Trienamine Catalysis for Asymmetric Diels-Alder Reactions of 2,4-Dienones: A Theoretical Investigation

Zhishan Su and Chan Kyung Kim*

Department of Chemistry and Chemical Engineering and Center for Design and Applications of Molecular Catalysts, Inha University, 100 Inha-ro, Incheon, 402-751, Korea

Supporting Information

Table S1. Activation energies and their energy components in the Diels-Alder reactions in the absence of a catalyst (in kcal mol^{-1}).

Pathway	Reaction	ΔE_{int}	ΔE_d			$\Delta E^{\neq d}$	$\Delta G^{\neq e}$
			Diene[a]	Dienophile[b]	Sum[c]		
2-B	R1a+R2→ 2-B-TS-1a	-13.4	30.0	13.2	39.2	25.8	32.4
	R1b+R2→ 2-B-TS-1b	-12.4	19.4	11.6	31.0	18.6	26.0
3-B-Path1	R1a+R3→ 3-B-TS-1a	-14.7	28.4	28.6	57.0	42.3	45.6
	R1b+R3→ 3-B-TS-1b	-14.9	24.0	23.2	47.2	32.3	36.7
3-B-Path2	R1a+R3→ 3-B-TS-1a'	-21.4	26.2	26.5	52.7	31.3	36.5
	R1b+R3→ 3-B-TS-1b'	-14.6	20.6	21.0	41.6	27.0	30.1

[a]Deformation energy of the 2,4-dienone fragment (**R1a** or **R1b**). [b]Deformation energy of dienophile fragment (**R2** or **R3**). [c]Total deformation energy. [d]Activation energy in the gas phase. [e]Activation free energy in a toluene solvent at 298 K.

Table S2. Activation energies and their energy components (kcal mol^{-1}) in the Diels-Alder reaction by trienamine catalysis.

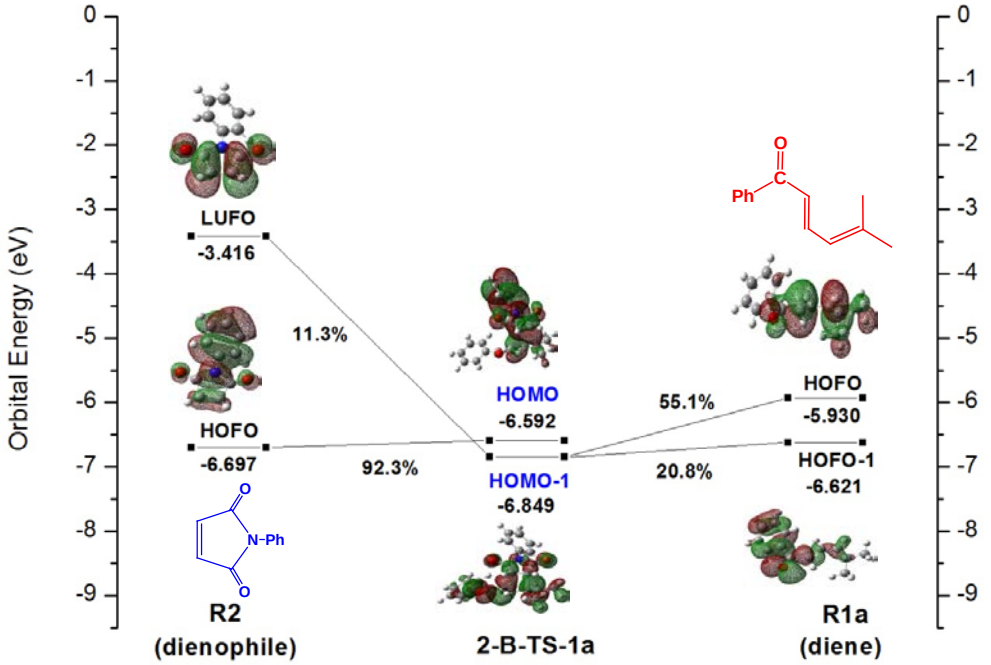
Path	Reactions	ΔE_{int}	ΔE_d			$\Delta_r E^{\neq d}$	$\Delta G^{\neq e}$
			Trienamine[a]	Dienophile (R2)[b]	Sum[c]		
1	2-1-COM-endo → 2-1-TS-endo	-14.5	9.5	16.0	25.4	10.9	12.1
2	2-2-COM-exo → 2-2-TS-exo	-10.5	9.0	15.2	24.1	14.0	14.0
3	2-3-COM-endo → 2-3-TS-endo	-11.2	9.4	14.3	23.6	12.4	15.0
4	2-4-COM-exo → 2-4-TS-exo	-15.0	10.7	21.8	32.5	19.1	18.1

[a]Deformation energy of trienamine fragment. [b]Deformation energies of dienophile (**R2**).[c] Total deformation energy. [d]Activation energy in the gas phase. [e]Activation free energy in a toluene solvent at 333 K.

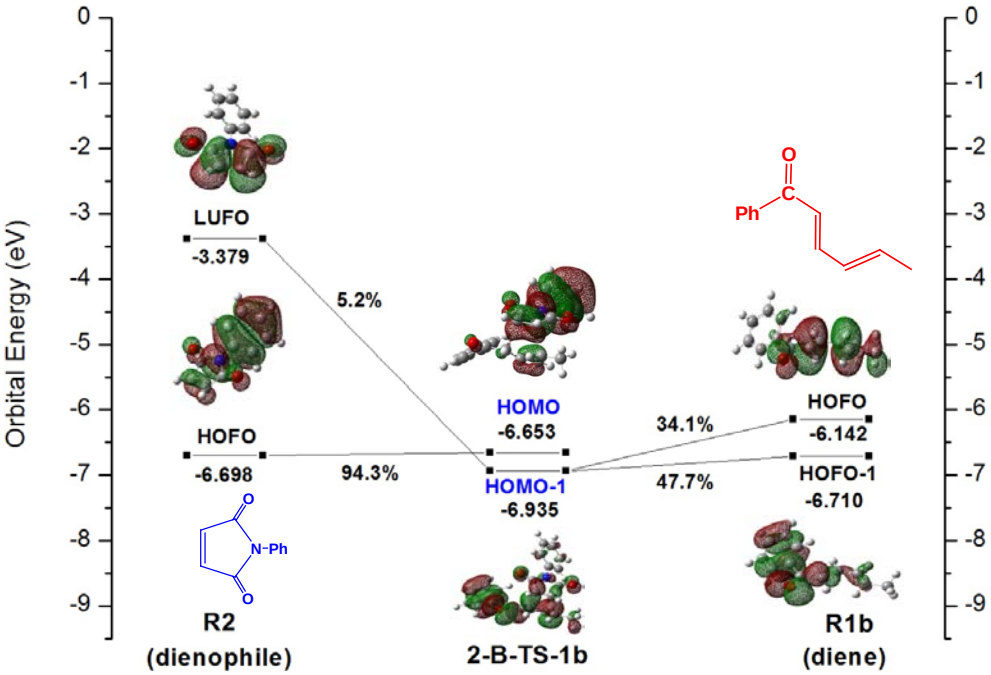
Table S3. Experimental and calculated enantiomeric transition state energy differences, ΔG^{TS}(kcal mol^{-1}), in the Diels-Alder reaction by trienamine catalysis.

Reactant	Selectivity	T(K)	ΔG^{TS}(exp.)	ΔG^{TS}(calc.)
R2	92 ~ 94[a]	333	2.1~2.3	2.9
	> 90[b]	333	> 2.0	1.9
R3	90%[a]	353	2.1	5.1
	> 90%[b]	353	> 2.1	0.3

[a]Enantiomeric excess %. [b]Diastereomeric ratio %.



(a)



(b)

Figure S1. Orbital interaction diagrams for transition states. (a) **2-B-TS-1a** and (b) **2-B-TS-1b**.

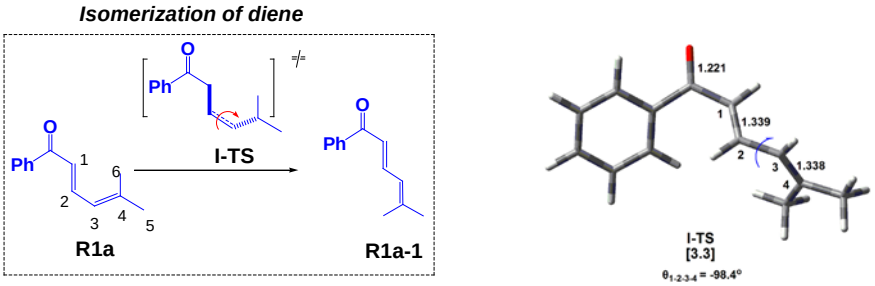


Figure S2. Optimized geometries of transition state **I-TS** in the isomerization reaction between **R1a** and **R1a-1** by C2-C3 single bond rotation. Activation free energies at 298 K ($\Delta G^{\neq}$, kcal mol^{-1}) are given in brackets.

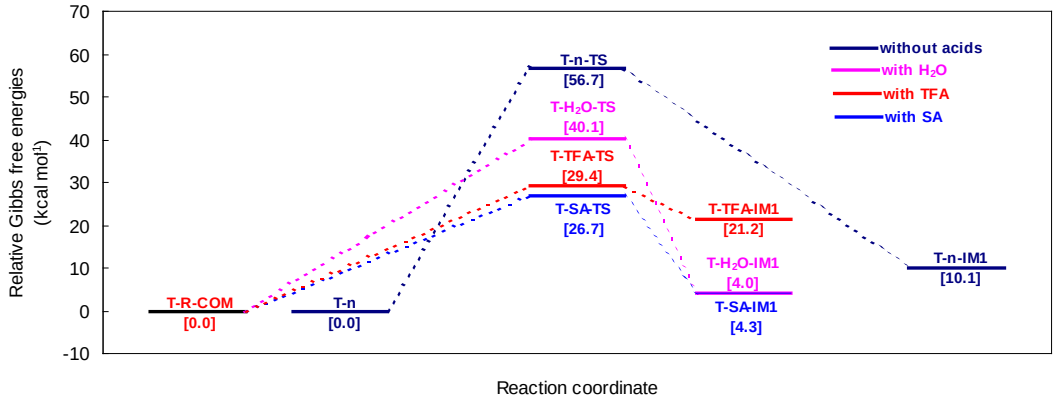


Figure S3. Gibbs energy profiles at 298 K for isomerization of trienamine intermediates in the absence of acidic additives and in the presence of water, acidic additives - trifluoroacetic acid (**TFA**) or salicylic acid (**SA**). Activation free energies ($\Delta G^{\neq}$, kcal mol^{-1}) are given in brackets.

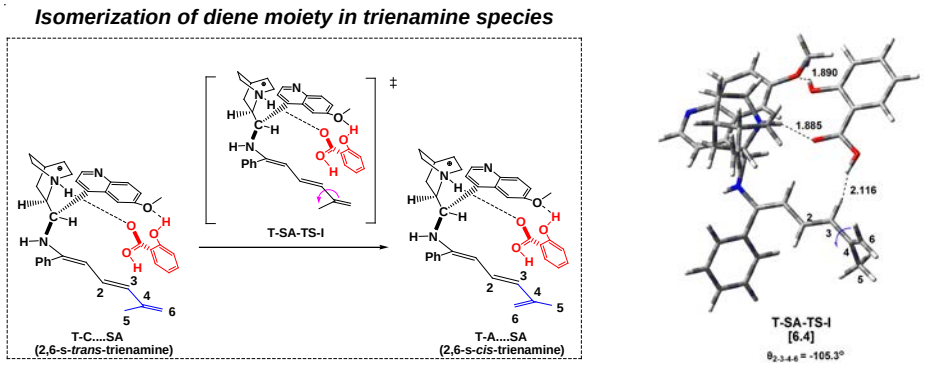


Figure S4. Optimized geometries of transition state **T-SA-TS-I** in the isomerization reaction from all *trans*-comformation to 2,6-s-*cis*-comformer by rotation of C3-C4 single bond. Activation free energies at 298 K ($\Delta G^{\neq}$, kcal mol^{-1}) are given in brackets.

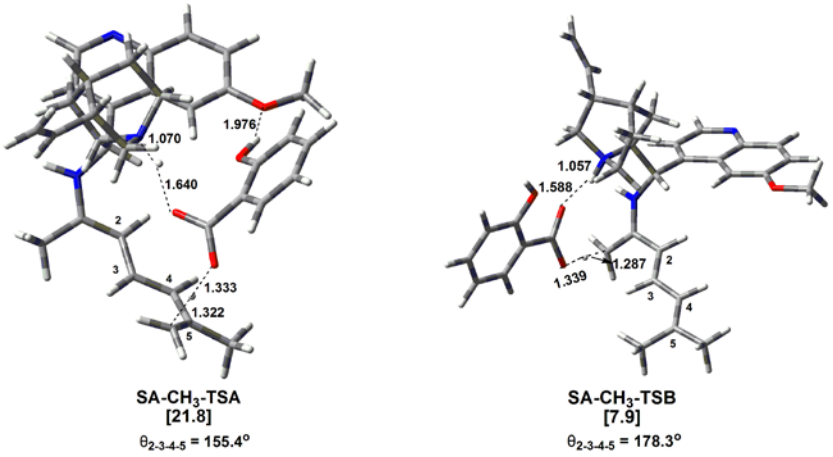


Figure S5. Optimized geometries for **SA-CH$_3$-TSA** and **SA-CH$_3$-TSB** and their relative energies (kcal mol^{-1}). Activation free energies at 298 K ($\Delta G^{\neq}$, kcal mol^{-1}) are given in brackets.

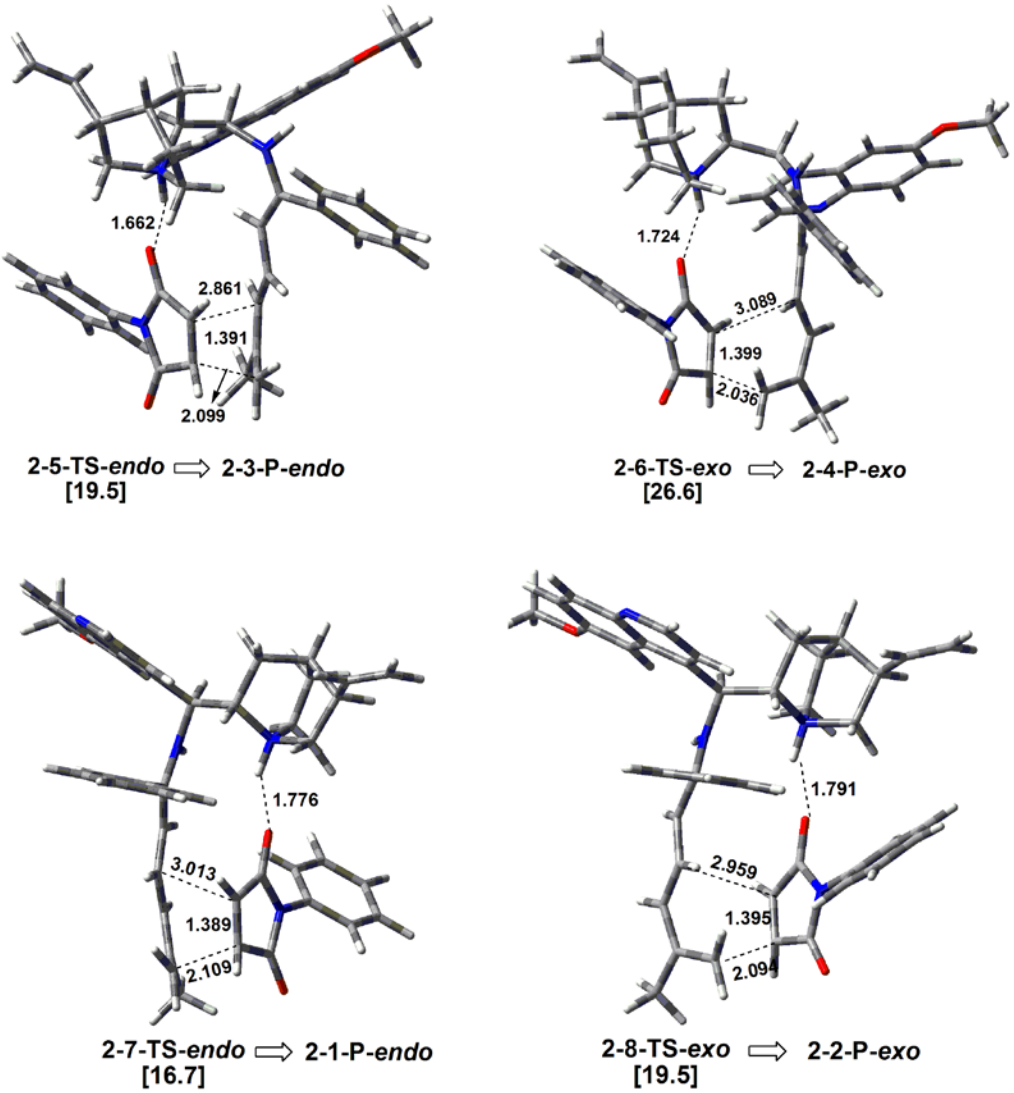
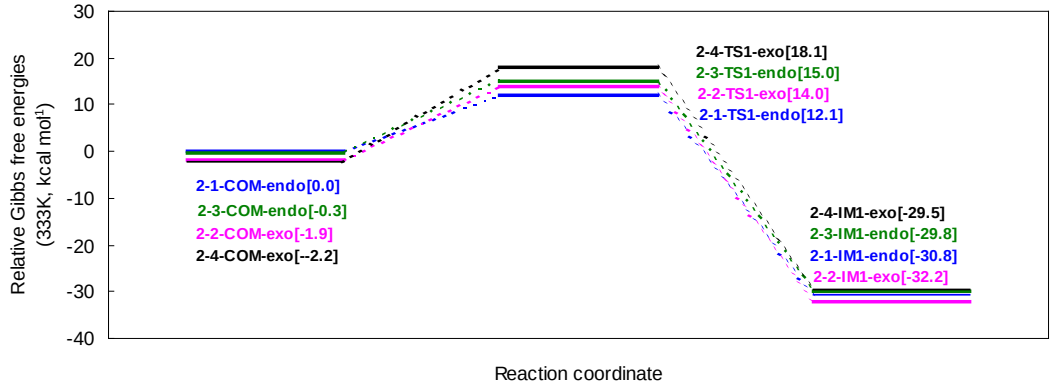
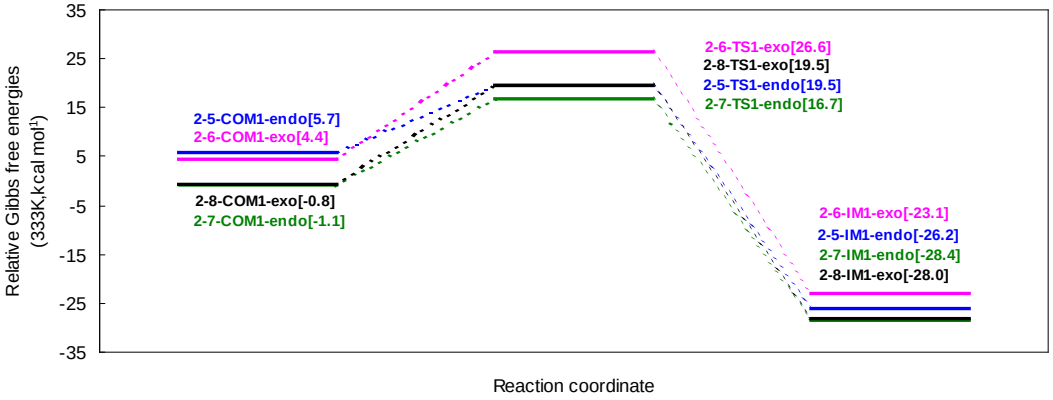


Figure S6. Optimized geometries for the transition states in **paths 5~8** and their relative Gibbs free energies at 333 K in kcal mol^{-1}.



(a)



(b)

Figure S7. Energy profiles for stereoselective Diels-Alder reaction of *N*-phenylmaleimide (**R2**) along eight lower energy pathways by trienamine catalysis at 333 K. Calculated at the M06-2X/6-311++G**(SMD,toluene) level. (a) Paths 1-4; (b) Paths 5-8.

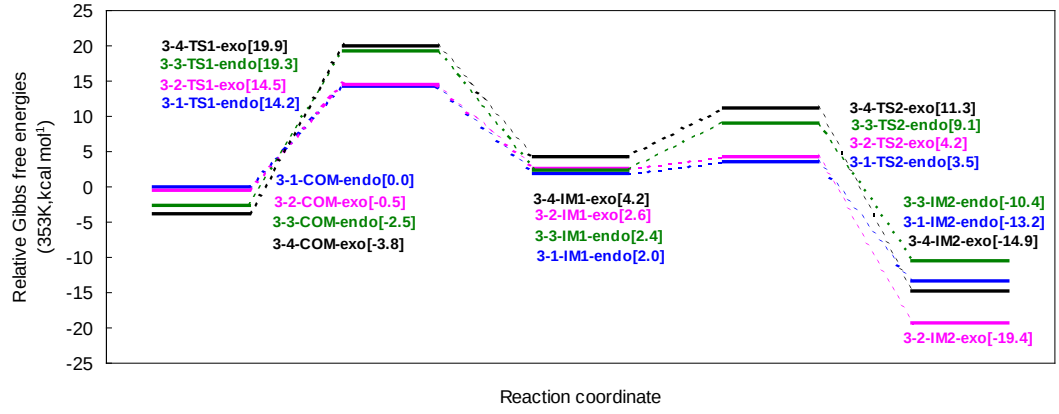
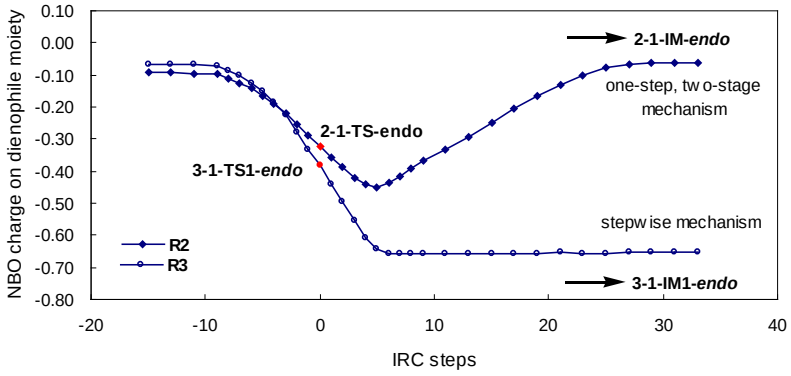
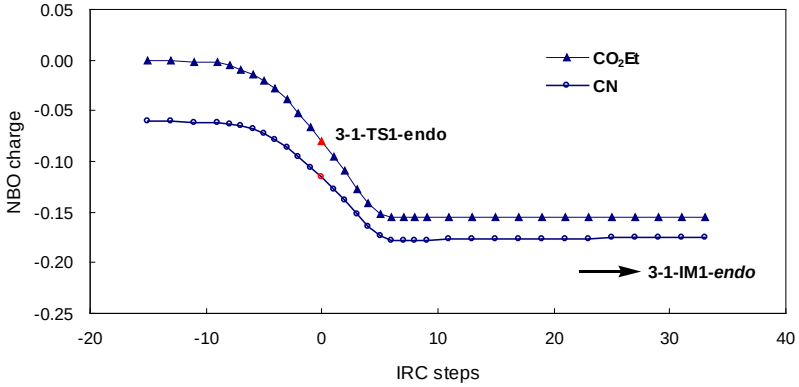


Figure S8. Energy profiles for stereoselective Diels-Alder reaction of benzylidenecyanoacetate (**R3**) along four lower energies pathways by trienamine catalysis at 353 K. Calculated at the M06-2X/6-311++G**(SMD,toluene) level.

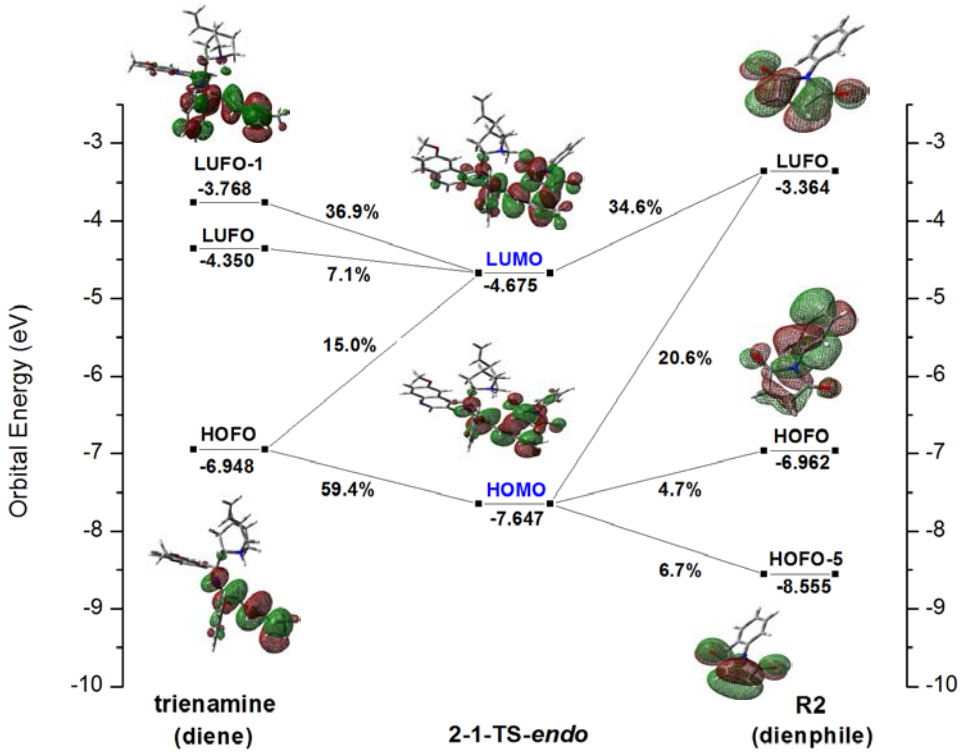


(a)

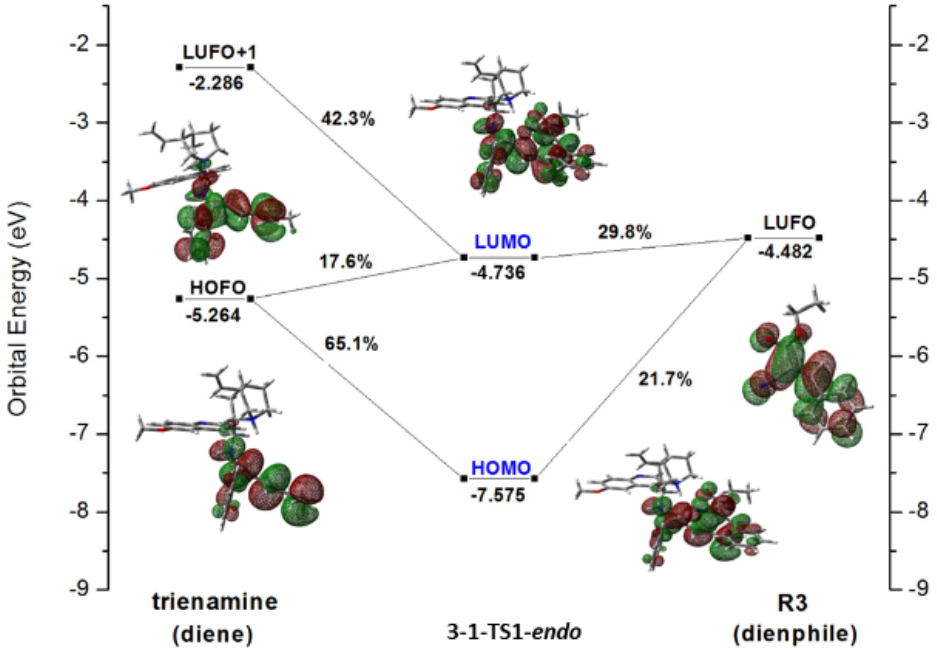


(b)

Figure S9. Evolution of charge in the formation of the C-C bond in Diels-Alder cycloadditon of dienophile *N*-phenylmaleimide (**R2**) and benzylidenecyanoacetate (**R3**) by trienamine catalysis. (a) The evolution of the charge populations for the dienophile moiety. (b) The evolution of NBO charge accumulated on -CO_2Et and -CN substituent in dienophile **R3**.



(a)



(b)

Figure S10. Orbital interaction diagrams for **2-1-TS-*endo*** and **3-1-TS1-*endo***. (a) **2-1-TS-*endo*** from trienamine and **R2** fragments. (b) **3-1-TS1-*endo*** from trienamine and **R3** fragments.

