Electronic Supplementary Material (ESI) for New Journal of Chemistry

DFT Investigation on C-H Bond Activation of Malononitrile in the Presence of Amines

Zhishan Su and Chan Kyung Kim*

Department of Chemistry, Inha University, Incheon 402-751, Korea

Supporting Information:

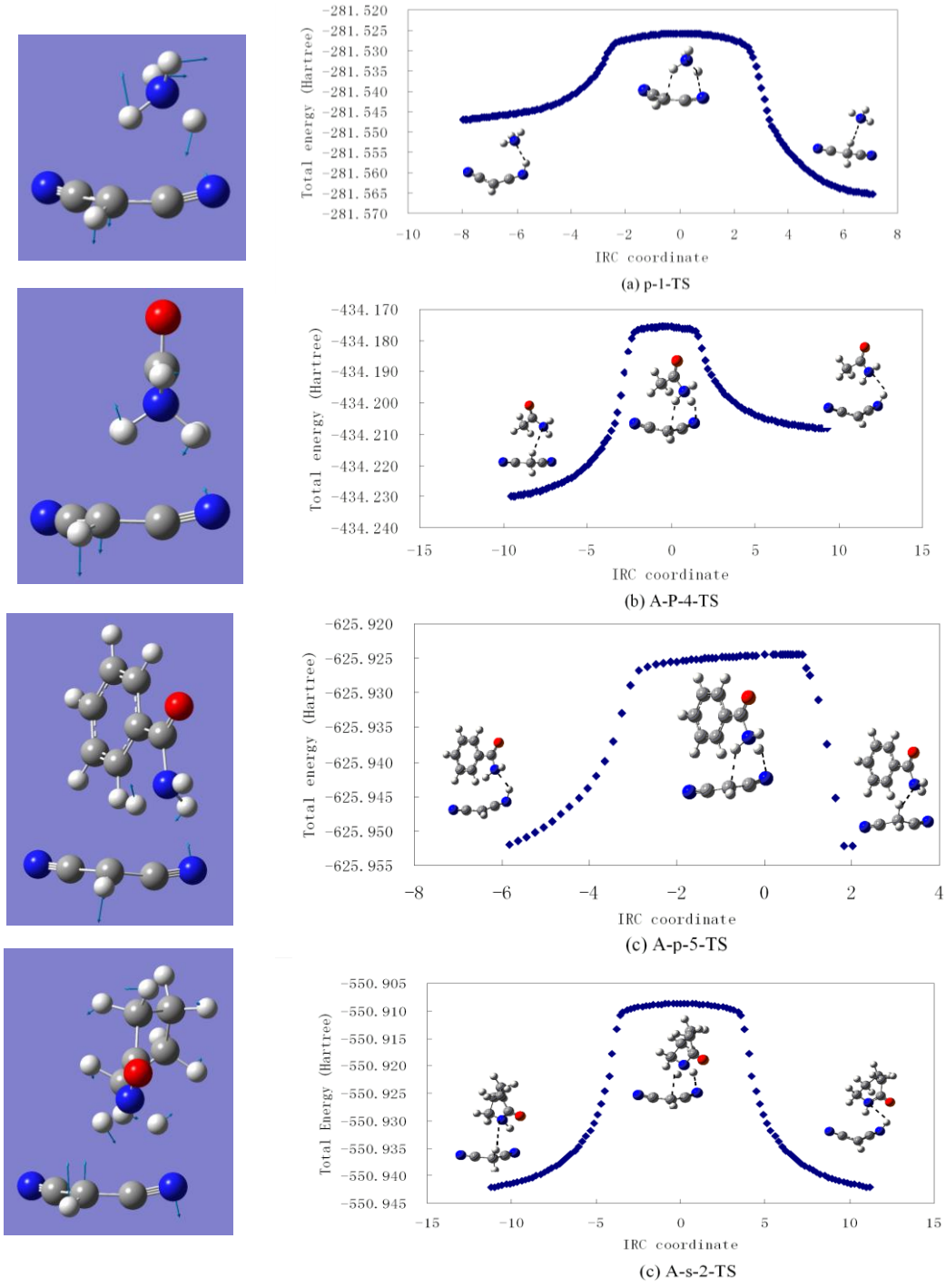
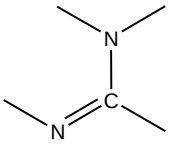


Fig. S1 Reaction-coordinate vectors of imaginary frequency at the TSs and potential energy profile along IRC paths for transition states, **p-1-TS**, **A-p-4-TS**, **A-p-5-TS**, and **A-s-2-TS**.



(*Z*)-*N*,*N*,*N*'-trimethylacetamidine
(**DBU-M**)

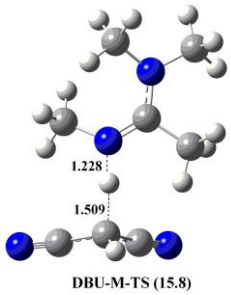
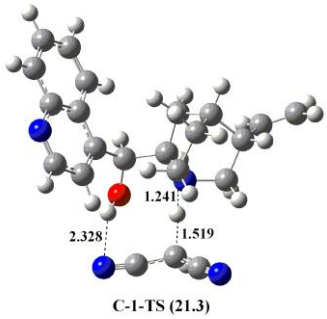


Fig. S2. Optimized geometries of transition states for deprotonation of malononitrile catalyzed by **DBU-M**. Relative Gibbs free energies are shown in parentheses (kcal mol^{-1}).



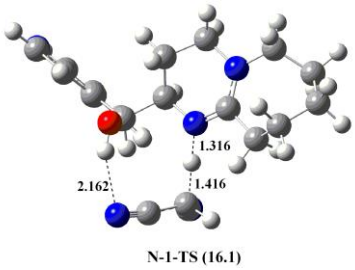


Fig. S3. Optimized geometries of transition states for deprotonation of malononitrile catalyzed by **C-1** and **N-1**. Relative Gibbs free energies are shown in parentheses (kcal mol^{-1}).

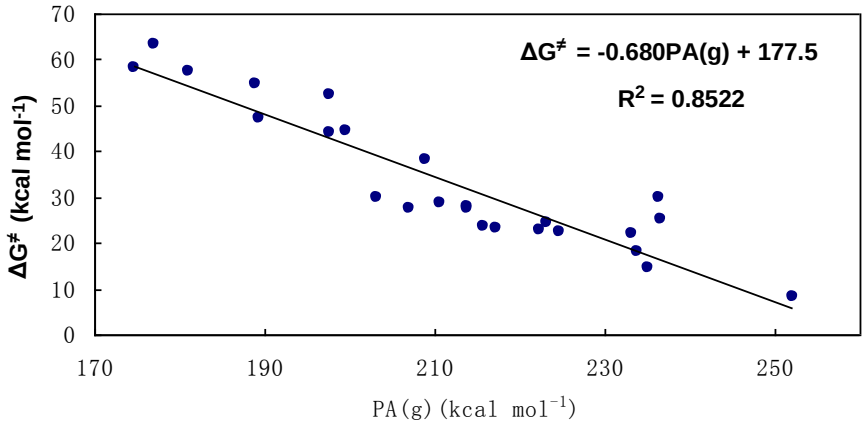
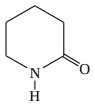
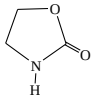
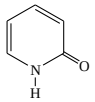
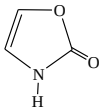
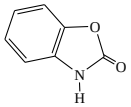


Fig. S4. A plot of activation free energy ($\Delta G^{\neq}$) *vs.* gas-phase proton affinity (PA) of amines.

Table S1 Calculated the pKa values and the corresponding experimental values.

Compound	pKa	
	Exp[ref.]	**Theor**
NH_3-**H**$^+$	10.5[32]	11.0
NH_2-**H**	41[40]	41.1
CH_3NH_2-**H**$^+$	11[32]	12.8
$PhNH_2$-**H**$^+$	3.6[32]	4.3
PhNH-**H**	30.6[38]	32.0
CH_3CONH-**H**	25.5[38]	25.4
PhCONH-**H**	23.35[38]	23.2
	26.4[32]	26.5
	24.2[32]	24.8
	20.8[33]	20.6
	17[32]	17.6
	15[34]	14.5
	12.1[34]	12.6

XYZ Coordinates and Energies of all the species studied in this work.

$CH_2(CN)_2$
Energy + zep (gas) = -224.94563 au
Gibbs free energy (gas) = -224.97337 au
Energy (sol) = -225.01181 au
Thermal correction to Gibbs free energy = 0.01682 au
Gibbs free energy (sol) = -224.99499 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.835130	0.000003
2	6	0	1.225517	0.023856	-0.000082

3	6	0	-1.225517	0.023856	0.000068
4	1	0	-0.000075	1.484662	-0.883538
5	1	0	0.000076	1.484636	0.883563
6	7	0	-2.208851	-0.590454	-0.000028
7	7	0	2.208851	-0.590454	0.000034

1-TS
Energy + zep (gas) = -224.82315 au
Gibbs free energy (gas) = -224.85109 au
Energy (sol) = -224.87047 au
Thermal correction to Gibbs free energy = 0.00943 au
Gibbs free energy (sol) = -224.86104 au
Number and value of imaginary frequency: 1, -1039.1cm^{-1}
Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.052431	0.749518	-0.080634
2	6	0	-1.272875	0.052950	-0.018553
3	6	0	1.178389	0.068899	-0.024904
4	1	0	-0.033309	1.827591	0.035959
5	1	0	1.291995	0.087464	1.125629
6	7	0	2.244276	-0.513111	-0.075558
7	7	0	-2.298159	-0.507354	0.015980

2-TS
Energy + zep (gas) = -674.75667 au
Gibbs free energy (gas) = -674.80381 au
Energy (sol) = -674.89990 au
Thermal correction to Gibbs free energy = 0.07553 au
Gibbs free energy (sol) = -449.86250 au
Number and value of imaginary frequency: 1, -1754.8cm^{-1}
Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.071083	3.233405	-1.551560
2	6	0	-1.033497	2.688315	-0.606406
3	6	0	-1.748358	1.489470	-0.619936
4	6	0	-1.121690	3.501538	0.573724
5	1	0	0.442164	2.175176	-0.623767
6	7	0	-1.126706	4.170340	1.526553
7	7	0	-2.286475	0.448033	-0.659911
8	7	0	1.533746	1.757469	-0.653956
9	1	0	-2.107176	-0.706357	-0.630437
10	6	0	2.167228	0.770872	-0.616640
11	6	0	2.848280	-0.447407	-0.606348
12	1	0	3.339584	-0.685014	-1.551850
13	1	0	1.663642	-1.469702	-0.626937
14	6	0	3.595104	-0.782026	0.573422
15	7	0	4.175419	-1.115838	1.525816
16	7	0	0.754358	-2.202233	-0.656348
17	6	0	-0.416562	-2.259055	-0.617167

18	6	0	-1.812251	-2.242025	-0.607131
19	1	0	-2.262548	-2.551492	-1.552281
20	6	0	-2.474908	-2.720814	0.573243
21	7	0	-3.053863	-3.056232	1.525885

3-TS
Energy + zep (gas) = -449.81375 au
Gibbs free energy (gas) = -449.85014 au
Energy (sol) = -449.90645 au
Thermal correction to Gibbs free energy = 0.04395 au
Gibbs free energy (sol) = -674.82437 au
Number and value of imaginary frequency: 1, -1281.7cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.961683	0.910118	-0.628241
2	7	0	0.040765	1.525607	-0.345253
3	6	0	1.004792	1.076331	0.158154
4	6	0	1.972157	0.264268	0.774390
5	6	0	3.172493	-0.031231	0.048021
6	1	0	2.094257	0.432917	1.844872
7	1	0	0.961727	-0.910065	0.628111
8	7	0	4.137838	-0.327599	-0.531628
9	7	0	-0.040738	-1.525579	0.345170
10	6	0	-1.004781	-1.076302	-0.158204
11	6	0	-1.972198	-0.264270	-0.774395
12	6	0	-3.172499	0.031216	-0.047965
13	1	0	-2.094363	-0.432943	-1.844866
14	7	0	-4.137825	0.327556	0.531729

p-1
Energy + zep (gas) = -56.53273 au
Gibbs free energy (gas) = -56.55076 au
Enthalpies (gas) = -56.52891 au
Energy (sol) = -56.57108 au
Thermal correction to Gibbs free energy = 0.01635 au
Gibbs free energy (sol) = -56.55473 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.108414
2	1	0	0.000000	0.949353	-0.252966
3	1	0	-0.822164	-0.474677	-0.252966
4	1	0	0.822164	-0.474677	-0.252966

p-1-COM
Energy + zep (gas) = -281.48684 au
Gibbs free energy (gas) = -281.52205 au
Energy (sol) = -281.57870 au
Thermal correction to Gibbs free energy = 0.04588 au

