0	0.108841	-1.954751	-1.606631

Zero-point correction= 0.532941 (Hartree/Particle)
Thermal correction to Energy= 0.561605
Thermal correction to Enthalpy= 0.562550
Thermal correction to Gibbs Free Energy= 0.471870

Sum of electronic and zero-point Energies= -1489.136543
Sum of electronic and thermal Energies= -1489.107879
Sum of electronic and thermal Enthalpies= -1489.106934
Sum of electronic and thermal Free Energies= -1489.197614
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1490.228844

TS(Ru)-Entry 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.362002	0.998349	-1.153065
2	6	0	-4.137698	-0.046219	-0.509817
3	6	0	-3.970459	0.101503	0.906005
4	6	0	-3.112901	1.256153	1.139124
5	6	0	-2.771829	1.830671	-0.133763
6	6	0	-3.332926	1.245553	-2.633182
7	1	0	-2.473631	1.851779	-2.932330
8	1	0	-3.292213	0.307606	-3.195462
9	1	0	-4.239140	1.781502	-2.949819
10	6	0	-4.975949	-1.079178	-1.202023
11	1	0	-6.016402	-0.738449	-1.303031
12	1	0	-4.596884	-1.293236	-2.205717
13	1	0	-4.977748	-2.021741	-0.648311
14	6	0	-4.614209	-0.742551	1.965728
15	1	0	-5.601239	-0.341463	2.237111
16	1	0	-4.746064	-1.772483	1.624718
17	1	0	-4.006390	-0.774240	2.874960
18	6	0	-2.777649	1.833523	2.482667
19	1	0	-3.570361	2.516382	2.820967
20	1	0	-2.672684	1.053444	3.243205
21	1	0	-1.844451	2.405057	2.455006
22	6	0	-2.029529	3.120510	-0.337825
23	1	0	-1.194499	3.224393	0.362853
24	1	0	-1.621493	3.202170	-1.349459
25	1	0	-2.694855	3.982711	-0.187740
26	17	0	-1.789345	-2.659212	0.150639
27	44	0	-2.034860	-0.256516	0.034240
28	6	0	0.827003	0.135468	-0.819286
29	6	0	0.279438	-0.110017	0.377613
30	6	0	1.730851	-0.906838	-0.436228
31	6	0	1.573537	-2.286667	-1.046117
32	1	0	1.888919	-3.074382	-0.351011
33	1	0	2.181622	-2.391740	-1.956613
34	6	0	3.002468	-0.660569	0.385908
35	1	0	2.891861	-1.221402	1.330979
36	6	0	3.325591	0.816977	0.753504
37	6	0	4.275403	-1.261797	-0.297150
38	1	0	2.449497	1.291855	1.206857
39	6	0	3.748351	1.633932	-0.487378
40	6	0	4.490092	0.831587	1.770017
41	1	0	4.082013	-2.299522	-0.586279
42	6	0	4.675694	-0.443130	-1.542111
43	6	0	5.438006	-1.243258	0.719645
44	1	0	3.958134	2.668906	-0.182734
45	1	0	2.933053	1.683187	-1.217560
46	6	0	4.999829	1.008206	-1.132886
47	1	0	4.209599	0.278635	2.677489
48	1	0	4.696526	1.865614	2.079352
49	6	0	5.750751	0.206384	1.137545
50	1	0	3.866594	-0.453207	-2.285089
51	1	0	5.549970	-0.906198	-2.020316
52	1	0	5.176627	-1.845987	1.600336
53	1	0	6.326971	-1.706684	0.269441
54	1	0	5.287332	1.587430	-2.020574
55	6	0	6.157230	1.015520	-0.112045
56	1	0	6.572045	0.213518	1.866465

57	1	0	7.062107	0.583615	-0.562009
58	1	0	6.403018	2.049033	0.169520
59	1	0	0.529332	-2.478870	-1.302060
60	6	0	0.404870	0.691057	-2.140522
61	1	0	0.035208	-0.108708	-2.795005
62	1	0	-0.385108	1.433708	-2.023216
63	1	0	1.265873	1.147067	-2.645410
64	6	0	0.329496	-0.300153	1.859817
65	1	0	1.350387	-0.313891	2.263012
66	1	0	-0.226199	0.491868	2.371575
67	1	0	-0.145395	-1.254064	2.113441

Zero-point correction= 0.590758 (Hartree/Particle)
Thermal correction to Energy= 0.622372
Thermal correction to Enthalpy= 0.623316
Thermal correction to Gibbs Free Energy= 0.528179
Sum of electronic and zero-point Energies= -1567.707058
Sum of electronic and thermal Energies= -1567.675444
Sum of electronic and thermal Enthalpies= -1567.674499
Sum of electronic and thermal Free Energies= -1567.769637
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in tetrahydrofuran solvent =-1568.81702