Cartesian coordinates of all the stational points

R1a

Energy + zep (gas) = -578.92656 au
Gibbs free energy (gas) = -578.96804 au
Gibbs free energy (in solvent) = -578.72407 au
Zero-point correction = 0.23220 au
Thermal correction to Gibbs free energy = 0.19073 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.180446	-0.238265	-0.569488
2	6	0	-0.740804	0.917189	-0.029609
3	6	0	0.671898	1.353877	0.044460
4	1	0	-0.432782	-0.926206	-0.956572
5	1	0	-1.433063	1.700890	0.254915
6	6	0	-2.556169	-0.665695	-0.783412
7	6	0	-3.663364	-0.373950	-0.069729
8	6	0	-3.685274	0.477829	1.171138
9	6	0	1.799164	0.358135	0.046006
10	6	0	3.022693	0.758188	-0.507357
11	6	0	1.704925	-0.904471	0.644486
12	6	0	4.116320	-0.098099	-0.497074
13	1	0	3.093500	1.750204	-0.936213
14	6	0	2.808515	-1.754795	0.672378
15	1	0	0.779763	-1.211995	1.115585
16	6	0	4.011296	-1.358223	0.093486
17	1	0	5.053971	0.216792	-0.941138
18	1	0	2.729303	-2.724556	1.150775
19	1	0	4.867022	-2.024031	0.109442
20	6	0	-4.999621	-0.930764	-0.483717
21	1	0	-4.935067	-1.517389	-1.401482
22	1	0	-5.418480	-1.565757	0.305833
23	1	0	-2.681591	-1.351713	-1.618401
24	1	0	-5.720781	-0.120520	-0.644382
25	1	0	-4.440390	0.109694	1.871943
26	1	0	-2.719963	0.500671	1.678108
27	1	0	-3.956268	1.513215	0.930869
28	8	0	0.920004	2.550621	0.086413

R1b

Energy + zep (gas) = -539.62795 au

Gibbs free energy (gas) = -539.66790 au
Gibbs free energy (in solvent) = -539.44229 au
Zero-point correction = 0.20402 au
Thermal correction to Gibbs free energy = 0.16406 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.516365	-0.218423	0.441118
2	6	0	-1.061432	0.899428	-0.155943
3	6	0	0.349396	1.343285	-0.217652
4	1	0	-0.793346	-0.887574	0.898756
5	1	0	-1.753563	1.648584	-0.528186
6	6	0	-2.914669	-0.615248	0.589734
7	6	0	-3.936144	-0.207972	-0.176626
8	6	0	1.482188	0.361111	-0.101351
9	6	0	1.418276	-0.943154	-0.607242
10	6	0	2.681503	0.812418	0.465282
11	6	0	2.527360	-1.783251	-0.530934
12	1	0	0.513607	-1.292385	-1.089049
13	6	0	3.779959	-0.032556	0.559349
14	1	0	2.730244	1.834142	0.821307
15	6	0	3.705044	-1.333940	0.060963
16	1	0	2.472298	-2.786367	-0.938694
17	1	0	4.698291	0.322890	1.013068
18	1	0	4.564982	-1.991223	0.126324
19	1	0	-3.118574	-1.331261	1.383381
20	8	0	0.590190	2.535164	-0.345286
21	1	0	-3.735590	0.470781	-1.003362
22	6	0	-5.360793	-0.628091	0.000664
23	1	0	-5.479430	-1.316382	0.840181
24	1	0	-6.003514	0.242077	0.177470
25	1	0	-5.742867	-1.116236	-0.903083

R2
Energy + zep (gas) = -590.48113 au
Gibbs free energy (gas) = -590.51737 au
Gibbs free energy (in solvent) = -590.30518 au
Zero-point correction = 0.14850 au
Thermal correction to Gibbs free energy = 0.11226 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.574283	-1.128773	0.239763
2	6	0	-2.991887	-0.650402	0.139495
3	6	0	-2.991899	0.650353	-0.139629
4	6	0	-1.574301	1.128758	-0.239865
5	7	0	-0.761528	0.000012	-0.000020
6	8	0	-1.197314	-2.248428	0.474384
7	8	0	-1.197375	2.248434	-0.474475
8	6	0	0.667050	0.000018	0.000016
9	6	0	1.363657	-1.065491	-0.574967
10	6	0	1.363640	1.065515	0.575050
11	6	0	2.755118	-1.062999	-0.564363
12	6	0	3.455903	0.000001	0.000093
13	6	0	2.755101	1.063007	0.564517
14	1	0	3.290768	-1.895805	-1.005316
15	1	0	0.821985	-1.893674	-1.009291
16	1	0	4.539761	-0.000006	0.000122
17	1	0	3.290740	1.895804	1.005503
18	1	0	0.821956	1.893698	1.009354
19	1	0	-3.822785	-1.324614	0.286449
20	1	0	-3.822810	1.324545	-0.286606

R1a-1

Energy + zep (gas) = -578.93322 au
Gibbs free energy (gas) = -578.97488 au
Gibbs free energy (in solvent) = -578.72955 au
Zero-point correction = 0.23201 au
Thermal correction to Gibbs free energy = 0.19035 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.288705	0.538383	-0.035938
2	6	0	0.491321	1.590217	-0.316722
3	6	0	-0.970483	1.660523	-0.112373
4	1	0	0.831026	-0.379977	0.314525
5	1	0	0.928416	2.541509	-0.608334
6	6	0	2.730159	0.578857	-0.147017
7	6	0	3.595402	-0.417990	0.135477

8	6	0	3.201000	-1.781875	0.633528
9	6	0	-1.810988	0.412790	-0.078441
10	6	0	-2.960499	0.420225	0.722080
11	6	0	-1.542876	-0.709511	-0.871787
12	6	0	-3.802433	-0.684178	0.758931
13	1	0	-3.176897	1.307738	1.303991
14	6	0	-2.399419	-1.808453	-0.850346
15	1	0	-0.683788	-0.711781	-1.531230
16	6	0	-3.523124	-1.802470	-0.027790
17	1	0	-4.681618	-0.672854	1.393375
18	1	0	-2.191998	-2.665811	-1.480902
19	1	0	-4.184976	-2.661138	-0.006130
20	6	0	5.076601	-0.214929	-0.036687
21	1	0	5.313361	0.786929	-0.398048
22	1	0	5.603666	-0.371962	0.911874
23	1	0	3.144619	1.521613	-0.497321
24	1	0	5.489677	-0.943132	-0.744775
25	1	0	3.664314	-1.977802	1.607390
26	1	0	2.125802	-1.915988	0.740807
27	1	0	3.572874	-2.556283	-0.047191
28	8	0	-1.499333	2.751175	0.050559

2-B-TS-1a

Energy + zep (gas) = -1169.36480 au
Gibbs free energy (gas) = -1169.42006 au
Gibbs free energy (in solvent) = -1169.98070 au
Zero-point correction = 0.38251 au
Thermal correction to Gibbs free energy = 0.32725 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.462164	-0.122969	1.341124
2	6	0	-0.216607	1.339259	1.508347
3	6	0	-1.352152	2.023395	1.047385
4	6	0	-2.347581	1.014392	0.603912
5	7	0	-1.703327	-0.249358	0.682518
6	8	0	0.242740	-1.038340	1.697287
7	8	0	-3.491807	1.187290	0.256660
8	6	0	-2.305302	-1.483356	0.291687
9	6	0	-2.167237	-2.624460	1.087255
10	6	0	-3.038662	-1.545868	-0.896865

11	6	0	-2.756276	-3.819575	0.683903
12	6	0	-3.491507	-3.885338	-0.496796
13	6	0	-3.632406	-2.743185	-1.281890
14	1	0	-2.640965	-4.701727	1.303288
15	1	0	-1.590723	-2.578339	1.999154
16	1	0	-3.952202	-4.817782	-0.802057
17	1	0	-4.205837	-2.781052	-2.201089
18	1	0	-3.157652	-0.659174	-1.503190
19	1	0	0.417408	1.659962	2.322034
20	1	0	-1.710702	2.951723	1.465635
21	6	0	1.458217	1.634982	0.130886
22	6	0	0.867598	1.435342	-1.124952
23	6	0	-0.270903	2.096520	-1.558997
24	6	0	-0.986778	3.118591	-0.897586
25	1	0	1.197592	0.590909	-1.718864
26	6	0	-2.354857	3.447913	-1.454154
27	1	0	-2.257049	4.248461	-2.198566
28	1	0	-3.027306	3.808609	-0.673709
29	1	0	-2.829496	2.589973	-1.927767
30	1	0	-0.773947	1.653046	-2.415242
31	6	0	2.664349	0.919093	0.664149
32	8	0	3.235658	1.431838	1.614722
33	6	0	3.244026	-0.300698	0.013339
34	6	0	2.483234	-1.335664	-0.544656
35	6	0	4.642193	-0.410185	0.016267
36	6	0	3.112104	-2.447474	-1.099960
37	1	0	1.404339	-1.311369	-0.494241
38	6	0	5.267033	-1.509993	-0.557187
39	1	0	5.221455	0.379680	0.478061
40	6	0	4.501875	-2.532091	-1.119054
41	1	0	2.512273	-3.252661	-1.508549
42	1	0	6.349161	-1.575994	-0.559595
43	1	0	4.987478	-3.395716	-1.559629
44	1	0	1.456724	2.624356	0.556959
45	6	0	-0.332149	4.336876	-0.269937
46	1	0	0.565701	4.142526	0.307279
47	1	0	-0.051942	5.019259	-1.081501
48	1	0	-1.040030	4.871483	0.367291

2-B-TS-1b

Energy + zep (gas) = -1130.07701 au
Gibbs free energy (gas) = -1130.13027 au
Gibbs free energy (in solvent) = -1129.70900 au
Zero-point correction = 0.35487 au

Thermal correction to Gibbs free energy = 0.30161 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.519015	-0.079823	1.337312
2	6	0	0.210655	-1.525678	1.494714
3	6	0	1.298033	-2.260392	1.008293
4	6	0	2.339448	-1.294452	0.555885
5	7	0	1.760633	-0.005923	0.663641
6	8	0	-0.134913	0.867388	1.707721
7	8	0	3.460567	-1.526867	0.172476
8	6	0	2.413484	1.203174	0.274945
9	6	0	2.349820	2.336654	1.090166
10	6	0	3.122000	1.247743	-0.929176
11	6	0	2.988240	3.507586	0.690917
12	6	0	3.699261	3.555484	-0.505353
13	6	0	3.765915	2.420258	-1.310066
14	1	0	2.930723	4.384505	1.325587
15	1	0	1.793140	2.304657	2.015037
16	1	0	4.198663	4.468751	-0.807647
17	1	0	4.319640	2.444342	-2.241708
18	1	0	3.183376	0.365587	-1.550645
19	1	0	-0.473520	-1.837249	2.269752
20	1	0	1.616290	-3.212945	1.406705
21	6	0	-1.475942	-1.731915	-0.000257
22	6	0	-0.838523	-1.428046	-1.204379
23	6	0	0.283871	-2.134904	-1.627066
24	6	0	0.824948	-3.197254	-0.894178
25	1	0	-1.132303	-0.543333	-1.756250
26	6	0	2.060596	-3.921995	-1.352602
27	1	0	0.128523	-3.800883	-0.322151
28	1	0	1.798609	-4.613435	-2.162208
29	1	0	2.503190	-4.513359	-0.549085
30	1	0	2.822662	-3.233123	-1.718319
31	1	0	0.847864	-1.751754	-2.472970
32	6	0	-2.705840	-1.086814	0.557761
33	8	0	-3.299679	-1.689879	1.439206
34	6	0	-3.275309	0.183658	0.003087
35	6	0	-2.502693	1.270446	-0.424627
36	6	0	-4.673580	0.284450	-0.035188
37	6	0	-3.120776	2.426826	-0.894933

38	1	0	-1.426290	1.247541	-0.332885
39	6	0	-5.286266	1.430363	-0.525245
40	1	0	-5.262571	-0.548679	0.327766
41	6	0	-4.509570	2.505185	-0.958592
42	1	0	-2.513473	3.270509	-1.202262
43	1	0	-6.368083	1.490699	-0.562373
44	1	0	-4.986243	3.403980	-1.333699
45	1	0	-1.433146	-2.752819	0.358136

R3

Energy + zep (gas) = -669.05635 au
Gibbs free energy (gas) = -669.09946 au
Gibbs free energy (in solvent) = -668.84095 au
Zero-point correction = 0.20343 au
Thermal correction to Gibbs free energy = 0.16032 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.100340	0.716002	-0.000022
2	8	0	-2.855582	1.655889	-0.000052
3	6	0	-0.609617	0.855144	-0.000004
4	6	0	0.207456	-0.229098	-0.000001
5	6	0	-0.156291	2.208283	0.000003
6	8	0	-2.499613	-0.571378	0.000032
7	6	0	1.657465	-0.358487	0.000003
8	6	0	2.173521	-1.670108	-0.000037
9	6	0	2.570072	0.715228	0.000043
10	6	0	3.541277	-1.906575	-0.000040
11	6	0	4.428900	-0.832328	0.000000
12	6	0	3.937326	0.473461	0.000042
13	1	0	3.914623	-2.923992	-0.000072
14	1	0	1.483410	-2.507101	-0.000066
15	1	0	5.498303	-1.010026	-0.000001
16	1	0	4.625430	1.310799	0.000075
17	1	0	2.216115	1.735882	0.000077
18	1	0	-0.321060	-1.175973	-0.000001
19	6	0	-3.934281	-0.788457	0.000019
20	6	0	-4.167976	-2.284445	0.000019
21	1	0	-4.358353	-0.304239	-0.882226
22	1	0	-4.358368	-0.304240	0.882257
23	1	0	-5.241605	-2.489251	0.000019
24	1	0	-3.731022	-2.748752	0.886812

25	1	0	-3.731022	-2.748754	-0.886773
26	7	0	0.222861	3.299693	-0.000013

3-B-TS-1a

Energy + zep (gas) = -1247.91375 au
Gibbs free energy (gas) = -1247.97399 au
Gibbs free energy (in solvent) = -1247.49532 au
Zero-point correction = 0.43745 au
Thermal correction to Gibbs free energy = 0.37721 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.192711	0.203554	-0.104129
2	6	0	-3.860166	-0.800350	-0.820733
3	6	0	-5.213872	-0.674154	-1.123769
4	6	0	-3.929862	1.330787	0.291485
5	6	0	-5.281183	1.456419	-0.014507
6	6	0	-5.931915	0.449543	-0.722699
7	1	0	-3.432546	2.124675	0.838536
8	1	0	-3.330375	-1.675051	-1.167277
9	1	0	-5.705198	-1.460889	-1.684984
10	1	0	-6.984428	0.541989	-0.964812
11	1	0	-5.822058	2.342609	0.298175
12	6	0	-0.952515	-1.072370	-1.767259
13	7	0	-1.150215	-1.909276	-2.542453
14	6	0	-0.732357	-0.089726	-0.764269
15	6	0	-1.726980	0.190629	0.250804
16	6	0	0.256900	0.945798	-1.153199
17	8	0	0.880243	0.943251	-2.187585
18	8	0	0.348677	1.950101	-0.236891
19	6	0	1.120489	3.104509	-0.655376
20	6	0	1.087012	4.111425	0.476023
21	1	0	2.135898	2.786129	-0.897189
22	1	0	0.674432	3.502927	-1.569470
23	1	0	1.651612	5.003350	0.192127
24	1	0	1.532496	3.700356	1.385205
25	1	0	0.062035	4.414064	0.701594
26	1	0	-1.472482	1.117736	0.748188
27	6	0	1.065547	-1.496616	0.453057
28	6	0	0.910368	-0.889756	1.693412
29	6	0	-0.311103	-0.664814	2.306638
30	6	0	-1.617312	-0.993256	1.822351

31	1	0	1.780125	-0.444575	2.162291
32	6	0	-2.718138	-0.528417	2.774008
33	1	0	-2.720873	-1.175322	3.657938
34	1	0	-3.703780	-0.592288	2.315607
35	1	0	-2.560265	0.498950	3.110951
36	1	0	-0.284542	-0.010246	3.174835
37	6	0	2.357130	-1.690359	-0.271737
38	8	0	2.427004	-2.644906	-1.029834
39	6	0	3.560433	-0.827489	-0.035022
40	6	0	3.497868	0.493670	0.424415
41	6	0	4.812415	-1.382245	-0.337164
42	6	0	4.664104	1.237469	0.590930
43	1	0	2.540464	0.954002	0.624863
44	6	0	5.974662	-0.644136	-0.158591
45	1	0	4.845947	-2.395761	-0.716457
46	6	0	5.903368	0.668827	0.308371
47	1	0	4.604251	2.263082	0.937521
48	1	0	6.936844	-1.087680	-0.387839
49	1	0	6.810051	1.247708	0.444226
50	1	0	0.338447	-2.201846	0.092074
51	6	0	-1.918681	-2.400114	1.298807
52	1	0	-1.415914	-2.670813	0.374853
53	1	0	-1.627344	-3.129076	2.061249
54	1	0	-2.989702	-2.509642	1.128364

3-B-TS-1b

Energy + zep (gas) = -1208.63110 au
Gibbs free energy (gas) = -1208.68986 au
Gibbs free energy (in solvent) = -1208.22775 au
Zero-point correction = 0.40914 au
Thermal correction to Gibbs free energy = 0.35039 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.187420	-0.328762	-0.110596
2	6	0	-3.231801	-1.721657	0.026325
3	6	0	-4.430845	-2.411777	-0.123806
4	6	0	-4.377604	0.350609	-0.399365
5	6	0	-5.576839	-0.339554	-0.555362
6	6	0	-5.607270	-1.724512	-0.414995
7	1	0	-4.361334	1.429760	-0.511311
8	1	0	-2.327805	-2.282021	0.232732

9	1	0	-4.441987	-3.490735	-0.021639
10	1	0	-6.538980	-2.265267	-0.535103
11	1	0	-6.485033	0.205626	-0.786364
12	6	0	-0.769140	-0.983082	-1.653964
13	7	0	-0.757707	-1.912530	-2.343169
14	6	0	-0.795572	0.159972	-0.810127
15	6	0	-1.922879	0.468290	0.043669
16	6	0	0.132407	1.242406	-1.205316
17	8	0	0.980105	1.168511	-2.066116
18	8	0	-0.081060	2.368437	-0.473709
19	6	0	0.755503	3.505526	-0.797882
20	6	0	0.225250	4.700448	-0.032615
21	1	0	1.786788	3.271651	-0.521678
22	1	0	0.728594	3.661012	-1.877748
23	1	0	0.836023	5.579827	-0.252474
24	1	0	0.256423	4.524578	1.045036
25	1	0	-0.805671	4.920488	-0.318368
26	1	0	-2.118555	1.535100	0.035373
27	6	0	0.825530	-0.913562	0.881766
28	6	0	0.916819	0.223504	1.670071
29	6	0	-0.220545	0.854917	2.157261
30	6	0	-1.539755	0.386810	1.902933
31	1	0	1.884834	0.686784	1.825841
32	6	0	-2.666952	1.119581	2.609521
33	1	0	-1.641047	-0.694874	1.957328
34	1	0	-2.618993	0.930341	3.685851
35	1	0	-3.645161	0.790651	2.259489
36	1	0	-2.590857	2.199915	2.456527
37	1	0	-0.103274	1.816728	2.647806
38	6	0	1.966324	-1.745697	0.395764
39	8	0	1.755409	-2.939781	0.255558
40	6	0	3.342890	-1.187597	0.214785
41	6	0	3.590521	0.086527	-0.307841
42	6	0	4.423676	-2.019969	0.537891
43	6	0	4.901102	0.523719	-0.488886
44	1	0	2.770392	0.707665	-0.641058
45	6	0	5.728172	-1.571083	0.379334
46	1	0	4.218160	-3.016504	0.908791
47	6	0	5.969412	-0.295635	-0.133277
48	1	0	5.086061	1.500985	-0.920242
49	1	0	6.558013	-2.216220	0.644687
50	1	0	6.987901	0.051636	-0.267067
51	1	0	-0.072083	-1.513277	0.918185

3-B-TS-1a'

Energy + zep (gas) = -1247.93146 au
Gibbs free energy (gas) = -1247.99084 au
Gibbs free energy (in solvent) = -1247.50989 au
Zero-point correction = 0.43721 au
Thermal correction to Gibbs free energy = 0.37783 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577914	1.730555	-0.803811
2	6	0	-0.416058	2.986334	-0.209640
3	6	0	-1.154749	4.079653	-0.651083
4	6	0	-1.508572	1.597489	-1.840959
5	6	0	-2.246473	2.691464	-2.285067
6	6	0	-2.071195	3.937759	-1.690393
7	1	0	-1.653141	0.629156	-2.308010
8	1	0	0.291701	3.124126	0.597600
9	1	0	-1.012129	5.045226	-0.179714
10	1	0	-2.645733	4.791518	-2.031325
11	1	0	-2.957978	2.567012	-3.093664
12	6	0	0.201903	0.503346	-0.385334
13	6	0	1.653125	0.522884	-0.548974
14	1	0	-0.193615	-0.363691	-0.898643
15	6	0	2.384714	-0.653907	-0.998625
16	8	0	3.580006	-0.699813	-1.230554
17	6	0	2.199816	-2.963124	-1.604541
18	1	0	3.192299	-3.039795	-1.159194
19	6	0	2.397013	1.715236	-0.486940
20	7	0	3.000895	2.700153	-0.366783
21	6	0	-0.275898	0.180456	1.311589
22	6	0	0.375974	-0.992528	1.833516
23	6	0	1.729220	-1.133404	2.080111
24	6	0	2.741611	-0.164923	2.118616
25	1	0	-0.205452	-1.906639	1.876274
26	6	0	4.149484	-0.610046	1.888412
27	1	0	4.403467	-0.426247	0.832041
28	1	0	4.275859	-1.680968	2.060370
29	1	0	4.862435	-0.051173	2.498423
30	1	0	2.078216	-2.161724	2.148572
31	6	0	-1.796031	0.188768	1.446290
32	8	0	-2.303828	1.111232	2.053832
33	6	0	-2.653463	-0.907179	0.877507

34	6	0	-2.176234	-1.951203	0.071015
35	6	0	-4.024611	-0.854603	1.170626
36	6	0	-3.050969	-2.915462	-0.424910
37	1	0	-1.127242	-2.024523	-0.183118
38	6	0	-4.893788	-1.818462	0.678774
39	1	0	-4.382009	-0.039071	1.786380
40	6	0	-4.408482	-2.853189	-0.121738
41	1	0	-2.669972	-3.714872	-1.050148
42	1	0	-5.950277	-1.764303	0.915474
43	1	0	-5.086279	-3.605917	-0.508526
44	1	0	0.068456	1.110723	1.750326
45	6	0	2.587833	1.236495	2.608534
46	1	0	1.569116	1.509473	2.869989
47	1	0	3.204910	1.334194	3.510259
48	1	0	2.987802	1.963551	1.889373
49	1	0	1.566145	-3.763625	-1.219555
50	8	0	1.569515	-1.748180	-1.135207
51	6	0	2.282221	-3.000567	-3.122058
52	1	0	2.696590	-3.959600	-3.446647
53	1	0	1.292162	-2.885697	-3.569798
54	1	0	2.932004	-2.205168	-3.489331

3-B-TS-1b'

Energy + zep (gas) = -1208.63926 au
Gibbs free energy (gas) = -1208.69747 au
Gibbs free energy (in solvent) = -1208.23829 au
Zero-point correction = 0.40950 au
Thermal correction to Gibbs free energy = 0.35132 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.223039	1.879783	0.645864
2	6	0	-0.087678	3.093306	0.021040
3	6	0	0.538077	4.272068	0.412682
4	6	0	1.189667	1.879107	1.659632
5	6	0	1.813022	3.059134	2.054465
6	6	0	1.488189	4.260851	1.431476
7	1	0	1.451840	0.945720	2.146192
8	1	0	-0.825157	3.130265	-0.770433
9	1	0	0.281337	5.202079	-0.081146
10	1	0	1.973983	5.181545	1.733769
11	1	0	2.553418	3.036970	2.846052

12	6	0	-0.413014	0.570959	0.280540
13	6	0	-1.851110	0.426938	0.270350
14	1	0	0.043128	-0.246778	0.821332
15	6	0	-2.481869	-0.834872	0.706012
16	8	0	-3.662433	-0.986216	0.927865
17	6	0	-2.083339	-3.128301	1.250275
18	1	0	-3.058565	-3.281709	0.787493
19	6	0	-2.722831	1.549025	0.277547
20	7	0	-3.445143	2.453229	0.240605
21	1	0	-1.371520	-3.849500	0.846551
22	8	0	-1.566803	-1.840604	0.828179
23	6	0	-2.176998	-3.222006	2.764086
24	1	0	-2.501033	-4.226271	3.052083
25	1	0	-1.207225	-3.028543	3.228774
26	1	0	-2.903994	-2.505127	3.147895
27	6	0	0.327083	0.176936	-1.459097
28	6	0	-0.244214	-1.014984	-1.981136
29	6	0	-1.594105	-1.124157	-2.284145
30	6	0	-2.484844	-0.072663	-2.132478
31	1	0	0.360022	-1.913665	-2.022948
32	6	0	-3.962552	-0.212615	-2.252965
33	1	0	-4.296165	0.211457	-3.208577
34	1	0	-4.469812	0.354458	-1.467350
35	1	0	-4.284266	-1.253444	-2.198286
36	1	0	-1.992975	-2.109113	-2.510195
37	6	0	1.835350	0.274277	-1.388415
38	8	0	2.370434	1.243722	-1.892524
39	6	0	2.662867	-0.795804	-0.734196
40	6	0	2.132588	-1.843029	0.033585
41	6	0	4.054292	-0.709840	-0.891349
42	6	0	2.977449	-2.780242	0.624741
43	1	0	1.065106	-1.934784	0.185245
44	6	0	4.893453	-1.648444	-0.307123
45	1	0	4.450579	0.110464	-1.476344
46	6	0	4.356172	-2.687679	0.453791
47	1	0	2.557028	-3.582204	1.220876
48	1	0	5.966512	-1.571249	-0.440210
49	1	0	5.010449	-3.420011	0.913413
50	1	0	-0.043282	1.094960	-1.907182
51	1	0	-2.105142	0.940195	-2.170485

I-TS

Energy + zep (gas) = -578.92163 au
Gibbs free energy (gas) = -578.96233 au
Gibbs free energy (in solvent) = -578.71888 au
Zero-point correction = 0.23102 au
Thermal correction to Gibbs free energy = 0.19031 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.252342	0.425083	-0.522245
2	6	0	-0.625826	1.316517	0.256136
3	6	0	0.846203	1.502386	0.369351
4	1	0	-0.656546	-0.295629	-1.080513
5	1	0	-1.194425	2.085400	0.771647
6	6	0	-2.717070	0.409599	-0.756301
7	6	0	-3.616079	-0.365386	-0.139452
8	6	0	-3.258127	-1.359298	0.934661
9	6	0	1.800379	0.368572	0.120511
10	6	0	3.080565	0.687156	-0.351993
11	6	0	1.496950	-0.966657	0.413228
12	6	0	4.023966	-0.310354	-0.561655
13	1	0	3.314141	1.727072	-0.544247
14	6	0	2.450741	-1.964065	0.221995
15	1	0	0.527186	-1.223818	0.819820
16	6	0	3.710633	-1.639722	-0.274742
17	1	0	5.006711	-0.054083	-0.941093
18	1	0	2.210790	-2.992951	0.465429
19	1	0	4.449473	-2.417919	-0.430504
20	6	0	-5.080934	-0.288440	-0.485582
21	1	0	-5.275833	0.445973	-1.269081
22	1	0	-5.452313	-1.261593	-0.827116
23	1	0	-3.068071	1.095242	-1.526714
24	1	0	-5.675970	-0.017582	0.394100
25	1	0	-3.561579	-2.370688	0.640609
26	1	0	-2.190207	-1.369061	1.153813
27	1	0	-3.791333	-1.131108	1.864569
28	8	0	1.275453	2.611049	0.645724

K-A

Energy + zep (gas) = -1519.35099 au
Gibbs free energy (gas) = -1519.42083 au
Gibbs free energy (in solvent) = -1519.84565 au

Zero-point correction = 0.64176 au
Thermal correction to Gibbs free energy = 0.57192 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.431654	-1.930954	-0.643060
2	6	0	2.270608	-0.669380	0.115872
3	6	0	2.474330	-1.676544	-2.102787
4	6	0	3.707107	-2.552558	-0.225310
5	6	0	0.798177	-0.172832	0.045315
6	6	0	3.323820	0.386837	-0.314543
7	6	0	3.687773	-0.781204	-2.487729
8	6	0	4.930033	-1.597864	-0.474074
9	6	0	0.529601	0.875576	1.117659
10	6	0	4.376172	-0.330609	-1.186620
11	6	0	0.472008	0.501194	2.441474
12	6	0	0.370167	2.261915	0.797897
13	6	0	0.264883	1.471272	3.447475
14	6	0	0.172536	3.158698	1.903363
15	7	0	0.122871	2.752497	3.199394
16	1	0	1.530443	-1.214687	-2.404579
17	1	0	2.519221	-2.646935	-2.601688
18	1	0	3.823653	-3.487042	-0.778216
19	1	0	3.629313	-2.812848	0.833184
20	1	0	0.598260	0.244283	-0.943441
21	1	0	3.778383	0.853025	0.561015
22	1	0	2.869227	1.194698	-0.895502
23	1	0	4.393543	-1.332451	-3.114576
24	1	0	3.361965	0.089188	-3.064010
25	1	0	5.619646	-2.082208	-1.172064
26	1	0	5.200786	0.349375	-1.407513
27	1	0	0.578419	-0.538665	2.730492
28	6	0	0.382466	2.797513	-0.510198
29	1	0	0.220776	1.166338	4.489539
30	6	0	0.016397	4.541717	1.641340
31	6	0	-3.546229	-0.476384	-0.240697
32	6	0	-2.215714	-0.391470	0.069288
33	6	0	-1.347778	-1.522394	0.137343
34	7	0	-0.034668	-1.387389	0.184620
35	1	0	-3.965831	-1.454221	-0.444810
36	1	0	-1.780362	0.587008	0.227059

37	1	0	0.549197	-2.229223	0.124198
38	6	0	-4.403135	0.659586	-0.330504
39	6	0	-5.728081	0.635996	-0.645683
40	6	0	0.040336	5.038037	0.362684
41	6	0	0.222389	4.154353	-0.732271
42	1	0	-0.123173	5.193528	2.494667
43	1	0	-0.079721	6.100025	0.198352
44	8	0	0.251196	4.551639	-2.027334
45	1	0	0.526644	2.177584	-1.384822
46	6	0	0.141590	5.941601	-2.337894
47	1	0	0.958584	6.515152	-1.890158
48	1	0	0.210205	6.003508	-3.421750
49	1	0	-0.820688	6.348916	-2.012786
50	6	0	-1.855179	-2.917261	0.153728
51	6	0	-1.317859	-3.870761	-0.724001
52	6	0	-2.840332	-3.306068	1.073845
53	6	0	-1.771585	-5.184694	-0.691701
54	1	0	-0.567380	-3.579507	-1.450097
55	6	0	-3.275397	-4.626778	1.112842
56	1	0	-3.236443	-2.585026	1.778492
57	6	0	-2.747488	-5.565253	0.227956
58	1	0	-1.364840	-5.910857	-1.385107
59	1	0	-4.022187	-4.924232	1.839172
60	1	0	-3.093356	-6.591640	0.256906
61	6	0	6.991428	-1.532675	0.960452
62	1	0	7.491954	-1.300202	1.893188
63	6	0	5.693505	-1.300113	0.787160
64	1	0	5.125599	-0.871700	1.612401
65	6	0	-6.508521	1.915042	-0.691342
66	1	0	-6.962146	2.049823	-1.679612
67	1	0	-7.338288	1.879492	0.023552
68	1	0	-3.950262	1.624861	-0.122180
69	1	0	7.602486	-1.965038	0.173846
70	1	0	-5.893585	2.786450	-0.467119
71	6	0	-6.514268	-0.600867	-0.962253
72	1	0	-5.941267	-1.524500	-0.909383
73	1	0	-7.364147	-0.684816	-0.276565
74	1	0	-6.940304	-0.520530	-1.968127
75	1	0	2.444540	-0.940896	1.161516

T-A

Energy + zep (gas) = -1519.31741 au
Gibbs free energy (gas) = -1519.38748 au
Gibbs free energy (in solvent) = -1519.82946 au

Zero-point correction = 0.64349 au
Thermal correction to Gibbs free energy = 0.57342 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.316743	-2.471983	-0.759964
2	7	0	2.154079	-1.926697	-1.020730
3	6	0	2.189524	-0.814241	0.026852
4	6	0	1.972666	-1.396453	-2.425381
5	6	0	3.421572	-2.737826	-0.934823
6	6	0	0.747517	-0.310689	0.265604
7	6	0	3.249687	0.216019	-0.413290
8	6	0	3.206766	-0.543741	-2.795353
9	6	0	4.645982	-1.796497	-1.164496
10	6	0	0.735386	0.714000	1.400432
11	6	0	4.099075	-0.391519	-1.548891
12	6	0	0.866682	0.293051	2.704722
13	6	0	0.612988	2.118877	1.155381
14	6	0	0.876055	1.230559	3.762229
15	6	0	0.634465	2.979375	2.305148
16	7	0	0.767188	2.524971	3.578883
17	1	0	1.041162	-0.833990	-2.442842
18	1	0	1.846920	-2.265446	-3.071345
19	1	0	3.355713	-3.524632	-1.686669
20	1	0	3.442248	-3.205114	0.049926
21	1	0	0.392878	0.167449	-0.645944
22	1	0	3.865867	0.493270	0.441680
23	1	0	2.774900	1.133930	-0.765938
24	1	0	3.764792	-1.015983	-3.606372
25	1	0	2.886888	0.436169	-3.153880
26	1	0	5.202817	-2.172901	-2.026326
27	1	0	4.940640	0.264811	-1.772026
28	1	0	0.952822	-0.759674	2.955408
29	6	0	0.468255	2.706913	-0.121880
30	1	0	0.976675	0.886401	4.787866
31	6	0	0.509947	4.377441	2.115731
32	6	0	-3.524609	-0.311406	-0.684405
33	6	0	-2.147127	-0.362818	-0.244454
34	6	0	-1.504309	-1.455747	0.228472
35	7	0	-0.090540	-1.499695	0.460428
36	1	0	-4.089102	-1.237831	-0.686081

37	1	0	-1.603539	0.572718	-0.327112
38	1	0	0.095819	-1.953981	1.350452
39	6	0	-4.130045	0.824427	-1.086781
40	6	0	-5.511455	0.947060	-1.573680
41	6	0	0.370627	4.923386	0.865257
42	6	0	0.347825	4.077764	-0.273665
43	1	0	0.528020	4.999800	3.001576
44	1	0	0.276619	5.995054	0.756663
45	8	0	0.213186	4.524610	-1.545180
46	1	0	0.432600	2.117619	-1.028977
47	6	0	0.061368	5.925744	-1.785134
48	1	0	0.939776	6.484670	-1.449097
49	1	0	-0.038594	6.026430	-2.863582
50	1	0	-0.837687	6.317223	-1.300367
51	6	0	-6.144230	-0.045026	-2.215502
52	6	0	-2.164478	-2.750172	0.544584
53	6	0	-1.686764	-3.958384	0.015261
54	6	0	-3.264457	-2.789529	1.413490
55	6	0	-2.298787	-5.167139	0.330898
56	1	0	-0.851396	-3.947834	-0.676669
57	6	0	-3.873156	-3.999991	1.733255
58	1	0	-3.633140	-1.866508	1.844611
59	6	0	-3.393472	-5.191174	1.193340
60	1	0	-1.928552	-6.089817	-0.101205
61	1	0	-4.720715	-4.012073	2.408511
62	1	0	-3.869911	-6.132353	1.441105
63	6	0	6.870860	-2.099544	-0.050253
64	1	0	7.507920	-2.069418	0.825481
65	6	0	5.581121	-1.785982	0.017591
66	1	0	5.157173	-1.500314	0.978971
67	6	0	-6.174272	2.282786	-1.327809
68	1	0	-5.601631	3.092060	-1.794569
69	1	0	-7.186753	2.307265	-1.732265
70	1	0	-3.569087	1.756424	-1.020986
71	1	0	7.339293	-2.396616	-0.983536
72	1	0	-6.225926	2.505781	-0.257025
73	1	0	-7.169616	0.064906	-2.548532
74	1	0	-5.655462	-0.985500	-2.441951
75	1	0	2.514982	-1.324078	0.937652

K-B

Energy + zep (gas) = -1519.34174 au
Gibbs free energy (gas) = -1519.41175 au
Gibbs free energy (in solvent) = -1519.84142 au