Gibbs free energy (sol) = -281.53283 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.859062	-0.047751	-0.121359
2	1	0	0.796850	-0.024271	0.481547
3	7	0	-1.324285	-2.189386	-0.379559
4	6	0	-0.891975	-1.209694	0.066778
5	6	0	-0.299055	0.000580	0.648578
6	6	0	-0.834746	1.237853	0.068025
7	1	0	-0.476643	0.004158	1.730773
8	7	0	-1.220305	2.237267	-0.377420
9	1	0	3.545520	-0.045984	0.629267
10	1	0	3.038581	-0.872190	-0.690073
11	1	0	3.049043	0.764952	-0.703437

p-1-TS

Energy + zep (gas) = -281.44396 au

Gibbs free energy (gas) = -281.47554 au

Energy (sol) = -281.55211 au

Thermal correction to Gibbs free energy = 0.05016 au

Gibbs free energy (sol) = -281.50195 au

Number and value of imaginary frequency: 1, -159.3cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.492842	1.479015	0.119867
2	1	0	0.663892	1.105073	0.656587
3	7	0	1.583034	-1.203283	-0.588491
4	6	0	0.562409	-1.093912	0.000872
5	6	0	-0.548485	-0.668619	0.724343
6	6	0	-1.609828	-0.023705	0.044923
7	1	0	-0.736618	-1.093730	1.704598
8	7	0	-2.441725	0.593513	-0.503001
9	1	0	2.161180	1.950438	0.726372
10	1	0	1.876502	0.569319	-0.285921
11	1	0	1.171406	2.101598	-0.621090

p-2

Energy + zep (gas) = -95.80797 au

Gibbs free energy (gas) = -95.83090 au

Enthalpies (gas) = -95.80360 au

Energy (sol) = -95.87568 au

Thermal correction to Gibbs free energy = 0.04108 au

Gibbs free energy (sol) = -95.83460 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.750529	-0.000007	-0.118799

2	1	0	1.159995	-0.817840	0.323960
3	1	0	1.159954	0.817845	0.323964
4	6	0	-0.709431	-0.000007	0.017726
5	1	0	-1.116459	0.881459	-0.487897
6	1	0	-1.116629	-0.880659	-0.489186
7	1	0	-1.083980	-0.000715	1.054395

p-2-COM
Energy + zep (gas) = -320.76244 au
Gibbs free energy (gas) = -320.80092 au
Energy (sol) = -320.88318 au
Thermal correction to Gibbs free energy = 0.07162 au
Gibbs free energy (sol) = -320.81157 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.176986	-0.374152	-0.553421
2	1	0	0.228509	-0.130429	0.266251
3	7	0	-2.212726	-2.058788	-0.238987
4	6	0	-1.620994	-1.127877	0.120654
5	6	0	-0.826174	0.014378	0.586865
6	6	0	-1.303977	1.299097	0.062317
7	1	0	-0.846008	0.043285	1.682987
8	7	0	-1.637598	2.332923	-0.345155
9	6	0	3.281276	0.055701	0.320683
10	1	0	4.280194	-0.046116	-0.126539
11	1	0	3.135647	1.104964	0.593630
12	1	0	2.293749	-1.348875	-0.821052
13	1	0	2.180800	0.161943	-1.418400
14	1	0	3.259685	-0.532442	1.242949

p-2-TS
Energy + zep (gas) = -320.72926 au
Gibbs free energy (gas) = -320.76292 au
Energy (sol) = -320.86335 au
Thermal correction to Gibbs free energy = 0.07774 au
Gibbs free energy (sol) = -320.78561 au
Number and value of imaginary frequency: 1, -86.6cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.661713	-0.010587	0.559915
2	1	0	-0.702070	-0.084630	0.990605
3	7	0	-0.204007	2.113398	-0.710043
4	6	0	0.593337	1.460424	-0.131855
5	6	0	1.310475	0.534047	0.628244
6	6	0	1.621743	-0.720982	0.056151
7	1	0	1.884503	0.878761	1.481597
8	7	0	1.786385	-1.791596	-0.393830
9	6	0	-1.965604	-1.197595	-0.295284
10	1	0	-2.896507	-1.022426	-0.835507

11	1	0	-1.138697	-1.331643	-0.992118
12	1	0	-2.360354	0.141475	1.287078
13	1	0	-1.541258	0.866018	-0.004566
14	1	0	-2.049990	-2.081430	0.337078

p-3
Energy + zep (gas) = -287.51422 au
Gibbs free energy (gas) = -287.54342 au
Enthalpies (gas) = -287. 50743au
Energy (sol) = -287.63579 au
Thermal correction to Gibbs free energy = 0.08771 au
Gibbs free energy (sol) = -287.54807 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.337165	0.000000	-0.072543
2	1	0	2.792422	-0.839051	0.260055
3	6	0	0.939298	0.000000	-0.007074
4	6	0	0.221723	1.209335	-0.004478
5	6	0	0.221722	-1.209335	-0.004478
6	6	0	-1.173128	1.203914	0.003133
7	1	0	0.762099	2.153078	-0.013098
8	6	0	-1.173128	-1.203913	0.003133
9	1	0	0.762098	-2.153078	-0.013099
10	6	0	-1.884233	0.000000	0.007433
11	1	0	-1.706585	2.150561	0.006789
12	1	0	-1.706585	-2.150561	0.006789
13	1	0	-2.969550	0.000000	0.014306
14	1	0	2.792423	0.839051	0.260051

p-3-COM
Energy + zep (gas) = -512.46526 au
Gibbs free energy (gas) = -512.50936 au
Energy (sol) = -512.63942 au
Thermal correction to Gibbs free energy = 0.11862 au
Gibbs free energy (sol) = -512.52080 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.265805	-1.514218	-1.289709
2	1	0	1.564326	-0.160332	-1.035504
3	7	0	3.320906	-1.526022	1.168621
4	6	0	2.989644	-0.748211	0.374329
5	6	0	2.545825	0.185816	-0.668839
6	6	0	2.451811	1.573376	-0.198459
7	1	0	3.248422	0.141080	-1.509892
8	7	0	2.374702	2.680480	0.138410
9	1	0	-0.528003	-1.684495	-2.254352
10	1	0	0.003837	-2.387003	-0.848369
11	6	0	-1.240908	-0.791736	-0.559327
12	6	0	-2.099211	0.104508	-1.214255

13	6	0	-1.308981	-0.907059	0.837667
14	6	0	-3.011495	0.865788	-0.482091
15	1	0	-2.050131	0.205696	-2.296002
16	6	0	-2.224703	-0.141373	1.561194
17	1	0	-0.643280	-1.593104	1.355954
18	6	0	-3.081670	0.749229	0.908887
19	1	0	-3.669801	1.553835	-1.004686
20	1	0	-2.264579	-0.243208	2.641810
21	1	0	-3.791288	1.343823	1.475144

p-3-TS
Energy + zep (gas) = -512.42380 au
Gibbs free energy (gas) = -512.46204 au
Energy (sol) = -512.60752 au
Thermal correction to Gibbs free energy = 0.12532 au
Gibbs free energy (sol) = -512.48220 au
Number and value of imaginary frequency: 1, -62.9cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.232627	-1.284016	-0.584826
2	1	0	1.013308	-0.662669	-0.943986
3	7	0	2.439830	-1.832369	1.143576
4	6	0	2.804908	-0.965389	0.429223
5	6	0	2.971412	0.032895	-0.534494
6	6	0	2.653436	1.371463	-0.207557
7	1	0	3.663174	-0.145549	-1.351892
8	7	0	2.300260	2.462922	0.033902
9	1	0	0.077922	-2.033679	-1.260748
10	1	0	0.713449	-1.700753	0.256081
11	6	0	-1.005289	-0.549760	-0.286643
12	6	0	-2.213393	-1.245981	-0.273214
13	6	0	-0.932627	0.813207	-0.006027
14	6	0	-3.387228	-0.552636	0.027611
15	1	0	-2.243976	-2.311233	-0.487800
16	6	0	-2.116948	1.491409	0.296743
17	1	0	0.016156	1.344766	-0.017219
18	6	0	-3.338920	0.815033	0.313162
19	1	0	-4.334319	-1.082461	0.039495
20	1	0	-2.073725	2.552926	0.517552
21	1	0	-4.253118	1.351442	0.547136

A-p-4
Energy + zep (gas) = -209.16466 au
Gibbs free energy (gas) = -209.19295 au
Enthalpies (gas) = -20915848 au
Energy (sol) = -209.24751 au
Thermal correction to Gibbs free energy = 0.04513 au
Gibbs free energy (sol) = -209.20239 au

Standard Orientation:

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

1	7	0	1.039893	-0.826248	-0.000031
2	1	0	2.007662	-0.538020	0.000476
3	1	0	0.824462	-1.809896	-0.000102
4	6	0	0.073930	0.143138	-0.000142
5	8	0	0.353861	1.336070	0.000006
6	6	0	-1.364431	-0.348112	-0.000010
7	1	0	-1.459317	-1.437566	-0.004573
8	1	0	-1.868551	0.051319	0.884321
9	1	0	-1.871395	0.059186	-0.879048

A-p-4-TS
Energy + zep (gas) = -434.05679 au
Gibbs free energy (gas) = -434.09299 au
Energy (sol) = -434.19258 au
Thermal correction to Gibbs free energy = 0.08244 au
Gibbs free energy (sol) = -434.11014 au
Number and value of imaginary frequency: 1, -106.6cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.002141	-0.824895	-0.645877
2	1	0	-0.092676	-0.409541	-1.016608
3	7	0	0.921700	-2.020972	0.962061
4	6	0	1.547444	-1.287578	0.275907
5	6	0	1.994137	-0.353560	-0.654878
6	6	0	2.067632	1.011982	-0.286113
7	1	0	2.589238	-0.694936	-1.495961
8	7	0	2.037547	2.148787	-0.006001
9	1	0	-1.485085	-1.344728	-1.381126
10	1	0	-0.569789	-1.485098	0.081188
11	6	0	-1.942490	0.187028	-0.062918
12	8	0	-3.045218	0.242691	-0.535105
13	6	0	-1.360401	0.993304	1.051202
14	1	0	-1.003505	0.331043	1.848723
15	1	0	-0.491205	1.563747	0.699864
16	1	0	-2.122913	1.670484	1.434273

B-p-4
Energy + zep (gas) = -209.14389 au
Gibbs free energy (gas) = -209.17072 au
Enthalpies (gas) = -209.13835 au
Energy (sol) = -209.22494 au
Thermal correction to Gibbs free energy = 0.04736 au
Gibbs free energy (sol) = -209.17758 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.795186	1.155619	0.000000
2	6	0	0.093423	0.092781	-0.000001
3	8	0	0.717571	-1.114169	0.000002

4	6	0	-1.402729	-0.069274	-0.000001
5	1	0	-1.716007	-0.636629	0.882195
6	1	0	1.672677	-0.934003	-0.000013
7	1	0	-1.715998	-0.636693	-0.882160
8	1	0	-1.902630	0.900842	-0.000033
9	1	0	0.210927	1.989457	0.000002

B-p-4-COM
Energy + zep (gas) = -434.09965 au
Gibbs free energy (gas) = -434.13914 au
Energy (sol) = -434.22896 au
Thermal correction to Gibbs free energy = 0.08045 au
Gibbs free energy (sol) = -434.14851 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.189658	-0.957097	0.403441
2	6	0	2.197893	-0.283063	-0.011117
3	8	0	2.075530	1.009464	-0.363631
4	6	0	3.618266	-0.754725	-0.177739
5	1	0	4.284842	-0.145447	0.440628
6	1	0	-1.055806	-0.829451	0.712746
7	7	0	-0.880020	2.120916	-0.082969
8	6	0	-1.395394	1.139144	0.258990
9	6	0	-1.924196	-0.148335	0.717907
10	6	0	-3.000752	-0.674016	-0.128744
11	1	0	-2.281950	-0.051218	1.749533
12	7	0	-3.852914	-1.119478	-0.777119
13	1	0	1.151984	1.307260	-0.258594
14	1	0	3.930566	-0.625427	-1.218657
15	1	0	3.724546	-1.803951	0.103051
16	1	0	1.469615	-1.911903	0.621078

B-p-4-TS
Energy + zep (gas) = -434.08371 au
Gibbs free energy (gas) = -434.12003au
Energy (sol) = -434.21412 au
Thermal correction to Gibbs free energy = 0.07916 au
Gibbs free energy (sol) = -434.13496 au
Number and value of imaginary frequency: 1, -1056cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.812804	-0.907236	0.488931
2	6	0	1.845495	-0.277879	0.009803
3	8	0	1.817721	0.969944	-0.386629
4	6	0	3.197509	-0.912208	-0.143499
5	1	0	3.932597	-0.332553	0.422395
6	1	0	-0.357696	-0.505366	0.631483
7	7	0	-0.628224	2.217530	-0.200841
8	6	0	-1.262854	1.317588	0.203909

9	6	0	-1.721949	0.078860	0.719271
10	6	0	-2.596529	-0.709115	-0.103803
11	1	0	-2.016946	0.117369	1.769377
12	7	0	-3.252533	-1.419162	-0.755366
13	1	0	0.925795	1.436805	-0.319132
14	1	0	3.492308	-0.875144	-1.196380
15	1	0	3.206402	-1.947337	0.200154
16	1	0	0.981409	-1.874728	0.741990

A-p-5
Energy + zep (gas) = -400.85811 au
Gibbs free energy (gas) = -400.89052 au
Enthalpies (gas) = -400.84958 au
Energy (sol) = -400.99441 au
Thermal correction to Gibbs free energy = 0.09502 au
Gibbs free energy (sol) = -400.89940 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.425827	1.011297	0.239619
2	1	0	3.427777	0.908015	0.317309
3	6	0	1.719416	-0.134248	-0.034473
4	8	0	2.289502	-1.188847	-0.300160
5	6	0	0.220315	-0.023423	-0.016732
6	6	0	-0.516387	-1.208653	0.121605
7	6	0	-0.460469	1.196512	-0.150802
8	6	0	-1.910066	-1.172891	0.147567
9	1	0	0.023889	-2.145643	0.204937
10	6	0	-1.856513	1.230099	-0.133321
11	1	0	0.088882	2.120643	-0.305304
12	6	0	-2.583306	0.046690	0.021969
13	1	0	-2.471868	-2.095167	0.262717
14	1	0	-2.374949	2.177317	-0.249526
15	1	0	-3.669022	0.073985	0.037675
16	1	0	2.000546	1.788031	0.721261