TS(Zn)-Entry 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.637944	-0.265936	-2.262748
2	6	0	-0.059545	-1.170968	-1.578447
3	6	0	0.901049	0.270572	-0.943655
4	1	0	1.236075	-0.263523	-3.170629
5	1	0	-0.000819	-2.244375	-1.793865
6	30	0	-1.589170	-1.103948	0.031184
7	17	0	-3.592416	-0.495976	-0.739749
8	17	0	-0.833625	-2.268047	1.796101
9	6	0	-0.026340	1.234917	-0.281842
10	6	0	-0.767483	2.138757	-1.062047
11	6	0	-0.164673	1.265236	1.120612
12	6	0	-1.629639	3.050480	-0.456448
13	1	0	-0.667809	2.117818	-2.142940
14	6	0	-1.037764	2.174847	1.718747
15	1	0	0.396209	0.567189	1.734483
16	6	0	-1.768546	3.069054	0.932814
17	1	0	-2.201335	3.738820	-1.071496
18	1	0	-1.150008	2.176434	2.798749
19	1	0	-2.450578	3.772360	1.401469
20	6	0	2.288246	0.117630	-0.432433
21	6	0	2.920457	1.166807	0.263629
22	6	0	3.022437	-1.052706	-0.699778
23	6	0	4.247463	1.046970	0.667438
24	1	0	2.375150	2.080673	0.471616
25	6	0	4.345124	-1.174213	-0.279839
26	1	0	2.544157	-1.883549	-1.207884
27	6	0	4.962836	-0.123587	0.400921
28	1	0	4.723262	1.868397	1.195351
29	1	0	4.889822	-2.092577	-0.478220
30	1	0	5.994299	-0.218007	0.728315

Zero-point correction= 0.220990 (Hartree/Particle)
Thermal correction to Energy= 0.238572
Thermal correction to Enthalpy= 0.239517
Thermal correction to Gibbs Free Energy= 0.171926
Sum of electronic and zero-point Energies= -1564.575151
Sum of electronic and thermal Energies= -1564.557569
Sum of electronic and thermal Enthalpies= -1564.556624
Sum of electronic and thermal Free Energies= -1564.624215
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1726.122768

TS(Zn)-Entry 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.344921	-1.582107	-0.453277
2	6	0	1.074484	-1.474829	0.023614
3	6	0	2.720752	-0.517500	0.363467
4	1	0	2.934143	-2.439168	-0.771788
5	1	0	0.630985	-2.409845	0.386638
6	30	0	-0.432083	0.111507	0.006912
7	17	0	0.504695	2.151537	-0.080369
8	17	0	-2.460822	-0.791189	0.033316
9	1	0	2.269360	0.470501	0.301586
10	1	0	3.541213	-0.646026	1.073300

Zero-point correction= 0.058851 (Hartree/Particle)
Thermal correction to Energy= 0.067228
Thermal correction to Enthalpy= 0.068172
Thermal correction to Gibbs Free Energy= 0.023039
Sum of electronic and zero-point Energies= -1102.629335
Sum of electronic and thermal Energies= -1102.620957
Sum of electronic and thermal Enthalpies= -1102.620013
Sum of electronic and thermal Free Energies= -1102.665146
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1264.2485

TS(Zn)-Entry 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.924799	-1.628937	-0.805627
2	6	0	-0.824570	-0.937524	-1.140885
3	6	0	-2.078295	-0.659704	0.228664
4	1	0	-2.671301	-2.165087	-1.387642
5	1	0	-0.670200	-0.741961	-2.209702
6	6	0	-3.202802	0.338578	0.139036
7	1	0	-3.817599	0.304816	1.046473
8	1	0	-2.767027	1.344942	0.076799
9	1	0	-3.836391	0.178543	-0.737631
10	6	0	-1.355303	-0.711746	1.552766
11	1	0	-1.031605	0.283472	1.877530
12	1	0	-2.076982	-1.072773	2.299921
13	1	0	-0.511811	-1.407160	1.544482
14	30	0	0.831216	0.150201	-0.220444
15	17	0	2.582976	-1.123423	0.286163
16	17	0	0.285321	2.321374	-0.035611

Zero-point correction= 0.114989 (Hartree/Particle)
Thermal correction to Energy= 0.126280
Thermal correction to Enthalpy= 0.127224
Thermal correction to Gibbs Free Energy= 0.075372
Sum of electronic and zero-point Energies= -1181.211661
Sum of electronic and thermal Energies= -1181.200370
Sum of electronic and thermal Enthalpies= -1181.199426
Sum of electronic and thermal Free Energies= -1181.251278
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1342.847352

TS(Zn)-Entry 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.347050	-1.881074	-0.901271
2	6	0	1.347448	-1.039565	-1.180947
3	6	0	0.066523	-0.915928	0.124505
4	1	0	-0.276286	-2.535420	-1.501871
5	1	0	1.547584	-0.802198	-2.232856