Zero-point correction = 0.64149 au
Thermal correction to Gibbs free energy = 0.57148 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.148961	2.369739	-0.765447
2	6	0	-0.825304	1.886969	0.230230
3	6	0	-0.261333	2.013599	-2.142982
4	6	0	0.200549	3.842434	-0.658750
5	6	0	-0.635752	0.371055	0.508146
6	6	0	-2.277681	2.270852	-0.176480
7	6	0	-1.611329	2.682254	-2.536980
8	6	0	-1.216534	4.496731	-0.863065
9	6	0	-1.668509	-0.199233	1.471597
10	6	0	-2.184093	3.350741	-1.275337
11	6	0	-1.802370	0.338282	2.733269
12	6	0	-2.508334	-1.301525	1.116303
13	6	0	-2.734552	-0.204565	3.646757
14	6	0	-3.419444	-1.770293	2.123348
15	7	0	-3.513688	-1.221091	3.363109
16	1	0	-0.322072	0.926568	-2.224754
17	1	0	0.545533	2.323385	-2.810628
18	1	0	0.905730	4.211045	-1.406984
19	1	0	0.607591	4.104515	0.321524
20	1	0	-0.665093	-0.162317	-0.435041
21	1	0	-2.837819	2.621545	0.691628
22	1	0	-2.824266	1.408043	-0.570581
23	1	0	-1.465051	3.426117	-3.324925
24	1	0	-2.314581	1.940020	-2.924965
25	1	0	-1.165624	5.193378	-1.705442
26	1	0	-3.174354	3.764839	-1.473985
27	1	0	-1.211437	1.192194	3.050816
28	6	0	-2.507397	-1.942823	-0.142638
29	1	0	-2.830889	0.225873	4.639805
30	6	0	-4.272101	-2.859300	1.820109
31	6	0	-4.247969	-3.469201	0.591476
32	6	0	-3.353180	-3.005557	-0.406798
33	1	0	-4.948206	-3.189844	2.598530
34	1	0	-4.913803	-4.297701	0.392486
35	8	0	-3.257866	-3.546154	-1.647187
36	1	0	-1.860509	-1.625870	-0.949286

37	6	0	-4.137868	-4.609367	-2.016612
38	1	0	-5.184876	-4.297629	-1.958723
39	1	0	-3.890443	-4.846846	-3.049021
40	1	0	-3.978145	-5.494610	-1.393618
41	6	0	-2.010482	6.560343	0.332253
42	1	0	-2.333025	7.071437	1.231966
43	6	0	-1.675595	5.273189	0.340499
44	1	0	-1.724328	4.729886	1.283995
45	1	0	-1.975252	7.151353	-0.577974
46	1	0	-0.577625	2.408158	1.161426
47	7	0	0.714125	0.163449	1.079539
48	1	0	0.804585	0.487581	2.036671
49	6	0	1.841919	-0.178847	0.481846
50	6	0	1.822690	-0.803899	-0.861475
51	6	0	2.539238	-0.231157	-1.920616
52	6	0	1.122584	-2.001666	-1.063496
53	6	0	2.541972	-0.845372	-3.168992
54	6	0	1.141187	-2.616383	-2.311808
55	6	0	1.846923	-2.037977	-3.365657
56	6	0	4.266213	-0.523435	0.826881
57	6	0	3.063031	0.004060	1.202975
58	6	0	5.473008	-0.341863	1.564613
59	6	0	6.689780	-0.862048	1.242485
60	6	0	7.875153	-0.592201	2.119497
61	1	0	3.062835	0.704848	-1.770326
62	1	0	0.584700	-2.462090	-0.243061
63	1	0	3.084519	-0.390794	-3.989327
64	1	0	0.602682	-3.544831	-2.458263
65	1	0	1.855662	-2.515848	-4.338092
66	1	0	4.298924	-1.120469	-0.076747
67	1	0	3.007105	0.577320	2.125061
68	1	0	5.405754	0.264094	2.464014
69	1	0	8.666460	-0.094845	1.547455
70	1	0	8.304320	-1.533992	2.479477
71	1	0	7.624998	0.027719	2.980279
72	6	0	6.966231	-1.718904	0.043560
73	1	0	7.338933	-2.696958	0.366717
74	1	0	6.105146	-1.879910	-0.601993
75	1	0	7.765151	-1.270152	-0.555964

T-B

Energy + zep (gas) = -1519.31553 au
Gibbs free energy (gas) = -1519.38429 au
Gibbs free energy (in solvent) = -1519.82615 au

Zero-point correction = 0.64340 au
Thermal correction to Gibbs free energy = 0.57464 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.039351	1.655043	-0.905233
2	6	0	-0.177727	1.729064	0.026290
3	6	0	0.675561	1.170376	-2.294465
4	6	0	1.677126	3.023462	-0.991178
5	6	0	-0.585688	0.319429	0.535043
6	6	0	-1.269589	2.530008	-0.715995
7	6	0	-0.240133	2.216638	-2.966349
8	6	0	0.627009	4.056458	-1.501408
9	6	0	-1.832281	0.439677	1.405377
10	6	0	-0.646218	3.267253	-1.917241
11	6	0	-1.804676	1.227075	2.535691
12	6	0	-3.042549	-0.259761	1.100274
13	6	0	-2.947070	1.334691	3.361506
14	6	0	-4.142679	-0.069129	2.004839
15	7	0	-4.077428	0.718976	3.110493
16	1	0	0.206085	0.195840	-2.183923
17	1	0	1.614889	1.022178	-2.826529
18	1	0	2.532703	2.936196	-1.661267
19	1	0	2.047270	3.268430	0.004426
20	1	0	-0.815564	-0.300285	-0.330407
21	1	0	-1.743013	3.223034	-0.021128
22	1	0	-2.057528	1.859823	-1.070747
23	1	0	0.274599	2.692709	-3.803777
24	1	0	-1.125662	1.723487	-3.371005
25	1	0	1.027609	4.522640	-2.405225
26	1	0	-1.369979	3.962279	-2.343708
27	1	0	-0.913702	1.777156	2.822837
28	6	0	-3.223553	-1.111624	-0.011792
29	1	0	-2.912865	1.955531	4.252681
30	6	0	-5.364619	-0.735184	1.744475
31	6	0	-5.516110	-1.556137	0.656108
32	6	0	-4.429976	-1.752117	-0.235280
33	1	0	-6.175854	-0.571879	2.442715
34	1	0	-6.462288	-2.051787	0.487929
35	8	0	-4.484809	-2.550400	-1.329154
36	1	0	-2.428229	-1.315731	-0.716102

37	6	0	-5.691635	-3.257341	-1.621554
38	1	0	-6.521680	-2.569228	-1.807648
39	1	0	-5.484769	-3.823764	-2.526944
40	1	0	-5.954468	-3.948050	-0.814806
41	6	0	0.530910	6.446191	-0.751655
42	1	0	0.325155	7.200637	-0.001885
43	6	0	0.370028	5.151552	-0.497840
44	1	0	0.030497	4.846652	0.490712
45	1	0	0.871978	6.801197	-1.719310
46	1	0	1.710523	0.990893	-0.488022
47	1	0	0.190189	2.297147	0.883229
48	7	0	0.478283	-0.354850	1.282008
49	1	0	0.636139	0.032424	2.202434
50	6	0	1.638038	-0.881372	0.668731
51	6	0	1.400719	-1.909249	-0.377191
52	6	0	2.205864	-1.995800	-1.525229
53	6	0	0.349656	-2.829512	-0.228644
54	6	0	1.974982	-2.975778	-2.486236
55	6	0	0.121544	-3.808423	-1.190669
56	6	0	0.932018	-3.885673	-2.322334
57	6	0	4.140219	-1.158911	0.901568
58	6	0	2.868992	-0.518274	1.142008
59	6	0	5.302524	-0.702465	1.415878
60	6	0	6.632376	-1.299731	1.238796
61	6	0	6.965542	-2.019405	0.157631
62	6	0	7.621616	-1.031291	2.348940
63	1	0	3.020704	-1.294340	-1.666163
64	1	0	-0.269249	-2.783164	0.658954
65	1	0	2.610088	-3.030050	-3.362948
66	1	0	-0.686353	-4.517180	-1.051606
67	1	0	0.754320	-4.650378	-3.069140
68	1	0	4.145688	-2.070597	0.314158
69	1	0	2.887016	0.288871	1.874817
70	1	0	5.265249	0.176156	2.059853
71	1	0	6.276059	-2.178323	-0.663511
72	1	0	7.949283	-2.462507	0.058571
73	1	0	7.775070	0.045268	2.482133
74	1	0	8.589571	-1.487795	2.140290
75	1	0	7.256235	-1.422658	3.303835

2-1-COM-endo

Energy + zep (gas) = -2109.81740 au
Gibbs free energy (gas) = -2109.90645 au
Gibbs free energy (in solvent) = -2109.15045 au

Zero-point correction = 0.79334 au
Thermal correction to Gibbs free energy = 0.70429 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.185144	-1.611365	-0.559098
2	6	0	1.298796	-1.459148	-0.866200
3	6	0	-1.059054	-1.450574	-1.782319
4	6	0	-0.423623	-2.971829	0.051451
5	6	0	1.654574	0.035535	-1.049902
6	6	0	1.627387	-2.385344	-2.055621
7	6	0	-0.753880	-2.597088	-2.771806
8	6	0	0.077808	-4.075786	-0.926860
9	6	0	3.124208	0.245232	-1.405071
10	6	0	0.469051	-3.381016	-2.261719
11	6	0	3.431347	0.794060	-2.629661
12	6	0	4.208848	-0.074454	-0.521659
13	6	0	4.776719	1.023316	-3.000450
14	6	0	5.533400	0.201041	-1.003082
15	7	0	5.794574	0.737969	-2.225556
16	1	0	-0.860217	-0.463842	-2.195737
17	1	0	-2.085175	-1.457580	-1.419976
18	1	0	-1.490658	-3.039916	0.256483
19	1	0	0.108909	-2.990777	1.002431
20	1	0	1.084926	0.392200	-1.906176
21	1	0	2.570577	-2.898142	-1.866507
22	1	0	1.771104	-1.800875	-2.968543
23	1	0	-1.618280	-3.258146	-2.863446
24	1	0	-0.554092	-2.189176	-3.764571
25	1	0	-0.762791	-4.740743	-1.142317
26	1	0	0.756829	-4.141768	-2.988128
27	1	0	2.644660	1.066560	-3.324787
28	6	0	4.074237	-0.623719	0.775202
29	1	0	5.003452	1.457673	-3.970310
30	6	0	6.641665	-0.092397	-0.172096
31	6	0	0.567719	2.051927	0.047289
32	7	0	1.205894	0.787201	0.127559
33	1	0	1.894698	0.783600	0.869331
34	6	0	6.482601	-0.627776	1.080993
35	6	0	5.178590	-0.898199	1.564762
36	1	0	7.625249	0.127790	-0.567694
37	1	0	7.351547	-0.836083	1.689754
38	8	0	4.917068	-1.426243	2.785480
39	1	0	3.112221	-0.847816	1.215870
40	6	0	6.000593	-1.700001	3.676125
41	1	0	6.554082	-0.788656	3.920640
42	1	0	5.541794	-2.095911	4.579530
43	1	0	6.680969	-2.448005	3.258148
44	6	0	0.519400	2.731273	1.371446
45	6	0	0.131953	2.031026	2.525568
46	6	0	0.919378	4.069237	1.502139
47	6	0	0.125571	2.659041	3.768726
48	1	0	-0.185922	0.998489	2.440407
49	6	0	0.912695	4.693349	2.746177

50	1	0	1.255813	4.611521	0.627011
51	6	0	0.513969	3.992527	3.882623
52	1	0	-0.182809	2.106737	4.649355
53	1	0	1.231532	5.725885	2.829147
54	1	0	0.513425	4.479583	4.850697
55	6	0	1.139620	-6.234748	-0.220368
56	1	0	1.962389	-6.795183	0.207193
57	6	0	1.182111	-4.910898	-0.330620
58	1	0	2.063330	-4.380272	0.026411
59	1	0	0.281216	-6.808689	-0.556017
60	1	0	-0.459145	-0.889733	0.123400
61	6	0	-0.818078	3.737622	-1.178236
62	6	0	0.023911	2.566347	-1.084780
63	1	0	-1.100936	4.227929	-0.252624
64	1	0	0.194444	2.058634	-2.029370
65	6	0	-1.293829	4.228088	-2.342002
66	6	0	-2.155860	5.406862	-2.506608
67	6	0	-2.175257	6.428101	-1.638007
68	6	0	-3.014472	5.416231	-3.750728
69	1	0	-3.689645	4.553927	-3.772218
70	1	0	-3.616084	6.323510	-3.816211
71	1	0	-1.042676	3.700030	-3.261919
72	1	0	-2.392454	5.356493	-4.650787
73	1	0	-1.522651	6.460888	-0.773264
74	1	0	-2.835828	7.275040	-1.781335
75	1	0	1.789032	-1.825048	0.034497
76	6	0	-3.257742	0.088834	1.297213
77	6	0	-3.497970	1.472266	1.815885
78	6	0	-4.811707	1.676876	1.902710
79	6	0	-5.528051	0.442382	1.446951
80	7	0	-4.502854	-0.490527	1.104768
81	8	0	-2.183051	-0.441740	1.069758
82	8	0	-6.705575	0.241189	1.362442
83	6	0	-4.740485	-1.817643	0.628202
84	6	0	-4.262609	-2.910048	1.353600
85	6	0	-5.469104	-2.010962	-0.545207
86	6	0	-4.500731	-4.201234	0.888739
87	6	0	-5.226800	-4.401158	-0.284840
88	6	0	-5.714599	-3.306187	-0.995316
89	1	0	-4.141733	-5.050772	1.458040
90	1	0	-3.728813	-2.747419	2.282046
91	1	0	-5.427663	-5.407155	-0.633849
92	1	0	-6.295294	-3.457616	-1.897441
93	1	0	-5.857112	-1.157277	-1.086456
94	1	0	-2.682265	2.140535	2.048987
95	1	0	-5.348581	2.555194	2.229287

2-1-TS-endo

Energy + zep (gas) = -2109.79910 au
Gibbs free energy (gas) = -2109.8798 au
Gibbs free energy (in solvent) = -2109.13113 au
Zero-point correction = 0.79425 au
Thermal correction to Gibbs free energy = 0.71359 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.169257	-1.746212	-0.337687
2	6	0	-1.606283	-1.427400	0.056835
3	6	0	0.555340	-2.534997	0.731981
4	6	0	-0.185324	-2.544148	-1.623711
5	6	0	-1.692425	-0.210096	1.023607
6	6	0	-2.232014	-2.745546	0.564883
7	6	0	-0.064609	-3.942642	0.832136
8	6	0	-1.077455	-3.808647	-1.450625
9	6	0	-3.008587	-0.145950	1.794660
10	6	0	-1.398537	-3.941945	0.063773
11	6	0	-2.973354	-0.240541	3.167134
12	6	0	-4.282538	0.040978	1.164669
13	6	0	-4.166337	-0.161622	3.923252
14	6	0	-5.425188	0.109906	2.030800
15	7	0	-5.349863	0.005392	3.384809
16	1	0	0.461054	-1.973923	1.661062
17	1	0	1.604645	-2.532102	0.447149
18	1	0	0.853740	-2.780669	-1.846621
19	1	0	-0.553414	-1.878890	-2.404858
20	1	0	-0.913179	-0.321849	1.776802
21	1	0	-3.266613	-2.799934	0.225956
22	1	0	-2.264083	-2.761323	1.657430
23	1	0	0.615080	-4.690735	0.417900
24	1	0	-0.227531	-4.201941	1.880102
25	1	0	-0.480929	-4.679609	-1.734589
26	1	0	-1.939761	-4.872668	0.236439
27	1	0	-2.031127	-0.370093	3.688775
28	6	0	-4.490704	0.165663	-0.228740
29	1	0	-4.125085	-0.238369	5.006274
30	6	0	-6.707604	0.295471	1.459746
31	6	0	-0.363549	1.883963	0.422673
32	7	0	-1.453512	1.046050	0.304602
33	1	0	-2.292568	1.507154	-0.018452
34	6	0	-6.883013	0.413317	0.104142
35	6	0	-5.758588	0.347817	-0.756557
36	1	0	-7.548279	0.342238	2.140532
37	1	0	-7.876848	0.555696	-0.297196
38	8	0	-5.829684	0.450562	-2.105187
39	1	0	-3.677214	0.129503	-0.940992
40	6	0	-7.099136	0.670932	-2.725373
41	1	0	-7.547769	1.609826	-2.388288

42	1	0	-6.894831	0.731580	-3.792015
43	1	0	-7.784558	-0.159970	-2.534372
44	6	0	-0.504872	3.124866	-0.388447
45	6	0	-0.847881	3.051158	-1.746730
46	6	0	-0.336363	4.384917	0.202288
47	6	0	-1.002299	4.211618	-2.499598
48	1	0	-0.971066	2.082613	-2.217922
49	6	0	-0.502323	5.543111	-0.551656
50	1	0	-0.096259	4.452227	1.256583
51	6	0	-0.831874	5.459476	-1.903147
52	1	0	-1.253755	4.141694	-3.551427
53	1	0	-0.381009	6.511553	-0.080814
54	1	0	-0.958536	6.362754	-2.488168
55	6	0	-2.594711	-4.725863	-3.223408
56	1	0	-3.489448	-4.670870	-3.831956
57	6	0	-2.299631	-3.784348	-2.332849
58	1	0	-2.974673	-2.937289	-2.221030
59	1	0	-1.953084	-5.588077	-3.376985
60	1	0	0.413947	-0.906767	-0.527326
61	6	0	1.996092	2.300912	1.012420
62	6	0	0.764014	1.600041	1.150963
63	1	0	2.013485	3.135325	0.325908
64	1	0	0.778887	0.723896	1.790466
65	6	0	3.141314	2.003473	1.729977
66	6	0	4.433587	2.488195	1.438298
67	6	0	4.679614	3.302035	0.323696
68	6	0	5.606723	2.001382	2.252579
69	1	0	5.329246	1.187866	2.924854
70	1	0	6.417886	1.655659	1.605404
71	1	0	3.063091	1.262170	2.521878
72	1	0	6.008677	2.817714	2.861764
73	1	0	3.912100	3.978154	-0.030555
74	1	0	5.694358	3.650650	0.165049
75	1	0	-2.076800	-1.135907	-0.880340
76	6	0	3.066816	0.261279	-1.014125
77	6	0	3.126521	1.619601	-1.478380
78	6	0	4.432587	2.088721	-1.367838
79	6	0	5.289409	0.920053	-0.962362
80	7	0	4.384496	-0.118264	-0.658730
81	8	0	2.105085	-0.514905	-0.942881
82	8	0	6.490277	0.851669	-0.884378
83	6	0	4.774224	-1.409607	-0.193594
84	6	0	5.633696	-2.195950	-0.960902
85	6	0	4.317133	-1.873827	1.041078

86	6	0	6.026876	-3.447415	-0.493999
87	6	0	5.559704	-3.920890	0.730219
88	6	0	4.704402	-3.131619	1.497297
89	1	0	6.702418	-4.051495	-1.088067
90	1	0	6.000318	-1.821541	-1.907892
91	1	0	5.871738	-4.893720	1.091543
92	1	0	4.358416	-3.485586	2.462017
93	1	0	3.682223	-1.237011	1.644833
94	1	0	2.281760	2.117250	-1.926677
95	1	0	4.869762	2.852427	-1.995969

2-1-IM-endo

Energy + zep (gas) = -2109.85212 au
Gibbs free energy (gas) = -2109.93193 au
Gibbs free energy (in solvent) = -2109.19949 au
Zero-point correction = 0.79993 au
Thermal correction to Gibbs free energy = 0.72013 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.167116	1.737945	0.111508
2	6	0	1.625973	1.388927	0.403971
3	6	0	-0.557783	2.250361	1.339473
4	6	0	0.130160	2.794921	-0.971414
5	6	0	1.778147	-0.008904	1.071714
6	6	0	2.221791	2.587029	1.173906
7	6	0	0.028660	3.620206	1.739447
8	6	0	0.981593	4.023891	-0.537643
9	6	0	3.144409	-0.181412	1.729109
10	6	0	1.339432	3.832675	0.962284
11	6	0	3.205416	-0.346255	3.094247
12	6	0	4.375937	-0.193922	0.994381
13	6	0	4.451746	-0.506750	3.743730
14	6	0	5.580735	-0.354937	1.758686
15	7	0	5.599754	-0.505540	3.110601
16	1	0	-0.432269	1.502630	2.121178
17	1	0	-1.611879	2.286411	1.073630
18	1	0	-0.919799	3.037945	-1.126873
19	1	0	0.509148	2.328232	-1.880553
20	1	0	1.048321	-0.084523	1.882441
21	1	0	3.244084	2.751236	0.832972

22	1	0	2.284481	2.366735	2.242881
23	1	0	-0.681219	4.420542	1.518851
24	1	0	0.214483	3.641585	2.814904
25	1	0	0.348292	4.912059	-0.610170
26	1	0	1.855124	4.722806	1.323960
27	1	0	2.298974	-0.358325	3.689786
28	6	0	4.483961	-0.062461	-0.409589
29	1	0	4.485322	-0.636582	4.822057
30	6	0	6.824448	-0.360185	1.082273
31	6	0	0.355048	-1.859202	0.067879
32	7	0	1.526645	-1.084596	0.105744
33	1	0	2.351292	-1.630048	-0.103054
34	6	0	6.903736	-0.221277	-0.280567
35	6	0	5.716675	-0.072085	-1.040890
36	1	0	7.714464	-0.481540	1.686871
37	1	0	7.870651	-0.231983	-0.764379
38	8	0	5.693528	0.066545	-2.389159
39	1	0	3.612521	0.020807	-1.044458
40	6	0	6.921620	0.022862	-3.118316
41	1	0	7.431031	-0.935687	-2.982427
42	1	0	6.643573	0.137700	-4.163725
43	1	0	7.586718	0.842059	-2.828864
44	6	0	0.510982	-3.050236	-0.823958
45	6	0	0.781341	-2.885885	-2.188435
46	6	0	0.436378	-4.345943	-0.297761
47	6	0	0.953362	-3.995319	-3.012895
48	1	0	0.850953	-1.886579	-2.603502
49	6	0	0.613323	-5.453567	-1.123086
50	1	0	0.251411	-4.481309	0.761940
51	6	0	0.868836	-5.280787	-2.482053
52	1	0	1.154856	-3.855872	-4.068747
53	1	0	0.558774	-6.451113	-0.702891
54	1	0	1.006840	-6.143633	-3.122979
55	6	0	2.416314	5.369318	-2.091561
56	1	0	3.295132	5.486154	-2.714377
57	6	0	2.179121	4.243009	-1.426871
58	1	0	2.884203	3.418750	-1.518204
59	1	0	1.741333	6.218063	-2.036711
60	1	0	-0.373146	0.930065	-0.240866
61	6	0	-2.115964	-2.255126	0.491782
62	6	0	-0.797784	-1.551567	0.692662
63	1	0	-1.913865	-3.285685	0.183445
64	1	0	-0.836070	-0.691699	1.352864
65	6	0	-2.962186	-2.302852	1.746045

66	6	0	-4.206190	-2.791977	1.712579
67	6	0	-4.745386	-3.237820	0.370305
68	6	0	-5.089273	-2.935260	2.917955
69	1	0	-4.594073	-2.587254	3.826437
70	1	0	-6.020744	-2.373420	2.789516
71	1	0	-2.515906	-1.978196	2.681613
72	1	0	-5.375257	-3.982619	3.066194
73	1	0	-4.311414	-4.205823	0.092055
74	1	0	-5.828268	-3.371650	0.400512
75	1	0	2.078874	1.322917	-0.583018
76	6	0	-3.098778	-0.165154	-0.693445
77	6	0	-2.958468	-1.678125	-0.712405
78	6	0	-4.411133	-2.204192	-0.726465
79	6	0	-5.279874	-0.962923	-0.553828
80	7	0	-4.432800	0.174710	-0.609605
81	8	0	-2.192526	0.655946	-0.749611
82	8	0	-6.467021	-0.914750	-0.392636
83	6	0	-4.921039	1.524281	-0.557241
84	6	0	-4.655383	2.395838	-1.612750
85	6	0	-5.676547	1.940409	0.537213
86	6	0	-5.143316	3.698664	-1.563952
87	6	0	-5.899563	4.123585	-0.472785
88	6	0	-6.167004	3.243275	0.573249
89	1	0	-4.946996	4.376029	-2.386804
90	1	0	-4.083871	2.052005	-2.465753
91	1	0	-6.288835	5.134430	-0.443708
92	1	0	-6.765275	3.566087	1.416905
93	1	0	-5.893085	1.247314	1.339424
94	1	0	-2.423301	-1.935063	-1.629957
95	1	0	-4.663252	-2.624291	-1.704782

2-2-COM-exo

Energy + zep (gas) = -2109.81795 au
Gibbs free energy (gas) = -2109.90805 au
Gibbs free energy (in solvent) = -2109.15351 au
Zero-point correction = 0.79279 au
Thermal correction to Gibbs free energy = 0.70269 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.139761	-0.644348	-0.934817

2	6	0	4.885586	-2.066784	-1.392011
3	7	0	4.513046	-0.728088	-1.058905
4	8	0	2.510009	0.362761	-0.644581
5	8	0	6.006693	-2.456842	-1.547205
6	6	0	5.439508	0.348853	-0.875250
7	6	0	6.399571	0.265853	0.131269
8	6	0	5.389256	1.457605	-1.719219
9	6	0	7.313209	1.303647	0.293680
10	6	0	7.261071	2.420818	-0.536887
11	6	0	6.298301	2.496879	-1.541881
12	1	0	8.067751	1.236220	1.068185
13	1	0	6.438431	-0.607691	0.769731
14	1	0	7.975688	3.225163	-0.408951
15	1	0	6.267332	3.356566	-2.201026
16	1	0	4.658446	1.493414	-2.518013
17	6	0	2.588186	-2.007339	-1.217870
18	6	0	3.599912	-2.831255	-1.486811
19	1	0	1.528795	-2.216582	-1.177803
20	1	0	3.581296	-3.882903	-1.731562
21	7	0	0.405880	2.135345	-0.224854
22	6	0	-0.889361	2.185547	0.576139
23	6	0	0.158976	2.125264	-1.716696
24	6	0	1.259022	3.326072	0.139347
25	6	0	-1.512666	0.773202	0.650596
26	6	0	-1.746913	3.329639	-0.005063
27	6	0	-0.458830	3.475928	-2.135858
28	6	0	0.452573	4.636765	-0.113773
29	6	0	-2.912035	0.822568	1.267744
30	6	0	-0.853279	4.247762	-0.864071
31	6	0	-3.060594	0.985580	2.626293
32	6	0	-4.096073	0.719237	0.470164
33	6	0	-4.349654	1.050618	3.202776
34	6	0	-5.352067	0.795273	1.161506
35	7	0	-5.457894	0.962065	2.506359
36	1	0	-0.493371	1.280166	-1.929127
37	1	0	1.122660	1.922100	-2.178886
38	1	0	2.165229	3.260095	-0.461160
39	1	0	1.540348	3.209807	1.186111
40	1	0	-1.593681	0.381496	-0.361791
41	1	0	-2.216732	3.877523	0.811456
42	1	0	-2.557875	2.935191	-0.621179
43	1	0	0.252159	4.055849	-2.728651
44	1	0	-1.335310	3.303273	-2.763088
45	1	0	1.038501	5.265772	-0.789101

46	1	0	-1.396852	5.155780	-1.126627
47	1	0	-2.201560	1.054546	3.285796
48	6	0	-4.111152	0.545437	-0.932985
49	1	0	-4.454148	1.178918	4.276721
50	6	0	-6.551286	0.692277	0.415199
51	6	0	-1.014561	-3.534165	-0.133494
52	6	0	-1.193072	-2.148728	0.240297
53	6	0	-0.504303	-1.478950	1.200169
54	7	0	-0.549585	-0.071422	1.352503
55	1	0	-0.226489	-4.092438	0.361816
56	1	0	-1.937465	-1.611598	-0.339033
57	1	0	-0.430650	0.194875	2.323063
58	6	0	-1.748863	-4.153120	-1.082569
59	6	0	-1.616518	-5.551172	-1.515608
60	6	0	-6.538648	0.523677	-0.946199
61	6	0	-5.300529	0.447296	-1.633812
62	1	0	-7.482190	0.751321	0.965077
63	1	0	-7.473160	0.447304	-1.484655
64	8	0	-5.188105	0.279687	-2.974682
65	1	0	-3.202005	0.468898	-1.514909
66	6	0	-6.370480	0.140490	-3.764813
67	1	0	-6.995486	1.036879	-3.709235
68	1	0	-6.023227	0.007342	-4.787133
69	1	0	-6.950331	-0.736688	-3.462803
70	6	0	-1.136718	-6.520899	-0.723467
71	6	0	0.413154	-2.121718	2.179090
72	6	0	1.677380	-1.574206	2.451356
73	6	0	0.008340	-3.257865	2.895711
74	6	0	2.518404	-2.160086	3.393293
75	1	0	2.006619	-0.696165	1.908452
76	6	0	0.851066	-3.840912	3.837183
77	1	0	-0.979196	-3.668889	2.725905
78	6	0	2.109520	-3.296973	4.087170
79	1	0	3.495053	-1.730035	3.584856
80	1	0	0.518899	-4.715069	4.385042
81	1	0	2.763209	-3.751605	4.822233
82	6	0	0.594643	6.684838	1.325930
83	1	0	0.396015	7.213436	2.250564
84	6	0	0.217520	5.422437	1.151169
85	1	0	-0.296897	4.910586	1.962942
86	6	0	-2.089912	-5.844721	-2.920901
87	1	0	-3.148123	-5.584584	-3.034760
88	1	0	-1.535764	-5.252819	-3.657330
89	1	0	-2.506451	-3.569573	-1.604954

90	1	0	1.115073	7.238353	0.550287
91	1	0	-1.972712	-6.899658	-3.171292
92	1	0	-0.848662	-6.334490	0.304643
93	1	0	-1.038624	-7.539896	-1.078848
94	1	0	0.920356	1.270098	0.005229
95	1	0	-0.568472	2.447659	1.587669

2-2-TS-exo

Energy + zep (gas) = -2109.79572 au

Gibbs free energy (gas) = -2109.87850 au

Gibbs free energy (in solvent) = -2109.12808 au

Zero-point correction = 0.79279 au

Thermal correction to Gibbs free energy = 0.71001 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.797554	0.095393	-1.233601
2	6	0	4.820058	-0.964179	-1.594678
3	7	0	4.144346	0.009826	-0.815760
4	8	0	1.987178	0.905681	-0.750079
5	8	0	5.996789	-1.208813	-1.548123
6	6	0	4.778195	0.837717	0.158614
7	6	0	5.661965	0.270560	1.079380
8	6	0	4.540736	2.214364	0.177127
9	6	0	6.300929	1.079986	2.013670
10	6	0	6.054090	2.450739	2.047085
11	6	0	5.171532	3.012710	1.127018
12	1	0	6.996705	0.635056	2.715414
13	1	0	5.865288	-0.791008	1.049172
14	1	0	6.555569	3.077753	2.774896
15	1	0	4.986603	4.080912	1.134619
16	1	0	3.870644	2.653002	-0.548824
17	6	0	2.595296	-0.881580	-2.262378
18	6	0	3.763331	-1.615514	-2.452621
19	1	0	1.671038	-0.971411	-2.807486
20	1	0	4.073155	-2.057650	-3.388437
21	7	0	-0.528338	1.722079	-1.254704
22	6	0	-1.726589	1.789464	-0.315040
23	6	0	-0.851169	1.017124	-2.549891
24	6	0	-0.072883	3.134359	-1.553117
25	6	0	-2.011360	0.444397	0.404078

26	6	0	-2.918215	2.348886	-1.131152
27	6	0	-1.891157	1.836702	-3.342942
28	6	0	-1.237173	3.956137	-2.179980
29	6	0	-3.312087	0.537610	1.198479
30	6	0	-2.409688	2.972773	-2.444323
31	6	0	-3.435012	1.472933	2.203448
32	6	0	-4.416916	-0.336262	0.949625
33	6	0	-4.626254	1.555745	2.959899
34	6	0	-5.578719	-0.157133	1.776153
35	7	0	-5.663345	0.778193	2.758341
36	1	0	-1.204191	0.019252	-2.295833
37	1	0	0.095556	0.905425	-3.076520
38	1	0	0.786933	3.046742	-2.215658
39	1	0	0.276888	3.557280	-0.611644
40	1	0	-2.117038	-0.331745	-0.347671
41	1	0	-3.460087	3.075416	-0.526486
42	1	0	-3.628083	1.550613	-1.364753
43	1	0	-1.444369	2.244008	-4.252607
44	1	0	-2.715994	1.191559	-3.651813
45	1	0	-0.902608	4.332016	-3.150472
46	1	0	-3.221127	3.506052	-2.940710
47	1	0	-2.630233	2.162986	2.438951
48	6	0	-4.443024	-1.345197	-0.038324
49	1	0	-4.712694	2.294889	3.751599
50	6	0	-6.701562	-0.994301	1.567209
51	6	0	1.187558	-2.513766	-0.332689
52	6	0	0.036004	-1.783308	0.048419
53	6	0	0.029133	-0.905882	1.113999
54	7	0	-0.909440	0.078132	1.293257
55	1	0	2.088340	-2.294150	0.227290
56	1	0	-0.839774	-1.862729	-0.587268
57	1	0	-0.976580	0.440096	2.233864
58	6	0	1.254549	-3.493951	-1.309938
59	6	0	2.458310	-4.015745	-1.825065
60	6	0	-6.702018	-1.966076	0.599245
61	6	0	-5.555993	-2.147939	-0.217121
62	1	0	-7.561791	-0.836269	2.205418
63	1	0	-7.575903	-2.588867	0.466898
64	8	0	-5.463576	-3.081096	-1.194490
65	1	0	-3.598121	-1.542690	-0.684465
66	6	0	-6.561665	-3.966180	-1.426457
67	1	0	-7.457510	-3.417732	-1.732474
68	1	0	-6.243810	-4.617062	-2.237975
69	1	0	-6.778841	-4.571244	-0.541311