A-p-5-TS
Energy + zep (gas) = -625.75182 au
Gibbs free energy (gas) = -625.79334 au
Energy (sol) = -625.94183 au
Thermal correction to Gibbs free energy = 0.13102 au
Gibbs free energy (sol) = -625.81081 au
Number and value of imaginary frequency: 1, -91.8cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.794781	1.780947	-0.146908
2	1	0	-1.102089	2.713319	-0.433661
3	6	0	0.691206	1.747371	-0.331666
4	8	0	1.196239	2.784670	-0.697846
5	6	0	1.368945	0.478044	-0.055076

6	6	0	2.775019	0.463718	-0.163617
7	6	0	0.679140	-0.699216	0.285697
8	6	0	3.473595	-0.714464	0.068806
9	1	0	3.291953	1.379228	-0.429740
10	6	0	1.387214	-1.878941	0.506049
11	1	0	-0.400586	-0.724449	0.365841
12	6	0	2.780238	-1.886434	0.401296
13	1	0	4.555870	-0.725948	-0.011829
14	1	0	0.845131	-2.786968	0.746827
15	1	0	3.328848	-2.807460	0.574336
16	1	0	-1.380827	1.052880	-0.672445
17	7	0	-2.641515	0.885858	1.794097
18	6	0	-2.955232	0.338296	0.795425
19	6	0	-3.073337	-0.158385	-0.506009
20	6	0	-2.693205	-1.498989	-0.776618
21	1	0	-3.841251	0.276053	-1.140982
22	7	0	-2.322790	-2.582340	-1.018063
23	1	0	-1.154850	1.608731	0.834820

B-p-5
Energy + zep (gas) = -400.83723 au
Gibbs free energy (gas) = -400.86981 au
Enthalpies (gas) = -400.82896 au
Energy (sol) = -400.97172 au
Thermal correction to Gibbs free energy = 0.09507 au
Gibbs free energy (sol) = -400.87665 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.485533	1.091671	0.197613
2	6	0	-1.712169	0.093365	0.010506
3	8	0	-2.273263	-1.126666	-0.203997
4	1	0	-3.234097	-0.995294	-0.148324
5	1	0	-1.970787	1.950560	0.378226
6	6	0	-0.222839	0.043917	-0.003919
7	6	0	0.529683	1.225107	-0.100693
8	6	0	0.448905	-1.185825	0.086386
9	6	0	1.922887	1.180787	-0.092504
10	1	0	0.030708	2.184790	-0.198129
11	6	0	1.844135	-1.227855	0.098339
12	1	0	-0.127334	-2.101111	0.152443
13	6	0	2.584849	-0.046830	0.009553
14	1	0	2.491350	2.102468	-0.173116
15	1	0	2.351949	-2.184726	0.175423
16	1	0	3.670342	-0.081062	0.016141

B-p-5-COM
Energy + zep (gas) = -625.79297 au
Gibbs free energy (gas) = -625.83786 au
Energy (sol) = -625.97562 au
Thermal correction to Gibbs free energy = 0.12834 au
Gibbs free energy (sol) = -625.84728 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.484053	-0.681699	-0.365662
2	6	0	-0.425965	0.210769	-0.207626
3	8	0	-0.098522	1.515846	-0.150530
4	1	0	2.736920	-0.973064	-0.517943
5	7	0	3.015099	2.068456	-0.298168
6	6	0	3.375238	0.970940	-0.408436
7	6	0	3.704973	-0.447195	-0.576413
8	6	0	4.633484	-0.955955	0.439149
9	1	0	4.127081	-0.609804	-1.574951
10	7	0	5.364834	-1.391253	1.226934
11	1	0	0.870029	1.620668	-0.200348
12	1	0	0.080252	-1.616055	-0.347297
13	6	0	-1.894119	-0.007124	-0.058599
14	6	0	-2.487696	-1.207747	-0.479258
15	6	0	-2.700779	0.988824	0.514830
16	6	0	-3.856686	-1.415656	-0.316902
17	1	0	-1.888197	-1.977996	-0.955935
18	6	0	-4.069773	0.775797	0.682690
19	1	0	-2.247541	1.921197	0.830395
20	6	0	-4.651174	-0.425324	0.268956
21	1	0	-4.303924	-2.345943	-0.653863
22	1	0	-4.682072	1.549866	1.135531
23	1	0	-5.717289	-0.588134	0.396584

B-p-5-TS
Energy + zep (gas) = -625.77753 au
Gibbs free energy (gas) = -625.81896 au
Energy (sol) = -625.96010 au
Thermal correction to Gibbs free energy = 0.12731 au
Gibbs free energy (sol) = -625.83279 au
Number and value of imaginary frequency: 1, -1100.3cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.692323	-0.647665	-0.323986
2	6	0	-0.199174	0.293148	-0.183666
3	8	0	0.115546	1.567831	-0.124555
4	1	0	1.928795	-0.546787	-0.487957
5	7	0	2.823607	2.157370	-0.152848
6	6	0	3.226862	1.073168	-0.346708
7	6	0	3.382193	-0.313515	-0.606508
8	6	0	4.034041	-1.114548	0.392311
9	1	0	3.697184	-0.538586	-1.627038
10	7	0	4.494667	-1.823273	1.195156
11	1	0	1.099190	1.774628	-0.120295
12	1	0	0.331531	-1.594105	-0.283225
13	6	0	-1.654678	0.027719	-0.066716
14	6	0	-2.218558	-1.161936	-0.556768
15	6	0	-2.481009	0.982239	0.548781
16	6	0	-3.585111	-1.398610	-0.420537

17	1	0	-1.605033	-1.893826	-1.074018
18	6	0	-3.846051	0.736315	0.691180
19	1	0	-2.045678	1.903815	0.916987
20	6	0	-4.400088	-0.452509	0.208811
21	1	0	-4.014228	-2.315714	-0.811550
22	1	0	-4.476709	1.473908	1.177497
23	1	0	-5.464166	-0.639821	0.316699

s-1
Energy + zep (gas) = -408.92378 au
Gibbs free energy (gas) = -408.958825 au
Enthalpies (gas) = -408.911694 au
Energy (sol) = -409.20695 au
Thermal correction to Gibbs free energy = 0.23467 au
Gibbs free energy (sol) = -408.97228 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.010981	-0.631864	0.717932
2	6	0	1.291722	-0.228401	0.088623
3	6	0	-1.278371	-0.249600	0.077253
4	6	0	1.329621	1.299581	-0.282882
5	6	0	-1.125928	1.028034	-0.799304
6	6	0	2.390735	-0.540782	1.118957
7	6	0	1.555347	-1.085792	-1.165940
8	6	0	-1.819946	-1.419857	-0.766924
9	6	0	-2.279466	0.018634	1.217583
10	6	0	-0.057906	1.961821	-0.223721
11	1	0	1.738679	1.415738	-1.294907
12	1	0	-0.845628	0.750123	-1.824055
13	1	0	-2.095586	1.535151	-0.874525
14	1	0	2.017044	1.831344	0.386539
15	1	0	-0.040808	2.914331	-0.766119
16	1	0	-3.285969	0.179501	0.818264
17	1	0	-2.002928	0.906390	1.799031
18	1	0	-2.318931	-0.838650	1.899057
19	1	0	2.236622	0.029674	2.043813
20	1	0	3.375554	-0.269402	0.724098
21	1	0	2.396013	-1.606325	1.369977
22	1	0	0.858639	-0.857569	-1.977301
23	1	0	2.566043	-0.893447	-1.543641
24	1	0	-1.980100	-2.299787	-0.135680
25	1	0	-1.125027	-1.699692	-1.561979
26	1	0	0.012377	-0.287468	1.673625
27	1	0	-2.773838	-1.146756	-1.234794
28	1	0	1.467865	-2.149722	-0.924807
29	1	0	-0.311728	2.207788	0.816011

s-COM
Energy + zep (gas) = -633.87542 au
Gibbs free energy (gas) = -633.92364 au
Energy (sol) = -634.21947 au
Thermal correction to Gibbs free energy = 0.26743 au

Gibbs free energy (sol) = -633.95204 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.493749	-0.023421	-0.234637
2	6	0	1.127862	1.319728	-0.083476
3	6	0	1.227354	-1.235880	0.257898
4	6	0	2.602943	1.346890	-0.623572
5	6	0	2.764989	-1.003940	0.280537
6	6	0	0.266792	2.300740	-0.897844
7	6	0	1.094470	1.758718	1.393478
8	6	0	0.729774	-1.630120	1.661489
9	6	0	0.889952	-2.383382	-0.713404
10	6	0	3.195375	-0.056233	-0.840878
11	1	0	3.233044	1.897031	0.086582
12	1	0	3.069211	-0.580656	1.246790
13	1	0	3.273846	-1.971599	0.197335
14	1	0	2.643530	1.908520	-1.564431
15	1	0	4.287872	0.005542	-0.898396
16	1	0	1.291071	-3.330838	-0.340389
17	1	0	1.316574	-2.208868	-1.708078
18	1	0	-0.193897	-2.498462	-0.823381
19	1	0	0.221578	2.004146	-1.953170
20	1	0	0.699000	3.305835	-0.858235
21	1	0	-0.756214	2.356805	-0.513263
22	1	0	1.756362	1.157474	2.022262
23	1	0	1.425856	2.799255	1.477223
24	1	0	-0.329484	-1.907342	1.635525
25	1	0	0.852762	-0.817783	2.381462
26	1	0	0.329418	-0.154431	-1.230699
27	1	0	-1.673311	-0.051600	0.335807
28	7	0	-3.600401	-2.186157	-0.948405
29	6	0	-3.254085	-1.282733	-0.308205
30	6	0	-2.763999	-0.168274	0.511706
31	6	0	-3.444535	1.098541	0.219294
32	1	0	-2.903738	-0.413775	1.571367
33	7	0	-3.950531	2.120793	0.007364
34	1	0	1.292380	-2.494539	2.032649
35	1	0	0.079098	1.691793	1.797607
36	1	0	2.863963	-0.459341	-1.806958

s-1-TS
Energy + zep (gas) = -633.85745 au
Gibbs free energy (gas) = -633.90224 au
Energy (sol) = -634.21252 au
Thermal correction to Gibbs free energy = 0.26837 au
Gibbs free energy (sol) = -633.94415 au
Number and value of imaginary frequency: 1, -639.2cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.293687	0.038556	-0.255384

2	6	0	-0.817605	-1.386938	-0.105888
3	6	0	-1.105144	1.222781	0.293076
4	6	0	-2.307352	-1.477485	-0.569591
5	6	0	-2.603126	0.842511	0.361953
6	6	0	0.061612	-2.268801	-1.008762
7	6	0	-0.657656	-1.830765	1.357614
8	6	0	-0.584643	1.631853	1.679869
9	6	0	-0.889144	2.383097	-0.695325
10	6	0	-2.997234	-0.117673	-0.760481
11	1	0	-2.860630	-2.054387	0.180461
12	1	0	-2.831913	0.379908	1.330431
13	1	0	-3.188062	1.767544	0.315581
14	1	0	-2.364569	-2.050981	-1.500781
15	1	0	-4.082894	-0.257737	-0.783671
16	1	0	-1.352320	3.291264	-0.298749
17	1	0	-1.349796	2.175046	-1.668293
18	1	0	0.174440	2.587406	-0.852365
19	1	0	0.003049	-1.943839	-2.055077
20	1	0	-0.307608	-3.298103	-0.967560
21	1	0	1.109879	-2.275281	-0.701440
22	1	0	-1.317675	-1.280886	2.033159
23	1	0	-0.919875	-2.890066	1.435426
24	1	0	0.426585	2.041606	1.627475
25	1	0	-0.587769	0.798666	2.386508
26	1	0	-0.189333	0.199513	-1.259032
27	1	0	0.849942	0.097835	0.134449
28	7	0	2.805233	2.308902	-1.083074
29	6	0	2.697693	1.395306	-0.361327
30	6	0	2.382565	0.298811	0.504729
31	6	0	3.079484	-0.929935	0.269837
32	1	0	2.397569	0.583009	1.559693
33	7	0	3.549583	-1.984200	0.087341
34	1	0	-1.239586	2.411770	2.081348
35	1	0	0.374974	-1.716972	1.699026
36	1	0	-2.729009	0.315314	-1.733008

A-s-2
Energy + zep (gas) = -325.83041 au
Gibbs free energy (gas) = -325.86164 au
Enthalpies (gas) = -325.82283 au
Energy (sol) = -325.99841au
Thermal correction to Gibbs free energy = 0.10874 au
Gibbs free energy (sol) = -325.88967 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.402618	-1.162729	-0.105569
2	6	0	-0.986922	-1.220338	0.340657
3	6	0	1.149075	-0.021397	0.010555
4	6	0	-1.798265	-0.069444	-0.280393
5	6	0	0.334883	1.175193	0.480742
6	6	0	-1.021637	1.277919	-0.250472
7	1	0	-2.750405	0.013311	0.255603
8	1	0	0.171192	1.065566	1.562267