6	30	0	2.849134	0.213341	-0.194141
7	17	0	4.700282	-0.894829	0.347407
8	17	0	2.115237	2.328663	-0.050576
9	6	0	0.761568	-0.972834	1.470070
10	1	0	1.669120	-1.581473	1.434761
11	1	0	0.988056	0.026174	1.859857
12	1	0	0.078656	-1.448845	2.185890
13	6	0	-1.101194	0.062466	-0.004749
14	1	0	-0.579366	1.026607	-0.132492
15	6	0	-1.993252	0.209433	1.266161
16	6	0	-2.027987	-0.150521	-1.231453
17	1	0	-1.363447	0.348508	2.150855
18	6	0	-2.896151	-1.029222	1.449238
19	6	0	-2.876910	1.464871	1.090697
20	1	0	-1.420263	-0.279373	-2.136641
21	6	0	-2.943335	-1.380968	-1.034046
22	6	0	-2.912219	1.106090	-1.397787
23	1	0	-3.496439	-0.911434	2.361102
24	1	0	-2.291396	-1.937482	1.587105
25	6	0	-3.817048	-1.192339	0.222060
26	1	0	-2.244393	2.356036	0.986411
27	1	0	-3.485896	1.608427	1.993336
28	6	0	-3.787253	1.302569	-0.142513
29	1	0	-2.357517	-2.304707	-0.935403
30	1	0	-3.576954	-1.507787	-1.922006
31	1	0	-2.281674	1.989271	-1.564753
32	1	0	-3.546372	0.992900	-2.287246
33	1	0	-4.458110	-2.072739	0.358297
34	6	0	-4.691489	0.068021	0.054480
35	1	0	-4.406187	2.200541	-0.263837
36	1	0	-5.361934	-0.052903	-0.807337
37	1	0	-5.329507	0.204513	0.938265

Zero-point correction= 0.312276 (Hartree/Particle)
Thermal correction to Energy= 0.329153
Thermal correction to Enthalpy= 0.330097
Thermal correction to Gibbs Free Energy= 0.265188
Sum of electronic and zero-point Energies= -1531.212764
Sum of electronic and thermal Energies= -1531.195887
Sum of electronic and thermal Enthalpies= -1531.194943
Sum of electronic and thermal Free Energies= -1531.259852
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1692.878863

TS(Zn)-Entry 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440130	1.944339	-0.074632
2	6	0	1.472242	1.316957	0.521450
3	6	0	0.001485	0.671601	-0.593040
4	30	0	2.719609	-0.400823	0.067208
5	17	0	4.651826	0.083590	-0.944601
6	17	0	1.852952	-2.305394	0.920734
7	6	0	0.658923	0.095219	-1.828881
8	1	0	1.582149	0.620916	-2.084985
9	1	0	0.835642	-0.984551	-1.759264
10	1	0	-0.038087	0.241663	-2.667047
11	6	0	-1.170476	-0.128538	-0.029157
12	1	0	-0.622478	-0.886228	0.560071
13	6	0	-2.017433	-0.941498	-1.058927
14	6	0	-2.143340	0.599263	0.935978
15	1	0	-1.359810	-1.455291	-1.766017
16	6	0	-2.997359	-0.024539	-1.820586
17	6	0	-2.818611	-2.008532	-0.278582
18	1	0	-1.571427	1.196307	1.657044
19	6	0	-3.133297	1.499945	0.160212

20	6	0	-2.947965	-0.471642	1.709154
21	1	0	-3.560778	-0.620361	-2.550905
22	1	0	-2.452687	0.741094	-2.392628
23	6	0	-3.961394	0.651989	-0.824773
24	1	0	-2.129197	-2.684941	0.242765
25	1	0	-3.392994	-2.620173	-0.987271
26	6	0	-3.770689	-1.327117	0.723713
27	1	0	-2.604794	2.283725	-0.394781
28	1	0	-3.795798	2.010233	0.872645
29	1	0	-2.266075	-1.108161	2.288230
30	1	0	-3.615101	0.021446	2.429013
31	1	0	-4.657095	1.302285	-1.370670
32	6	0	-4.752081	-0.420949	-0.047911
33	1	0	-4.328937	-2.091065	1.279557
34	1	0	-5.452231	0.060781	0.648365
35	1	0	-5.355266	-1.021948	-0.741989
36	6	0	1.938018	1.701928	1.920350
37	1	0	1.710660	0.886913	2.619673
38	1	0	3.026814	1.836778	1.935315
39	1	0	1.467489	2.617803	2.297247
40	6	0	-0.210888	3.270661	0.178214
41	1	0	-0.679249	3.655699	-0.733373
42	1	0	-0.983103	3.228784	0.953672
43	1	0	0.549255	3.989116	0.499328

Zero-point correction= 0.369150 (Hartree/Particle)
Thermal correction to Energy= 0.389257
Thermal correction to Enthalpy= 0.390201
Thermal correction to Gibbs Free Energy= 0.318976
Sum of electronic and zero-point Energies= -1609.792335
Sum of electronic and thermal Energies= -1609.772228
Sum of electronic and thermal Enthalpies= -1609.771284
Sum of electronic and thermal Free Energies= -1609.842509
M06/6-311++G(d,p)-SDD/SMD//B3LYP/6-31G(d)-LANL2DZ energy in dichloromethane solvent = -1771.471433