70	6	0	3.701608	-3.478319	-1.468481
71	6	0	1.039822	-0.955724	2.203055
72	6	0	1.700519	0.206139	2.628674
73	6	0	1.298120	-2.167776	2.860383
74	6	0	2.607910	0.152360	3.681156
75	1	0	1.544899	1.136880	2.097708
76	6	0	2.198015	-2.213727	3.920600
77	1	0	0.774463	-3.064473	2.552046
78	6	0	2.854132	-1.055406	4.332205
79	1	0	3.136289	1.049411	3.980303
80	1	0	2.381369	-3.153018	4.428864
81	1	0	3.558336	-1.093886	5.154978
82	6	0	-1.623260	6.400412	-1.772564
83	1	0	-1.913892	7.223479	-1.130763
84	6	0	-1.619325	5.145024	-1.336250
85	1	0	-1.908814	4.944510	-0.305960
86	6	0	2.394744	-5.062130	-2.909545
87	1	0	2.511374	-6.061995	-2.476801
88	1	0	1.440778	-5.045955	-3.440936
89	1	0	0.325763	-3.828709	-1.766021
90	1	0	-1.336386	6.652589	-2.788851
91	1	0	3.201365	-4.936005	-3.635977
92	1	0	3.829073	-3.034893	-0.488839
93	1	0	4.602879	-3.935310	-1.861431
94	1	0	0.311283	1.236578	-0.848732
95	1	0	-1.422667	2.507879	0.448096

2-2-IM-exo

Energy + zep (gas) = -2109.85143 au

Gibbs free energy (gas) = -2109.93432 au

Gibbs free energy (in solvent) = -2109.20173 au

Zero-point correction = 0.79894 au

Thermal correction to Gibbs free energy = 0.71605 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.858750	-0.044937	-1.058656
2	6	0	4.786327	-1.335395	-1.274509
3	7	0	4.224053	-0.088904	-0.873035
4	8	0	2.160984	0.937814	-0.844365
5	8	0	5.933784	-1.640645	-1.116226

6	6	0	5.006604	0.988425	-0.331141
7	6	0	5.689226	0.803975	0.868699
8	6	0	5.092549	2.194443	-1.023576
9	6	0	6.463487	1.842127	1.379409
10	6	0	6.548428	3.054776	0.698953
11	6	0	5.862352	3.229714	-0.501380
12	1	0	7.004201	1.699878	2.307425
13	1	0	5.624374	-0.143414	1.387917
14	1	0	7.154924	3.858970	1.098440
15	1	0	5.936418	4.167899	-1.038592
16	1	0	4.571546	2.314773	-1.965274
17	6	0	2.381820	-1.401578	-1.545403
18	6	0	3.674624	-2.153875	-1.919511
19	1	0	1.730542	-1.256331	-2.410645
20	1	0	3.833650	-2.069446	-2.999602
21	7	0	-0.447476	1.867441	-0.855910
22	6	0	-1.731975	1.811711	-0.031760
23	6	0	-0.669961	1.436887	-2.288879
24	6	0	0.079700	3.285657	-0.829579
25	6	0	-2.065855	0.380532	0.466910
26	6	0	-2.824886	2.523660	-0.860118
27	6	0	-1.558676	2.474851	-3.004249
28	6	0	-1.016804	4.264916	-1.343051
29	6	0	-3.437757	0.392154	1.135471
30	6	0	-2.166181	3.404813	-1.940640
31	6	0	-3.626675	1.125687	2.287716
32	6	0	-4.550362	-0.337611	0.609627
33	6	0	-4.890200	1.147692	2.921011
34	6	0	-5.787539	-0.236475	1.333598
35	7	0	-5.936389	0.499566	2.466679
36	1	0	-1.128060	0.450079	-2.259281
37	1	0	0.320106	1.334373	-2.728393
38	1	0	0.979786	3.292718	-1.441972
39	1	0	0.375404	3.493056	0.198545
40	1	0	-2.101924	-0.299438	-0.383667
41	1	0	-3.452884	3.111071	-0.191185
42	1	0	-3.480972	1.792942	-1.341365
43	1	0	-0.975370	3.049735	-3.727273
44	1	0	-2.346745	1.963527	-3.560295
45	1	0	-0.588058	4.848406	-2.161927
46	1	0	-2.909396	4.062941	-2.391771
47	1	0	-2.815798	1.694823	2.731012
48	6	0	-4.514487	-1.140013	-0.552318
49	1	0	-5.028144	1.727073	3.829898

50	6	0	-6.919387	-0.939243	0.854024
51	6	0	1.561161	-2.167097	-0.451748
52	6	0	0.296588	-1.438971	-0.086954
53	6	0	0.005905	-0.949103	1.135811
54	7	0	-1.050089	-0.069536	1.421177
55	1	0	2.198983	-2.216941	0.438394
56	1	0	-0.389673	-1.267579	-0.911598
57	1	0	-1.401082	-0.168469	2.363162
58	6	0	1.341793	-3.579078	-0.962767
59	6	0	2.350421	-4.286092	-1.480139
60	6	0	-6.858647	-1.710694	-0.278475
61	6	0	-5.638001	-1.816453	-0.993598
62	1	0	-7.837015	-0.844134	1.420823
63	1	0	-7.741734	-2.235470	-0.616038
64	8	0	-5.482069	-2.557305	-2.117794
65	1	0	-3.610407	-1.274322	-1.131208
66	6	0	-6.587392	-3.309809	-2.620706
67	1	0	-7.419055	-2.657385	-2.903439
68	1	0	-6.213463	-3.819174	-3.506225
69	1	0	-6.927636	-4.052692	-1.893146
70	6	0	3.724811	-3.652410	-1.531941
71	6	0	0.822375	-1.236644	2.354151
72	6	0	1.350011	-0.188873	3.121146
73	6	0	1.035748	-2.556161	2.773516
74	6	0	2.090677	-0.456021	4.269024
75	1	0	1.191537	0.835949	2.806504
76	6	0	1.771788	-2.820984	3.925494
77	1	0	0.611606	-3.372766	2.200968
78	6	0	2.302812	-1.772662	4.673934
79	1	0	2.503553	0.363035	4.846561
80	1	0	1.923287	-3.846248	4.242375
81	1	0	2.874842	-1.980094	5.570716
82	6	0	-1.420451	6.556112	-0.408196
83	1	0	-1.767279	7.215137	0.378720
84	6	0	-1.471560	5.234025	-0.281911
85	1	0	-1.866551	4.808546	0.639102
86	6	0	2.215656	-5.701815	-1.962970
87	1	0	2.891690	-6.366795	-1.413912
88	1	0	1.197555	-6.074796	-1.839325
89	1	0	0.346237	-4.002413	-0.874479
90	1	0	-1.030916	7.029819	-1.304121
91	1	0	2.488237	-5.783912	-3.021043
92	1	0	4.200964	-3.753780	-0.548912
93	1	0	4.375598	-4.184911	-2.227321

94	1	0	0.300497	1.260123	-0.478183
95	1	0	-1.496542	2.395782	0.858421

2-3-COM-endo

Energy + zep (gas) = -2109.81356 au
Gibbs free energy (gas) = -2109.90085 au
Gibbs free energy (in solvent) = -2109.15090 au
Zero-point correction = 0.79261 au
Thermal correction to Gibbs free energy = 0.70532 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.021840	1.262977	-0.944912
2	6	0	-1.175302	1.517501	-0.030091
3	6	0	-0.388082	0.752514	-2.310211
4	6	0	0.803729	2.553566	-1.098125
5	6	0	-1.804654	0.212455	0.535484
6	6	0	-2.163638	2.412663	-0.817063
7	6	0	-1.178543	1.856666	-3.043168
8	6	0	-0.118877	3.667189	-1.670780
9	6	0	-2.992148	0.598505	1.419462
10	6	0	-1.467294	3.002712	-2.057432
11	6	0	-2.776931	1.334340	2.564409
12	6	0	-4.335409	0.214349	1.110679
13	6	0	-3.858525	1.690605	3.401925
14	6	0	-5.356574	0.639287	2.027880
15	7	0	-5.103654	1.365284	3.149240
16	1	0	-0.966391	-0.155520	-2.155240
17	1	0	0.536047	0.472506	-2.811780
18	1	0	1.645307	2.324394	-1.747407
19	1	0	1.201942	2.802887	-0.114657
20	1	0	-2.162565	-0.385355	-0.300100
21	1	0	-2.543151	3.195885	-0.161679
22	1	0	-3.030857	1.827918	-1.135138
23	1	0	-0.611955	2.227820	-3.899940
24	1	0	-2.113595	1.446602	-3.429417
25	1	0	0.335948	4.042732	-2.591297
26	1	0	-2.112139	3.747451	-2.525354
27	1	0	-1.780613	1.655181	2.853208
28	6	0	-4.717724	-0.541715	-0.020001
29	1	0	-3.675303	2.267084	4.304790

30	6	0	-6.702469	0.289235	1.762561
31	6	0	-7.048272	-0.444899	0.656489
32	6	0	-6.042432	-0.870127	-0.248701
33	1	0	-7.449562	0.623730	2.471302
34	1	0	-8.085715	-0.697252	0.485493
35	8	0	-6.289421	-1.605084	-1.361581
36	1	0	-3.995606	-0.911002	-0.735434
37	6	0	-7.631937	-1.988673	-1.662518
38	1	0	-8.270773	-1.114366	-1.819887
39	1	0	-7.571386	-2.560243	-2.586159
40	1	0	-8.052958	-2.619394	-0.873792
41	6	0	0.002072	6.093326	-1.045028
42	1	0	-0.134070	6.900265	-0.334914
43	6	0	-0.268272	4.831836	-0.725571
44	1	0	-0.626861	4.607199	0.277604
45	1	0	0.365851	6.367685	-2.030567
46	1	0	0.662173	0.570794	-0.535448
47	1	0	-0.746179	2.070017	0.808140
48	7	0	-0.873921	-0.616021	1.286525
49	1	0	-0.623625	-0.274945	2.202348
50	6	0	-0.049423	-1.626234	0.766458
51	6	0	-0.642833	-2.489838	-0.289776
52	6	0	0.053327	-2.762807	-1.476344
53	6	0	-1.911394	-3.061938	-0.106426
54	6	0	-0.500192	-3.593203	-2.448636
55	6	0	-2.460535	-3.892710	-1.078223
56	6	0	-1.757316	-4.160888	-2.252348
57	6	0	2.046830	-2.966129	1.089940
58	6	0	1.180210	-1.837735	1.312677
59	6	0	3.266591	-3.100574	1.657087
60	6	0	4.196433	-4.224175	1.480037
61	6	0	4.189031	-5.023416	0.402151
62	6	0	5.191739	-4.425006	2.599653
63	1	0	1.024717	-2.308472	-1.633083
64	1	0	-2.454268	-2.869031	0.811489
65	1	0	0.049826	-3.796628	-3.360551
66	1	0	-3.436555	-4.334890	-0.916252
67	1	0	-2.185969	-4.809574	-3.007184
68	1	0	1.677279	-3.760744	0.449943
69	1	0	1.523383	-1.110787	2.047876
70	1	0	3.593509	-2.328706	2.353662
71	1	0	3.500770	-4.872926	-0.422049
72	1	0	4.870502	-5.861580	0.318596
73	1	0	5.800754	-3.526115	2.746842

74	1	0	5.862746	-5.259883	2.395124
75	1	0	4.679700	-4.620429	3.547427
76	6	0	3.735179	-0.315650	-1.105354
77	6	0	4.496453	-1.483944	-1.645394
78	6	0	5.777713	-1.365507	-1.300290
79	6	0	5.948966	-0.111615	-0.499472
80	7	0	4.647465	0.468061	-0.415804
81	8	0	2.547575	-0.076008	-1.251097
82	8	0	6.943406	0.348410	-0.015660
83	6	0	4.352681	1.694515	0.260341
84	6	0	4.722490	2.908525	-0.316164
85	6	0	3.720449	1.664545	1.502933
86	6	0	4.448065	4.099607	0.351688
87	6	0	3.805343	4.077007	1.588309
88	6	0	3.443544	2.859447	2.163710
89	1	0	4.016901	-2.264513	-2.216089
90	1	0	6.607707	-2.022898	-1.511450
91	1	0	5.233978	2.915745	-1.271126
92	1	0	3.473790	0.710372	1.952577
93	1	0	4.746747	5.043332	-0.088711
94	1	0	3.603495	5.004707	2.110585
95	1	0	2.970029	2.838624	3.138535

2-3-TS-endo

Energy + zep (gas) = -2109.79250 au
Gibbs free energy (gas) = -2109.87371 au
Gibbs free energy (in solvent) = -2109.12661 au
Zero-point correction = 0.79390 au
Thermal correction to Gibbs free energy = 0.71269 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.284376	-0.612705	-1.042295
2	6	0	3.538797	-1.943043	-1.505075
3	6	0	4.840520	-2.317112	-1.187435
4	6	0	5.512613	-1.093009	-0.613309
5	7	0	4.497081	-0.128774	-0.473594
6	8	0	2.252362	0.068139	-1.128085
7	8	0	6.674733	-0.946911	-0.323505
8	6	0	4.683888	1.171150	0.077902
9	6	0	5.756120	1.962253	-0.339259

10	6	0	3.800549	1.650844	1.048512
11	6	0	5.936631	3.227478	0.213216
12	6	0	5.049617	3.715067	1.170075
13	6	0	3.981246	2.922433	1.585865
14	1	0	2.824208	-2.517955	-2.070541
15	1	0	5.446009	-2.994076	-1.774912
16	1	0	6.449741	1.582013	-1.076544
17	1	0	2.988031	1.019737	1.383288
18	1	0	6.775260	3.833568	-0.108574
19	1	0	5.195593	4.700375	1.596569
20	1	0	3.299951	3.287326	2.346742
21	7	0	-0.145600	1.365206	-0.987803
22	6	0	-1.326665	1.593841	-0.048087
23	6	0	-0.576066	0.844769	-2.342245
24	6	0	0.599237	2.676152	-1.162634
25	6	0	-1.911634	0.289330	0.568584
26	6	0	-2.358564	2.450806	-0.823880
27	6	0	-1.396922	1.931162	-3.067109
28	6	0	-0.363473	3.766745	-1.711368
29	6	0	-3.132587	0.650730	1.415190
30	6	0	-1.700253	3.066410	-2.073708
31	6	0	-2.978207	1.445581	2.529886
32	6	0	-4.446832	0.185108	1.096563
33	6	0	-4.094325	1.784046	3.328263
34	6	0	-5.508102	0.600266	1.971948
35	7	0	-5.315946	1.386197	3.064179
36	1	0	-1.140434	-0.069785	-2.171010
37	1	0	0.343562	0.574533	-2.857257
38	1	0	1.434382	2.461606	-1.825998
39	1	0	1.014832	2.935531	-0.189180
40	1	0	-2.214675	-0.377937	-0.234658
41	1	0	-2.757726	3.219259	-0.162935
42	1	0	-3.207943	1.835319	-1.131886
43	1	0	-0.846034	2.317124	-3.927497
44	1	0	-2.326132	1.501363	-3.446214
45	1	0	0.062714	4.157400	-2.639171
46	1	0	-2.375583	3.793547	-2.526016
47	1	0	-2.006191	1.830480	2.823488
48	6	0	-4.765458	-0.639079	-0.005893
49	1	0	-3.960073	2.408055	4.207698
50	6	0	-6.829506	0.175194	1.693369
51	6	0	-7.114145	-0.620726	0.613109
52	6	0	-6.068107	-1.037721	-0.249815
53	1	0	-7.608061	0.504449	2.369961

54	1	0	-8.134556	-0.927900	0.429855
55	8	0	-6.254316	-1.829984	-1.333879
56	1	0	-4.010359	-1.007377	-0.687439
57	6	0	-7.570388	-2.287784	-1.648827
58	1	0	-8.243792	-1.451570	-1.859560
59	1	0	-7.460517	-2.895069	-2.544667
60	1	0	-7.982133	-2.902881	-0.843096
61	6	0	-0.264796	6.190076	-1.070758
62	1	0	-0.402462	6.990708	-0.353874
63	6	0	-0.523508	4.924282	-0.759112
64	1	0	-0.875398	4.690927	0.244723
65	1	0	0.093937	6.473951	-2.055367
66	1	0	0.551691	0.695908	-0.620029
67	1	0	-0.899797	2.177113	0.770613
68	7	0	-0.938987	-0.435755	1.383935
69	1	0	-0.634097	0.054334	2.213991
70	6	0	-0.075217	-1.422351	0.933714
71	6	0	-0.637480	-2.387486	-0.051960
72	6	0	-0.061117	-2.583914	-1.311411
73	6	0	-1.774380	-3.130425	0.301767
74	6	0	-0.602697	-3.513743	-2.197507
75	6	0	-2.305901	-4.064176	-0.581919
76	6	0	-1.721672	-4.258939	-1.833103
77	6	0	2.214498	-2.436876	1.219820
78	6	0	1.169863	-1.514667	1.499505
79	6	0	3.425620	-2.334434	1.881364
80	6	0	4.653005	-2.945191	1.546876
81	6	0	4.825029	-3.691086	0.372611
82	6	0	5.866526	-2.648660	2.391475
83	1	0	0.797201	-1.989608	-1.593521
84	1	0	-2.226596	-2.984934	1.275755
85	1	0	-0.150677	-3.655377	-3.172711
86	1	0	-3.176271	-4.641053	-0.292607
87	1	0	-2.138097	-4.986639	-2.519573
88	1	0	2.045351	-3.221347	0.492302
89	1	0	1.417022	-0.745677	2.229967
90	1	0	3.465888	-1.621563	2.701562
91	1	0	3.985490	-4.219256	-0.059094
92	1	0	5.784146	-4.175283	0.223284
93	1	0	5.630879	-1.985196	3.224389
94	1	0	6.651398	-2.180735	1.788719
95	1	0	6.281446	-3.575013	2.800304

2-3-IM-endo

Energy + zep (gas) = -2109.84825 au
Gibbs free energy (gas) = -2109.92899 au
Gibbs free energy (in solvent) = -2109.19792 au
Zero-point correction = 0.79947 au
Thermal correction to Gibbs free energy = 0.71874 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.129699	1.534077	-0.641137
2	6	0	-1.390137	1.657588	0.218602
3	6	0	-0.433890	1.118388	-2.061946
4	6	0	0.593884	2.867564	-0.642640
5	6	0	-2.026453	0.293267	0.612210
6	6	0	-2.357943	2.611731	-0.527934
7	6	0	-1.279519	2.215379	-2.744791
8	6	0	-0.323157	3.973587	-1.235835
9	6	0	-3.253367	0.577882	1.480197
10	6	0	-1.636343	3.292007	-1.704064
11	6	0	-3.092156	1.174012	2.711485
12	6	0	-4.580683	0.238078	1.067562
13	6	0	-4.211621	1.440175	3.532135
14	6	0	-5.644127	0.565944	1.976568
15	7	0	-5.444248	1.157397	3.184448
16	1	0	-0.941343	0.156712	-2.016858
17	1	0	0.533154	0.963094	-2.538299
18	1	0	1.512285	2.718277	-1.205123
19	1	0	0.871614	3.070975	0.391562
20	1	0	-2.344693	-0.215893	-0.295785
21	1	0	-2.757036	3.345465	0.171879
22	1	0	-3.214634	2.051041	-0.909978
23	1	0	-0.726444	2.658960	-3.575525
24	1	0	-2.189601	1.778528	-3.160585
25	1	0	0.166439	4.381494	-2.124330
26	1	0	-2.288553	4.042542	-2.152335
27	1	0	-2.109983	1.448422	3.083727
28	6	0	-4.909979	-0.385832	-0.156781
29	1	0	-4.070276	1.906434	4.503588
30	6	0	-6.976767	0.261435	1.608210
31	6	0	-7.271034	-0.339029	0.410396
32	6	0	-6.223334	-0.671538	-0.486084
33	1	0	-7.756398	0.521528	2.313132

34	1	0	-8.300066	-0.558280	0.160742
35	8	0	-6.418330	-1.273016	-1.686056
36	1	0	-4.155001	-0.685553	-0.871187
37	6	0	-7.744786	-1.611812	-2.091361
38	1	0	-8.374520	-0.721492	-2.182322
39	1	0	-7.640442	-2.078894	-3.068370
40	1	0	-8.205034	-2.322669	-1.398349
41	6	0	-0.251096	6.380684	-0.534956
42	1	0	-0.430989	7.165823	0.189664
43	6	0	-0.537571	5.110212	-0.269862
44	1	0	-0.954038	4.855756	0.703499
45	1	0	0.172722	6.684149	-1.487360
46	1	0	0.532424	0.839971	-0.261826
47	1	0	-1.029644	2.128543	1.135780
48	6	0	3.374866	-0.324877	-0.510261
49	6	0	3.080261	-1.808947	-0.683270
50	6	0	4.470976	-2.470417	-0.779934
51	6	0	5.452195	-1.365034	-0.398012
52	7	0	4.727347	-0.146212	-0.315400
53	8	0	2.555002	0.582407	-0.546943
54	8	0	6.632424	-1.464260	-0.215233
55	6	0	5.350656	1.123305	-0.063463
56	6	0	6.315643	1.601742	-0.946666
57	6	0	5.001013	1.850990	1.072357
58	6	0	6.930543	2.824041	-0.690727
59	6	0	6.579843	3.563223	0.436860
60	6	0	5.615558	3.075505	1.316908
61	1	0	2.530120	-1.906411	-1.620919
62	1	0	4.696490	-2.723977	-1.821069
63	1	0	6.591552	1.018373	-1.815922
64	1	0	4.267701	1.453660	1.763052
65	1	0	7.687695	3.194865	-1.371125
66	1	0	7.063863	4.512237	0.634810
67	1	0	5.351740	3.641480	2.202582
68	7	0	-1.120071	-0.619362	1.304350
69	1	0	-0.737698	-0.252338	2.165191
70	6	0	-0.235414	-1.471815	0.599509
71	6	0	-0.901138	-2.422869	-0.335385
72	6	0	-0.411066	-2.673619	-1.624436
73	6	0	-2.054492	-3.104002	0.085412
74	6	0	-1.042199	-3.589861	-2.463652
75	6	0	-2.680256	-4.022193	-0.750736
76	6	0	-2.176521	-4.269201	-2.027484
77	6	0	2.168486	-2.400607	0.463412

78	6	0	1.080038	-1.453608	0.893824
79	6	0	3.009609	-2.836078	1.649721
80	6	0	4.173093	-3.476014	1.501671
81	6	0	4.684867	-3.714532	0.099441
82	6	0	5.000317	-3.979404	2.648603
83	1	0	0.459690	-2.137669	-1.982049
84	1	0	-2.445149	-2.913792	1.077329
85	1	0	-0.649865	-3.769447	-3.458068
86	1	0	-3.562343	-4.547882	-0.404451
87	1	0	-2.666990	-4.983619	-2.678053
88	1	0	1.703530	-3.289850	0.022081
89	1	0	1.405469	-0.690156	1.598869
90	1	0	2.602824	-2.657644	2.640630
91	1	0	4.167913	-4.569968	-0.351950
92	1	0	5.749887	-3.954826	0.104476
93	1	0	4.529513	-3.770038	3.610656
94	1	0	5.995128	-3.521163	2.638861
95	1	0	5.152114	-5.061803	2.570916

2-4-COM-exo

Energy + zep (gas) = -2109.82024 au
Gibbs free energy (gas) = -2109.90989 au
Gibbs free energy (in solvent) = -2109.15401 au
Zero-point correction = 0.79322 au
Thermal correction to Gibbs free energy = 0.70358 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.028402	1.670863	1.044233
2	6	0	0.410804	2.122621	0.847004
3	6	0	-1.380143	1.464621	2.498137
4	6	0	-1.951422	2.702105	0.441994
5	6	0	1.390999	0.943758	1.027869
6	6	0	0.654608	3.334774	1.771931
7	6	0	-1.303571	2.821600	3.233211
8	6	0	-1.696785	4.087703	1.108059
9	6	0	2.839414	1.370058	0.794474
10	6	0	-0.699334	3.869219	2.280671
11	6	0	3.350676	1.814149	-0.470877
12	6	0	3.717376	1.299812	1.852703
13	6	0	4.743318	2.160994	-0.517724

14	6	0	5.073471	1.667272	1.692054
15	7	0	5.575629	2.085734	0.555884
16	1	0	-0.689616	0.725173	2.897826
17	1	0	-2.377351	1.026220	2.508236
18	1	0	-2.967052	2.338580	0.589002
19	1	0	-1.754232	2.718294	-0.629984
20	1	0	1.332547	0.617209	2.067828
21	1	0	1.211546	4.100195	1.231308
22	1	0	1.273206	3.045908	2.625852
23	1	0	-2.297025	3.135970	3.560503
24	1	0	-0.686806	2.723811	4.128599
25	1	0	-2.638394	4.429940	1.545609
26	1	0	-0.552851	4.814052	2.805119
27	6	0	2.599874	1.927031	-1.665295
28	1	0	3.380230	0.952552	2.823365
29	6	0	5.301116	2.606646	-1.740676
30	1	0	5.753490	1.607983	2.537613
31	7	0	0.935581	-0.205412	0.216736
32	1	0	1.101017	-0.038029	-0.769634
33	6	0	-1.870232	6.286756	-0.084510
34	1	0	-1.506376	7.008811	-0.805740
35	6	0	-1.249988	5.127911	0.113160
36	1	0	-0.360407	4.900849	-0.472298
37	1	0	-2.763965	6.558792	0.468834
38	1	0	-1.169346	0.772372	0.550133
39	1	0	0.439559	2.446316	-0.192790
40	6	0	1.421217	-1.502397	0.560250
41	6	0	1.160118	-1.946207	1.956182
42	6	0	-0.143551	-1.953821	2.475793
43	6	0	2.210968	-2.378804	2.776891
44	6	0	-0.389039	-2.392559	3.774358
45	6	0	1.964589	-2.810912	4.078446
46	6	0	0.665372	-2.819572	4.580888
47	6	0	2.348082	-3.680323	-0.257401
48	6	0	2.002986	-2.282764	-0.383203
49	6	0	2.953400	-4.387017	-1.234392
50	6	0	3.313377	-5.810940	-1.183243
51	6	0	2.629684	-6.706796	-0.457128
52	6	0	4.498279	-6.214900	-2.029743
53	1	0	-0.968514	-1.645030	1.843773
54	1	0	3.222902	-2.372365	2.389345
55	1	0	-1.404741	-2.416770	4.153462
56	1	0	2.788920	-3.142900	4.698907
57	1	0	0.473951	-3.162669	5.590817

58	1	0	2.110314	-4.175107	0.678869
59	1	0	2.203886	-1.829480	-1.353217
60	1	0	3.242165	-3.860987	-2.143906
61	1	0	1.747546	-6.433155	0.110229
62	1	0	2.927345	-7.748241	-0.423663
63	1	0	5.401527	-5.676025	-1.725432
64	1	0	4.322819	-5.972789	-3.083789
65	1	0	4.696252	-7.284802	-1.956365
66	6	0	4.548107	2.710673	-2.882739
67	6	0	3.174748	2.364766	-2.846744
68	8	0	2.346892	2.431510	-3.919022
69	6	0	2.869050	2.855267	-5.180098
70	1	0	3.656678	2.182110	-5.531154
71	1	0	2.029276	2.817529	-5.870577
72	1	0	5.007710	3.053188	-3.799480
73	1	0	6.353580	2.861089	-1.737407
74	1	0	1.547930	1.681347	-1.718061
75	1	0	3.250219	3.879546	-5.129485
76	6	0	-4.198616	-2.941922	-1.757875
77	6	0	-2.776370	-3.412486	-1.698232
78	6	0	-2.041104	-2.484261	-1.087999
79	6	0	-2.930228	-1.341244	-0.704636
80	7	0	-4.205759	-1.658273	-1.132040
81	8	0	-5.154429	-3.497098	-2.217777
82	8	0	-2.608616	-0.319184	-0.116940
83	6	0	-5.370376	-0.838545	-0.977443
84	6	0	-5.401229	0.434216	-1.546413
85	6	0	-6.471146	-1.331410	-0.279280
86	6	0	-6.537950	1.224075	-1.399091
87	6	0	-7.642789	0.738163	-0.702120
88	6	0	-7.608994	-0.539945	-0.148857
89	1	0	-2.476648	-4.366964	-2.105086
90	1	0	-0.983859	-2.490224	-0.862964
91	1	0	-4.549688	0.792705	-2.111581
92	1	0	-6.441611	-2.327006	0.144693
93	1	0	-6.567521	2.211169	-1.845439
94	1	0	-8.531398	1.349667	-0.599902
95	1	0	-8.469922	-0.925239	0.384118

2-4-TS-exo

Energy + zep (gas) = -2109.78958 au
Gibbs free energy (gas) = -2109.87100 au
Gibbs free energy (in solvent) = -2109.12166 au
Zero-point correction = 0.79349 au

Thermal correction to Gibbs free energy = 0.71207 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.488174	1.625659	-0.609428
2	6	0	1.901898	1.215401	-0.206055
3	6	0	-0.146814	2.572800	0.387838
4	6	0	0.549848	2.292590	-1.968025
5	6	0	1.920505	0.133019	0.913021
6	6	0	2.670942	2.513115	0.131991
7	6	0	0.621464	3.911244	0.373519
8	6	0	1.528939	3.500441	-1.924589
9	6	0	3.326451	-0.094313	1.468872
10	6	0	1.916261	3.729473	-0.437848
11	6	0	4.407338	-0.640001	0.701861
12	6	0	3.562165	0.215261	2.789088
13	6	0	5.655756	-0.821161	1.388102
14	6	0	4.837687	0.000882	3.361263
15	7	0	5.850345	-0.498074	2.694886
16	1	0	-0.120981	2.081555	1.358409
17	1	0	-1.190764	2.661987	0.093885
18	1	0	-0.471711	2.578704	-2.210898
19	1	0	0.861589	1.529588	-2.681345
20	1	0	1.317431	0.497690	1.744406
21	1	0	3.683237	2.443037	-0.266365
22	1	0	2.772332	2.626023	1.214543
23	1	0	0.006670	4.701442	-0.063390
24	1	0	0.853707	4.214901	1.396095
25	1	0	0.984733	4.387382	-2.259679
26	1	0	2.539297	4.621387	-0.363308
27	6	0	4.338542	-1.014340	-0.660516
28	1	0	2.769513	0.616712	3.411105
29	6	0	6.756100	-1.364538	0.681286
30	1	0	5.010942	0.251313	4.404315
31	7	0	1.307346	-1.114010	0.470003
32	1	0	1.808923	-1.631230	-0.237780
33	6	0	3.049070	4.170966	-3.802337
34	1	0	3.913895	4.002897	-4.432947
35	6	0	2.711854	3.317177	-2.841136
36	1	0	3.317744	2.424826	-2.692505
37	1	0	2.473577	5.071472	-3.994075

38	1	0	-0.155825	0.821936	-0.721340
39	1	0	2.312420	0.773835	-1.113030
40	6	0	0.040419	-1.566426	0.763058
41	6	0	-0.587207	-1.058631	2.023275
42	6	0	-1.704065	-0.217149	2.045182
43	6	0	-0.031977	-1.485722	3.239996
44	6	0	-2.256975	0.187620	3.260713
45	6	0	-0.590077	-1.083496	4.449283
46	6	0	-1.704204	-0.244703	4.462872
47	6	0	-1.853434	-2.993561	0.043846
48	6	0	-0.512774	-2.551582	-0.019637
49	6	0	-2.376538	-4.046744	-0.689178
50	6	0	-3.750725	-4.271450	-0.902523
51	6	0	-4.700254	-3.291929	-0.579960
52	6	0	-4.185939	-5.486871	-1.680327
53	1	0	-2.133191	0.129665	1.115132
54	1	0	0.825716	-2.148570	3.233091
55	1	0	-3.122387	0.840134	3.258833
56	1	0	-0.160715	-1.433660	5.380771
57	1	0	-2.139890	0.064651	5.405636
58	1	0	-2.506951	-2.472771	0.734506
59	1	0	0.102909	-2.953222	-0.822403
60	1	0	-1.677959	-4.692539	-1.216175
61	1	0	-4.496056	-2.604050	0.231602
62	1	0	-5.753117	-3.514112	-0.714936
63	1	0	-4.564150	-6.256156	-0.998077
64	1	0	-3.363208	-5.927662	-2.246677
65	1	0	-4.999136	-5.250219	-2.371753
66	6	0	6.660495	-1.721537	-0.639773
67	6	0	5.432698	-1.543383	-1.324789
68	8	0	5.238160	-1.859338	-2.627918
69	6	0	6.315883	-2.420469	-3.381651
70	1	0	6.640207	-3.376288	-2.960090
71	1	0	5.917695	-2.583989	-4.380592
72	1	0	7.520836	-2.134977	-1.147597
73	1	0	7.681065	-1.488066	1.230432
74	1	0	3.438732	-0.903235	-1.251005
75	1	0	7.163134	-1.730748	-3.437744
76	6	0	-5.187474	-0.732766	-1.379471
77	6	0	-4.426149	-1.847054	-2.054822
78	6	0	-3.098276	-1.425391	-2.145534
79	6	0	-2.932183	-0.194066	-1.438586
80	7	0	-4.209898	0.199317	-0.955966
81	8	0	-6.373487	-0.633280	-1.203456