9	1	0	0.940398	2.071770	0.334157
10	1	0	-2.039177	-0.330859	-1.316085
11	1	0	-1.624487	2.061012	0.220920
12	1	0	0.906560	-2.008108	-0.338754
13	1	0	-0.833025	1.611033	-1.276332
14	1	0	-1.402178	-2.187750	0.046385
15	1	0	-1.039299	-1.169963	1.438645
16	8	0	2.348662	0.020186	-0.249295

A-s-2-TS
Energy + zep (gas) = -550.72383 au
Gibbs free energy (gas) = -550.76427 au
Energy (sol) = -550.95824 au
Thermal correction to Gibbs free energy = 0.14437 au
Gibbs free energy (sol) = -550.81387 au
Number and value of imaginary frequency: 1, -82.4cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.289160	0.244956	-0.034592
2	6	0	0.467095	-1.243642	0.061656
3	6	0	1.451734	1.007888	-0.559143
4	6	0	1.722442	-1.545024	0.876646
5	6	0	2.662915	0.158434	-0.832523
6	6	0	2.983402	-0.826294	0.318670
7	1	0	1.865760	-2.629307	0.894357
8	1	0	2.459580	-0.401697	-1.756483
9	1	0	3.497468	0.829949	-1.042590
10	1	0	1.541174	-1.241207	1.913458
11	1	0	3.710605	-1.553039	-0.053947
12	1	0	-0.032782	0.624840	0.912624
13	1	0	-0.601460	0.482876	-0.570869
14	7	0	-1.494202	0.952799	1.992166
15	6	0	-2.162330	0.874192	1.018979
16	6	0	-2.675506	0.716486	-0.265237
17	6	0	-3.079227	-0.569194	-0.700987
18	1	0	-3.062230	1.586617	-0.785818
19	7	0	-3.335629	-1.643567	-1.090888
20	1	0	3.480586	-0.276565	1.123171
21	1	0	-0.435662	-1.641891	0.527086
22	1	0	0.518240	-1.638234	-0.956291
23	8	0	1.327532	2.192658	-0.722484

B-s-2
Energy + zep (gas) = -325.81680 au
Gibbs free energy (gas) = -325.84681 au
Enthalpies (gas) = -325.80956 au
Energy (sol) = -325.96208 au
Thermal correction to Gibbs free energy = 0.10970 au
Gibbs free energy (sol) = -325.85238 au

Standard Orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.453398	-1.209314	-0.082200
2	6	0	0.988983	-0.060112	0.004987
3	8	0	2.347300	0.042788	0.057259
4	6	0	0.315812	1.289153	0.072740
5	1	0	0.850664	1.980519	-0.587454
6	6	0	-1.172995	1.182462	-0.288324
7	1	0	2.691085	-0.866197	0.030391
8	6	0	-1.767582	-0.078137	0.349174
9	6	0	-1.005553	-1.322492	-0.127109
10	1	0	0.446675	1.677380	1.091928
11	1	0	-1.282733	1.124354	-1.379448
12	1	0	-1.705040	2.082817	0.036814
13	1	0	-1.699074	-0.001537	1.443198
14	1	0	-2.830650	-0.180923	0.101710
15	1	0	-1.288868	-1.563575	-1.162268
16	1	0	-1.286240	-2.195179	0.473647

B-s-2-COM
Energy + zep (gas) = -550.77122 au
Gibbs free energy (gas) = -550.81427 au
Energy (sol) = -550.96506 au
Thermal correction to Gibbs free energy = 0.14210 au
Gibbs free energy (sol) = -550.82297 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.621056	-0.180890	0.230077
2	6	0	1.334325	0.825044	-0.103685
3	8	0	0.776584	2.041227	-0.302504
4	6	0	2.825944	0.865646	-0.341480
5	1	0	3.224987	1.764768	0.139730
6	6	0	3.518073	-0.411036	0.152255
7	1	0	-1.516183	-0.567432	0.618948
8	7	0	-2.533672	2.257455	0.014668
9	6	0	-2.615083	1.135804	0.301572
10	6	0	-2.582119	-0.278788	0.685029
11	6	0	-3.400604	-1.138400	-0.176692
12	1	0	-2.907654	-0.385099	1.726361
13	7	0	-4.032391	-1.849644	-0.840228
14	1	0	-0.189529	1.992523	-0.188348
15	6	0	2.658384	-1.626535	-0.206618
16	6	0	1.267168	-1.486986	0.421618
17	1	0	2.980634	1.004738	-1.419874
18	1	0	3.647094	-0.364394	1.241768
19	1	0	4.520008	-0.487986	-0.282564
20	1	0	2.563586	-1.700744	-1.298500
21	1	0	3.122693	-2.557242	0.138873
22	1	0	1.327285	-1.675091	1.503968
23	1	0	0.592928	-2.250798	0.016053

B-s-2-TS

Energy + zep (gas) = -550.75870 au
Gibbs free energy (gas) = -550.79811 au
Energy (sol) = -550.95315 au
Thermal correction to Gibbs free energy = 0.14185 au
Gibbs free energy (sol) = -550.81129 au
Number and value of imaginary frequency: 1, -1114.7cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.393553	-0.151415	0.301382
2	6	0	1.038854	0.897190	-0.096512
3	8	0	0.462952	2.066933	-0.321391
4	6	0	2.519946	0.927736	-0.379711
5	1	0	2.920823	1.849673	0.053403
6	6	0	3.255290	-0.321151	0.121374
7	1	0	-0.858063	-0.211823	0.514138
8	7	0	-2.372054	2.219364	-0.017657
9	6	0	-2.487800	1.096434	0.295978
10	6	0	-2.301346	-0.261030	0.683417
11	6	0	-2.811133	-1.278137	-0.196418
12	1	0	-2.524203	-0.446645	1.736241
13	7	0	-3.138113	-2.145943	-0.903004
14	1	0	-0.525652	2.096146	-0.205745
15	6	0	2.412410	-1.566901	-0.167863
16	6	0	1.056248	-1.448921	0.525408
17	1	0	2.623334	1.036047	-1.467613
18	1	0	3.431787	-0.240337	1.201696
19	1	0	4.237698	-0.386905	-0.356039
20	1	0	2.265667	-1.675765	-1.250282
21	1	0	2.914722	-2.474947	0.181361
22	1	0	1.167650	-1.585105	1.609422
23	1	0	0.364095	-2.221160	0.175465

A-s-3
Energy + zep (gas) = -286.54488 au
Gibbs free energy (gas) = -286.57372 au
Enthalpies (gas) = -286.53851au
Energy (sol) = -286.68618 au
Thermal correction to Gibbs free energy = 0.08205 au
Gibbs free energy (sol) = -286.60414 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.086811	-1.097613	-0.073024
2	6	0	-1.330058	-0.817384	0.130779
3	6	0	0.903868	0.001523	-0.006514
4	6	0	-1.415538	0.695558	-0.185897
5	6	0	-0.006148	1.224466	0.136864
6	1	0	-2.208738	1.187683	0.382332
7	1	0	0.077650	1.580775	1.171192
8	1	0	0.334689	2.031313	-0.515515
9	1	0	-1.631106	0.832285	-1.250610

10	1	0	0.485703	-2.025308	-0.033937
11	1	0	-1.953715	-1.421019	-0.535835
12	1	0	-1.633629	-1.029619	1.166345
13	8	0	2.126091	-0.012225	-0.040525

A-s-3-TS
Energy + zep (gas) = -511.43760 au
Gibbs free energy (gas) = -511.47584 au
Energy (sol) = -511.64606 au
Thermal correction to Gibbs free energy = 0.11721 au
Gibbs free energy (sol) = -511.52886 au
Number and value of imaginary frequency: 1, -90.7cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.527515	-0.189468	0.067503
2	6	0	-0.700088	1.216740	0.565744
3	6	0	-1.809484	-0.625868	-0.557818
4	6	0	-2.215843	1.336679	0.797474
5	6	0	-2.829185	0.465479	-0.310137
6	1	0	-2.544746	2.376792	0.756227
7	1	0	-2.949031	1.023521	-1.249081
8	1	0	-3.797913	0.021031	-0.071250
9	1	0	-2.479822	0.940341	1.783506
10	1	0	-0.192830	-0.839365	0.845788
11	1	0	-0.092252	1.358025	1.459567
12	1	0	-0.342484	1.895216	-0.212193
13	8	0	-1.898385	-1.672260	-1.133942
14	1	0	0.323785	-0.298724	-0.570269
15	7	0	1.335739	-1.510849	1.662997
16	6	0	1.937575	-1.170175	0.703640
17	6	0	2.357497	-0.660101	-0.522856
18	6	0	2.804594	0.682270	-0.606386
19	1	0	2.665140	-1.354813	-1.298134
20	7	0	3.095611	1.812590	-0.700584

B-s-3
Energy + zep (gas) = -286.52356 au
Gibbs free energy (gas) = -286.55241 au
Enthalpies (gas) = -286.51721 au
Energy (sol) = -286.64072 au
Thermal correction to Gibbs free energy = 0.08172 au
Gibbs free energy (sol) = -286.55900 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.136571	-1.161276	-0.026313
2	6	0	-0.746737	-0.043052	0.000372
3	8	0	-2.090913	0.079210	-0.039301
4	6	0	0.084451	1.211273	0.113032
5	1	0	-0.032963	1.640298	1.116596

6	1	0	-2.461190	-0.817885	-0.081186
7	6	0	1.496181	0.639022	-0.141088
8	6	0	1.306673	-0.891688	0.079342
9	1	0	1.652247	-1.208672	1.072503
10	1	0	2.258490	1.069732	0.513753
11	1	0	1.800027	0.835102	-1.174568
12	1	0	1.852507	-1.492890	-0.654842
13	1	0	-0.229227	1.976238	-0.603610

B-s-3-COM
Energy + zep (gas) = -511.48004 au
Gibbs free energy (gas) = -511.52117 au
Energy (sol) = -511.64460 au
Thermal correction to Gibbs free energy = 0.11502 au
Gibbs free energy (sol) = -511.52958 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.873713	-0.351447	0.277743
2	6	0	1.639636	0.599365	-0.113714
3	8	0	1.253973	1.855699	-0.367563
4	6	0	3.078484	-1.262323	-0.191828
5	6	0	1.708823	-1.551621	0.482246
6	1	0	3.098676	-1.692858	-1.198267
7	1	0	1.815415	-1.729141	1.561395
8	1	0	-1.316104	-0.723489	0.626491
9	7	0	-1.827876	2.237034	0.086626
10	6	0	-2.108008	1.140709	0.343840
11	6	0	-2.320697	-0.267401	0.688929
12	6	0	-3.259255	-0.954466	-0.204610
13	1	0	-2.673831	-0.343638	1.723847
14	7	0	-3.993845	-1.529500	-0.893674
15	1	0	0.296539	1.965778	-0.211318
16	1	0	1.211317	-2.431038	0.060017
17	1	0	3.920569	-1.681651	0.364894
18	6	0	3.106446	0.276144	-0.274345
19	1	0	3.669886	0.740747	0.545252
20	1	0	3.509229	0.674648	-1.209777

B-s-3-TS
Energy + zep (gas) = -511.46696 au
Gibbs free energy (gas) = -511.50482 au
Energy (sol) = -511.63239 au
Thermal correction to Gibbs free energy = 0.11417 au
Gibbs free energy (sol) = -511.51726 au
Number and value of imaginary frequency: 1, -1139.9cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.621155	-0.307463	0.319452
2	6	0	1.370146	0.664320	-0.106369

3	8	0	1.003102	1.890071	-0.384820
4	6	0	2.766154	-1.250913	-0.173765
5	6	0	1.423013	-1.525766	0.544903
6	1	0	2.743590	-1.680212	-1.180021
7	1	0	1.551068	-1.673526	1.624404
8	1	0	-0.630983	-0.306030	0.538451
9	7	0	-1.724311	2.293038	-0.018357
10	6	0	-2.032743	1.208075	0.300377
11	6	0	-2.069980	-0.157459	0.695534
12	6	0	-2.717028	-1.089514	-0.187738
13	1	0	-2.326314	-0.301643	1.747057
14	7	0	-3.166412	-1.899260	-0.895593
15	1	0	0.025184	2.076176	-0.254989
16	1	0	0.891470	-2.394724	0.148473
17	1	0	3.618132	-1.683336	0.355145
18	6	0	2.821672	0.287373	-0.258511
19	1	0	3.386248	0.742414	0.565432
20	1	0	3.236363	0.679407	-1.190485

A-s-4
Energy + zep (gas) = -322.47365 au
Gibbs free energy (gas) = -322.50208 au
Enthalpies (gas) = -322.46768 au
Energy (sol) = -322.59691 au
Thermal correction to Gibbs free energy = 0.05908 au
Gibbs free energy (sol) = -322.53783 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.030520	1.084121	-0.175208
2	6	0	-1.347320	0.744167	0.148396
3	6	0	0.862785	-0.006316	-0.011805
4	6	0	-1.300212	-0.772860	-0.112990
5	8	0	0.081756	-1.130599	0.087154
6	1	0	-1.910334	-1.357200	0.577041
7	1	0	0.423615	1.994327	0.015325
8	1	0	-1.595667	0.970566	1.194769
9	8	0	2.070046	-0.022634	0.031276
10	1	0	-1.575250	-1.013689	-1.145600
11	1	0	-2.061943	1.253074	-0.504116

A-s-4-TS
Energy + zep (gas) = -547.36458 au
Gibbs free energy (gas) = -547.40261 au
Energy (sol) = -547.55168 au
Thermal correction to Gibbs free energy = 0.09397 au
Gibbs free energy (sol) = -547.45771 au
Number and value of imaginary frequency: 1, -119.1cm^{-1}

Standard Orientation:

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

1	7	0	-0.525307	-0.186481	0.076905
2	6	0	-0.660624	1.220197	0.555309
3	6	0	-1.817280	-0.568234	-0.535777
4	6	0	-2.181965	1.347368	0.704550
5	8	0	-2.720333	0.367983	-0.222306
6	1	0	-2.535899	1.090711	1.706668
7	1	0	-0.197617	-0.849062	0.853143
8	1	0	-0.110857	1.355949	1.486696
9	8	0	-1.980663	-1.546659	-1.197103
10	1	0	0.319065	-0.319890	-0.575043
11	7	0	1.302047	-1.538986	1.646249
12	6	0	1.905784	-1.203785	0.686075
13	6	0	2.309765	-0.678802	-0.540888
14	6	0	2.744762	0.670214	-0.600819
15	1	0	2.628408	-1.360386	-1.323212
16	7	0	3.012023	1.808173	-0.667427
17	1	0	-2.566126	2.323775	0.411797
18	1	0	-0.252996	1.887626	-0.205568

B-s-4

Energy + zep (gas) = -322.44756 au

Gibbs free energy (gas) = -322.47543 au

Enthalpies (gas) = -322.44216 au

Energy (sol) = -322.54334 au

Thermal correction to Gibbs free energy = 0.05888 au

Gibbs free energy (sol) = -322.48445 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.076244	1.166435	0.004610
2	6	0	-0.704903	0.057206	0.000644
3	8	0	-2.030681	-0.109715	0.000681
4	8	0	-0.033074	-1.114649	-0.007487
5	1	0	-2.426586	0.774992	0.002402
6	6	0	1.374100	-0.745005	0.007054
7	6	0	1.350638	0.812979	-0.005474
8	1	0	1.835487	1.224263	-0.897710
9	1	0	1.842965	-1.187611	-0.874999
10	1	0	1.819788	-1.171303	0.909290
11	1	0	1.853073	1.238450	0.869856

B-s-4-COM

Energy + zep (gas) = -547.40470 au

Gibbs free energy (gas) = -547.44614 au

Energy (sol) = -547.54769 au

Thermal correction to Gibbs free energy = 0.09104 au

Gibbs free energy (sol) = -547.45665 au

Standard Orientation:

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

1	7	0	0.866277	-0.418580	0.210029
2	6	0	1.651771	0.540190	-0.127734
3	8	0	1.354179	1.815362	-0.322188
4	8	0	2.962799	0.285559	-0.330094
5	6	0	3.149600	-1.111820	0.014159
6	6	0	1.703227	-1.630866	0.235766
7	1	0	3.677360	-1.593033	-0.811432
8	1	0	1.599013	-2.153550	1.192308
9	1	0	-1.386378	-0.821424	0.632220
10	7	0	-1.606119	2.176562	0.086965
11	6	0	-1.985933	1.113031	0.351792
12	6	0	-2.334827	-0.264766	0.707947
13	6	0	-3.354341	-0.855447	-0.166129
14	1	0	-2.676451	-0.299786	1.748981
15	7	0	-4.156825	-1.353603	-0.838901
16	1	0	0.394967	1.962464	-0.205315
17	1	0	1.388444	-2.321341	-0.556276
18	1	0	3.766911	-1.153284	0.916314

B-s-4-TS
Energy + zep (gas) = -547.38956 au
Gibbs free energy (gas) = -547.42750 au
Energy (sol) = -547.53251au
Thermal correction to Gibbs free energy = 0.09019 au
Gibbs free energy (sol) = -547.44232 au
Number and value of imaginary frequency: 1, -1123.0cm^{-1}
Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.617399	-0.355146	0.317739
2	6	0	1.379754	0.605939	-0.133124
3	8	0	1.086776	1.844791	-0.376766
4	8	0	2.648911	0.277294	-0.380620
5	6	0	2.832483	-1.099359	0.063473
6	6	0	1.394970	-1.602566	0.326298
7	1	0	3.357182	-1.633166	-0.728951
8	1	0	1.301727	-2.112211	1.288680
9	1	0	-0.617299	-0.325865	0.548324
10	7	0	-1.581802	2.295286	-0.003112
11	6	0	-1.952964	1.231147	0.319947
12	6	0	-2.062462	-0.127005	0.720436
13	6	0	-2.742945	-1.034029	-0.162290
14	1	0	-2.320248	-0.257227	1.773042
15	7	0	-3.220299	-1.827776	-0.870093
16	1	0	0.110124	2.066143	-0.248532
17	1	0	1.033302	-2.275376	-0.458785
18	1	0	3.449615	-1.070290	0.965135

A-s-5
Energy + zep (gas) = -323.45097 au
Gibbs free energy (gas) = -323.47991 au
Enthalpies (gas) = -323.44473au
Energy (sol) = -323.57042 au

Thermal correction to Gibbs free energy = 0.06461 au
Gibbs free energy (sol) = -323.50582 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.303310	-1.124861	0.000060
2	6	0	1.060803	-1.191101	-0.000132
3	6	0	-1.063181	0.063470	-0.000064
4	6	0	1.806667	-0.047463	0.000090
5	6	0	-0.248889	1.265695	0.000126
6	6	0	1.117607	1.203665	-0.000221
7	1	0	-0.784166	2.208151	-0.000219
8	1	0	2.888127	-0.099372	0.000771
9	1	0	1.695568	2.124185	0.000048
10	1	0	-0.856422	-1.974063	-0.000181
11	1	0	1.491576	-2.186186	-0.000145
12	8	0	-2.293694	0.004464	0.000064

A-s-5-TS
Energy + zep (gas) = -548.32188 au
Gibbs free energy (gas) = -548.36003 au
Energy (sol) = -548.49741 au
Thermal correction to Gibbs free energy = 0.09752 au
Gibbs free energy (sol) = -548.39989 au
Number and value of imaginary frequency: 1, -168.6cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.410431	-0.131665	0.186655
2	6	0	-0.647488	1.223006	0.601197
3	6	0	-1.510051	-0.940163	-0.421573
4	6	0	-1.875838	1.762165	0.505042
5	6	0	-2.802349	-0.288260	-0.462333
6	6	0	-2.973484	0.988374	-0.026586
7	1	0	-3.613960	-0.877348	-0.873244
8	1	0	-2.034281	2.784431	0.827541
9	1	0	-3.955798	1.447933	-0.082017
10	1	0	0.079133	-0.710550	0.995021
11	1	0	0.227840	1.734425	0.984026
12	8	0	-1.223304	-2.049358	-0.818904
13	1	0	0.475929	-0.198769	-0.448605
14	7	0	1.464369	-1.354051	1.709922
15	6	0	2.064127	-1.063036	0.731625
16	6	0	2.417413	-0.582460	-0.523003
17	6	0	2.933285	0.734103	-0.646968
18	1	0	2.621297	-1.295055	-1.316467
19	7	0	3.282146	1.843919	-0.765066

B-s-5
Energy + zep (gas) = -323.45041 au
Gibbs free energy (gas) = -323.47922 au

Enthalpies (gas) = -323.44424 au
Energy (sol) = -323.54898 au
Thermal correction to Gibbs free energy = 0.06458 au
Gibbs free energy (sol) = -323.48440 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.338636	-1.172580	-0.000073
2	6	0	0.903613	0.031227	-0.000515
3	8	0	2.259385	0.084632	0.000268
4	6	0	0.186002	1.237594	-0.000189
5	1	0	0.713951	2.184148	-0.000154
6	6	0	-1.200412	1.155575	0.000183
7	1	0	2.576036	-0.832934	0.000522
8	6	0	-1.819317	-0.102471	0.000064
9	6	0	-1.004183	-1.230445	0.000098
10	1	0	-1.797055	2.063052	0.000331
11	1	0	-2.899120	-0.202848	-0.000042
12	1	0	-1.433564	-2.229301	-0.000132

B-s-5-COM

Energy + zep (gas) = -548.40331 au

Gibbs free energy (gas) = -548.44560 au

Energy (sol) = -548.55112 au

Thermal correction to Gibbs free energy = 0.09638 au

Gibbs free energy (sol) = -548.45474 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.782087	-0.269966	0.149775
2	6	0	1.571052	0.773760	-0.118309
3	8	0	1.021797	1.997384	-0.253939
4	6	0	2.966262	0.672271	-0.270176
5	6	0	3.546460	-0.579252	-0.135928
6	1	0	0.055283	1.953474	-0.148282
7	6	0	2.735290	-1.689728	0.142196
8	6	0	1.369495	-1.477470	0.273379
9	1	0	3.544621	1.562797	-0.487023
10	1	0	4.620526	-0.695047	-0.247509
11	1	0	3.151130	-2.685078	0.251679
12	1	0	0.702112	-2.309716	0.487364
13	1	0	-1.485973	-0.725455	0.542331
14	7	0	-2.175327	2.233648	0.088559
15	6	0	-2.371656	1.116593	0.333027
16	6	0	-2.497630	-0.306700	0.662029
17	6	0	-3.453900	-1.022325	-0.190548
18	1	0	-2.791561	-0.414214	1.712731
19	7	0	-4.201438	-1.619214	-0.846020

B-s-5-TS

Energy + zep (gas) = -548.38368 au
Gibbs free energy (gas) = -548.42165 au
Energy (sol) = -548.53191 au
Thermal correction to Gibbs free energy = 0.09674 au
Gibbs free energy (sol) = -548.43517 au
Number and value of imaginary frequency: 1, -785.4cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.502665	-0.224913	0.234956
2	6	0	1.235258	0.859318	-0.100926
3	8	0	0.696704	2.055141	-0.253431
4	6	0	2.626470	0.726758	-0.295568
5	6	0	3.214818	-0.515064	-0.150845
6	1	0	-0.300031	2.114497	-0.172166
7	6	0	2.431337	-1.635639	0.187197
8	6	0	1.080126	-1.444317	0.370821
9	1	0	3.192148	1.611785	-0.560561
10	1	0	4.284250	-0.624082	-0.303007
11	1	0	2.865039	-2.621863	0.298999
12	1	0	0.397721	-2.247645	0.629521
13	1	0	-0.685271	-0.222711	0.454592
14	7	0	-2.069371	2.251581	-0.025839
15	6	0	-2.279016	1.140679	0.288884
16	6	0	-2.207498	-0.218842	0.680556
17	6	0	-2.765684	-1.210251	-0.192641
18	1	0	-2.414639	-0.388477	1.738302
19	7	0	-3.137253	-2.066452	-0.892417

A-s-6
Energy + zep (gas) = -321.27187 au
Gibbs free energy (gas) = -321.29970 au
Enthalpies (gas) = -321.26629 au
Energy (sol) = -321.36195 au
Thermal correction to Gibbs free energy = 0.03519 au
Gibbs free energy (sol) = -321.32676 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.050308	1.081337	-0.000088
2	6	0	-1.380326	0.652948	0.000042
3	6	0	0.802626	-0.002402	-0.000087
4	6	0	-1.340303	-0.689279	-0.000036
5	8	0	-0.024693	-1.116667	-0.000048
6	1	0	-2.103143	-1.449333	0.000146
7	1	0	0.287848	2.030131	-0.000295
8	1	0	-2.216063	1.333878	0.000579
9	8	0	2.011135	-0.039789	0.000131

A-s-6-TS
Energy + zep (gas) = -546.14976 au

Gibbs free energy (gas) = -546.18660 au
Energy (sol) = -546.29751 au
Thermal correction to Gibbs free energy = 0.06853 au
Gibbs free energy (sol) = -546.22898 au
Number and value of imaginary frequency: 1, -258.6cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.592042	-0.040276	0.202371
2	6	0	-0.908342	1.269427	0.724558
3	6	0	-1.815127	-0.516000	-0.446359
4	6	0	-2.184046	1.511578	0.426930
5	8	0	-2.755860	0.456018	-0.270785
6	1	0	-2.828506	2.353082	0.623907
7	1	0	-0.152415	-0.760202	0.941804
8	1	0	-0.168927	1.858735	1.243391
9	8	0	-1.953173	-1.550962	-1.021590
10	1	0	0.291821	-0.082138	-0.450182
11	7	0	1.122990	-1.588820	1.524448
12	6	0	1.763803	-1.229999	0.594781
13	6	0	2.158358	-0.619894	-0.590043
14	6	0	2.843205	0.626079	-0.541997
15	1	0	2.302241	-1.244750	-1.467215
16	7	0	3.337757	1.684480	-0.521094

B-s-6
Energy + zep (gas) = -321.25419 au
Gibbs free energy (gas) = -321.28188 au
Enthalpies (gas) = -321.24870 au
Energy (sol) = -321.32460 au
Thermal correction to Gibbs free energy = 0.03552 au
Gibbs free energy (sol) = -321.28908 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.040959	1.154192	0.000143
2	6	0	-0.637958	0.049759	-0.000095
3	8	0	-1.962033	-0.115452	0.000016
4	8	0	0.081238	-1.084715	-0.000109
5	1	0	-2.364390	0.766171	0.000156
6	6	0	1.398152	-0.639325	0.000176
7	6	0	1.367948	0.713807	-0.000163
8	1	0	2.161281	-1.398832	0.000325
9	1	0	2.193907	1.409211	-0.000248

B-s-6-COM
Energy + zep (gas) = -546.21160 au
Gibbs free energy (gas) = -546.25166 au
Energy (sol) = -546.32927 au
Thermal correction to Gibbs free energy = 0.06880 au