82	8	0	-1.903269	0.467995	-1.224934
83	6	0	-4.509367	1.413539	-0.275757
84	6	0	-4.055804	2.634450	-0.782949
85	6	0	-5.289338	1.388401	0.882540
86	6	0	-4.361537	3.818996	-0.117380
87	6	0	-5.134620	3.795841	1.042110
88	6	0	-5.604666	2.579233	1.532207
89	1	0	-4.943567	-2.419976	-2.811460
90	1	0	-2.294224	-1.887593	-2.692524
91	1	0	-3.490962	2.650868	-1.706073
92	1	0	-5.667508	0.444953	1.253994
93	1	0	-4.019595	4.765042	-0.522072
94	1	0	-5.385176	4.720389	1.548547
95	1	0	-6.225705	2.554417	2.420075

2-4-IM-exo

Energy + zep (gas) = -2109.84909 au
Gibbs free energy (gas) = -2109.92898 au
Gibbs free energy (in solvent) = -2109.19746 au
Zero-point correction = 0.79967 au
Thermal correction to Gibbs free energy = 0.71978 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.463365	1.638661	-0.060983
2	6	0	1.937314	1.259214	0.118739
3	6	0	-0.100251	2.368758	1.140673
4	6	0	0.335041	2.516110	-1.289461
5	6	0	2.138766	0.016644	1.039676
6	6	0	2.674153	2.538818	0.577193
7	6	0	0.601148	3.737049	1.272481
8	6	0	1.250512	3.765883	-1.146817
9	6	0	3.614721	-0.186361	1.380648
10	6	0	1.798342	3.776408	0.306062
11	6	0	4.617186	-0.524029	0.413124
12	6	0	4.004966	-0.062320	2.694459
13	6	0	5.955549	-0.697883	0.903662
14	6	0	5.355773	-0.254586	3.066532
15	7	0	6.302189	-0.558028	2.211744
16	1	0	0.052630	1.727933	2.006610
17	1	0	-1.171692	2.444555	0.966049

18	1	0	-0.720097	2.767218	-1.373842
19	1	0	0.605598	1.900004	-2.147306
20	1	0	1.635494	0.222504	1.986982
21	1	0	3.633471	2.602387	0.063545
22	1	0	2.899453	2.483655	1.645491
23	1	0	-0.095807	4.547331	1.047056
24	1	0	0.939178	3.881249	2.300383
25	1	0	0.625561	4.654954	-1.266067
26	1	0	2.379786	4.685607	0.462772
27	6	0	4.390156	-0.703069	-0.971681
28	1	0	3.278311	0.174434	3.464072
29	6	0	6.983988	-1.035174	-0.009451
30	1	0	5.648821	-0.152170	4.107971
31	7	0	1.548862	-1.218688	0.524475
32	1	0	1.966841	-1.555243	-0.331251
33	6	0	2.496918	4.832828	-3.042727
34	1	0	3.289811	4.830225	-3.781105
35	6	0	2.324911	3.817103	-2.202856
36	1	0	2.994818	2.961364	-2.266948
37	1	0	1.852931	5.706796	-3.022163
38	1	0	-0.127139	0.809200	-0.225012
39	1	0	2.255512	0.992969	-0.888477
40	6	0	0.158142	-1.457751	0.618313
41	6	0	-0.375683	-1.445166	2.013911
42	6	0	-1.537245	-0.748041	2.373733
43	6	0	0.311047	-2.162801	3.005839
44	6	0	-2.008913	-0.781870	3.685244
45	6	0	-0.166059	-2.201212	4.311912
46	6	0	-1.328085	-1.511407	4.656352
47	6	0	-1.954994	-2.290182	-0.584652
48	6	0	-0.542886	-1.787903	-0.486036
49	6	0	-2.031956	-3.728815	-1.071078
50	6	0	-3.201197	-4.270691	-1.421842
51	6	0	-4.443175	-3.410461	-1.323001
52	6	0	-3.363940	-5.696990	-1.861696
53	1	0	-2.065513	-0.162941	1.631473
54	1	0	1.213413	-2.698610	2.737598
55	1	0	-2.907492	-0.234843	3.947018
56	1	0	0.366805	-2.774910	5.061407
57	1	0	-1.698110	-1.541539	5.674446
58	1	0	-2.429037	-2.239335	0.402123
59	1	0	-0.006282	-1.766104	-1.435354
60	1	0	-1.114804	-4.308452	-1.088747
61	1	0	-4.753642	-3.350903	-0.271970

62	1	0	-5.283644	-3.855724	-1.857031
63	1	0	-4.051782	-6.232808	-1.198128
64	1	0	-2.411243	-6.229029	-1.865626
65	1	0	-3.794368	-5.749948	-2.867832
66	6	0	6.734712	-1.202447	-1.348266
67	6	0	5.416333	-1.034971	-1.839498
68	8	0	5.067479	-1.179238	-3.142465
69	6	0	6.064176	-1.554107	-4.095243
70	1	0	6.499785	-2.527993	-3.853276
71	1	0	5.545417	-1.619128	-5.049252
72	1	0	7.544195	-1.462315	-2.016310
73	1	0	7.980608	-1.158613	0.395441
74	1	0	3.409584	-0.600370	-1.415987
75	1	0	6.853859	-0.799886	-4.163687
76	6	0	-5.164273	-0.964704	-1.291860
77	6	0	-4.190943	-1.983575	-1.865118
78	6	0	-2.791826	-1.407276	-1.569611
79	6	0	-3.049713	-0.011852	-1.026238
80	7	0	-4.409694	0.172142	-0.877323
81	8	0	-6.353331	-1.060127	-1.180810
82	8	0	-2.201550	0.821170	-0.737276
83	6	0	-5.013587	1.363892	-0.349184
84	6	0	-4.809880	2.584283	-0.991476
85	6	0	-5.817109	1.282444	0.786337
86	6	0	-5.405489	3.734244	-0.481360
87	6	0	-6.207748	3.662575	0.656014
88	6	0	-6.414796	2.436947	1.284851
89	1	0	-4.359545	-1.995145	-2.946126
90	1	0	-2.206016	-1.304593	-2.486931
91	1	0	-4.202735	2.628579	-1.887009
92	1	0	-5.988217	0.324997	1.260941
93	1	0	-5.255370	4.683534	-0.982077
94	1	0	-6.679062	4.557660	1.044297
95	1	0	-7.048775	2.375049	2.161236

2-5-COM-endo

Energy + zep (gas) = -2109.80412 au
Gibbs free energy (gas) = -2109.89170 au
Gibbs free energy (in solvent) = -2109.14140 au

Zero-point correction = 0.79345 au

Thermal correction to Gibbs free energy = 0.70588 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.083605	1.459225	-0.865213
2	6	0	-2.858346	2.708042	-1.659748
3	6	0	-3.811190	3.588204	-1.353749
4	6	0	-4.724232	2.980011	-0.333797
5	7	0	-4.210138	1.667714	-0.093296
6	8	0	-2.409394	0.439666	-0.884194
7	8	0	-5.685492	3.454960	0.198239
8	6	0	-4.793211	0.726519	0.815428
9	6	0	-4.816426	1.010074	2.179983
10	6	0	-5.358617	-0.450007	0.325134
11	6	0	-5.404976	0.103571	3.058462
12	6	0	-5.958680	-1.080968	2.577205
13	6	0	-5.934780	-1.356710	1.211126
14	1	0	-5.434504	0.327159	4.118109
15	1	0	-4.392785	1.936994	2.546215
16	1	0	-6.419179	-1.781535	3.263596
17	1	0	-6.382966	-2.267740	0.832236
18	1	0	-5.366523	-0.639211	-0.741616
19	1	0	-2.022298	2.816359	-2.334271
20	7	0	-0.770780	-1.780322	-1.290753
21	6	0	0.141943	-2.554029	-0.335031
22	6	0	-0.178524	-1.567119	-2.670928
23	6	0	-2.064310	-2.559091	-1.427472
24	6	0	1.302031	-1.784375	0.357370
25	6	0	0.631543	-3.799870	-1.106573
26	6	0	0.012415	-2.935414	-3.357437
27	6	0	-1.766710	-3.995733	-1.947481
28	6	0	0.901363	-0.926446	1.563523
29	6	0	-0.263247	-4.050231	-2.333768
30	6	0	-0.401656	-0.578884	1.838320
31	6	0	1.905998	-0.520410	2.504320
32	6	0	-0.717730	0.185102	2.986834
33	6	0	1.472908	0.255058	3.631964
34	7	0	0.175268	0.600988	3.850586
35	1	0	0.746804	-1.017866	-2.537691
36	1	0	-0.883677	-0.922474	-3.194708
37	1	0	-2.693547	-1.989066	-2.108619
38	1	0	-2.545541	-2.557079	-0.450120
39	1	0	1.857286	-2.619260	0.802501
40	1	0	0.635065	-4.656670	-0.430540
41	1	0	1.660401	-3.647000	-1.442137

42	1	0	-0.657698	-3.033719	-4.214485
43	1	0	1.032471	-3.017243	-3.737288
44	1	0	-2.342990	-4.147963	-2.863989
45	1	0	-0.040495	-5.025534	-2.767911
46	1	0	-1.226580	-0.852520	1.192770
47	6	0	3.272994	-0.855519	2.407792
48	1	0	-1.753411	0.451895	3.179674
49	6	0	2.431253	0.672743	4.586084
50	6	0	3.756472	0.338812	4.465983
51	6	0	4.185319	-0.444408	3.364544
52	1	0	2.073165	1.259788	5.422465
53	1	0	4.462357	0.668974	5.215533
54	8	0	5.467170	-0.835224	3.167790
55	1	0	3.663921	-1.441975	1.588917
56	6	0	6.470019	-0.454138	4.110394
57	1	0	6.257197	-0.858333	5.104651
58	1	0	7.397151	-0.884633	3.738318
59	1	0	6.572974	0.633881	4.165004
60	6	0	-3.024493	-6.050100	-1.250032
61	1	0	-3.288149	-6.799734	-0.513548
62	6	0	-2.183663	-5.060750	-0.965425
63	1	0	-1.760267	-5.002554	0.036013
64	1	0	-3.479021	-6.149811	-2.231057
65	1	0	-1.026533	-0.855132	-0.922662
66	1	0	-0.530172	-2.867763	0.464160
67	6	0	2.337838	0.131385	-1.043970
68	7	0	2.260713	-1.196456	-0.587767
69	1	0	3.172473	-1.624726	-0.541483
70	6	0	3.568703	0.372929	-1.848743
71	6	0	4.383104	1.483094	-1.582707
72	6	0	3.963360	-0.522355	-2.855205
73	6	0	5.546840	1.699327	-2.314305
74	1	0	4.107839	2.165353	-0.788219
75	6	0	5.125274	-0.301416	-3.589031
76	1	0	3.349281	-1.388469	-3.075957
77	6	0	5.919911	0.811030	-3.320954
78	1	0	6.167230	2.559769	-2.092276
79	1	0	5.408658	-0.995356	-4.372001
80	1	0	6.826055	0.981979	-3.890122
81	6	0	1.347410	2.390192	-1.437528
82	6	0	1.388740	1.080057	-0.826755
83	1	0	2.020957	2.582789	-2.266933
84	1	0	0.584841	0.862921	-0.135064
85	6	0	0.527050	3.383390	-1.031444

86	6	0	0.410269	4.712236	-1.649530
87	6	0	0.567516	4.917917	-2.966168
88	6	0	0.083464	5.846495	-0.705557
89	1	0	0.871150	5.969307	0.044817
90	1	0	-0.034104	6.791530	-1.237298
91	1	0	-0.073170	3.221494	-0.136504
92	1	0	-0.843538	5.644678	-0.157070
93	1	0	0.764733	4.102569	-3.653202
94	1	0	0.508367	5.912694	-3.392251
95	1	0	-3.962998	4.589890	-1.727514

2-5-TS-endo

Energy + zep (gas) = -2109.78524 au
Gibbs free energy (gas) = -2109.86494 au
Gibbs free energy (in solvent) = -2109.11934 au
Zero-point correction = 0.79418 au
Thermal correction to Gibbs free energy = 0.71448 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.776995	0.002023	-0.924129
2	6	0	2.693762	-0.619456	-2.217510
3	6	0	3.708836	-1.562988	-2.341572
4	6	0	4.567242	-1.450410	-1.108227
5	7	0	3.895523	-0.541359	-0.258568
6	8	0	2.063967	0.885528	-0.418954
7	8	0	5.603932	-2.011005	-0.861111
8	6	0	4.368789	-0.135928	1.028010
9	6	0	4.729742	-1.099692	1.970261
10	6	0	4.495144	1.221199	1.332824
11	6	0	5.209566	-0.704088	3.215500
12	6	0	5.321867	0.648073	3.530032
13	6	0	4.963343	1.607508	2.585263
14	1	0	5.497298	-1.456889	3.939893
15	1	0	4.654192	-2.149201	1.723454
16	1	0	5.695788	0.952134	4.500523
17	1	0	5.063434	2.661682	2.817080
18	1	0	4.234436	1.964273	0.591812
19	1	0	1.990918	-0.308438	-2.973533
20	7	0	-0.024882	2.459276	-0.878297
21	6	0	-1.326539	2.546733	-0.087934

22	6	0	-0.229502	2.325315	-2.371947
23	6	0	0.754332	3.729948	-0.609954
24	6	0	-2.070249	1.229417	0.285258
25	6	0	-2.225990	3.556988	-0.833708
26	6	0	-0.885306	3.607664	-2.925408
27	6	0	-0.107136	4.973904	-0.980727
28	6	0	-1.615696	0.578298	1.596332
29	6	0	-1.363785	4.458959	-1.736831
30	6	0	-0.390210	0.824288	2.172702
31	6	0	-2.523000	-0.280502	2.299502
32	6	0	-0.045167	0.225293	3.407780
33	6	0	-2.071514	-0.825494	3.547814
34	7	0	-0.844650	-0.570431	4.076542
35	1	0	-0.836196	1.440514	-2.528589
36	1	0	0.759372	2.140201	-2.789845
37	1	0	1.667133	3.662007	-1.200328
38	1	0	1.037024	3.718235	0.442356
39	1	0	-3.070612	1.611310	0.517675
40	1	0	-2.786942	4.138037	-0.099567
41	1	0	-2.959024	3.030703	-1.452873
42	1	0	-0.178750	4.171745	-3.538566
43	1	0	-1.727876	3.345073	-3.568728
44	1	0	0.466813	5.580823	-1.685881
45	1	0	-1.946674	5.310999	-2.088225
46	1	0	0.361936	1.436249	1.690965
47	6	0	-3.821448	-0.605675	1.853270
48	1	0	0.932660	0.418689	3.839866
49	6	0	-2.942090	-1.667016	4.281417
50	6	0	-4.201783	-1.966586	3.827755
51	6	0	-4.652477	-1.426917	2.595912
52	1	0	-2.574487	-2.061540	5.220383
53	1	0	-4.843132	-2.609878	4.414344
54	8	0	-5.877826	-1.663839	2.069446
55	1	0	-4.215763	-0.235991	0.916968
56	6	0	-6.799951	-2.489576	2.782406
57	1	0	-7.044193	-2.061916	3.759396
58	1	0	-7.697508	-2.520247	2.168574
59	1	0	-6.411939	-3.505066	2.906966
60	6	0	-0.115365	7.131832	0.295592
61	1	0	-0.367864	7.718897	1.170492
62	6	0	-0.422552	5.841363	0.211255
63	1	0	-0.933965	5.368732	1.048193
64	1	0	0.400403	7.650279	-0.506936
65	1	0	0.608995	1.666964	-0.604481

66	1	0	-1.025474	2.988240	0.861236
67	6	0	-1.565006	-0.760649	-1.296048
68	7	0	-2.308405	0.325847	-0.852949
69	1	0	-3.265321	0.310157	-1.171287
70	6	0	-2.111866	-1.380602	-2.532142
71	6	0	-2.167217	-2.778398	-2.656196
72	6	0	-2.629571	-0.597683	-3.578211
73	6	0	-2.697266	-3.369447	-3.798372
74	1	0	-1.822493	-3.398379	-1.838692
75	6	0	-3.154896	-1.191375	-4.721261
76	1	0	-2.611191	0.483816	-3.507651
77	6	0	-3.187746	-2.579556	-4.836141
78	1	0	-2.739982	-4.449758	-3.871471
79	1	0	-3.537421	-0.570893	-5.523252
80	1	0	-3.601472	-3.042091	-5.724361
81	6	0	0.509196	-2.148368	-1.181543
82	6	0	-0.444882	-1.225827	-0.657888
83	1	0	0.489236	-2.358221	-2.244591
84	1	0	-0.230668	-0.849820	0.330430
85	6	0	1.389457	-2.845735	-0.372795
86	6	0	2.506728	-3.585346	-0.813381
87	6	0	2.952399	-3.510789	-2.138167
88	6	0	3.334600	-4.346840	0.190890
89	1	0	3.169768	-5.423085	0.071463
90	1	0	4.402452	-4.168333	0.039024
91	1	0	1.250737	-2.760435	0.701914
92	1	0	3.072204	-4.085720	1.217546
93	1	0	2.248556	-3.324160	-2.938780
94	1	0	3.813180	-4.106131	-2.423569
95	1	0	4.185998	-1.845556	-3.269587

2-5-IM-endo

Energy + zep (gas) = -2109.84134 au
Gibbs free energy (gas) = -2109.92112 au
Gibbs free energy (in solvent) = -2109.19222 au
Zero-point correction = 0.80013 au
Thermal correction to Gibbs free energy = 0.72035 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.643822	-0.605679	-0.718419

2	6	0	1.948342	-1.575614	-1.664468
3	6	0	2.922493	-2.771293	-1.771513
4	6	0	3.986231	-2.502803	-0.711221
5	7	0	3.771519	-1.194397	-0.200194
6	8	0	2.290932	0.538386	-0.448419
7	8	0	4.863699	-3.233324	-0.348525
8	6	0	4.641252	-0.574553	0.763152
9	6	0	4.756840	-1.129515	2.035108
10	6	0	5.374073	0.555002	0.406227
11	6	0	5.614837	-0.541083	2.960282
12	6	0	6.345591	0.593978	2.615909
13	6	0	6.224052	1.140809	1.339822
14	1	0	5.714925	-0.974191	3.948292
15	1	0	4.191247	-2.016125	2.291323
16	1	0	7.015058	1.046813	3.337613
17	1	0	6.800393	2.016706	1.066190
18	1	0	5.287417	0.962342	-0.593559
19	1	0	1.834083	-1.060147	-2.621721
20	7	0	0.400669	2.472546	-0.900758
21	6	0	-0.896612	2.796230	-0.156591
22	6	0	0.211814	2.330210	-2.398895
23	6	0	1.377063	3.597459	-0.631892
24	6	0	-1.855125	1.622889	0.197837
25	6	0	-1.586387	3.917953	-0.962566
26	6	0	-0.180174	3.695292	-2.999323
27	6	0	0.743279	4.958733	-1.048949
28	6	0	-1.567061	0.929521	1.536905
29	6	0	-0.552631	4.642485	-1.846615
30	6	0	-0.348511	0.991929	2.173322
31	6	0	-2.622110	0.217997	2.198119
32	6	0	-0.146970	0.340535	3.413323
33	6	0	-2.307298	-0.405201	3.452059
34	7	0	-1.078558	-0.341749	4.033125
35	1	0	-0.549836	1.572058	-2.543026
36	1	0	1.158391	1.951241	-2.782202
37	1	0	2.280065	3.365260	-1.195067
38	1	0	1.628482	3.562253	0.427848
39	1	0	-2.790726	2.164519	0.374667
40	1	0	-2.073484	4.602946	-0.266316
41	1	0	-2.368379	3.493501	-1.599105
42	1	0	0.640299	4.114132	-3.586649
43	1	0	-1.027697	3.568250	-3.675670
44	1	0	1.435086	5.451506	-1.737194
45	1	0	-0.970957	5.571610	-2.234951

46	1	0	0.500573	1.508658	1.741614
47	6	0	-3.942580	0.113384	1.710273
48	1	0	0.827600	0.390401	3.891768
49	6	0	-3.321846	-1.114269	4.138927
50	6	0	-4.596801	-1.206182	3.640348
51	6	0	-4.916974	-0.577005	2.410452
52	1	0	-3.052345	-1.574812	5.081126
53	1	0	-5.349934	-1.750977	4.192810
54	8	0	-6.148612	-0.600861	1.846784
55	1	0	-4.251503	0.571195	0.780549
56	6	0	-7.212505	-1.280724	2.514204
57	1	0	-7.412670	-0.841028	3.495926
58	1	0	-8.084968	-1.151081	1.877550
59	1	0	-6.998546	-2.348521	2.620989
60	6	0	1.046994	7.107357	0.207039
61	1	0	0.861034	7.742615	1.064788
62	6	0	0.530401	5.885728	0.120900
63	1	0	-0.088070	5.518648	0.938167
64	1	0	1.674527	7.519149	-0.577506
65	1	0	0.855780	1.594961	-0.586024
66	1	0	-0.556195	3.206866	0.793515
67	6	0	-1.514345	-0.451385	-1.294758
68	7	0	-2.173789	0.748792	-0.941672
69	1	0	-3.166040	0.682552	-1.112812
70	6	0	-2.240805	-1.185104	-2.374162
71	6	0	-2.551527	-2.543586	-2.222421
72	6	0	-2.667487	-0.525538	-3.536198
73	6	0	-3.248642	-3.226601	-3.215074
74	1	0	-2.260698	-3.058250	-1.314512
75	6	0	-3.360882	-1.210895	-4.529964
76	1	0	-2.451217	0.528781	-3.667502
77	6	0	-3.651430	-2.564265	-4.372830
78	1	0	-3.485845	-4.275377	-3.079176
79	1	0	-3.674217	-0.688673	-5.426608
80	1	0	-4.194760	-3.097218	-5.144224
81	6	0	0.506076	-2.013468	-1.192854
82	6	0	-0.345701	-0.852121	-0.759356
83	1	0	0.063833	-2.458011	-2.090532
84	1	0	0.035011	-0.313217	0.093666
85	6	0	0.609699	-3.096174	-0.133309
86	6	0	1.424505	-4.142990	-0.302255
87	6	0	2.289903	-4.158836	-1.543560
88	6	0	1.536870	-5.288625	0.661060
89	1	0	1.285704	-6.234904	0.168686

90	1	0	2.564145	-5.390552	1.027110
91	1	0	-0.028230	-3.015861	0.741118
92	1	0	0.871810	-5.162970	1.517269
93	1	0	1.694871	-4.432354	-2.423437
94	1	0	3.091343	-4.894950	-1.459127
95	1	0	3.439192	-2.761582	-2.736349

2-6-COM-exo

Energy + zep (gas) = -2109.80482 au
Gibbs free energy (gas) = -2109.89180 au
Gibbs free energy (in solvent) = -2109.14351 au
Zero-point correction = 0.79323 au
Thermal correction to Gibbs free energy = 0.70624 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.886593	-0.694551	-2.033721
2	6	0	-2.834536	-1.511619	-3.287260
3	6	0	-3.853281	-2.370215	-3.285053
4	6	0	-4.645132	-2.177268	-2.025834
5	7	0	-3.986286	-1.125706	-1.319179
6	8	0	-2.111296	0.189511	-1.703407
7	8	0	-5.624075	-2.755409	-1.653330
8	6	0	-4.409944	-0.618955	-0.047245
9	6	0	-5.131380	0.573294	0.012364
10	6	0	-4.121011	-1.337810	1.111100
11	6	0	-5.555631	1.057866	1.247867
12	6	0	-5.267844	0.346354	2.412385
13	6	0	-4.555554	-0.850055	2.342069
14	1	0	-6.132873	1.973761	1.297879
15	1	0	-5.377835	1.097918	-0.903503
16	1	0	-5.615424	0.713973	3.370836
17	1	0	-4.346865	-1.412364	3.244459
18	1	0	-3.572667	-2.269965	1.043595
19	1	0	-2.061676	-1.370190	-4.028252
20	1	0	-4.130291	-3.109259	-4.022297
21	7	0	-0.876011	2.054886	0.019115
22	6	0	0.527196	2.655164	-0.114992
23	6	0	-1.254104	1.695877	1.445332
24	6	0	-1.868308	3.072237	-0.509500
25	6	0	1.750285	1.694472	-0.120708

26	6	0	0.637885	3.748475	0.970548
27	6	0	-1.334240	2.986235	2.286471
28	6	0	-1.719387	4.413256	0.266065
29	6	0	2.032483	0.982008	-1.449245
30	6	0	-0.763393	4.153557	1.462713
31	6	0	1.116108	0.912525	-2.473421
32	6	0	3.333302	0.424089	-1.688435
33	6	0	1.444645	0.274406	-3.692910
34	6	0	3.553464	-0.204872	-2.959937
35	7	0	2.607731	-0.276735	-3.935280
36	1	0	-0.504958	0.998354	1.802501
37	1	0	-2.206584	1.171771	1.378283
38	1	0	-2.854185	2.625972	-0.389350
39	1	0	-1.675559	3.185007	-1.576108
40	1	0	2.569810	2.418701	-0.033490
41	1	0	1.181156	4.601245	0.559474
42	1	0	1.217015	3.372047	1.817660
43	1	0	-2.367462	3.193822	2.573751
44	1	0	-0.763645	2.859733	3.208519
45	1	0	-2.697168	4.669653	0.682433
46	1	0	-0.700947	5.054765	2.073632
47	1	0	0.114373	1.311489	-2.386254
48	6	0	4.407554	0.480038	-0.775610
49	1	0	0.704388	0.228306	-4.487962
50	6	0	4.822989	-0.765182	-3.238316
51	6	0	5.849422	-0.703439	-2.330345
52	6	0	5.643796	-0.062981	-1.082229
53	1	0	4.954813	-1.235969	-4.204425
54	1	0	6.809427	-1.135881	-2.576334
55	8	0	6.599039	0.062566	-0.130320
56	1	0	4.313113	0.946371	0.194297
57	6	0	7.905051	-0.461849	-0.373586
58	1	0	8.372958	0.019435	-1.237657
59	1	0	8.480972	-0.234133	0.520710
60	1	0	7.878451	-1.545870	-0.520314
61	6	0	-1.959371	6.693256	-0.749647
62	1	0	-1.607744	7.489008	-1.395375
63	6	0	-1.289972	5.551894	-0.623687
64	1	0	-0.371261	5.416244	-1.191945
65	1	0	-2.883879	6.875850	-0.210367
66	1	0	-0.999086	1.210251	-0.554433
67	1	0	0.512824	3.126077	-1.098284
68	6	0	1.459721	-0.434463	1.321441
69	7	0	1.873442	0.889620	1.100676

70	1	0	2.694133	1.115978	1.640875
71	6	0	1.949736	-0.957234	2.628627
72	6	0	2.582999	-2.206229	2.703509
73	6	0	1.830962	-0.194938	3.801273
74	6	0	3.066150	-2.683743	3.918000
75	1	0	2.709431	-2.792813	1.802082
76	6	0	2.310868	-0.676640	5.015777
77	1	0	1.345776	0.774326	3.766880
78	6	0	2.929352	-1.923363	5.077641
79	1	0	3.557568	-3.648928	3.956530
80	1	0	2.199391	-0.080275	5.914031
81	1	0	3.306122	-2.297705	6.022200
82	6	0	0.053707	-2.421939	0.782103
83	6	0	0.660404	-1.145572	0.481727
84	1	0	0.142168	-2.790514	1.799181
85	1	0	0.438860	-0.737825	-0.496873
86	6	0	-0.613070	-3.176981	-0.117694
87	6	0	-1.289446	-4.452477	0.157464
88	6	0	-1.811807	-4.762243	1.354618
89	6	0	-1.374139	-5.411695	-1.007696
90	1	0	-0.374426	-5.698672	-1.349707
91	1	0	-1.920757	-6.317925	-0.744616
92	1	0	-0.620692	-2.850837	-1.157253
93	1	0	-1.878161	-4.946030	-1.862147
94	1	0	-1.782842	-4.070650	2.189297
95	1	0	-2.276863	-5.724175	1.534833

2-6-TS-exo

Energy + zep (gas) = -2109.77475 au
Gibbs free energy (gas) = -2109.85753 au
Gibbs free energy (in solvent) = -2109.10812 au
Zero-point correction = 0.79340 au
Thermal correction to Gibbs free energy = 0.71062 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.397956	-0.826830	-1.651634
2	6	0	-1.863489	-1.942564	-2.357121
3	6	0	-2.720279	-3.041558	-2.229893
4	6	0	-3.950061	-2.539572	-1.500546
5	7	0	-3.652960	-1.215424	-1.111750

6	8	0	-1.932688	0.313994	-1.499363
7	8	0	-4.971619	-3.130047	-1.264978
8	6	0	-4.523522	-0.376754	-0.360462
9	6	0	-4.895571	0.874095	-0.861294
10	6	0	-5.022628	-0.811978	0.868616
11	6	0	-5.746006	1.691552	-0.120615
12	6	0	-6.242874	1.260203	1.108589
13	6	0	-5.885103	0.004588	1.595065
14	1	0	-6.044687	2.654645	-0.519201
15	1	0	-4.535654	1.187499	-1.832804
16	1	0	-6.919204	1.890513	1.673940
17	1	0	-6.281600	-0.344962	2.541160
18	1	0	-4.752155	-1.791719	1.240794
19	1	0	-0.955943	-1.875920	-2.933871
20	1	0	-2.873971	-3.778419	-3.007798
21	7	0	-0.586631	2.260648	-0.358026
22	6	0	0.866429	2.644840	-0.106135
23	6	0	-1.410212	2.097623	0.905718
24	6	0	-1.211762	3.356250	-1.195619
25	6	0	1.900840	1.521193	0.216298
26	6	0	0.845172	3.777833	0.943923
27	6	0	-1.519943	3.453642	1.629966
28	6	0	-1.056130	4.728039	-0.472594
29	6	0	2.531317	0.865427	-1.012704
30	6	0	-0.545167	4.441602	0.967396
31	6	0	1.932949	0.858473	-2.252233
32	6	0	3.838895	0.287579	-0.899243
33	6	0	2.593128	0.282218	-3.363365
34	6	0	4.417118	-0.259060	-2.093402
35	7	0	3.786032	-0.258733	-3.298248
36	1	0	-0.920010	1.334551	1.498228
37	1	0	-2.368973	1.703241	0.576847
38	1	0	-2.251811	3.069782	-1.340410
39	1	0	-0.719455	3.343494	-2.168103
40	1	0	2.720522	2.108147	0.646174
41	1	0	1.632737	4.494417	0.704092
42	1	0	1.066712	3.384973	1.941514
43	1	0	-2.542808	3.833251	1.580093
44	1	0	-1.275712	3.333503	2.687947
45	1	0	-2.051645	5.169497	-0.377536
46	1	0	-0.507327	5.376884	1.526952
47	1	0	0.939399	1.257559	-2.414464
48	6	0	4.583347	0.234931	0.297864
49	1	0	2.103620	0.277141	-4.333553

50	6	0	5.713519	-0.824207	-2.027695
51	6	0	6.421603	-0.858131	-0.853086
52	6	0	5.851416	-0.320572	0.329680
53	1	0	6.126622	-1.225101	-2.944803
54	1	0	7.411250	-1.293431	-0.837535
55	8	0	6.473268	-0.312085	1.531806
56	1	0	4.191615	0.612659	1.232432
57	6	0	7.790673	-0.853458	1.646140
58	1	0	8.499775	-0.311754	1.013176
59	1	0	8.068231	-0.723811	2.689838
60	1	0	7.806608	-1.918758	1.397103
61	6	0	-0.602440	6.908563	-1.624948
62	1	0	0.050404	7.577075	-2.173337
63	6	0	-0.200226	5.700383	-1.243913
64	1	0	0.808328	5.379550	-1.499949
65	1	0	-1.600044	7.275191	-1.403071
66	1	0	-0.719339	1.370858	-0.881656
67	1	0	1.194634	3.066898	-1.055450
68	6	0	0.931276	-0.638028	1.301492
69	7	0	1.511205	0.619837	1.312847
70	1	0	1.858454	0.899978	2.217476
71	6	0	0.470726	-1.091441	2.640583
72	6	0	0.612380	-2.439534	3.014553
73	6	0	-0.043274	-0.193720	3.593963
74	6	0	0.220025	-2.875645	4.275361
75	1	0	1.065863	-3.138868	2.325085
76	6	0	-0.434798	-0.631829	4.853977
77	1	0	-0.154100	0.856101	3.351891
78	6	0	-0.309472	-1.976295	5.197935
79	1	0	0.345545	-3.918007	4.543339
80	1	0	-0.840734	0.075752	5.567366
81	1	0	-0.611181	-2.317148	6.181187
82	6	0	0.002982	-2.564063	0.025015
83	6	0	0.852593	-1.435666	0.180272
84	1	0	-0.850815	-2.631050	0.692085
85	1	0	1.470632	-1.181775	-0.666870
86	6	0	0.218247	-3.605310	-0.861979
87	6	0	-0.731245	-4.595805	-1.185702
88	6	0	-2.086823	-4.417700	-0.869539
89	6	0	-0.336841	-5.725135	-2.101037
90	1	0	0.731220	-5.717061	-2.322198
91	1	0	-0.585970	-6.693037	-1.656802
92	1	0	1.173737	-3.639333	-1.380020
93	1	0	-0.880669	-5.666889	-3.051720