Gibbs free energy (sol) = -546.26047 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.952437	-0.507907	0.191290
2	6	0	1.757689	0.470631	-0.122142
3	8	0	1.507728	1.755403	-0.312071
4	8	0	3.047828	0.120365	-0.276680
5	1	0	-1.423293	-0.939885	0.577356
6	7	0	-1.380044	2.092699	0.122334
7	6	0	-1.840444	1.056395	0.364196
8	6	0	-2.306781	-0.294004	0.689709
9	6	0	-3.400229	-0.758265	-0.171913
10	1	0	-2.624651	-0.327947	1.738414
11	7	0	-4.265088	-1.154721	-0.834683
12	1	0	0.553715	1.940375	-0.190503
13	6	0	3.065975	-1.244511	-0.033309
14	6	0	1.798999	-1.621551	0.248813
15	1	0	4.021527	-1.734947	-0.107668
16	1	0	1.425862	-2.606418	0.487698

B-s-6-TS

Energy + zep (gas) = -546.19112 au

Gibbs free energy (gas) = -546.22765 au

Energy (sol) = -546.30769 au

Thermal correction to Gibbs free energy = 0.06754 au

Gibbs free energy (sol) = -546.240147 au

Number and value of imaginary frequency: 1, -938.8cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.652476	-0.446763	0.275993
2	6	0	1.472178	0.515828	-0.127277
3	8	0	1.264038	1.767720	-0.369985
4	8	0	2.716071	0.059804	-0.295390
5	1	0	-0.538877	-0.372570	0.515156
6	7	0	-1.320653	2.285114	-0.008608
7	6	0	-1.790061	1.259730	0.317816
8	6	0	-2.023866	-0.075799	0.719831
9	6	0	-2.771724	-0.929756	-0.157721
10	1	0	-2.268787	-0.189846	1.776802
11	7	0	-3.315093	-1.684264	-0.861088
12	1	0	0.285731	2.047736	-0.254274
13	6	0	2.683425	-1.293596	0.019278
14	6	0	1.423104	-1.610058	0.368054
15	1	0	3.612705	-1.829675	-0.066923
16	1	0	0.992909	-2.552546	0.668272

A-s-7

Energy + zep (gas) = -474.89208 au

Gibbs free energy (gas) = -474.92364 au

Enthalpies (gas) = -474.88416 au
Energy (sol) = -474.02773 au
Thermal correction to Gibbs free energy = 0.07876 au
Gibbs free energy (sol) = -474. 94897 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.194589	1.102885	-0.000056
2	6	0	0.147143	0.725006	0.000021
3	6	0	-2.014412	-0.011097	0.000006
4	6	0	0.132084	-0.673920	-0.000013
5	8	0	-1.174271	-1.120984	0.000060
6	1	0	-1.574139	2.036671	0.000140
7	8	0	-3.218334	-0.072400	-0.000031
8	6	0	1.286398	-1.433236	-0.000020
9	6	0	2.500653	-0.727387	-0.000014
10	6	0	2.527028	0.672549	-0.000013
11	6	0	1.344789	1.428974	0.000027
12	1	0	1.370201	2.513717	0.000083
13	1	0	3.481995	1.188348	-0.000039
14	1	0	3.434218	-1.280532	-0.000034
15	1	0	1.248586	-2.516672	0.000039

A-s-7-TS
Energy + zep (gas) = -699.77106 au
Gibbs free energy (gas) = -699.811395 au
Energy (sol) = -699.96511 au
Thermal correction to Gibbs free energy = 0.11276 au
Gibbs free energy (sol) = -699.85235 au
Number and value of imaginary frequency: 1, -196.6 cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.239734	0.790105	0.118918
2	6	0	0.792342	-0.221865	0.170558
3	6	0	0.441367	2.027847	-0.309948
4	6	0	1.983363	0.404609	-0.166970
5	8	0	1.765264	1.751952	-0.446934
6	1	0	-0.828401	0.921368	1.047254
7	8	0	-0.093675	3.074798	-0.500340
8	1	0	-1.111208	0.543530	-0.494446
9	7	0	-2.271389	0.755707	1.880082
10	6	0	-2.782192	0.394015	0.875012
11	6	0	-3.016567	0.022181	-0.445205
12	6	0	-3.017709	-1.358474	-0.786878
13	1	0	-3.586076	0.699865	-1.075296
14	7	0	-2.951792	-2.485827	-1.088113
15	6	0	3.190455	-0.264667	-0.214642
16	6	0	3.145325	-1.632178	0.097484
17	6	0	1.944888	-2.272262	0.431442
18	6	0	0.730710	-1.571733	0.475220
19	1	0	-0.204316	-2.064512	0.717598

20	1	0	1.948593	-3.332975	0.657700
21	1	0	4.065712	-2.206348	0.073519
22	1	0	4.111491	0.240348	-0.480776

B-s-7
Energy + zep (gas) = -474.87040 au
Gibbs free energy (gas) = -474.90178 au
Enthalpies (gas) = -474.86259 au
Energy (sol) = -474.98802 au
Thermal correction to Gibbs free energy = 0.07901 au
Gibbs free energy (sol) = -474.90901 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.191346	1.166299	-0.000041
2	6	0	1.858378	0.058368	0.000018
3	8	0	3.178013	-0.107573	0.000081
4	8	0	1.154298	-1.100942	-0.000124
5	1	0	3.582897	0.773497	0.000162
6	6	0	-0.165392	-0.667738	-0.000004
7	6	0	-0.143513	0.734419	-0.000028
8	6	0	-1.318566	-1.430947	0.000035
9	6	0	-1.345665	1.442394	-0.000020
10	6	0	-2.519984	-0.708606	0.000041
11	6	0	-2.529875	0.697109	0.000024
12	1	0	-1.294332	-2.514889	0.000019
13	1	0	-3.461335	-1.248870	0.000055
14	1	0	-3.482917	1.217218	0.000033
15	1	0	-1.354523	2.527074	-0.000036

B-s-7-COM
Energy + zep (gas) = -699.82791 au
Gibbs free energy (gas) = -699.87154 au
Energy (sol) = -699.99234 au
Thermal correction to Gibbs free energy = 0.11227 au
Gibbs free energy (sol) = -699.88007 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.061573	0.319791	0.115197
2	6	0	0.438568	1.548948	-0.094355
3	8	0	-0.282194	2.648699	-0.178729
4	8	0	1.771177	1.759950	-0.252988
5	1	0	-2.021293	-1.035169	0.442919
6	7	0	-3.069731	1.847646	0.242341
7	6	0	-3.118873	0.700705	0.404166
8	6	0	-3.066485	-0.746785	0.625829
9	6	0	-3.972133	-1.503550	-0.246578
10	1	0	-3.300113	-0.962743	1.675046
11	7	0	-4.678255	-2.128871	-0.920857
12	1	0	-1.234475	2.447969	-0.059549

13	6	0	2.322565	0.495410	-0.129470
14	6	0	1.267927	-0.398632	0.097898
15	6	0	3.653708	0.129645	-0.208560
16	6	0	1.542280	-1.757517	0.258875
17	6	0	3.916789	-1.237349	-0.044473
18	6	0	2.880870	-2.158804	0.184055
19	1	0	4.440734	0.853779	-0.386789
20	1	0	4.942208	-1.589085	-0.096366
21	1	0	3.126207	-3.209535	0.304380
22	1	0	0.748457	-2.476800	0.433014

B-s-7-TS
Energy + zep (gas) = -699.80723 au
Gibbs free energy (gas) = -699.84741 au
Energy (sol) = -699.96890 au
Thermal correction to Gibbs free energy = 0.11078 au
Gibbs free energy (sol) = -699.85812 au
Number and value of imaginary frequency: 1, -1029.9 cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.199639	-0.278602	0.166536
2	6	0	0.012809	-1.564730	-0.096191
3	8	0	0.859239	-2.531522	-0.203809
4	8	0	-1.278501	-1.886736	-0.276459
5	1	0	1.253660	0.297425	0.417992
6	7	0	3.327233	-1.589194	0.121753
7	6	0	3.174808	-0.451209	0.366247
8	6	0	2.650674	0.828016	0.665743
9	6	0	2.888808	1.899608	-0.258400
10	1	0	2.742366	1.112535	1.715176
11	7	0	2.993465	2.792112	-1.001097
12	1	0	1.835462	-2.238807	-0.098815
13	6	0	-1.989670	-0.699945	-0.121548
14	6	0	-1.073677	0.315078	0.153084
15	6	0	-3.354487	-0.503972	-0.218228
16	6	0	-1.503001	1.626106	0.343214
17	6	0	-3.787083	0.813935	-0.021164
18	6	0	-2.880702	1.852426	0.251383
19	1	0	-4.039355	-1.315575	-0.434665
20	1	0	-4.847169	1.035999	-0.085063
21	1	0	-3.258400	2.860168	0.390340
22	1	0	-0.805700	2.432214	0.541990

DBU
Energy + zep (gas) = -461.87605 au
Gibbs free energy (gas) = -461.91135 au
Enthalpies (gas) = -461.26699 au
Energy (sol) = -462.14633 au
Thermal correction to Gibbs free energy = 0.20998 au
Gibbs free energy (sol) = -461.93635 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.451097	-1.431565	-0.320648
2	6	0	-2.715997	-0.715420	-0.387657
3	6	0	-0.368586	-0.738108	-0.179382
4	6	0	-2.729165	0.477817	0.568123
5	7	0	-0.326850	0.645423	-0.050499
6	1	0	-2.896334	-0.365530	-1.418129
7	1	0	-3.523793	-1.416200	-0.150337
8	6	0	0.920086	-1.554525	-0.154347
9	6	0	-1.563857	1.395909	0.216594
10	1	0	-2.622488	0.111223	1.596313
11	6	0	0.851424	1.522756	-0.028326
12	1	0	-3.668867	1.039076	0.513224
13	1	0	-1.369114	2.094936	1.042664
14	6	0	2.125764	1.008277	-0.701226
15	6	0	2.924406	0.005938	0.146212
16	6	0	2.027015	-1.063288	0.790231
17	1	0	0.544377	2.442072	-0.545039
18	1	0	1.076717	1.819217	1.011120
19	1	0	2.755686	1.878649	-0.921533
20	1	0	1.863024	0.573000	-1.672438
21	1	0	3.481055	0.541248	0.926363
22	1	0	3.675017	-0.476241	-0.493319
23	1	0	1.569617	-0.669919	1.707083
24	1	0	2.642123	-1.915105	1.102631
25	1	0	0.590755	-2.558159	0.120956
26	1	0	1.311473	-1.639107	-1.177545
27	1	0	-1.810163	2.007699	-0.665320

DBU-COM
Energy + zep (gas) = -686.83398 au
Gibbs free energy (gas) = -686.88290 au
Energy (sol) = -687.13555 au
Thermal correction to Gibbs free energy = 0.24207 au
Gibbs free energy (sol) = -686.89348 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.373989	0.956218	-0.322663
2	6	0	0.237007	2.406299	-0.254949
3	6	0	-0.686498	0.227932	-0.134604
4	6	0	-1.082488	2.862864	-0.875037
5	7	0	-1.950585	0.738577	0.081196
6	1	0	0.291148	2.741203	0.793562
7	1	0	1.089424	2.860730	-0.772524
8	6	0	-0.453184	-1.279114	-0.173699
9	6	0	-2.223151	2.168787	-0.142041
10	1	0	-1.093582	2.589811	-1.937014
11	6	0	-3.170816	0.008990	0.466451
12	1	0	-1.210403	3.948844	-0.810405
13	1	0	-3.153386	2.250060	-0.720436
14	6	0	-2.990722	-1.318842	1.204261

15	6	0	-2.651993	-2.503154	0.286983
16	6	0	-1.581215	-2.144475	-0.755260
17	1	0	-3.720320	0.692276	1.126266
18	1	0	-3.808204	-0.138679	-0.421017
19	1	0	-3.925772	-1.527780	1.737468
20	1	0	-2.225244	-1.193446	1.979077
21	1	0	-3.560109	-2.849926	-0.222286
22	1	0	-2.303737	-3.341068	0.903864
23	1	0	-2.039089	-1.619707	-1.603441
24	1	0	-1.148950	-3.062844	-1.167188
25	1	0	0.455655	-1.405307	-0.764091
26	1	0	-0.200098	-1.624985	0.837564
27	1	0	2.305597	0.361561	-0.379649
28	7	0	3.554584	-2.482080	-0.919679
29	6	0	3.505232	-1.349577	-0.670557
30	6	0	3.388926	0.085708	-0.392036
31	6	0	3.998335	0.471788	0.884966
32	1	0	3.865953	0.648184	-1.203702
33	7	0	4.457913	0.815158	1.893733
34	1	0	-2.406779	2.652719	0.828973

DBU-TS
Energy + zep (gas) = -686.82366 au
Gibbs free energy (gas) = -686.86987 au
Energy (sol) = -687.15967 au
Thermal correction to Gibbs free energy = 0.24124 au
Gibbs free energy (sol) = -686.91842 au
Number and value of imaginary frequency: 1, -1023.7cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.684175	0.706141	0.285689
2	6	0	-0.978322	2.113412	0.029236
3	6	0	0.529796	0.220411	0.183446
4	6	0	0.202082	2.969852	0.473855
5	7	0	1.598961	0.995939	-0.133049
6	1	0	-1.187286	2.262064	-1.039063
7	1	0	-1.893985	2.368061	0.568749
8	6	0	0.659225	-1.270833	0.461408
9	6	0	1.463361	2.465637	-0.216845
10	1	0	0.315138	2.901611	1.562086
11	6	0	2.974757	0.544021	-0.439104
12	1	0	0.044840	4.023192	0.222337
13	1	0	2.354372	2.904235	0.246932
14	6	0	3.128390	-0.868648	-1.006086
15	6	0	3.086494	-1.975638	0.057739
16	6	0	1.976682	-1.743016	1.092684
17	1	0	3.344643	1.255794	-1.185068
18	1	0	3.604367	0.671892	0.453991
19	1	0	4.086495	-0.906258	-1.537099
20	1	0	2.356510	-1.029876	-1.767762
21	1	0	4.055381	-2.038907	0.568417
22	1	0	2.932968	-2.940350	-0.440206
23	1	0	2.303820	-1.014371	1.845244

24	1	0	1.785164	-2.672543	1.638633
25	1	0	-0.171773	-1.516698	1.123735
26	1	0	0.452598	-1.820438	-0.465083
27	1	0	-1.683274	-0.023203	0.455604
28	7	0	-2.320192	-2.986718	-0.698291
29	6	0	-2.673686	-2.012059	-0.160082
30	6	0	-2.951920	-0.781495	0.526677
31	6	0	-3.905343	0.093438	-0.100207
32	1	0	-3.176278	-0.941853	1.584921
33	7	0	-4.603386	0.888756	-0.593883
34	1	0	1.468741	2.758328	-1.275957

t-1
Energy + zep (gas) = -329.14153 au
Gibbs free energy (gas) = -329.17213 au
Enthalpies (gas) = -329.50672 au
Energy (sol) = -329.33903 au
Thermal correction to Gibbs free energy = 0.16412 au
Gibbs free energy (sol) = -329.17491 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.292125	0.023180	0.007208
2	6	0	-0.803335	-0.648964	1.224355
3	6	0	-0.818235	-0.711753	-1.178996
4	6	0	-0.772823	1.401951	-0.032545
5	6	0	0.757666	-0.651762	1.295806
6	6	0	0.740632	-0.819167	-1.207593
7	6	0	0.787742	1.431328	-0.100572
8	1	0	-1.284259	-1.703657	-1.171232
9	1	0	-1.194419	-0.188519	-2.065508
10	1	0	-1.216894	1.906322	-0.898203
11	1	0	-1.138552	1.919818	0.861447
12	6	0	1.295378	-0.022782	-0.007145
13	1	0	1.112548	-0.076142	2.159956
14	1	0	1.145052	-1.671430	1.411990
15	1	0	1.145611	-0.420442	-2.145843
16	1	0	1.132180	1.885032	-1.038287
17	1	0	1.206074	2.031668	0.716649
18	1	0	1.063622	-1.865612	-1.140301
19	1	0	2.390910	-0.042444	-0.012867
20	1	0	-1.199857	-1.670702	1.220884
21	1	0	-1.239294	-0.139259	2.091006

t-1-COM
Energy + zep (gas) = -554.09658 au
Gibbs free energy (gas) = -554.14109 au
Energy (sol) = -554.34591 au
Thermal correction to Gibbs free energy = 0.19574 au
Gibbs free energy (sol) = -554.15017 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.491416	0.013565	-0.238870
2	6	0	-0.703115	-0.163021	1.215997
3	6	0	-1.095194	1.294262	-0.669028
4	6	0	-1.135244	-1.101949	-0.966861
5	6	0	-2.221292	-0.176289	1.576945
6	6	0	-2.630387	1.328115	-0.388405
7	6	0	-2.669312	-1.161920	-0.685030
8	1	0	-0.576671	2.101096	-0.140326
9	1	0	-0.885245	1.420713	-1.737056
10	1	0	-0.934555	-0.962703	-2.035060
11	1	0	-0.639195	-2.029839	-0.662413
12	6	0	-3.027522	-0.007423	0.273165
13	1	0	-2.496204	-1.116143	2.069886
14	1	0	-2.463095	0.632912	2.275981
15	1	0	-3.194083	1.468474	-1.318338
16	1	0	-3.241089	-1.069613	-1.615998
17	1	0	-2.945438	-2.122650	-0.234777
18	1	0	-2.887434	2.165890	0.270300
19	1	0	-4.101093	-0.016420	0.489506
20	1	0	-0.180060	0.650656	1.729749
21	1	0	1.559712	0.013112	-0.562468
22	7	0	3.557652	-2.225516	0.413435
23	6	0	3.188222	-1.229008	-0.052427
24	6	0	2.671896	0.001189	-0.662754
25	6	0	3.216104	1.218226	-0.050418
26	1	0	2.911066	-0.000842	-1.733075
27	7	0	3.608699	2.204858	0.417496
28	1	0	-0.216090	-1.098093	1.512568

t-1-TS
Energy + zep (gas) = -554.08091 au
Gibbs free energy (gas) = -554.12215au
Energy (sol) = -554.33876 au
Thermal correction to Gibbs free energy = 0.19747 au
Gibbs free energy (sol) = -554.14129 au
Number and value of imaginary frequency: 1, -183.2cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.255747	-0.009676	-0.308560
2	6	0	-0.362035	-0.005599	1.188650
3	6	0	-0.890489	1.221578	-0.875347
4	6	0	-0.899746	-1.238790	-0.868254
5	6	0	-1.855734	-0.087790	1.601424
6	6	0	-2.374766	1.295784	-0.428925
7	6	0	-2.423116	-1.209994	-0.571958
8	1	0	-0.300557	2.073540	-0.530102
9	1	0	-0.785717	1.161563	-1.962102
10	1	0	-0.680853	-1.259647	-1.939256
11	1	0	-0.397546	-2.094209	-0.410688
12	6	0	-2.729181	0.002038	0.332812

13	1	0	-2.056445	-1.026129	2.129193
14	1	0	-2.102355	0.726260	2.290512
15	1	0	-3.027819	1.414959	-1.299681
16	1	0	-2.995385	-1.137180	-1.503112
17	1	0	-2.728545	-2.138964	-0.080018
18	1	0	-2.536775	2.166413	0.215066
19	1	0	-3.788793	0.006711	0.605903
20	1	0	0.122749	0.909732	1.535208
21	1	0	0.883996	-0.010128	-0.582204
22	7	0	2.905086	-2.243343	0.486217
23	6	0	2.786589	-1.215289	-0.059430
24	6	0	2.476448	0.004361	-0.737320
25	6	0	2.757864	1.231114	-0.059723
26	1	0	2.757092	0.007648	-1.791536
27	7	0	2.849962	2.262379	0.485086
28	1	0	0.226839	-0.850561	1.552035

t-2
Energy + zep (gas) = -292.24067 au
Gibbs free energy (gas) = -292.27459 au
Enthalpies (gas) = -292.60181 au
Energy (sol) = -292.45737 au
Thermal correction to Gibbs free energy = 0.17144 au
Gibbs free energy (sol) = -292.28593 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000322	-0.000298	0.010161
2	6	0	-1.210018	-0.716430	0.438567
3	6	0	-0.015388	1.405939	0.438206
4	6	0	-1.534320	-1.933553	-0.430351
5	1	0	-2.460581	-2.407587	-0.086076
6	1	0	-1.663223	-1.632465	-1.474658
7	1	0	-0.745191	-2.691290	-0.393701
8	1	0	1.007964	1.788351	0.380781
9	6	0	-0.908181	2.295311	-0.429987
10	1	0	-0.316241	1.490010	1.501879
11	1	0	-1.134279	-1.018364	1.502497
12	1	0	-2.051621	-0.020144	0.379715
13	1	0	-0.862096	3.333316	-0.081202
14	1	0	-1.957828	1.985865	-0.399254
15	1	0	-0.578915	2.262611	-1.473282
16	6	0	1.225485	-0.690500	0.437514
17	6	0	2.442475	-0.360691	-0.429596
18	1	0	1.448165	-0.475106	1.501989
19	1	0	1.043345	-1.767378	0.376041
20	1	0	2.703805	0.701751	-0.393220
21	1	0	3.316425	-0.924901	-0.084555
22	1	0	2.247695	-0.623033	-1.474197

t-2-COM
Energy + zep (gas) = -517.19186 au
Gibbs free energy (gas) = -517.23875 au

Energy (sol) = -517.45103 au
Thermal correction to Gibbs free energy = 0.20417 au
Gibbs free energy (sol) = -517.24687 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.386484	-0.001407	0.127725
2	6	0	-1.483934	-0.619273	1.469157
3	6	0	-2.162269	-0.785693	-0.856761
4	6	0	-0.387106	-0.185155	2.442998
5	1	0	0.755341	0.001615	-0.481313
6	7	0	2.925298	-2.212284	0.122646
7	6	0	2.461030	-1.222922	-0.266806
8	6	0	1.827892	0.000557	-0.773148
9	6	0	2.462842	1.223964	-0.268811
10	1	0	1.872545	0.000133	-1.869064
11	7	0	2.927797	2.214404	0.117050
12	1	0	-0.548840	-0.663244	3.414916
13	1	0	0.602336	-0.486809	2.086475
14	1	0	-0.373577	0.896047	2.610003
15	1	0	-2.335632	-0.152440	-1.731131
16	6	0	-1.468633	-2.067815	-1.321694
17	1	0	-3.160942	-1.026553	-0.446284
18	1	0	-2.479287	-0.413088	1.905889
19	1	0	-1.421982	-1.703638	1.344365
20	1	0	-2.109825	-2.598208	-2.033816
21	1	0	-1.255760	-2.756095	-0.498494
22	1	0	-0.522282	-1.845010	-1.824973
23	6	0	-1.865176	1.397772	0.167490
24	6	0	-1.386991	2.257880	-1.003981
25	1	0	-2.969968	1.417784	0.223334
26	1	0	-1.502439	1.850692	1.093843
27	1	0	-1.702335	1.861836	-1.974519
28	1	0	-1.803186	3.266902	-0.914375
29	1	0	-0.296374	2.349200	-1.007483

t-2-TS
Energy + zep (gas) = -517.17495 au
Gibbs free energy (gas) = -517.21833 au
Energy (sol) = -517.46140 au
Thermal correction to Gibbs free energy = 0.20559 au
Gibbs free energy (sol) = -517.25581 au
Number and value of imaginary frequency: 1, -592.6cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.000741	-0.026631	0.149619
2	6	0	0.865721	0.507660	1.549197
3	6	0	1.894529	0.840160	-0.686691
4	6	0	0.011493	-0.346627	2.484624
5	1	0	-0.096415	0.001686	-0.359439
6	7	0	-2.358341	2.327508	-0.055827

7	6	0	-2.058405	1.279640	-0.478227
8	6	0	-1.534572	0.039771	-0.969119
9	6	0	-2.123280	-1.164479	-0.463620
10	1	0	-1.427313	0.032178	-2.056641
11	7	0	-2.483205	-2.184049	-0.019414
12	1	0	-0.167402	0.228644	3.397895
13	1	0	-0.961659	-0.586408	2.048586
14	1	0	0.501397	-1.279052	2.776002
15	1	0	1.828294	0.455377	-1.706183
16	6	0	1.532697	2.325295	-0.687239
17	1	0	2.926319	0.691529	-0.341208
18	1	0	1.877931	0.634795	1.956086
19	1	0	0.411065	1.494382	1.455978
20	1	0	2.117556	2.819467	-1.469102
21	1	0	1.771176	2.818472	0.258140
22	1	0	0.473636	2.490982	-0.903097
23	6	0	1.454746	-1.457984	0.140612
24	6	0	1.573728	-2.075856	-1.251766
25	1	0	2.412780	-1.511303	0.675121
26	1	0	0.715316	-2.019688	0.711374
27	1	0	2.403634	-1.666809	-1.833626
28	1	0	1.751706	-3.148967	-1.136003
29	1	0	0.647668	-1.958569	-1.821157

t-3
Energy + zep (gas) = -370.81477 au
Gibbs free energy (gas) = -370.85182 au
Enthalpies (gas) = 370.17862 au
Energy (sol) = -371.08761 au
Thermal correction to Gibbs free energy = 0.22399 au
Gibbs free energy (sol) = -370.86362 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.005899	0.264863	0.165485
2	6	0	-1.031521	-0.796137	0.208836
3	6	0	1.402114	-0.162802	0.067499
4	6	0	-2.138729	-0.427751	1.211748
5	1	0	-2.873202	-1.237152	1.297906
6	1	0	-1.710287	-0.234863	2.199351
7	1	0	-2.677841	0.473528	0.896789
8	1	0	1.973977	0.765751	-0.042247
9	6	0	1.884605	-0.814274	1.373352
10	6	0	1.752350	-1.045606	-1.150965
11	6	0	-1.649615	-1.197902	-1.150428
12	1	0	-0.527729	-1.684181	0.605456
13	1	0	2.962915	-1.004994	1.328754
14	1	0	1.393626	-1.776387	1.559576
15	1	0	1.680164	-0.158462	2.224668
16	1	0	2.837127	-1.190236	-1.213547
17	1	0	1.424877	-0.585553	-2.089269
18	1	0	1.293384	-2.037696	-1.076896
19	1	0	-2.259899	-0.392075	-1.573023
20	1	0	-0.886693	-1.464207	-1.886254