94	1	0	-2.348733	-3.822558	-0.002942
95	1	0	-2.781452	-5.227836	-1.063959

2-6-IM-exo

Energy + zep (gas) = -2109.83741 au
Gibbs free energy (gas) = -2109.91690 au
Gibbs free energy (in solvent) = -2109.18735 au
Zero-point correction = 0.80017 au
Thermal correction to Gibbs free energy = 0.72069 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.485757	-0.775871	-1.074662
2	6	0	-1.507249	-1.869136	-1.453542
3	6	0	-2.394369	-3.098138	-1.738035
4	6	0	-3.758226	-2.724692	-1.175670
5	7	0	-3.736839	-1.325313	-0.894763
6	8	0	-2.227776	0.413564	-0.939511
7	8	0	-4.704305	-3.434855	-0.988527
8	6	0	-4.896616	-0.586052	-0.478818
9	6	0	-5.348764	0.478943	-1.256980
10	6	0	-5.571092	-0.957292	0.682576
11	6	0	-6.480683	1.184633	-0.859463
12	6	0	-7.160886	0.821669	0.301750
13	6	0	-6.706923	-0.249651	1.067788
14	1	0	-6.839798	2.007954	-1.465725
15	1	0	-4.825417	0.743747	-2.167071
16	1	0	-8.048398	1.365598	0.602799
17	1	0	-7.240057	-0.542380	1.964405
18	1	0	-5.222503	-1.799603	1.265647
19	1	0	-0.967771	-1.542621	-2.345703
20	1	0	-2.533939	-3.195830	-2.819664
21	7	0	-0.620564	2.369954	0.062049
22	6	0	0.843098	2.805050	0.133247
23	6	0	-1.250169	2.130734	1.425180
24	6	0	-1.391231	3.465884	-0.642080
25	6	0	1.925899	1.693814	0.271865
26	6	0	0.917648	3.881634	1.236542
27	6	0	-1.339627	3.465303	2.189674
28	6	0	-1.171462	4.820027	0.098631
29	6	0	2.501688	1.189773	-1.060901

30	6	0	-0.476636	4.503517	1.453527
31	6	0	1.867966	1.364744	-2.270796
32	6	0	3.782997	0.546431	-1.075373
33	6	0	2.453703	0.894010	-3.469559
34	6	0	4.282570	0.107341	-2.347536
35	7	0	3.611020	0.280802	-3.517560
36	1	0	-0.624087	1.401096	1.924343
37	1	0	-2.219490	1.680740	1.222560
38	1	0	-2.433930	3.152434	-0.648972
39	1	0	-1.041070	3.500044	-1.673858
40	1	0	2.753995	2.251065	0.722836
41	1	0	1.655506	4.631336	0.944898
42	1	0	1.263452	3.438042	2.175144
43	1	0	-2.375002	3.807497	2.255732
44	1	0	-0.981367	3.327689	3.212013
45	1	0	-2.156226	5.233139	0.332095
46	1	0	-0.396060	5.420578	2.037928
47	1	0	0.899115	1.845512	-2.345638
48	6	0	4.584344	0.339979	0.067934
49	1	0	1.933135	1.035525	-4.413269
50	6	0	5.546044	-0.528763	-2.405026
51	6	0	6.303838	-0.721944	-1.277885
52	6	0	5.821205	-0.275377	-0.021138
53	1	0	5.894743	-0.849770	-3.378568
54	1	0	7.267313	-1.206462	-1.357130
55	8	0	6.502334	-0.410607	1.141631
56	1	0	4.271662	0.654694	1.053703
57	6	0	7.791330	-1.025939	1.132075
58	1	0	8.496870	-0.463240	0.513458
59	1	0	8.128254	-1.010921	2.166253
60	1	0	7.735648	-2.062092	0.784864
61	6	0	-0.922126	7.040751	-1.037320
62	1	0	-0.359171	7.744199	-1.639097
63	6	0	-0.442205	5.836748	-0.742423
64	1	0	0.538017	5.555934	-1.123861
65	1	0	-1.895869	7.369141	-0.686797
66	1	0	-0.768513	1.494343	-0.466477
67	1	0	1.019280	3.289709	-0.825352
68	6	0	0.930790	-0.551684	1.097945
69	7	0	1.601003	0.681678	1.285119
70	1	0	2.297112	0.617808	2.012571
71	6	0	0.790849	-1.297613	2.386102
72	6	0	0.994005	-2.684299	2.444198
73	6	0	0.499645	-0.623774	3.584255

74	6	0	0.883015	-3.373275	3.648523
75	1	0	1.262462	-3.225804	1.547330
76	6	0	0.385533	-1.313546	4.787360
77	1	0	0.360480	0.450413	3.579889
78	6	0	0.573655	-2.693003	4.823699
79	1	0	1.051077	-4.443809	3.668943
80	1	0	0.151156	-0.772825	5.697089
81	1	0	0.489568	-3.230906	5.760621
82	6	0	-0.437425	-2.168029	-0.349641
83	6	0	0.437014	-0.968619	-0.086959
84	1	0	-0.976247	-2.430525	0.570549
85	1	0	0.694651	-0.405222	-0.972216
86	6	0	0.319304	-3.399417	-0.830808
87	6	0	-0.344911	-4.486418	-1.234635
88	6	0	-1.858287	-4.442590	-1.191675
89	6	0	0.316658	-5.750176	-1.702544
90	1	0	1.404726	-5.673004	-1.668317
91	1	0	0.013743	-6.601674	-1.082975
92	1	0	1.403551	-3.360152	-0.843697
93	1	0	0.020391	-5.990018	-2.729753
94	1	0	-2.195982	-4.573479	-0.156038
95	1	0	-2.298324	-5.266680	-1.754581

2-7-COM-endo

Energy + zep (gas) = -2109.81547 au
Gibbs free energy (gas) = -2109.90504 au
Gibbs free energy (in solvent) = -2109.15224 au
Zero-point correction = 0.79325 au
Thermal correction to Gibbs free energy = 0.70368 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.353577	1.698658	-0.141241
2	6	0	0.060986	2.153411	-0.477619
3	6	0	-1.823548	2.165747	1.216113
4	6	0	-2.300517	2.203321	-1.200925
5	6	0	1.069196	1.350281	0.364144
6	6	0	0.112945	3.688284	-0.292909
7	6	0	-1.863947	3.709452	1.235237
8	6	0	-2.261200	3.760605	-1.238145
9	6	0	2.522542	1.713969	0.093937

10	6	0	-1.314369	4.237830	-0.101692
11	6	0	2.961123	2.166796	-1.128481
12	6	0	3.497369	1.540568	1.131255
13	6	0	4.332390	2.449950	-1.336630
14	6	0	4.858097	1.857519	0.809090
15	7	0	5.252197	2.304747	-0.413868
16	1	0	-1.144982	1.750279	1.958384
17	1	0	-2.797892	1.704208	1.367088
18	1	0	-3.285106	1.808725	-0.954418
19	1	0	-1.980815	1.761430	-2.144334
20	1	0	0.872301	1.612935	1.406190
21	1	0	0.600615	4.147861	-1.152305
22	1	0	0.720325	3.944860	0.579513
23	1	0	-2.886689	4.059061	1.390715
24	1	0	-1.265326	4.090918	2.064855
25	1	0	-3.261147	4.134612	-1.002052
26	1	0	-1.292013	5.328233	-0.091290
27	1	0	2.280809	2.304423	-1.959524
28	6	0	3.204207	1.083489	2.434686
29	1	0	4.664940	2.808406	-2.307363
30	6	0	5.851251	1.704930	1.806252
31	6	0	5.541132	1.260195	3.067009
32	6	0	4.196954	0.944128	3.389367
33	1	0	6.868915	1.954931	1.533549
34	1	0	6.323909	1.156021	3.805699
35	8	0	3.793916	0.499126	4.605176
36	1	0	2.198137	0.831209	2.744750
37	6	0	4.758207	0.338327	5.646526
38	1	0	5.239049	1.289198	5.894901
39	1	0	4.198748	-0.017669	6.508954
40	1	0	5.516802	-0.402638	5.376807
41	6	0	-2.626741	5.133358	-3.305168
42	1	0	-2.311532	5.487539	-4.279383
43	6	0	-1.887107	4.282350	-2.601345
44	1	0	-0.948045	3.926331	-3.022091
45	1	0	-3.574858	5.509764	-2.933249
46	1	0	0.175026	1.881340	-1.526671
47	1	0	-1.367369	0.666624	-0.132349
48	7	0	0.767803	-0.111451	0.280912
49	1	0	0.922208	-0.524809	1.192502
50	6	0	1.399589	-0.934958	-0.707722
51	6	0	0.996087	-0.719150	-2.124107
52	6	0	1.960673	-0.532402	-3.124878
53	6	0	-0.357105	-0.738164	-2.498650

54	6	0	1.584915	-0.363950	-4.455888
55	6	0	-0.731338	-0.575804	-3.830573
56	6	0	0.238699	-0.382899	-4.813769
57	6	0	2.768178	-2.993853	-1.129546
58	6	0	2.233783	-1.928082	-0.313605
59	6	0	3.621424	-3.927763	-0.660494
60	6	0	4.183098	-5.051953	-1.422177
61	6	0	3.528909	-5.637134	-2.435348
62	6	0	5.542872	-5.532981	-0.971602
63	1	0	3.008899	-0.514547	-2.852420
64	1	0	-1.116024	-0.919378	-1.746122
65	1	0	2.346277	-0.221248	-5.214093
66	1	0	-1.779421	-0.620598	-4.105990
67	1	0	-0.052211	-0.260319	-5.850448
68	1	0	2.466990	-3.033598	-2.171292
69	1	0	2.507153	-1.957557	0.740229
70	1	0	3.964813	-3.837765	0.369684
71	1	0	2.530593	-5.331552	-2.726499
72	1	0	3.970575	-6.455511	-2.991712
73	1	0	6.287536	-4.733768	-1.045774
74	1	0	5.886164	-6.378209	-1.569215
75	1	0	5.515506	-5.847015	0.077712
76	6	0	-3.113224	-1.823609	0.498368
77	6	0	-2.216801	-3.023670	0.510242
78	6	0	-2.902925	-4.067301	0.973194
79	6	0	-4.297866	-3.622971	1.299052
80	7	0	-4.345981	-2.234575	0.970705
81	8	0	-2.823386	-0.690381	0.146801
82	8	0	-5.203709	-4.264693	1.747197
83	6	0	-5.508863	-1.408902	1.105729
84	6	0	-6.110390	-1.265069	2.354808
85	6	0	-6.042439	-0.777412	-0.017605
86	6	0	-7.254343	-0.480923	2.477140
87	6	0	-7.786594	0.163206	1.362394
88	6	0	-7.178520	0.015572	0.116931
89	1	0	-1.188496	-2.973125	0.182367
90	1	0	-2.584465	-5.088785	1.120123
91	1	0	-5.696966	-1.773898	3.216279
92	1	0	-5.581325	-0.920233	-0.987129
93	1	0	-7.731020	-0.377939	3.444582
94	1	0	-8.679081	0.769567	1.461518
95	1	0	-7.599908	0.501591	-0.755196

2-7-TS-endo

Energy + zep (gas) = -2109.78640 au
Gibbs free energy (gas) = -2109.86763 au
Gibbs free energy (in solvent) = -2109.12382 au
Zero-point correction = 0.79384 au
Thermal correction to Gibbs free energy = 0.71261 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.053569	2.118750	0.021984
2	6	0	1.448339	1.778941	-0.489724
3	6	0	0.043854	2.566023	1.462408
4	6	0	-0.529566	3.217084	-0.845196
5	6	0	2.094931	0.593505	0.274937
6	6	0	2.301323	3.075512	-0.411747
7	6	0	1.018656	3.753204	1.629415
8	6	0	0.234900	4.546620	-0.614052
9	6	0	3.406026	0.132162	-0.369008
10	6	0	1.489278	4.212611	0.236842
11	6	0	3.707767	0.337148	-1.693986
12	6	0	4.378149	-0.540105	0.443508
13	6	0	4.941334	-0.111279	-2.223795
14	6	0	5.594166	-0.948404	-0.198138
15	7	0	5.854357	-0.729685	-1.515546
16	1	0	0.305655	1.709212	2.079825
17	1	0	-0.990104	2.825251	1.687857
18	1	0	-1.587681	3.275958	-0.597886
19	1	0	-0.448041	2.871474	-1.876006
20	1	0	2.374351	0.985421	1.256555
21	1	0	2.642640	3.361432	-1.407187
22	1	0	3.202318	2.888924	0.176992
23	1	0	0.520136	4.569921	2.154543
24	1	0	1.879148	3.461557	2.236230
25	1	0	-0.395722	5.215234	-0.020762
26	1	0	2.113482	5.102288	0.328560
27	1	0	3.015461	0.819267	-2.371947
28	6	0	4.217014	-0.817849	1.817465
29	1	0	5.163747	0.053872	-3.274565
30	6	0	6.584801	-1.607940	0.568399
31	6	0	6.406305	-1.863543	1.904746
32	6	0	5.204934	-1.462273	2.542411
33	1	0	7.492803	-1.901517	0.056716

34	1	0	7.183461	-2.368306	2.461915
35	8	0	4.938005	-1.671095	3.854362
36	1	0	3.318782	-0.549320	2.357255
37	6	0	5.907164	-2.332519	4.669540
38	1	0	6.842461	-1.766611	4.714589
39	1	0	5.467508	-2.380476	5.663385
40	1	0	6.102943	-3.347510	4.311103
41	6	0	0.126795	6.466022	-2.224556
42	1	0	0.379582	6.926642	-3.172021
43	6	0	0.540179	5.241401	-1.914862
44	1	0	1.138533	4.686246	-2.635634
45	1	0	-0.478821	7.054839	-1.542495
46	1	0	1.274616	1.484984	-1.522297
47	1	0	-0.602344	1.319039	-0.082576
48	7	0	1.170219	-0.498705	0.594699
49	1	0	0.957563	-0.589742	1.576751
50	6	0	0.383377	-1.290763	-0.220849
51	6	0	0.728117	-1.415218	-1.670861
52	6	0	1.639033	-2.402300	-2.064383
53	6	0	0.139492	-0.603720	-2.646640
54	6	0	1.963470	-2.564770	-3.408266
55	6	0	0.470361	-0.764439	-3.991977
56	6	0	1.384361	-1.743778	-4.374315
57	6	0	-1.687415	-2.676036	-0.329435
58	6	0	-0.656483	-1.975310	0.349451
59	6	0	-2.770938	-3.191944	0.358531
60	6	0	-4.005683	-3.610616	-0.182439
61	6	0	-4.310203	-3.477038	-1.542236
62	6	0	-5.096136	-4.062749	0.756770
63	1	0	2.091733	-3.041678	-1.315869
64	1	0	-0.597507	0.133539	-2.352079
65	1	0	2.668489	-3.334090	-3.700054
66	1	0	0.004083	-0.134167	-4.740893
67	1	0	1.636442	-1.873737	-5.420203
68	1	0	-1.615797	-2.785536	-1.404586
69	1	0	-0.789132	-1.861856	1.424493
70	1	0	-2.712657	-3.169620	1.444026
71	1	0	-3.519496	-3.500484	-2.280362
72	1	0	-5.261946	-3.866162	-1.887249
73	1	0	-4.781206	-4.013061	1.799791
74	1	0	-5.384880	-5.095167	0.536913
75	1	0	-5.990852	-3.443908	0.636295
76	6	0	-3.197150	0.007549	-0.719249
77	6	0	-3.380215	-0.754616	-1.917610

78	6	0	-4.601616	-1.415166	-1.874271
79	6	0	-5.305477	-0.948267	-0.625761
80	7	0	-4.368262	-0.157481	0.069081
81	8	0	-2.253615	0.739997	-0.383336
82	8	0	-6.432975	-1.188278	-0.269422
83	6	0	-4.603376	0.461226	1.330745
84	6	0	-3.636513	0.382222	2.336635
85	6	0	-5.803570	1.134593	1.568873
86	6	0	-3.864963	0.988666	3.568728
87	6	0	-5.061393	1.661670	3.809568
88	6	0	-6.028479	1.725653	2.809161
89	1	0	-2.680328	-0.738924	-2.736129
90	1	0	-5.205169	-1.658983	-2.737486
91	1	0	-2.720427	-0.161991	2.149899
92	1	0	-6.558608	1.177562	0.796351
93	1	0	-3.116559	0.917247	4.350283
94	1	0	-5.243364	2.122286	4.773373
95	1	0	-6.965510	2.238470	2.991551

2-7-IM-endo

Energy + zep (gas) = -2109.84213 au
Gibbs free energy (gas) = -2109.92296 au
Gibbs free energy (in solvent) = -2109.19572 au
Zero-point correction = 0.79970 au
Thermal correction to Gibbs free energy = 0.71887 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.003872	1.901664	-0.197500
2	6	0	1.410288	1.610221	-0.699048
3	6	0	-0.024592	2.569906	1.155995
4	6	0	-0.709500	2.789166	-1.205814
5	6	0	2.188023	0.632416	0.217930
6	6	0	2.126362	2.980045	-0.866901
7	6	0	0.839193	3.848155	1.096660
8	6	0	-0.075872	4.204416	-1.209348
9	6	0	3.559517	0.287359	-0.372405
10	6	0	1.225426	4.124301	-0.368802
11	6	0	3.828038	0.310419	-1.720191
12	6	0	4.623821	-0.084852	0.513724
13	6	0	5.117875	-0.020490	-2.199805

14	6	0	5.892996	-0.389544	-0.080646
15	7	0	6.118871	-0.353784	-1.422346
16	1	0	0.332800	1.848430	1.888324
17	1	0	-1.073882	2.767935	1.371638
18	1	0	-1.762378	2.788961	-0.933764
19	1	0	-0.608364	2.294033	-2.172633
20	1	0	2.397361	1.177891	1.142050
21	1	0	2.408566	3.133433	-1.908941
22	1	0	3.057993	2.976635	-0.297559
23	1	0	0.281623	4.689722	1.511784
24	1	0	1.740188	3.730800	1.703087
25	1	0	-0.756287	4.894089	-0.701219
26	1	0	1.762401	5.070968	-0.440261
27	1	0	3.068146	0.557363	-2.450932
28	6	0	4.500645	-0.168767	1.917151
29	1	0	5.311903	-0.003471	-3.269029
30	6	0	6.974618	-0.745777	0.759865
31	6	0	6.832717	-0.810929	2.123381
32	6	0	5.576849	-0.519688	2.713576
33	1	0	7.921322	-0.965664	0.282434
34	1	0	7.679387	-1.086187	2.737008
35	8	0	5.339255	-0.564319	4.048260
36	1	0	3.562878	0.017244	2.422749
37	6	0	6.395658	-0.934216	4.934625
38	1	0	7.229468	-0.227722	4.879095
39	1	0	5.963491	-0.901907	5.932531
40	1	0	6.753222	-1.947649	4.728468
41	6	0	-0.419999	5.825419	-3.091976
42	1	0	-0.235863	6.154896	-4.107539
43	6	0	0.127199	4.713199	-2.612295
44	1	0	0.767069	4.115757	-3.259893
45	1	0	-1.070120	6.450237	-2.487269
46	1	0	1.240513	1.133591	-1.664113
47	1	0	-0.566084	1.036706	-0.140835
48	7	0	1.440346	-0.561842	0.652830
49	1	0	1.111103	-0.484890	1.604622
50	6	0	0.520899	-1.258847	-0.169892
51	6	0	1.059868	-1.837273	-1.433242
52	6	0	2.186625	-2.669397	-1.381876
53	6	0	0.452872	-1.601798	-2.673027
54	6	0	2.678812	-3.263476	-2.538297
55	6	0	0.954475	-2.187271	-3.834792
56	6	0	2.066393	-3.022624	-3.768329
57	6	0	-1.825800	-2.312490	-0.298136

58	6	0	-0.734177	-1.455479	0.281535
59	6	0	-2.420247	-3.238626	0.747178
60	6	0	-3.546243	-3.922836	0.523246
61	6	0	-4.261968	-3.707608	-0.791540
62	6	0	-4.138324	-4.900151	1.496513
63	1	0	2.667690	-2.849366	-0.428327
64	1	0	-0.412318	-0.950202	-2.733462
65	1	0	3.543971	-3.913552	-2.481471
66	1	0	0.476267	-1.992757	-4.787978
67	1	0	2.454880	-3.483577	-4.668861
68	1	0	-1.400174	-2.923431	-1.102171
69	1	0	-0.988627	-0.987722	1.231270
70	1	0	-1.866738	-3.373297	1.671605
71	1	0	-3.762974	-4.269858	-1.590099
72	1	0	-5.290727	-4.070191	-0.744892
73	1	0	-3.529620	-4.994070	2.397463
74	1	0	-4.229917	-5.892469	1.040985
75	1	0	-5.148883	-4.593837	1.787486
76	6	0	-3.325052	-0.205117	-0.205488
77	6	0	-2.956139	-1.457235	-0.991819
78	6	0	-4.289430	-2.213965	-1.164503
79	6	0	-5.281262	-1.460628	-0.281920
80	7	0	-4.641607	-0.283635	0.191032
81	8	0	-2.584778	0.738869	0.037892
82	8	0	-6.411279	-1.765742	-0.025263
83	6	0	-5.308503	0.704807	0.992514
84	6	0	-4.842733	0.982343	2.276171
85	6	0	-6.429298	1.357228	0.484345
86	6	0	-5.499900	1.933005	3.051673
87	6	0	-6.620177	2.593114	2.550090
88	6	0	-7.084769	2.301473	1.269466
89	1	0	-2.563535	-1.117329	-1.952732
90	1	0	-4.657262	-2.107711	-2.190153
91	1	0	-3.986023	0.447453	2.666708
92	1	0	-6.791967	1.118569	-0.507377
93	1	0	-5.145789	2.147039	4.053242
94	1	0	-7.135747	3.325606	3.159780
95	1	0	-7.961824	2.804765	0.880672

2-8-COM-exo

Energy + zep (gas) = -2109.81450 au
Gibbs free energy (gas) = -2109.90414 au
Gibbs free energy (in solvent) = -2109.15176 au
Zero-point correction = 0.79304 au

Thermal correction to Gibbs free energy = 0.70341 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.227558	0.841712	2.360219
2	6	0	2.786247	1.583303	3.584379
3	6	0	3.668736	2.544645	3.850068
4	6	0	4.754696	2.501340	2.816625
5	7	0	4.414224	1.423493	1.946124
6	8	0	2.655267	-0.089743	1.819004
7	8	0	5.715216	3.207772	2.708046
8	6	0	5.199877	1.017550	0.819933
9	6	0	5.755424	-0.261364	0.788472
10	6	0	5.425261	1.915054	-0.222383
11	6	0	6.527549	-0.648103	-0.303560
12	6	0	6.757256	0.243950	-1.349781
13	6	0	6.211054	1.525119	-1.304214
14	1	0	1.878836	1.325654	4.110281
15	1	0	3.674194	3.272925	4.647534
16	1	0	5.600198	-0.936252	1.621564
17	1	0	5.003177	2.911083	-0.178949
18	1	0	6.967837	-1.638050	-0.326746
19	1	0	7.372007	-0.053811	-2.190909
20	1	0	6.400518	2.226751	-2.107819
21	7	0	0.987073	-2.018258	0.500422
22	6	0	-0.275326	-2.162077	-0.340744
23	6	0	0.916772	-2.770591	1.807734
24	6	0	2.171528	-2.501464	-0.298787
25	6	0	-1.402532	-1.322608	0.287360
26	6	0	-0.566088	-3.673284	-0.487710
27	6	0	0.795848	-4.282082	1.515652
28	6	0	1.961736	-3.995976	-0.685453
29	6	0	-2.710994	-1.384544	-0.488709
30	6	0	0.652427	-4.483599	-0.003314
31	6	0	-2.757756	-1.565729	-1.851549
32	6	0	-3.953614	-1.206807	0.204285
33	6	0	-4.000030	-1.581989	-2.529474
34	6	0	-5.151691	-1.242690	-0.582961
35	7	0	-5.156101	-1.429446	-1.930637
36	1	0	0.069152	-2.377833	2.365785
37	1	0	1.819698	-2.502901	2.352863

38	1	0	3.053615	-2.338562	0.317608
39	1	0	2.245717	-1.853054	-1.171110
40	1	0	-1.601124	-1.761991	1.267767
41	1	0	-0.805575	-3.903618	-1.525346
42	1	0	-1.444912	-3.950689	0.101278
43	1	0	1.674888	-4.812399	1.888045
44	1	0	-0.071886	-4.695532	2.033453
45	1	0	2.782893	-4.578521	-0.258894
46	1	0	0.506702	-5.540889	-0.227892
47	1	0	-1.856113	-1.687818	-2.438568
48	6	0	-4.070011	-1.001222	1.596728
49	1	0	-4.021903	-1.728210	-3.606309
50	6	0	-6.400525	-1.078933	0.063001
51	6	0	-6.487898	-0.882814	1.418489
52	6	0	-5.305611	-0.842434	2.200310
53	1	0	-7.287222	-1.114305	-0.557494
54	1	0	-7.458114	-0.761728	1.880229
55	8	0	-5.291605	-0.652756	3.543097
56	1	0	-3.206321	-0.964486	2.248483
57	6	0	-6.527991	-0.488241	4.239039
58	1	0	-7.162432	-1.374027	4.139272
59	1	0	-6.258276	-0.355145	5.284541
60	1	0	-7.067844	0.396930	3.889331
61	6	0	2.779501	-5.062193	-2.803731
62	1	0	2.750354	-5.182826	-3.880057
63	6	0	1.981828	-4.202615	-2.178209
64	1	0	1.292532	-3.598860	-2.766134
65	1	0	3.490852	-5.679553	-2.263462
66	1	0	0.003741	-1.723638	-1.298299
67	1	0	1.099390	-1.018700	0.723107
68	7	0	-0.912757	0.058333	0.583907
69	1	0	-1.325014	0.367803	1.455618
70	6	0	-1.060391	1.101897	-0.390382
71	6	0	-0.172741	1.028610	-1.582304
72	6	0	-0.696530	1.118800	-2.880149
73	6	0	1.217293	0.898028	-1.433004
74	6	0	0.141354	1.071020	-3.992568
75	6	0	2.055225	0.855468	-2.544823
76	6	0	1.518419	0.935990	-3.829898
77	6	0	-2.004683	3.369357	-0.887670
78	6	0	-1.896478	2.137645	-0.141184
79	6	0	-2.893999	4.338680	-0.588890
80	6	0	-3.044559	5.623787	-1.285499
81	6	0	-2.018883	6.245372	-1.884321

82	6	0	-4.431520	6.223004	-1.260565
83	1	0	-1.766957	1.219436	-3.012572
84	1	0	1.646112	0.872104	-0.437649
85	1	0	-0.283493	1.142156	-4.987307
86	1	0	3.128125	0.780053	-2.405913
87	1	0	2.169372	0.905684	-4.695865
88	1	0	-1.337604	3.509690	-1.731811
89	1	0	-2.533247	2.061761	0.738960
90	1	0	-3.598345	4.156007	0.222160
91	1	0	-1.011502	5.846515	-1.856134
92	1	0	-2.157546	7.185766	-2.404771
93	1	0	-5.159114	5.551600	-1.728189
94	1	0	-4.463054	7.180046	-1.782546
95	1	0	-4.764837	6.386573	-0.229765

2-8-TS-exo

Energy + zep (gas) = -2109.78291 au
Gibbs free energy (gas) = -2109.86428 au
Gibbs free energy (in solvent) = -2109.11941 au
Zero-point correction = 0.79350 au
Thermal correction to Gibbs free energy = 0.71214 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.022037	-0.613217	-1.297116
2	6	0	3.147979	-1.872709	-1.965066
3	6	0	4.313734	-2.514431	-1.545071
4	6	0	5.045721	-1.541697	-0.653358
5	7	0	4.167469	-0.445445	-0.477139
6	8	0	2.117172	0.236269	-1.368072
7	8	0	6.139175	-1.648846	-0.163243
8	6	0	4.477573	0.702017	0.307479
9	6	0	4.430108	1.977042	-0.261537
10	6	0	4.864934	0.549087	1.640373
11	6	0	4.743976	3.093726	0.508892
12	6	0	5.125855	2.944004	1.840920
13	6	0	5.194178	1.669143	2.399279
14	1	0	2.456054	-2.192072	-2.725755
15	1	0	4.906941	-3.178605	-2.157389
16	1	0	4.170555	2.083722	-1.306768
17	1	0	4.929048	-0.441810	2.070522

18	1	0	4.714480	4.080285	0.060350
19	1	0	5.386429	3.812832	2.433774
20	1	0	5.511300	1.542429	3.427873
21	7	0	-0.108899	1.842962	-1.441377
22	6	0	-1.176103	1.835564	-0.351540
23	6	0	-0.685905	1.920963	-2.832980
24	6	0	0.806740	3.028862	-1.217040
25	6	0	-2.110684	0.604394	-0.460653
26	6	0	-1.944347	3.182893	-0.438212
27	6	0	-1.630947	3.139150	-2.920144
28	6	0	0.048654	4.350035	-1.508252
29	6	0	-3.067954	0.484627	0.726908
30	6	0	-1.456021	3.995496	-1.651858
31	6	0	-2.795527	1.013830	1.966079
32	6	0	-4.314526	-0.201962	0.549421
33	6	0	-3.727173	0.874479	3.022241
34	6	0	-5.183541	-0.278755	1.687836
35	7	0	-4.876726	0.256712	2.900144
36	1	0	-1.181282	0.975990	-3.044841
37	1	0	0.167622	1.999393	-3.506052
38	1	0	1.671537	2.879220	-1.859720
39	1	0	1.152334	2.965214	-0.185575
40	1	0	-2.744343	0.785615	-1.332797
41	1	0	-1.817891	3.748035	0.485847
42	1	0	-3.015125	2.990333	-0.534466
43	1	0	-1.400119	3.722441	-3.813341
44	1	0	-2.670389	2.814587	-3.010609
45	1	0	0.384961	4.743964	-2.472019
46	1	0	-2.038857	4.913342	-1.737745
47	1	0	-1.866739	1.527514	2.177853
48	6	0	-4.736546	-0.794418	-0.659866
49	1	0	-3.496487	1.293750	3.997797
50	6	0	-6.429691	-0.937181	1.554630
51	6	0	-6.820034	-1.501515	0.366346
52	6	0	-5.962059	-1.430922	-0.760594
53	1	0	-7.065218	-0.976029	2.430467
54	1	0	-7.779294	-1.995718	0.297708
55	8	0	-6.258937	-1.960426	-1.971911
56	1	0	-4.123448	-0.783150	-1.551504
57	6	0	-7.505044	-2.635664	-2.154306
58	1	0	-8.350833	-1.961586	-1.989377
59	1	0	-7.506802	-2.968400	-3.189960
60	1	0	-7.587184	-3.504597	-1.494635
61	6	0	0.861192	6.588499	-0.722155

62	1	0	1.043055	7.310345	0.065034
63	6	0	0.339042	5.393998	-0.462567
64	1	0	0.100322	5.132484	0.566860
65	1	0	1.123958	6.891208	-1.731166
66	1	0	-0.599508	1.767882	0.567928
67	1	0	0.498239	1.001167	-1.379474
68	7	0	-1.401043	-0.632543	-0.804135
69	1	0	-1.665749	-1.031595	-1.692642
70	6	0	-0.525273	-1.419495	-0.089356
71	6	0	-0.148053	-1.056032	1.312370
72	6	0	-0.777521	-1.753521	2.352398
73	6	0	0.831024	-0.106107	1.628165
74	6	0	-0.461767	-1.479816	3.679740
75	6	0	1.150541	0.159975	2.959522
76	6	0	0.498838	-0.518178	3.987110
77	6	0	1.132615	-3.222762	-0.271358
78	6	0	-0.051788	-2.567843	-0.680143
79	6	0	1.653431	-4.372158	-0.841349
80	6	0	2.986741	-4.802482	-0.686865
81	6	0	3.951760	-3.978522	-0.092859
82	6	0	3.424669	-6.084230	-1.348345
83	1	0	-1.519326	-2.507084	2.116774
84	1	0	1.382537	0.384181	0.835935
85	1	0	-0.961765	-2.023785	4.472369
86	1	0	1.927490	0.880977	3.185927
87	1	0	0.751211	-0.312678	5.020872
88	1	0	1.667096	-2.771871	0.557408
89	1	0	-0.502808	-2.884612	-1.618886
90	1	0	1.026603	-4.925805	-1.536331
91	1	0	3.646918	-3.256061	0.654529
92	1	0	4.956239	-4.361936	0.048279
93	1	0	4.434129	-5.999035	-1.758675
94	1	0	2.746154	-6.385472	-2.148979
95	1	0	3.448029	-6.897787	-0.614764