21	1	0	-2.306541	-2.065518	-1.019195
22	6	0	-0.336089	1.448202	-0.630443
23	6	0	0.159216	2.758049	-0.004204
24	1	0	0.042628	1.373598	-1.667252
25	1	0	-1.424861	1.508718	-0.715244
26	1	0	1.249357	2.783409	0.094244
27	1	0	-0.133137	3.610968	-0.628391
28	1	0	-0.270560	2.890640	0.993791

t-3-COM

Energy + zep (gas) = -595.76319 au

Gibbs free energy (gas) = -595.81312 au

Energy (sol) = -596.07832 au

Thermal correction to Gibbs free energy = 0.25728 au

Gibbs free energy (sol) = -595.82104 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.989862	-0.180724	-0.081584
2	6	0	1.254673	0.058067	1.369593
3	6	0	1.612613	0.800770	-1.010836
4	6	0	0.011302	-0.278501	2.208268
5	1	0	-1.299936	0.110203	-0.434952
6	7	0	-3.276530	2.372943	0.553729
7	6	0	-2.900348	1.408771	0.029584
8	6	0	-2.382752	0.215301	-0.650809
9	6	0	-3.074060	-1.015572	-0.247669
10	1	0	-2.490474	0.347327	-1.734326
11	7	0	-3.590160	-2.010301	0.052131
12	1	0	0.214612	-0.121870	3.273201
13	1	0	-0.835266	0.357927	1.936706
14	1	0	-0.290300	-1.324471	2.083407
15	1	0	1.335603	0.453448	-2.011777
16	6	0	1.000763	2.202061	-0.857498
17	6	0	3.153768	0.888632	-0.977788
18	6	0	2.494070	-0.653278	1.957427
19	1	0	1.424424	1.133860	1.470859
20	1	0	1.360985	2.852059	-1.661928
21	1	0	1.278012	2.678845	0.088158
22	1	0	-0.091138	2.174418	-0.910687
23	1	0	3.506253	1.505114	-1.812170
24	1	0	3.627206	-0.093478	-1.073988
25	1	0	3.511925	1.354471	-0.053638
26	1	0	2.342280	-1.734389	2.043377
27	1	0	3.395210	-0.484029	1.364062
28	1	0	2.683114	-0.272709	2.966971
29	6	0	1.204534	-1.585877	-0.477128
30	6	0	0.518318	-2.002624	-1.782127
31	1	0	2.276944	-1.835224	-0.547946
32	1	0	0.801232	-2.211565	0.324479
33	1	0	0.913814	-1.480888	-2.658675
34	1	0	0.678332	-3.073551	-1.946329
35	1	0	-0.562330	-1.835429	-1.740841

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t-3-TS
Energy + zep (gas) = -595.74689 au
Gibbs free energy (gas) = -595.79175 au
Energy (sol) = -596.08978 au
Thermal correction to Gibbs free energy = 0.26045 au
Gibbs free energy (sol) = -595.82933 au
Number and value of imaginary frequency: 1, -847.9cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.626409	0.224741	0.070940
2	6	0	-0.707512	-0.728992	1.255446
3	6	0	-1.442623	-0.146638	-1.157509
4	6	0	0.353175	-0.392514	2.314841
5	1	0	0.531584	0.099954	-0.345544
6	7	0	2.391417	-2.600812	-0.477774
7	6	0	2.261955	-1.456439	-0.673994
8	6	0	1.948671	-0.074162	-0.902790
9	6	0	2.742810	0.888703	-0.193462
10	1	0	1.884996	0.156280	-1.970007
11	7	0	3.284389	1.725657	0.415527
12	1	0	0.469882	-1.263000	2.966684
13	1	0	1.331193	-0.176556	1.881151
14	1	0	0.058719	0.451155	2.946816
15	1	0	-0.935768	0.399602	-1.960877
16	6	0	-1.327177	-1.638292	-1.494069
17	6	0	-2.908369	0.310270	-1.147839
18	6	0	-2.094784	-0.837339	1.901779
19	1	0	-0.438754	-1.699360	0.834030
20	1	0	-1.722304	-1.794549	-2.502516
21	1	0	-1.914567	-2.263797	-0.815114
22	1	0	-0.293563	-1.992195	-1.483600
23	1	0	-3.329102	0.121106	-2.140679
24	1	0	-3.022567	1.378384	-0.948832
25	1	0	-3.515653	-0.239108	-0.426047
26	1	0	-2.466537	0.133027	2.246295
27	1	0	-2.840120	-1.280121	1.238765
28	1	0	-2.016282	-1.484840	2.780697
29	6	0	-0.761246	1.667190	0.462686
30	6	0	-0.438992	2.661663	-0.654107
31	1	0	-1.767701	1.844694	0.854931
32	1	0	-0.056666	1.830410	1.278059
33	1	0	-1.148635	2.624114	-1.484624
34	1	0	-0.480542	3.670504	-0.232493
35	1	0	0.571170	2.516499	-1.043840

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t-4
Energy + zep (gas) = -867.32286 au
Gibbs free energy (gas) = -867.37301 au
Enthalpies (gas) = -867.68018 au
Energy (sol) = -867.69187 au
Thermal correction to Gibbs free energy = 0.31447 au

Gibbs free energy (sol) = -867.37740 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.194003	-0.240339	-0.614263
2	6	0	-0.926035	-1.490557	-0.384427
3	6	0	-0.062154	0.563399	0.605015
4	1	0	0.663962	0.127867	1.314451
5	1	0	-1.036037	0.534593	1.107857
6	1	0	-0.851207	-2.078187	-1.308234
7	1	0	-0.472688	-2.106321	0.412786
8	6	0	1.063058	-0.422375	-1.366716
9	1	0	0.797093	-0.899623	-2.317196
10	1	0	1.444155	0.575611	-1.604554
11	6	0	-2.395155	-1.272978	-0.066408
12	6	0	-3.202314	-0.501999	-0.916694
13	6	0	-2.982388	-1.869463	1.056220
14	6	0	-4.561890	-0.333915	-0.650473
15	1	0	-2.752143	-0.028753	-1.784747
16	6	0	-4.345250	-1.705316	1.326384
17	1	0	-2.367856	-2.466016	1.726559
18	6	0	-5.138952	-0.936536	0.473098
19	1	0	-5.173105	0.265744	-1.319391
20	1	0	-4.782385	-2.173838	2.203741
21	1	0	-6.197055	-0.805177	0.680656
22	6	0	2.164830	-1.230547	-0.690038
23	6	0	3.145605	-0.596880	0.088703
24	6	0	2.226436	-2.626256	-0.825445
25	6	0	4.146806	-1.334484	0.726666
26	1	0	3.131512	0.485876	0.184125
27	6	0	3.224699	-3.369270	-0.190289
28	1	0	1.492683	-3.137225	-1.444314
29	6	0	4.186976	-2.724803	0.592329
30	1	0	4.898709	-0.822946	1.321316
31	1	0	3.255881	-4.448466	-0.312489
32	1	0	4.966184	-3.299902	1.084245
33	6	0	0.299214	2.015447	0.345919
34	6	0	1.203240	2.680709	1.184633
35	6	0	-0.302331	2.735999	-0.696536
36	6	0	1.499576	4.033975	0.993080
37	1	0	1.678336	2.135284	1.996979
38	6	0	-0.005512	4.085974	-0.894187
39	1	0	-0.999566	2.224577	-1.353084
40	6	0	0.896564	4.741212	-0.049428
41	1	0	2.203753	4.531454	1.654285
42	1	0	-0.479969	4.628548	-1.707422
43	1	0	1.127618	5.791263	-0.204153

t-4-COM

Energy + zep (gas) = -1092.27191 au

Gibbs free energy (gas) = -1092.33470 au

Energy (sol) = -1092.69135 au

Thermal correction to Gibbs free energy = 0.34748 au

Gibbs free energy (sol) = -1092.34386 au

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.332257	-0.308338	0.037074
2	6	0	-0.278389	-1.786560	0.043998
3	6	0	-0.382537	0.243881	-1.333111
4	1	0	-1.391622	0.159226	-1.767774
5	1	0	0.276331	-0.376633	-1.946759
6	1	0	-0.344702	-2.098155	1.093127
7	1	0	-1.146856	-2.227176	-0.472013
8	6	0	-1.391956	0.220688	0.932087
9	1	0	-1.133857	-0.094156	1.950068
10	1	0	-1.318813	1.313227	0.900513
11	6	0	0.993816	-2.349849	-0.559335
12	6	0	2.231788	-2.168279	0.075556
13	6	0	0.957196	-3.085746	-1.751276
14	6	0	3.402845	-2.694176	-0.471940
15	1	0	2.279764	-1.619590	1.011937
16	6	0	2.126773	-3.617508	-2.304065
17	1	0	0.004612	-3.245257	-2.251183
18	6	0	3.353351	-3.419804	-1.666931
19	1	0	4.350862	-2.540819	0.035283
20	1	0	2.077382	-4.183877	-3.229715
21	1	0	4.263771	-3.830472	-2.093569
22	6	0	-2.831917	-0.191043	0.647614
23	6	0	-3.669966	0.602604	-0.150263
24	6	0	-3.363637	-1.369526	1.195314
25	6	0	-4.988198	0.221528	-0.415673
26	1	0	-3.294639	1.539634	-0.551295
27	6	0	-4.679971	-1.756379	0.933839
28	1	0	-2.747457	-1.984857	1.845898
29	6	0	-5.495673	-0.963959	0.121271
30	1	0	-5.619335	0.854426	-1.033220
31	1	0	-5.070496	-2.670613	1.371691
32	1	0	-6.520567	-1.261292	-0.080515
33	6	0	0.100446	1.680079	-1.418493
34	6	0	-0.760077	2.723229	-1.782982
35	6	0	1.449381	1.983903	-1.171355
36	6	0	-0.296738	4.040464	-1.875713
37	1	0	-1.800353	2.504436	-2.009157
38	6	0	1.917744	3.295704	-1.261303
39	1	0	2.138902	1.180613	-0.924424
40	6	0	1.042231	4.331238	-1.608686
41	1	0	-0.981530	4.834842	-2.158851
42	1	0	2.966410	3.507654	-1.072415
43	1	0	1.405470	5.352225	-1.681186
44	1	0	1.220887	0.734720	1.448444
45	7	0	4.321668	1.213914	1.846614
46	6	0	3.180578	1.231019	2.054605
47	6	0	1.729732	1.261074	2.277353
48	6	0	1.339785	0.643944	3.551759
49	1	0	1.386025	2.302009	2.255854
50	7	0	0.993473	0.150242	4.542833

t-4-TS
Energy + zep (gas) = -1092.25146 au
Gibbs free energy (gas) = -1092.30946 au
Energy (sol) = -1092.67421 au
Thermal correction to Gibbs free energy = 0.34962 au
Gibbs free energy (sol) = -1092.32459 au
Number and value of imaginary frequency: 1, -805.5cm^{-1}

Standard Orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.194553	-0.087291	0.201941
2	6	0	-0.072919	-1.582507	-0.018982
3	6	0	-0.060178	0.691138	-1.080230
4	1	0	-0.936418	0.476968	-1.701716
5	1	0	0.812911	0.279185	-1.587982
6	1	0	-0.110662	-2.027531	0.978622
7	1	0	-0.959018	-1.907716	-0.570325
8	6	0	-1.447317	0.244317	0.991446
9	1	0	-1.234709	-0.073021	2.015227
10	1	0	-1.520558	1.333938	0.991242
11	6	0	1.175304	-2.028701	-0.746929
12	6	0	2.397620	-2.166661	-0.074041
13	6	0	1.113296	-2.361922	-2.109620
14	6	0	3.537855	-2.598912	-0.754247
15	1	0	2.461854	-1.944531	0.985621
16	6	0	2.250432	-2.801370	-2.790393
17	1	0	0.166685	-2.284223	-2.639671
18	6	0	3.467887	-2.914770	-2.113329
19	1	0	4.477786	-2.687140	-0.218634
20	1	0	2.184592	-3.057434	-3.843819
21	1	0	4.354980	-3.253403	-2.640371
22	6	0	-2.740658	-0.390685	0.527013
23	6	0	-3.531604	0.189954	-0.476350
24	6	0	-3.198438	-1.568772	1.139613
25	6	0	-4.732112	-0.402479	-0.876154
26	1	0	-3.221942	1.122898	-0.935937
27	6	0	-4.398620	-2.162671	0.744268
28	1	0	-2.615223	-2.018443	1.939131
29	6	0	-5.166371	-1.583791	-0.269912
30	1	0	-5.331537	0.064918	-1.651886
31	1	0	-4.735935	-3.071671	1.233261
32	1	0	-6.101695	-2.042579	-0.576280
33	6	0	0.121556	2.183381	-0.893975
34	6	0	-0.914521	3.081825	-1.186690
35	6	0	1.360745	2.697161	-0.479774
36	6	0	-0.730412	4.460061	-1.044726
37	1	0	-1.869642	2.708215	-1.545359
38	6	0	1.545365	4.072739	-0.330991
39	1	0	2.189891	2.026244	-0.274972
40	6	0	0.499311	4.957902	-0.608944
41	1	0	-1.544188	5.140110	-1.278810
42	1	0	2.510413	4.449268	-0.005605
43	1	0	0.645562	6.028175	-0.497076
44	1	0	0.660159	0.223682	1.013393

45	7	0	3.960175	0.880994	1.542151
46	6	0	2.872178	0.712134	1.932619
47	6	0	1.497669	0.535195	2.299181
48	6	0	1.201854	-0.578527	3.153551
49	1	0	1.054534	1.464537	2.667682
50	7	0	0.859323	-1.515800	3.763026