2-8-IM-exo

Energy + zep (gas) = -2109.84123 au

Gibbs free energy (gas) = -2109.92208 au

Gibbs free energy (in solvent) = -2109.19512 au

Zero-point correction = 0.79938 au

Thermal correction to Gibbs free energy = 0.71853 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.223701	-0.511712	-1.036310
2	6	0	2.915126	-1.942340	-1.436264
3	6	0	4.235989	-2.707528	-1.227301
4	6	0	5.136305	-1.730156	-0.485542
5	7	0	4.487458	-0.459903	-0.482370
6	8	0	2.474572	0.448647	-1.149683
7	8	0	6.199378	-1.944400	0.023706
8	6	0	5.084746	0.726300	0.064939
9	6	0	5.269063	1.844513	-0.746895
10	6	0	5.492072	0.739067	1.397715
11	6	0	5.852868	2.989631	-0.212704
12	6	0	6.259880	3.012524	1.120000
13	6	0	6.082604	1.886441	1.920666
14	1	0	2.614283	-1.943119	-2.486870
15	1	0	4.710756	-2.880294	-2.198089
16	1	0	4.968441	1.812133	-1.786608
17	1	0	5.367337	-0.143998	2.010649
18	1	0	6.003494	3.858641	-0.842331
19	1	0	6.724178	3.901617	1.529931
20	1	0	6.410614	1.895693	2.953247
21	7	0	-0.146272	1.703983	-1.137226
22	6	0	-1.298529	1.680809	-0.130540
23	6	0	-0.622217	1.823865	-2.563816
24	6	0	0.765642	2.874272	-0.807006
25	6	0	-2.283868	0.507149	-0.356446
26	6	0	-2.003624	3.064685	-0.213820
27	6	0	-1.552210	3.051458	-2.678479
28	6	0	0.060418	4.209033	-1.152417
29	6	0	-3.342508	0.452743	0.752450
30	6	0	-1.438431	3.884706	-1.387720
31	6	0	-3.116246	0.891954	2.035095
32	6	0	-4.634294	-0.093420	0.452008
33	6	0	-4.136121	0.803128	3.012908
34	6	0	-5.593330	-0.129086	1.517799
35	7	0	-5.330119	0.317557	2.776194
36	1	0	-1.110412	0.888827	-2.831141
37	1	0	0.276647	1.916253	-3.173223
38	1	0	1.691336	2.715657	-1.353414
39	1	0	0.994046	2.791786	0.255915
40	1	0	-2.832848	0.746804	-1.270494
41	1	0	-1.889443	3.605015	0.726738

42	1	0	-3.076240	2.918496	-0.352404
43	1	0	-1.267807	3.648430	-3.546963
44	1	0	-2.587189	2.737138	-2.831395
45	1	0	0.467759	4.590617	-2.093685
46	1	0	-2.001226	4.813006	-1.492252
47	1	0	-2.159690	1.296117	2.341722
48	6	0	-5.016150	-0.593301	-0.811707
49	1	0	-3.940022	1.151375	4.023604
50	6	0	-6.883602	-0.651129	1.261081
51	6	0	-7.233068	-1.125236	0.021419
52	6	0	-6.285872	-1.097592	-1.033110
53	1	0	-7.586339	-0.661554	2.084846
54	1	0	-8.227537	-1.517396	-0.140966
55	8	0	-6.536082	-1.547159	-2.288106
56	1	0	-4.335188	-0.614558	-1.652110
57	6	0	-7.819265	-2.094839	-2.591806
58	1	0	-8.612075	-1.352316	-2.459179
59	1	0	-7.771449	-2.385846	-3.639017
60	1	0	-8.031110	-2.977464	-1.980709
61	6	0	0.880849	6.427815	-0.319852
62	1	0	1.027197	7.148794	0.475481
63	6	0	0.307549	5.250375	-0.093072
64	1	0	-0.012085	5.002616	0.917675
65	1	0	1.223176	6.716758	-1.308837
66	1	0	-0.793079	1.551174	0.824476
67	1	0	0.432162	0.852362	-1.052076
68	7	0	-1.675165	-0.807618	-0.620877
69	1	0	-1.868106	-1.152822	-1.549240
70	6	0	-0.437269	-1.258964	-0.116315
71	6	0	-0.246497	-1.172195	1.364065
72	6	0	-1.145240	-1.835806	2.209194
73	6	0	0.824728	-0.471590	1.934334
74	6	0	-0.965964	-1.814006	3.588503
75	6	0	0.993792	-0.437098	3.318244
76	6	0	0.101469	-1.112022	4.147694
77	6	0	1.726252	-2.539216	-0.613030
78	6	0	0.444269	-1.838540	-0.956191
79	6	0	1.687709	-4.034595	-0.882901
80	6	0	2.804306	-4.766028	-0.836774
81	6	0	4.105886	-4.068347	-0.501434
82	6	0	2.838274	-6.252643	-1.044976
83	1	0	-1.980078	-2.374018	1.776829
84	1	0	1.530184	0.048866	1.296077
85	1	0	-1.661553	-2.344339	4.228309

86	1	0	1.825870	0.111315	3.745017
87	1	0	0.237220	-1.093813	5.222717
88	1	0	1.943309	-2.387988	0.450982
89	1	0	0.183955	-1.861238	-2.015327
90	1	0	0.723604	-4.490855	-1.082531
91	1	0	4.154088	-3.907482	0.582907
92	1	0	4.966559	-4.692221	-0.746356
93	1	0	1.843678	-6.655449	-1.243355
94	1	0	3.242395	-6.760215	-0.161994
95	1	0	3.491795	-6.515846	-1.884053

3-1-COM-endo

Energy + zep (gas) = -2188.40122 au
Gibbs free energy (gas) = -2188.49345 au
Gibbs free energy (in solvent) = -2187.70558 au
Zero-point correction = 0.84845 au
Thermal correction to Gibbs free energy = 0.75623 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.684540	2.219285	0.825087
2	7	0	-1.453695	2.637151	0.277577
3	6	0	-2.388424	1.527018	-0.196517
4	6	0	-0.822961	3.405455	-0.868668
5	6	0	-2.245939	3.585847	1.141934
6	6	0	-1.588611	0.249104	-0.542561
7	6	0	-3.293823	2.129817	-1.285541
8	6	0	-1.924638	4.177022	-1.623617
9	6	0	-3.479430	4.105241	0.337209
10	6	0	-2.412419	-0.743413	-1.369431
11	6	0	-3.294020	3.666537	-1.144361
12	6	0	-3.572211	-1.430124	-0.881850
13	6	0	-2.017380	-0.990278	-2.664766
14	6	0	-4.218356	-2.334542	-1.791496
15	6	0	-2.733202	-1.900108	-3.476965
16	7	0	-3.791753	-2.554248	-3.064864
17	1	0	-0.285555	2.688469	-1.485343
18	1	0	-0.078961	4.057587	-0.414190
19	1	0	-1.572362	4.391352	1.434334
20	1	0	-2.539351	3.042288	2.040003
21	1	0	-0.734609	0.531563	-1.163767

22	1	0	-4.295413	1.710392	-1.188628
23	1	0	-2.935957	1.858176	-2.281693
24	1	0	-1.835358	5.251728	-1.448422
25	1	0	-1.814102	4.015677	-2.697560
26	1	0	-3.452858	5.197853	0.357223
27	1	0	-4.094442	4.098748	-1.745617
28	6	0	-4.127865	-1.278278	0.409329
29	1	0	-1.146118	-0.490441	-3.075589
30	6	0	-5.367895	-3.039413	-1.359269
31	1	0	-2.407082	-2.086852	-4.496839
32	7	0	-1.022911	-0.257410	0.709728
33	1	0	-1.720366	-0.499315	1.401632
34	6	0	-5.737279	4.511129	1.347638
35	1	0	-6.669519	4.153957	1.768687
36	6	0	-4.790315	3.671056	0.941971
37	1	0	-4.959755	2.600315	1.041994
38	1	0	-5.617393	5.587581	1.271618
39	1	0	-2.993827	1.307378	0.683403
40	6	0	2.038465	-2.253417	-0.297106
41	6	0	0.795923	-1.517060	-0.324323
42	6	0	0.068505	-1.150405	0.761200
43	1	0	2.469203	-2.473997	0.674641
44	1	0	0.450214	-1.217525	-1.306511
45	6	0	2.689436	-2.677725	-1.401493
46	6	0	3.973272	-3.392777	-1.428659
47	6	0	4.922576	-3.229504	-0.494651
48	6	0	0.354872	-1.610519	2.148174
49	6	0	0.479072	-0.689450	3.199279
50	6	0	0.462393	-2.978611	2.434767
51	6	0	0.719791	-1.126914	4.498624
52	1	0	0.415696	0.371227	2.987216
53	6	0	0.699418	-3.413071	3.735986
54	1	0	0.345367	-3.699535	1.634595
55	6	0	0.829665	-2.489438	4.771007
56	1	0	0.826874	-0.403667	5.299348
57	1	0	0.775340	-4.474545	3.941807
58	1	0	1.014065	-2.829163	5.783612
59	6	0	4.171368	-4.332427	-2.596321
60	1	0	4.076877	-3.797935	-3.548440
61	1	0	5.153372	-4.806378	-2.569211
62	1	0	2.214102	-2.522905	-2.370088
63	1	0	3.409384	-5.118621	-2.599068
64	1	0	4.805365	-2.529329	0.324737
65	1	0	5.844691	-3.798469	-0.524329

66	6	0	-5.883100	-2.875300	-0.098207
67	6	0	-5.256232	-1.977599	0.801465
68	8	0	-5.692606	-1.739756	2.063427
69	6	0	-6.820801	-2.461337	2.560932
70	1	0	-6.634004	-3.539256	2.561999
71	1	0	-6.956946	-2.118764	3.584478
72	1	0	-7.723011	-2.240438	1.982493
73	1	0	-6.762504	-3.429981	0.198667
74	1	0	-3.700964	-0.617290	1.150713
75	1	0	-5.827279	-3.715302	-2.069670
76	6	0	5.233921	1.243618	0.967510
77	6	0	4.742191	1.749590	2.188892
78	6	0	6.566879	0.783050	0.920895
79	6	0	5.557479	1.787561	3.309641
80	6	0	6.873226	1.323111	3.244456
81	6	0	7.377030	0.819279	2.046711
82	1	0	5.169767	2.181491	4.241529
83	1	0	3.728652	2.116657	2.265373
84	1	0	7.502676	1.356506	4.126098
85	1	0	8.397118	0.458977	1.991951
86	1	0	6.957520	0.391316	-0.011697
87	6	0	2.633356	1.276105	-1.944299
88	8	0	1.467845	1.484927	-2.229502
89	6	0	3.180558	1.449632	-0.564992
90	6	0	4.477891	1.160399	-0.264722
91	6	0	2.209624	1.913668	0.365230
92	8	0	3.555496	0.883589	-2.819228
93	6	0	3.126033	0.677583	-4.197590
94	6	0	4.356298	0.334352	-5.008407
95	1	0	2.639710	1.591097	-4.543754
96	1	0	2.389222	-0.127979	-4.203989
97	1	0	4.070939	0.165985	-6.049645
98	1	0	4.832672	-0.573075	-4.632665
99	1	0	5.082937	1.148642	-4.981424
100	7	0	1.381653	2.298448	1.075748
101	1	0	5.045530	0.792049	-1.112234

3-1-TS1-endo

Energy + zep (gas) = -2188.37895 au

Gibbs free energy (gas) = -2188.46510 au

Gibbs free energy (in solvent) = -2187.68300 au

Zero-point correction = 0.84877 au

Thermal correction to Gibbs free energy = 0.76263 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.257805	-1.365545	1.503855
2	7	0	-1.015378	-1.075910	2.159423
3	6	0	-2.180253	-0.426730	1.413662
4	6	0	-0.359447	-0.133947	3.152676
5	6	0	-1.535683	-2.290100	2.886450
6	6	0	-1.671279	0.433372	0.223736
7	6	0	-3.059251	0.271761	2.471318
8	6	0	-1.357956	0.187688	4.282247
9	6	0	-2.707826	-1.871586	3.828049
10	6	0	-2.618695	1.563094	-0.178847
11	6	0	-2.748537	-0.317145	3.862565
12	6	0	-3.927045	1.350823	-0.719602
13	6	0	-2.180920	2.859434	-0.029243
14	6	0	-4.673544	2.521715	-1.081563
15	6	0	-3.007429	3.942119	-0.413174
16	7	0	-4.205135	3.789748	-0.924331
17	1	0	-0.018520	0.738131	2.598208
18	1	0	0.531888	-0.652199	3.503538
19	1	0	-0.695212	-2.716126	3.434169
20	1	0	-1.850896	-3.012966	2.133529
21	1	0	-0.738161	0.909969	0.533758
22	1	0	-4.107176	0.147337	2.198128
23	1	0	-2.866386	1.347035	2.484180
24	1	0	-1.049478	-0.282767	5.218812
25	1	0	-1.381849	1.265138	4.455871
26	1	0	-2.463435	-2.212103	4.837541
27	1	0	-3.504139	0.003592	4.580455
28	6	0	-4.529963	0.087893	-0.913531
29	6	0	-5.970758	2.365758	-1.627268
30	7	0	-1.318438	-0.470346	-0.874145
31	1	0	-2.024745	-1.125672	-1.176050
32	6	0	-4.736380	-3.287913	4.237012
33	1	0	-5.678625	-3.715471	3.915585
34	6	0	-4.018166	-2.506011	3.437325
35	1	0	-4.389731	-2.296864	2.435495
36	1	0	-4.410260	-3.528552	5.244262
37	1	0	-2.729462	-1.275315	1.003594
38	6	0	1.922997	0.759384	-2.065592
39	6	0	0.558668	0.787931	-1.715519

40	6	0	-0.232448	-0.346869	-1.697472
41	1	0	2.345072	-0.216431	-2.281478
42	1	0	0.172327	1.701233	-1.281225
43	6	0	2.771350	1.853065	-2.094710
44	6	0	4.180130	1.769173	-2.053937
45	6	0	4.838883	0.572777	-1.750481
46	6	0	0.029281	-1.523878	-2.558990
47	6	0	-0.064962	-2.830243	-2.052761
48	6	0	0.340603	-1.343632	-3.915496
49	6	0	0.154801	-3.924796	-2.881051
50	1	0	-0.257999	-2.981372	-0.997941
51	6	0	0.553571	-2.442170	-4.742323
52	1	0	0.388951	-0.340434	-4.320434
53	6	0	0.461156	-3.733684	-4.228188
54	1	0	0.098895	-4.928035	-2.474808
55	1	0	0.783631	-2.289066	-5.790072
56	1	0	0.628621	-4.588337	-4.873137
57	6	0	4.984911	3.036489	-2.187859
58	1	0	4.395899	3.923201	-1.946480
59	1	0	5.872004	3.020204	-1.551066
60	1	0	2.327473	2.844647	-2.058080
61	1	0	5.332529	3.146422	-3.221391
62	1	0	4.358577	-0.373041	-1.963042
63	1	0	5.920435	0.547943	-1.823849
64	6	0	-6.531179	1.126623	-1.810341
65	6	0	-5.802473	-0.033075	-1.445033
66	1	0	-6.506159	3.268562	-1.893304
67	1	0	-7.524321	1.044047	-2.229705
68	8	0	-6.272549	-1.297918	-1.578119
69	1	0	-4.032378	-0.837099	-0.653778
70	6	0	-7.566742	-1.507303	-2.146604
71	1	0	-8.349550	-1.046383	-1.536787
72	1	0	-7.708270	-2.585829	-2.158680
73	1	0	-7.618314	-1.124459	-3.170123
74	1	0	-2.651828	4.961948	-0.292460
75	1	0	-1.195993	3.061687	0.379479
76	6	0	5.408157	-0.981822	0.463933
77	6	0	4.920281	-2.255409	0.133104
78	6	0	6.728157	-0.875966	0.929718
79	6	0	5.721627	-3.382196	0.283546
80	6	0	7.025103	-3.262995	0.763044
81	6	0	7.526436	-2.004064	1.085742
82	1	0	5.327867	-4.357672	0.022024
83	1	0	3.914309	-2.375390	-0.248589

84	1	0	7.646240	-4.143456	0.878597
85	1	0	8.539502	-1.899674	1.456499
86	1	0	7.126029	0.101382	1.181885
87	6	0	2.636497	1.668209	1.038217
88	8	0	1.454988	1.831927	1.335116
89	6	0	3.242147	0.382764	0.691390
90	6	0	4.614708	0.264641	0.340415
91	6	0	2.331175	-0.683139	0.798214
92	8	0	3.523411	2.685312	1.030096
93	6	0	3.029534	3.993363	1.413139
94	6	0	4.226939	4.900055	1.607867
95	1	0	2.440196	3.891130	2.325683
96	1	0	2.365614	4.358023	0.624442
97	1	0	3.888588	5.899277	1.893197
98	1	0	4.812091	4.987884	0.690315
99	1	0	4.877483	4.521235	2.398804
100	7	0	1.501055	-1.490136	0.912359
101	1	0	5.177891	1.151436	0.597993

3-1-IM1-endo

Energy + zep (gas) = -2188.39214 au
Gibbs free energy (gas) = -2188.47645 au
Gibbs free energy (in solvent) = -2187.70242 au
Zero-point correction = 0.85144 au
Thermal correction to Gibbs free energy = 0.76713 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.286993	-0.966084	-0.255755
2	6	0	5.025092	-1.604147	-1.473438
3	6	0	6.272107	-1.506576	0.577017
4	6	0	5.725527	-2.749729	-1.844275
5	6	0	6.703937	-3.277215	-1.004966
6	6	0	6.975196	-2.651217	0.208991
7	1	0	5.508504	-3.228379	-2.792640
8	1	0	4.266608	-1.214634	-2.143425
9	1	0	7.252570	-4.165338	-1.296485
10	1	0	7.737318	-3.050170	0.868838
11	1	0	6.491598	-1.025617	1.524680
12	6	0	2.490577	0.692365	1.705970
13	8	0	1.310760	0.563402	2.070077

14	6	0	3.102145	0.041150	0.581529
15	6	0	4.540724	0.287298	0.184947
16	6	0	2.261727	-0.865465	-0.052488
17	8	0	3.339933	1.515140	2.377467
18	6	0	2.821771	2.178336	3.552367
19	6	0	3.983873	2.853888	4.252380
20	1	0	2.337762	1.438024	4.192202
21	1	0	2.061235	2.901486	3.244615
22	1	0	3.628443	3.359308	5.153900
23	1	0	4.455367	3.599622	3.608899
24	1	0	4.739391	2.122357	4.546315
25	7	0	1.464688	-1.567032	-0.544000
26	1	0	5.038742	0.658501	1.080145
27	1	0	-0.086300	-2.041418	0.135872
28	7	0	-0.838608	-2.280903	0.831437
29	6	0	-2.007841	-1.301903	0.757715
30	6	0	-0.149247	-2.267179	2.184636
31	6	0	-1.364569	-3.664815	0.550297
32	6	0	-1.532720	0.146272	0.449990
33	6	0	-2.846720	-1.506776	2.036984
34	6	0	-1.116707	-2.815143	3.252165
35	6	0	-2.517443	-3.998702	1.547606
36	6	0	-2.469042	1.236483	0.966273
37	6	0	-2.524779	-2.890357	2.638131
38	6	0	-3.800031	1.443037	0.483180
39	6	0	-1.992552	2.075432	1.948393
40	6	0	-4.531524	2.535204	1.058753
41	6	0	-2.808605	3.117746	2.449898
42	7	0	-4.027264	3.350146	2.024833
43	1	0	0.184838	-1.246494	2.366134
44	1	0	0.745147	-2.877358	2.062669
45	1	0	-0.521825	-4.348837	0.648039
46	1	0	-1.698947	-3.687008	-0.487499
47	1	0	-0.567851	0.301166	0.942162
48	1	0	-3.903138	-1.402287	1.789304
49	1	0	-2.619372	-0.733264	2.773820
50	1	0	-0.799405	-3.802101	3.597309
51	1	0	-1.116176	-2.154925	4.121637
52	1	0	-2.267243	-4.940070	2.043635
53	1	0	-3.262078	-3.144772	3.400306
54	6	0	-4.438836	0.653424	-0.498087
55	1	0	-0.988141	1.943511	2.337985
56	6	0	-5.852046	2.784839	0.612723
57	1	0	-2.426027	3.776764	3.224695

58	7	0	-1.272906	0.245542	-0.998413
59	1	0	-1.915683	-0.224027	-1.620799
60	6	0	-4.570571	-5.298444	0.928431
61	1	0	-5.525099	-5.385600	0.423224
62	6	0	-3.845388	-4.186562	0.859448
63	1	0	-4.225660	-3.349195	0.276140
64	1	0	-4.237967	-6.163127	1.494514
65	1	0	-2.589551	-1.654330	-0.096762
66	6	0	1.879331	1.993964	-1.190347
67	6	0	0.541010	1.826655	-0.897454
68	6	0	-0.247772	0.882671	-1.587891
69	1	0	2.292934	1.350318	-1.958386
70	1	0	0.127468	2.305279	-0.018410
71	6	0	2.766771	2.932205	-0.587288
72	6	0	4.113439	2.732651	-0.513271
73	6	0	4.727743	1.433409	-0.915909
74	6	0	-0.035551	0.576987	-3.019115
75	6	0	-0.088176	-0.745300	-3.490518
76	6	0	0.181176	1.621127	-3.932170
77	6	0	0.072135	-1.012854	-4.844295
78	1	0	-0.177127	-1.560148	-2.783210
79	6	0	0.329883	1.346999	-5.287817
80	1	0	0.203506	2.644125	-3.578341
81	6	0	0.274877	0.032442	-5.745839
82	1	0	0.055999	-2.037454	-5.196468
83	1	0	0.483167	2.160667	-5.986522
84	1	0	0.396503	-0.179168	-6.801668
85	6	0	5.013009	3.745009	0.126269
86	1	0	4.465565	4.617645	0.484942
87	1	0	5.552566	3.298456	0.968446
88	1	0	2.334564	3.805305	-0.105652
89	1	0	5.772921	4.082146	-0.587634
90	1	0	4.304072	1.061506	-1.851425
91	1	0	5.802506	1.549876	-1.071650
92	6	0	-6.448387	2.004294	-0.345646
93	6	0	-5.734155	0.916889	-0.909012
94	8	0	-6.239110	0.082848	-1.851149
95	6	0	-7.566096	0.296473	-2.336904
96	1	0	-7.735052	-0.484401	-3.075190
97	1	0	-8.303812	0.201944	-1.534539
98	1	0	-7.459040	2.222620	-0.661766
99	1	0	-6.376401	3.618183	1.063345
100	1	0	-3.951762	-0.191593	-0.966085
101	1	0	-7.661381	1.274822	-2.817013

3-1-TS2-endo

Energy + zep (gas) = -2188.38627 au

Gibbs free energy (gas) = -2188.47045 au

Gibbs free energy (in solvent) = -2187.70002 au

Zero-point correction = 0.85162 au

Thermal correction to Gibbs free energy = 0.76744 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.183551	1.076927	0.259774
2	6	0	4.889308	1.703115	1.476657
3	6	0	6.072705	1.710527	-0.614217
4	6	0	5.466211	2.926532	1.807423
5	6	0	6.351564	3.545541	0.927831
6	6	0	6.653369	2.933444	-0.285744
7	1	0	5.226809	3.394109	2.755706
8	1	0	4.204474	1.241391	2.179728
9	1	0	6.805429	4.494573	1.188527
10	1	0	7.344956	3.403607	-0.975543
11	1	0	6.319357	1.238726	-1.559901
12	6	0	2.602220	-0.852568	-1.707391
13	8	0	1.475511	-0.704016	-2.166447
14	6	0	3.088774	-0.222421	-0.459431
15	6	0	4.586311	-0.270570	-0.126294
16	6	0	2.308584	0.917695	-0.150835
17	8	0	3.509810	-1.665357	-2.271339
18	6	0	3.101528	-2.381180	-3.468534
19	6	0	4.315707	-3.109583	-4.004023
20	1	0	2.704015	-1.659669	-4.184420
21	1	0	2.296775	-3.069403	-3.200048
22	1	0	4.043614	-3.659821	-4.908077
23	1	0	4.700919	-3.823856	-3.273637
24	1	0	5.112369	-2.407831	-4.259030
25	7	0	1.544736	1.755676	0.096762
26	1	0	5.082144	-0.587008	-1.042791
27	1	0	-0.254078	1.946083	-0.439429
28	7	0	-1.017162	2.103131	-1.129045
29	6	0	-2.181536	1.136400	-0.906767
30	6	0	-0.380669	1.943343	-2.496985
31	6	0	-1.533242	3.512309	-0.976549

32	6	0	-1.661351	-0.263951	-0.477826
33	6	0	-3.072139	1.210588	-2.162919
34	6	0	-1.391572	2.375831	-3.577983
35	6	0	-2.726083	3.738427	-1.955417
36	6	0	-2.618258	-1.411219	-0.795803
37	6	0	-2.775649	2.520119	-2.921506
38	6	0	-3.910045	-1.559303	-0.196510
39	6	0	-2.206540	-2.371345	-1.691992
40	6	0	-4.668266	-2.717885	-0.573024
41	6	0	-3.042402	-3.471708	-1.997034
42	7	0	-4.225769	-3.649257	-1.461176
43	1	0	-0.052895	0.909847	-2.583822
44	1	0	0.518257	2.558043	-2.477918
45	1	0	-0.696175	4.180061	-1.179443
46	1	0	-1.825519	3.642246	0.065775
47	1	0	-0.748007	-0.460450	-1.042405
48	1	0	-4.117283	1.140643	-1.860644
49	1	0	-2.880770	0.359789	-2.821095
50	1	0	-1.087892	3.318974	-4.038427
51	1	0	-1.423775	1.626639	-4.371263
52	1	0	-2.499024	4.621161	-2.558827
53	1	0	-3.540923	2.695577	-3.678311
54	6	0	-4.485075	-0.654512	0.723955
55	1	0	-1.234590	-2.295975	-2.168744
56	6	0	-5.949369	-2.913163	-0.002579
57	1	0	-2.707086	-4.224364	-2.705689
58	7	0	-1.257119	-0.196855	0.927676
59	1	0	-1.975158	0.027090	1.601540
60	6	0	-4.761155	5.094194	-1.401895
61	1	0	-5.694220	5.236123	-0.869777
62	6	0	-4.025191	3.999798	-1.236518
63	1	0	-4.372281	3.233538	-0.545002
64	1	0	-4.459367	5.888818	-2.077384
65	1	0	-2.717877	1.569327	-0.062008
66	6	0	2.162458	-1.585868	0.960713
67	6	0	0.753423	-1.520001	0.741497
68	6	0	-0.077927	-0.677417	1.444371
69	1	0	2.526291	-0.965733	1.772702
70	1	0	0.362839	-2.026330	-0.132568
71	6	0	2.966560	-2.760629	0.674095
72	6	0	4.314335	-2.695979	0.703083
73	6	0	4.956057	-1.364595	0.954443
74	6	0	0.203983	-0.233528	2.833926
75	6	0	0.005042	1.098137	3.229340

76	6	0	0.633099	-1.165480	3.791007
77	6	0	0.241401	1.488105	4.542708
78	1	0	-0.289337	1.835450	2.492977
79	6	0	0.864816	-0.772993	5.105988
80	1	0	0.757664	-2.201989	3.502511
81	6	0	0.669923	0.553336	5.484762
82	1	0	0.102170	2.523561	4.830990
83	1	0	1.186704	-1.505637	5.836661
84	1	0	0.849839	0.858398	6.508995
85	6	0	5.193914	-3.871285	0.402691
86	1	0	4.615027	-4.772628	0.194071
87	1	0	5.836113	-3.661365	-0.460362
88	1	0	2.458940	-3.675530	0.382925
89	1	0	5.863346	-4.080171	1.244349
90	1	0	4.656367	-0.982276	1.935361
91	1	0	6.044296	-1.448539	0.973366
92	6	0	-6.482901	-2.021069	0.893337
93	6	0	-5.742453	-0.869891	1.261854
94	8	0	-6.186752	0.072437	2.129525
95	6	0	-7.466839	-0.090229	2.743486
96	1	0	-6.494650	-3.798411	-0.305043
97	1	0	-3.977715	0.245460	1.045600
98	1	0	-7.464338	-2.201966	1.309654
99	1	0	-8.267708	-0.099337	1.998108
100	1	0	-7.506763	-1.003631	3.344167
101	1	0	-7.589750	0.773346	3.393476

3-1-IM2- endo

Energy + zep (gas) = -2188.39965 au

Gibbs free energy (gas) = -2188.48564 au

Gibbs free energy (in solvent) = -2187.72665 au

Zero-point correction = 0.85357 au

Thermal correction to Gibbs free energy = 0.76759 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.874340	0.931770	1.062114
2	6	0	-4.875753	2.226023	0.526724
3	6	0	-5.076476	0.784636	2.439256
4	6	0	-5.058787	3.336963	1.347013

5	6	0	-5.252201	3.174603	2.716428
6	6	0	-5.263735	1.892943	3.260828
7	1	0	-5.058536	4.329718	0.912093
8	1	0	-4.751261	2.375244	-0.539962
9	1	0	-5.403945	4.039042	3.352290
10	1	0	-5.427978	1.753762	4.323188
11	1	0	-5.097891	-0.209590	2.873861
12	6	0	-2.944694	-2.123088	-0.531775
13	8	0	-1.849298	-2.637925	-0.584958
14	6	0	-3.172827	-0.672594	-0.012431
15	6	0	-4.690798	-0.311080	0.197577
16	6	0	-2.403571	-0.604595	1.236394
17	8	0	-4.064862	-2.738457	-0.889171
18	6	0	-3.931728	-4.099008	-1.409539
19	6	0	-5.321881	-4.616398	-1.704782
20	1	0	-3.415584	-4.698307	-0.657724
21	1	0	-3.304367	-4.055490	-2.301511
22	1	0	-5.253731	-5.637377	-2.088063
23	1	0	-5.820526	-4.004229	-2.458560
24	1	0	-5.936667	-4.632459	-0.802688
25	7	0	-1.700303	-0.573719	2.150810
26	1	0	-5.127090	-1.143105	0.753314
27	1	0	0.466880	-0.718818	1.699898
28	7	0	1.220219	-1.411490	1.806598
29	6	0	2.366660	-1.104683	0.840354
30	6	0	0.611161	-2.782089	1.579270
31	6	0	1.749810	-1.325115	3.219241
32	6	0	1.808022	-0.616865	-0.523758
33	6	0	3.290830	-2.336602	0.834971
34	6	0	1.657384	-3.859747	1.930813
35	6	0	2.967340	-2.286986	3.373427
36	6	0	2.829275	-0.675858	-1.655276
37	6	0	3.026923	-3.178930	2.099708
38	6	0	4.034954	0.099092	-1.674347
39	6	0	2.574313	-1.497403	-2.729657
40	6	0	4.884265	-0.055066	-2.821168
41	6	0	3.483879	-1.570887	-3.810645
42	7	0	4.598514	-0.882804	-3.862784
43	1	0	0.270897	-2.823379	0.547551
44	1	0	-0.276642	-2.819649	2.207093
45	1	0	0.923828	-1.581560	3.881826
46	1	0	2.020658	-0.284676	3.398848
47	1	0	1.008345	-1.300128	-0.805029
48	1	0	4.326649	-2.001249	0.777654

49	1	0	3.111983	-2.949302	-0.052504
50	1	0	1.376741	-4.384962	2.846785
51	1	0	1.699074	-4.604123	1.133464
52	1	0	2.765023	-2.946321	4.221471
53	1	0	3.811119	-3.926340	2.224174
54	6	0	4.441386	0.994280	-0.657934
55	1	0	1.670012	-2.095604	-2.763384
56	6	0	6.088532	0.686535	-2.887157
57	1	0	3.269982	-2.223788	-4.652638
58	7	0	1.214731	0.708707	-0.337543
59	1	0	1.861393	1.476297	-0.458701
60	6	0	5.010281	-1.773125	4.731786
61	1	0	5.931906	-1.227641	4.895824
62	6	0	4.251908	-1.552338	3.662829
63	1	0	4.566373	-0.800726	2.940562
64	1	0	4.738709	-2.508781	5.482653
65	1	0	2.876243	-0.264643	1.308468
66	6	0	-2.515082	0.382520	-1.013829
67	6	0	-1.028589	0.193095	-1.141805
68	6	0	-0.118797	1.047404	-0.628014
69	1	0	-2.678875	1.342466	-0.516709
70	1	0	-0.708989	-0.767074	-1.523501
71	6	0	-3.294440	0.360419	-2.307630
72	6	0	-4.606627	0.114619	-2.379684
73	6	0	-5.434204	-0.227498	-1.164943
74	6	0	-0.425544	2.459067	-0.249355
75	6	0	-0.118446	2.953830	1.025341
76	6	0	-0.984205	3.331014	-1.193537
77	6	0	-0.382223	4.279828	1.353724
78	1	0	0.308063	2.290632	1.768341
79	6	0	-1.240356	4.659941	-0.866570
80	1	0	-1.199223	2.965412	-2.190843
81	6	0	-0.941922	5.136836	0.407838
82	1	0	-0.154799	4.644276	2.348830
83	1	0	-1.663402	5.324776	-1.610788
84	1	0	-1.140151	6.171626	0.661913
85	6	0	-5.356452	0.144192	-3.684360
86	1	0	-4.700016	0.384980	-4.522003
87	1	0	-5.831152	-0.822447	-3.886568
88	1	0	-2.736792	0.596501	-3.208991
89	1	0	-6.160665	0.887422	-3.656045
90	1	0	-6.241257	0.506497	-1.068282
91	1	0	-5.930315	-1.181842	-1.357756
92	6	0	6.461268	1.547251	-1.885487

93	6	0	5.626011	1.705311	-0.751536
94	8	0	5.907230	2.527129	0.289339
95	6	0	7.090291	3.327194	0.249719
96	1	0	6.706091	0.546455	-3.765473
97	1	0	3.847892	1.171221	0.228931
98	1	0	7.387306	2.099138	-1.969684
99	1	0	7.990669	2.706355	0.216864
100	1	0	7.078883	4.011874	-0.603416
101	1	0	7.083543	3.902616	1.172875

3-2-COM-exo

Energy + zep (gas) = -2188.40205 au
Gibbs free energy (gas) = -2188.49493 au
Gibbs free energy (in solvent) = -2187.70639 au
Zero-point correction = 0.84833 au
Thermal correction to Gibbs free energy = 0.75544 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.404586	-2.316079	0.378633
2	7	0	-1.349993	-2.494873	0.752275
3	6	0	-2.386502	-1.729760	-0.065309
4	6	0	-1.350860	-2.088431	2.211725
5	6	0	-1.640414	-3.971240	0.640401
6	6	0	-1.849812	-0.340773	-0.480351
7	6	0	-3.717501	-1.793199	0.712862
8	6	0	-2.683013	-2.521921	2.856808
9	6	0	-3.104687	-4.250233	1.098901
10	6	0	-2.982609	0.506046	-1.071571
11	6	0	-3.652202	-2.942978	1.739230
12	6	0	-3.412334	0.275243	-2.357997
13	6	0	-3.638958	1.531575	-0.318761
14	6	0	-4.479270	1.025574	-2.902547
15	6	0	-4.711352	2.228684	-0.970718
16	7	0	-5.114853	1.964097	-2.242074
17	1	0	-1.181405	-1.015715	2.247732
18	1	0	-0.479202	-2.565681	2.655740
19	1	0	-0.901261	-4.483865	1.254128
20	1	0	-1.471358	-4.254645	-0.398486
21	1	0	-1.447378	0.160829	0.399566
22	1	0	-4.538071	-1.926814	0.008210

23	1	0	-3.907157	-0.854083	1.236725
24	1	0	-2.524416	-3.347248	3.554890
25	1	0	-3.100053	-1.691275	3.428926
26	1	0	-3.069440	-5.005973	1.888123
27	1	0	-4.644669	-3.134584	2.148230
28	1	0	-2.937158	-0.471587	-2.985243
29	6	0	-3.300120	1.899955	1.003940
30	1	0	-4.809257	0.833075	-3.919975
31	6	0	-5.391938	3.249572	-0.264290
32	7	0	-0.722948	-0.584062	-1.378779
33	1	0	-0.988055	-1.137772	-2.186000
34	6	0	-4.613032	-5.954354	0.046846
35	1	0	-5.229775	-6.302540	-0.773096
36	6	0	-3.965375	-4.795117	-0.012327
37	1	0	-4.056192	-4.188497	-0.911879
38	1	0	-4.553612	-6.597573	0.919545
39	1	0	-2.484287	-2.315448	-0.983575
40	6	0	1.222308	2.673861	-1.299161
41	6	0	0.209957	1.655753	-1.142300
42	6	0	0.176863	0.446534	-1.755668
43	1	0	2.077088	2.449500	-1.928974
44	1	0	-0.562588	1.888364	-0.418012
45	6	0	1.159808	3.881944	-0.699154
46	6	0	2.164209	4.950813	-0.788138
47	6	0	3.468964	4.718236	-0.997526
48	6	0	1.089936	0.027366	-2.850723
49	6	0	1.674413	-1.249832	-2.851366
50	6	0	1.344516	0.876583	-3.938555
51	6	0	2.505059	-1.652613	-3.893074
52	1	0	1.483470	-1.920251	-2.021525
53	6	0	2.176307	0.471523	-4.978028
54	1	0	0.869925	1.849162	-3.975311
55	6	0	2.762150	-0.792581	-4.958724
56	1	0	2.955835	-2.638756	-3.873359
57	1	0	2.357238	1.141171	-5.810860
58	1	0	3.407367	-1.107060	-5.770695
59	6	0	1.634516	6.355476	-0.610067
60	1	0	1.136571	6.462437	0.360117
61	1	0	2.432961	7.096584	-0.665963
62	1	0	0.269002	4.119236	-0.118914
63	1	0	0.889531	6.593542	-1.376342
64	1	0	3.867233	3.713627	-1.080286
65	1	0	4.177196	5.533692	-1.088540
66	6	0	-5.048547	3.585359	1.020808

67	6	0	-3.985093	2.904116	1.666246
68	8	0	-3.573698	3.172451	2.930703
69	6	0	-4.207533	4.220165	3.664397
70	1	0	-6.196222	3.757533	-0.781655
71	1	0	-5.589145	4.370959	1.530548
72	1	0	-2.486422	1.431318	1.542286
73	1	0	-5.269009	4.009197	3.827307
74	1	0	-3.696683	4.253710	4.624368
75	1	0	-4.094434	5.184994	3.160715
76	6	0	2.623336	-2.621492	0.780870
77	8	0	1.460084	-2.975629	0.638089
78	6	0	3.010251	-1.265778	1.250979
79	6	0	4.316845	-0.881965	1.333537
80	6	0	1.897201	-0.454909	1.613815
81	8	0	3.661816	-3.411155	0.528033
82	6	0	4.928726	0.371061	1.716805
83	6	0	6.331002	0.368075	1.879137
84	6	0	4.230735	1.581315	1.913865
85	6	0	7.009572	1.519553	2.248717
86	6	0	6.302299	2.705391	2.443001
87	6	0	4.916940	2.733178	2.267355
88	1	0	8.084930	1.497891	2.377162
89	1	0	6.880658	-0.552668	1.716750
90	1	0	6.829387	3.610343	2.722087
91	1	0	4.372342	3.660338	2.395877
92	1	0	3.160749	1.632034	1.771003
93	1	0	5.021442	-1.662557	1.067319
94	6	0	3.386678	-4.763968	0.055684
95	6	0	4.718206	-5.435459	-0.197610
96	1	0	2.779474	-4.692243	-0.848473
97	1	0	2.803484	-5.278227	0.822034
98	1	0	4.549541	-6.454734	-0.553140
99	1	0	5.312184	-5.487525	0.716729
100	1	0	5.289998	-4.899147	-0.957259
101	7	0	0.957898	0.147639	1.915208

3-2-TS1-exo

Energy + zep (gas) = -2188.37706 au
Gibbs free energy (gas) = -2188.46328 au
Gibbs free energy (in solvent) = -2187.68242 au
Zero-point correction = 0.84889 au
Thermal correction to Gibbs free energy = 0.76266 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.625360	-1.392730	1.445971
2	7	0	-1.515869	-1.153510	1.932175
3	6	0	-2.662756	-0.924182	0.947606
4	6	0	-1.222253	0.078004	2.770792
5	6	0	-1.903536	-2.292861	2.842559
6	6	0	-2.157613	-0.297808	-0.383563
7	6	0	-3.786352	-0.209636	1.725133
8	6	0	-2.406923	0.351369	3.715342
9	6	0	-3.278662	-1.979197	3.511633
10	6	0	-3.285609	0.403573	-1.140122
11	6	0	-3.604044	-0.483247	3.233429
12	6	0	-4.231757	-0.341563	-1.807134
13	6	0	-3.408787	1.829470	-1.162126
14	6	0	-5.295301	0.294339	-2.485978
15	6	0	-4.532497	2.365905	-1.880586
16	7	0	-5.450430	1.596376	-2.523667
17	1	0	-1.018974	0.895571	2.084818
18	1	0	-0.290340	-0.131712	3.293641
19	1	0	-1.102295	-2.401623	3.573045
20	1	0	-1.935880	-3.199042	2.237384
21	1	0	-1.368027	0.418009	-0.158544
22	1	0	-4.750177	-0.565487	1.361474
23	1	0	-3.762610	0.867857	1.547313
24	1	0	-2.153183	0.096174	4.747171
25	1	0	-2.647973	1.415738	3.696625
26	1	0	-3.151967	-2.084557	4.592237
27	1	0	-4.509162	-0.208296	3.775750
28	1	0	-4.183597	-1.425279	-1.834092
29	6	0	-2.512237	2.726636	-0.535481
30	1	0	-6.035863	-0.303934	-3.009997
31	6	0	-4.704778	3.769813	-1.930403
32	7	0	-1.541555	-1.379387	-1.154126
33	1	0	-2.138038	-2.165020	-1.370689
34	6	0	-5.066578	-3.685361	3.934217
35	1	0	-5.849903	-4.349065	3.588017
36	6	0	-4.367449	-2.932937	3.090417
37	1	0	-4.591129	-2.994428	2.026634
38	1	0	-4.884708	-3.662797	5.004346
39	1	0	-3.004883	-1.931821	0.701050
40	6	0	1.783759	-0.168405	-2.137614

41	6	0	0.379567	-0.182828	-1.989033
42	6	0	-0.349068	-1.344253	-1.826440
43	1	0	2.295084	-1.124077	-2.088632
44	1	0	-0.108348	0.769419	-1.815814
45	6	0	2.549160	0.973731	-2.277088
46	6	0	3.939241	1.046341	-2.033653
47	6	0	4.632206	0.026442	-1.372849
48	6	0	0.093453	-2.659122	-2.350716
49	6	0	-0.081931	-3.837186	-1.605921
50	6	0	0.648632	-2.752203	-3.636342
51	6	0	0.292628	-5.069639	-2.130563
52	1	0	-0.473880	-3.778081	-0.597690
53	6	0	1.023744	-3.986650	-4.157264
54	1	0	0.758305	-1.855702	-4.233436
55	6	0	0.845808	-5.147810	-3.408330
56	1	0	0.160236	-5.969699	-1.541111
57	1	0	1.442083	-4.042588	-5.155257
58	1	0	1.133020	-6.108955	-3.818194
59	6	0	4.660332	2.328930	-2.355627
60	1	0	3.989650	3.190253	-2.335644
61	1	0	5.486827	2.511350	-1.667571
62	1	0	2.035956	1.905280	-2.499911
63	1	0	5.081650	2.266666	-3.366032
64	1	0	4.251894	-0.986999	-1.385599
65	1	0	5.711949	0.104696	-1.307804
66	6	0	-3.826537	4.621375	-1.310296
67	6	0	-2.713375	4.095651	-0.605199
68	8	0	-1.795442	4.864853	0.028434
69	6	0	-1.918813	6.285570	-0.017040
70	1	0	-5.559597	4.144378	-2.479417
71	1	0	-3.986874	5.689194	-1.367899
72	1	0	-1.627640	2.395590	-0.004890
73	1	0	-2.847735	6.622746	0.453431
74	1	0	-1.071591	6.668807	0.547705
75	1	0	-1.866996	6.659179	-1.044380
76	6	0	2.264462	-1.436647	0.951402
77	8	0	1.091440	-1.775430	1.164003
78	6	0	2.732382	-0.070925	0.812342
79	6	0	4.116820	0.235468	0.668171
80	6	0	1.696954	0.886614	0.868559
81	8	0	3.242942	-2.353716	0.830886
82	6	0	4.770098	1.499879	1.079841
83	6	0	6.109474	1.424994	1.500190
84	6	0	4.144746	2.756572	1.086409

85	6	0	6.797778	2.556286	1.921725
86	6	0	6.161214	3.795970	1.928153
87	6	0	4.835478	3.888453	1.509149
88	1	0	7.827590	2.470026	2.248392
89	1	0	6.611700	0.462899	1.503459
90	1	0	6.693073	4.681048	2.257088
91	1	0	4.333083	4.848998	1.510935
92	1	0	3.117881	2.861788	0.765564
93	1	0	4.737938	-0.627322	0.872481
94	6	0	2.897804	-3.746503	1.044610
95	6	0	4.184270	-4.544668	1.006771
96	1	0	2.203404	-4.056772	0.261385
97	1	0	2.390448	-3.835190	2.007567
98	1	0	3.964164	-5.603726	1.162763
99	1	0	4.870587	-4.219917	1.791315
100	1	0	4.683803	-4.439605	0.041545
101	7	0	0.792988	1.614603	0.908818

3-2-IM1-exo

Energy + zep (gas) = -2188.38941 au
Gibbs free energy (gas) = -2188.47395 au
Gibbs free energy (in solvent) = -2187.70145 au
Zero-point correction = 0.85153 au
Thermal correction to Gibbs free energy = 0.76699 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.360015	-1.278415	1.500535
2	7	0	-1.280234	-1.092289	1.990402
3	6	0	-2.451958	-1.011962	1.015684
4	6	0	-1.105685	0.186590	2.789328
5	6	0	-1.546852	-2.232925	2.939884
6	6	0	-2.050396	-0.381068	-0.352115
7	6	0	-3.637867	-0.389789	1.783167
8	6	0	-2.305231	0.371284	3.737433
9	6	0	-2.939023	-2.040483	3.617538
10	6	0	-3.252483	0.217284	-1.081015
11	6	0	-3.416316	-0.594998	3.297063
12	6	0	-4.170052	-0.609426	-1.690320
13	6	0	-3.472792	1.630557	-1.131744
14	6	0	-5.301685	-0.065816	-2.338194

15	6	0	-4.661729	2.068574	-1.812118
16	7	0	-5.548724	1.221216	-2.397598
17	1	0	-0.983237	0.998131	2.077709
18	1	0	-0.155021	0.085398	3.311632
19	1	0	-0.731764	-2.236505	3.662944
20	1	0	-1.488537	-3.158192	2.366454
21	1	0	-1.292743	0.384100	-0.183677
22	1	0	-4.563931	-0.851847	1.441604
23	1	0	-3.723852	0.678466	1.572372
24	1	0	-2.020192	0.177533	4.774373
25	1	0	-2.652974	1.404743	3.686744
26	1	0	-2.792081	-2.097922	4.699210
27	1	0	-4.340745	-0.394112	3.839455
28	1	0	-4.049333	-1.687779	-1.693082
29	6	0	-2.613161	2.601661	-0.566926
30	1	0	-6.019311	-0.726631	-2.816944
31	6	0	-4.934278	3.455410	-1.885471
32	7	0	-1.412817	-1.443818	-1.147704
33	1	0	-1.912178	-2.320905	-1.199754
34	6	0	-4.525622	-3.917918	4.114371
35	1	0	-5.240156	-4.669032	3.799294
36	6	0	-3.930064	-3.112075	3.240911
37	1	0	-4.170503	-3.218913	2.184125
38	1	0	-4.323180	-3.854334	5.179124
39	1	0	-2.697305	-2.057304	0.811636
40	6	0	1.781511	-0.106318	-2.208178
41	6	0	0.404936	-0.180707	-2.091167
42	6	0	-0.260570	-1.392133	-1.837409
43	1	0	2.352402	-1.020400	-2.093991
44	1	0	-0.155327	0.744350	-2.019769
45	6	0	2.493540	1.095427	-2.484336
46	6	0	3.793355	1.316555	-2.131101
47	6	0	4.526582	0.373733	-1.238941
48	6	0	0.232052	-2.690882	-2.347236
49	6	0	0.148305	-3.853753	-1.563077
50	6	0	0.737885	-2.784984	-3.653231
51	6	0	0.558914	-5.078409	-2.075760
52	1	0	-0.178416	-3.780733	-0.532913
53	6	0	1.144417	-4.014219	-4.161945
54	1	0	0.781271	-1.899319	-4.274063
55	6	0	1.053957	-5.161838	-3.377379
56	1	0	0.505599	-5.967118	-1.457876
57	1	0	1.521578	-4.076924	-5.175596
58	1	0	1.369993	-6.118369	-3.776581

59	6	0	4.500582	2.567552	-2.556147
60	1	0	3.841258	3.257205	-3.085198
61	1	0	4.943821	3.081092	-1.698936
62	1	0	1.939497	1.900593	-2.959725
63	1	0	5.329770	2.305314	-3.224686
64	1	0	4.369472	-0.664607	-1.542790
65	1	0	5.599967	0.571289	-1.278031
66	6	0	-4.091229	4.380433	-1.324919
67	6	0	-2.913423	3.951424	-0.659779
68	8	0	-2.025333	4.798777	-0.088227
69	6	0	-2.252181	6.206022	-0.157067
70	1	0	-5.836213	3.756316	-2.403510
71	1	0	-4.328379	5.432831	-1.398830
72	1	0	-1.684355	2.344461	-0.071743
73	1	0	-3.180971	6.487352	0.348965
74	1	0	-1.410048	6.661235	0.359656
75	1	0	-2.273624	6.557521	-1.193282
76	6	0	2.300853	-1.335227	0.803647
77	8	0	1.145848	-1.770421	1.039435
78	6	0	2.658324	0.015787	0.547132
79	6	0	4.093899	0.429858	0.305171
80	6	0	1.588468	0.914642	0.621412
81	8	0	3.342303	-2.201647	0.741494
82	6	0	4.545557	1.719819	0.980008
83	6	0	5.691117	1.682221	1.784320
84	6	0	3.892884	2.948971	0.822753
85	6	0	6.173523	2.828233	2.411735
86	6	0	5.512945	4.042677	2.247542
87	6	0	4.370977	4.096912	1.452088
88	1	0	7.062179	2.769965	3.029974
89	1	0	6.212640	0.740446	1.924057
90	1	0	5.882724	4.937092	2.735429
91	1	0	3.846097	5.036422	1.319790
92	1	0	2.998961	3.020952	0.216578
93	1	0	4.698009	-0.365514	0.740191
94	6	0	3.097483	-3.584629	1.078937
95	6	0	4.435117	-4.296785	1.073373
96	1	0	2.410780	-4.012957	0.345291
97	1	0	2.618004	-3.631242	2.059578
98	1	0	4.294677	-5.351731	1.322445
99	1	0	5.113569	-3.859505	1.808574
100	1	0	4.906214	-4.237758	0.089935
101	7	0	0.646896	1.600591	0.655497

3-2-TS2-exo

Energy + zep (gas) = -2188.38345 au
Gibbs free energy (gas) = -2188.46754 au
Gibbs free energy (in solvent) = -2187.69889 au
Zero-point correction = 0.85164 au
Thermal correction to Gibbs free energy = 0.76755 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.450615	-1.370192	-1.143795
2	1	0	-2.037438	-2.097146	-1.527943
3	6	0	2.297157	-1.375604	0.696265
4	8	0	1.171616	-1.721303	1.065084
5	8	0	3.279767	-2.268024	0.499834
6	6	0	3.002634	-3.662050	0.802771
7	6	0	4.286633	-4.436344	0.593581
8	1	0	2.205751	-4.005961	0.141254
9	1	0	2.647613	-3.726342	1.833499
10	1	0	4.115994	-5.493927	0.809573
11	1	0	5.075770	-4.076207	1.256483
12	1	0	4.632030	-4.350488	-0.438526
13	6	0	1.973841	-0.062828	-1.743444
14	6	0	0.548597	-0.131599	-1.681807
15	6	0	-0.186927	-1.291639	-1.680209
16	1	0	2.505035	-0.997643	-1.886630
17	1	0	0.041504	0.802175	-1.467633
18	6	0	2.627449	1.132621	-2.251394
19	6	0	3.946040	1.367437	-2.081742
20	6	0	4.724820	0.431907	-1.211544
21	6	0	0.285644	-2.564227	-2.285474
22	6	0	0.024828	-3.802842	-1.677621
23	6	0	0.941703	-2.550735	-3.525954
24	6	0	0.421649	-4.989945	-2.284894
25	1	0	-0.465410	-3.832613	-0.711814
26	6	0	1.338652	-3.739428	-4.130632
27	1	0	1.109866	-1.605662	-4.027037
28	6	0	1.081149	-4.961494	-3.512968
29	1	0	0.220138	-5.937920	-1.799298
30	1	0	1.835337	-3.711382	-5.093294
31	1	0	1.384893	-5.886565	-3.988579
32	6	0	4.638906	2.561102	-2.668040

33	1	0	5.424190	2.238120	-3.361144
34	1	0	3.948617	3.206854	-3.213671
35	1	0	2.002893	1.863132	-2.757532
36	1	0	5.133342	3.149725	-1.889127
37	1	0	4.686004	-0.585400	-1.617107
38	1	0	5.776783	0.717985	-1.162913
39	6	0	2.684898	-0.009704	0.336366
40	6	0	4.176462	0.345710	0.269767
41	6	0	1.739796	0.949562	0.789393
42	7	0	0.898263	1.690028	1.083563
43	1	0	4.698305	-0.510851	0.693703
44	6	0	4.595186	1.551053	1.104810
45	6	0	4.129054	2.850039	0.867480
46	6	0	5.518730	1.359298	2.138688
47	6	0	4.576937	3.919710	1.639026
48	6	0	5.498790	3.713510	2.662819
49	6	0	5.968534	2.427116	2.911889
50	1	0	4.200529	4.916831	1.440646
51	1	0	3.401703	3.034414	0.087044
52	1	0	5.846137	4.547681	3.261301
53	1	0	6.685694	2.252558	3.705881
54	1	0	5.895563	0.361224	2.339143
55	1	0	-0.597307	-1.504786	1.400918
56	7	0	-1.470113	-1.277266	1.915159
57	6	0	-2.633698	-1.027671	0.955394
58	6	0	-1.151689	-0.060457	2.766222
59	6	0	-1.840648	-2.431244	2.813722
60	6	0	-2.142884	-0.349869	-0.352874
61	6	0	-3.746284	-0.334502	1.767863
62	6	0	-2.320244	0.207517	3.732611
63	6	0	-3.197317	-2.122584	3.521079
64	6	0	-3.295870	0.300989	-1.113632
65	6	0	-3.527456	-0.623049	3.268220
66	6	0	-3.449975	1.722075	-1.183576
67	6	0	-4.231818	-0.487123	-1.745648
68	6	0	-4.582678	2.209652	-1.922514
69	6	0	-5.307767	0.102202	-2.446523
70	7	0	-5.484671	1.398949	-2.536478
71	1	0	-0.949940	0.767141	2.091559
72	1	0	-0.213354	-0.285495	3.270547
73	1	0	-1.022833	-2.557172	3.522938
74	1	0	-1.893855	-3.325740	2.192696
75	1	0	-1.407859	0.407735	-0.092646
76	1	0	-4.715059	-0.694808	1.422467

77	1	0	-3.736480	0.745383	1.601680
78	1	0	-2.047686	-0.054561	4.757798
79	1	0	-2.560830	1.272075	3.725698
80	1	0	-3.044234	-2.240940	4.596872
81	1	0	-4.419668	-0.354706	3.834730
82	6	0	-2.578444	2.659495	-0.581986
83	1	0	-4.168873	-1.570832	-1.725406
84	6	0	-4.782873	3.607342	-2.023038
85	1	0	-6.038857	-0.529109	-2.944344
86	6	0	-4.979657	-3.829192	3.965190
87	1	0	-5.771413	-4.488092	3.629163
88	6	0	-4.296948	-3.070013	3.114066
89	1	0	-4.542047	-3.120971	2.054449
90	1	0	-4.775214	-3.817420	5.031407
91	1	0	-2.970661	-2.029339	0.679808
92	6	0	-3.925703	4.498074	-1.429176
93	6	0	-2.806977	4.020867	-0.698457
94	8	0	-1.911249	4.828681	-0.083605
95	6	0	-2.068341	6.244765	-0.167014
96	1	0	-1.235790	6.662312	0.395030
97	1	0	-3.009629	6.570554	0.286393
98	1	0	-5.642915	3.944814	-2.587704
99	1	0	-4.107721	5.559715	-1.524359
100	1	0	-1.697244	2.366364	-0.024678
101	1	0	-2.015836	6.592412	-1.203348

3-2-IM2-exo

Energy + zep (gas) = -2188.40936 au
Gibbs free energy (gas) = -2188.49491 au
Gibbs free energy (in solvent) = -2187.73648 au
Zero-point correction = 0.85333 au
Thermal correction to Gibbs free energy = 0.76779 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.457194	0.273104	1.502878
2	1	0	-1.985412	0.237719	2.363551
3	6	0	2.733025	0.639024	0.146135
4	8	0	1.991820	1.545382	-0.190109
5	8	0	3.607407	0.724136	1.132194
6	6	0	3.713760	2.000915	1.837478

7	6	0	4.775256	1.845887	2.903180
8	1	0	2.734675	2.230432	2.260633
9	1	0	3.967350	2.767002	1.103270
10	1	0	4.876384	2.785264	3.452294
11	1	0	5.742615	1.604555	2.459911
12	1	0	4.505050	1.062008	3.613033
13	6	0	1.722064	-1.627660	0.477534
14	6	0	0.327541	-1.053801	0.500058
15	6	0	-0.271157	-0.475852	1.563015
16	1	0	2.157206	-1.531977	1.476014
17	1	0	-0.183685	-1.069887	-0.456839
18	6	0	1.751928	-3.082645	0.054819
19	6	0	2.712469	-3.657271	-0.673812
20	6	0	3.913077	-2.883078	-1.162578
21	6	0	0.281869	-0.509353	2.951347
22	6	0	0.420504	0.672887	3.693463
23	6	0	0.623360	-1.726128	3.556611
24	6	0	0.914339	0.640979	4.994847
25	1	0	0.141588	1.619757	3.245466
26	6	0	1.113339	-1.756901	4.859445
27	1	0	0.485300	-2.651368	3.010087
28	6	0	1.264476	-0.574312	5.580469
29	1	0	1.021207	1.563561	5.553922
30	1	0	1.365976	-2.707026	5.315371
31	1	0	1.641924	-0.600332	6.595933
32	6	0	2.659821	-5.106933	-1.071659
33	1	0	3.518814	-5.654311	-0.668537
34	1	0	1.748320	-5.591361	-0.718085
35	1	0	0.903934	-3.675126	0.385929
36	1	0	2.703366	-5.211940	-2.161318
37	1	0	4.823954	-3.458967	-0.965970
38	1	0	3.859592	-2.790692	-2.254109
39	6	0	2.687363	-0.773185	-0.457664
40	6	0	4.079609	-1.496852	-0.513089
41	6	0	2.090973	-0.680860	-1.793188
42	7	0	1.605867	-0.635176	-2.837960
43	1	0	4.344780	-1.651081	0.535101
44	6	0	5.206884	-0.693823	-1.147987
45	6	0	5.198668	-0.325445	-2.499598
46	6	0	6.321171	-0.349954	-0.374111
47	6	0	6.267116	0.378474	-3.051473
48	6	0	7.368182	0.716087	-2.268350
49	6	0	7.394269	0.345263	-0.926235
50	1	0	6.241819	0.653297	-4.099799

51	1	0	4.362898	-0.589457	-3.135859
52	1	0	8.202071	1.255398	-2.702371
53	1	0	8.251377	0.591739	-0.309820
54	1	0	6.351028	-0.637755	0.671413
55	7	0	-0.756589	2.110722	-0.867419
56	6	0	-2.135788	1.891154	-0.245014
57	6	0	-0.667567	1.555468	-2.276647
58	6	0	-0.468281	3.595501	-0.892711
59	6	0	-2.309169	0.456007	0.320861
60	6	0	-3.173546	2.349860	-1.293986
61	6	0	-1.582138	2.377114	-3.205699
62	6	0	-1.605872	4.338245	-1.654554
63	6	0	-3.767018	0.218616	0.704109
64	6	0	-2.492605	3.258872	-2.336531
65	6	0	-4.538273	-0.850212	0.147160
66	6	0	-4.368369	1.038704	1.635538
67	6	0	-5.894771	-0.972615	0.606600
68	6	0	-5.711578	0.821228	2.017483
69	7	0	-6.454643	-0.141072	1.524802
70	1	0	-0.952438	0.507197	-2.229246
71	1	0	0.381608	1.586331	-2.556067
72	1	0	0.505205	3.713926	-1.366440
73	1	0	-0.381847	3.920738	0.143862
74	1	0	-2.031457	-0.262901	-0.447831
75	1	0	-3.991964	2.859147	-0.786507
76	1	0	-3.612866	1.486350	-1.801345
77	1	0	-0.987707	2.991818	-3.885391
78	1	0	-2.177723	1.702093	-3.822727
79	1	0	-1.143851	4.927788	-2.450710
80	1	0	-3.246383	3.752187	-2.950983
81	6	0	-4.062235	-1.778505	-0.804780
82	1	0	-3.828240	1.861584	2.092635
83	6	0	-6.701052	-2.013111	0.085340
84	1	0	-6.176254	1.473053	2.752412
85	6	0	-2.498241	6.590691	-1.009040
86	1	0	-3.066846	7.235697	-0.349821
87	6	0	-2.371059	5.289297	-0.770369
88	1	0	-2.847528	4.869093	0.113902
89	1	0	-2.040765	7.060131	-1.874525
90	1	0	-2.147170	2.564436	0.613261
91	1	0	-0.010038	1.664029	-0.315375
92	6	0	-6.215449	-2.901184	-0.840328
93	6	0	-4.875695	-2.785954	-1.293024
94	8	0	-4.310878	-3.618880	-2.199794

95	6	0	-5.081396	-4.692263	-2.742297
96	1	0	-5.403382	-5.386663	-1.960456
97	1	0	-4.415757	-5.208739	-3.430395
98	1	0	-6.857549	-3.685297	-1.217254
99	1	0	-3.046830	-1.752709	-1.177207
100	1	0	-7.718438	-2.080547	0.449630
101	1	0	-5.951644	-4.320606	-3.291666

3-3-COM-endo

Energy + zep (gas) = -2188.40796 au
Gibbs free energy (gas) = -2188.50338 au
Gibbs free energy (in solvent) = -2187.70960 au
Zero-point correction = 0.84823 au
Thermal correction to Gibbs free energy = 0.75281 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.400742	-1.911114	-1.106212
2	7	0	0.361090	-2.601507	-1.004609
3	6	0	1.224987	-2.147551	0.165876
4	6	0	1.129278	-2.676720	-2.300538
5	6	0	-0.239456	-3.946558	-0.684472
6	6	0	1.549623	-0.644059	0.058614
7	6	0	2.445879	-3.093189	0.249284
8	6	0	2.254022	-3.728440	-2.158836
9	6	0	0.894855	-4.991516	-0.470343
10	6	0	2.300780	-0.207762	1.319678
11	6	0	2.251348	-4.275766	-0.719259
12	6	0	1.636729	-0.168407	2.526283
13	6	0	3.684803	0.158242	1.301510
14	6	0	2.319782	0.213258	3.702998
15	6	0	4.276367	0.522003	2.559276
16	7	0	3.589941	0.541417	3.733001
17	1	0	1.498447	-1.677410	-2.519482
18	1	0	0.402742	-2.935300	-3.070941
19	1	0	-0.901425	-4.204747	-1.509980
20	1	0	-0.853689	-3.813125	0.205284
21	1	0	2.188273	-0.478802	-0.807889
22	1	0	2.576089	-3.437105	1.275345
23	1	0	3.359827	-2.557325	-0.016396
24	1	0	2.105184	-4.540667	-2.873577

25	1	0	3.220333	-3.274034	-2.385737
26	1	0	0.793611	-5.768699	-1.232917
27	1	0	3.061734	-4.994746	-0.592549
28	1	0	0.582315	-0.414833	2.597189
29	6	0	4.497264	0.183356	0.144685
30	1	0	1.786647	0.240055	4.650038
31	6	0	5.645545	0.880336	2.593423
32	7	0	0.297505	0.086335	-0.201468
33	1	0	-0.334657	0.039461	0.594264
34	6	0	6.414203	0.889909	1.456973
35	6	0	5.832289	0.539526	0.212139
36	1	0	6.062726	1.148390	3.556038
37	1	0	7.456819	1.169965	1.518631
38	8	0	6.511387	0.529439	-0.963490
39	1	0	4.106823	-0.048690	-0.836870
40	6	0	7.888260	0.903793	-0.977563
41	1	0	8.201283	0.825198	-2.016628
42	1	0	8.026084	1.934326	-0.635895
43	1	0	8.493496	0.227008	-0.366356
44	6	0	0.698045	-6.970248	1.058767
45	1	0	0.638143	-7.403413	2.050085
46	6	0	0.796291	-5.657206	0.877883
47	1	0	0.806954	-5.002877	1.748176
48	1	0	0.676095	-7.662152	0.222296
49	1	0	0.575971	-2.284210	1.033630
50	6	0	0.398196	1.417029	-0.695958
51	6	0	-6.244720	-0.483636	-0.432826
52	6	0	-5.952686	-0.972145	-1.723679
53	6	0	-7.578395	-0.131843	-0.134681
54	6	0	-6.960152	-1.101997	-2.666821
55	6	0	-8.275401	-0.753170	-2.350605
56	6	0	-8.583439	-0.267552	-1.081126
57	6	0	-3.140165	-0.267599	1.925012
58	8	0	-1.936665	-0.447411	1.987455
59	6	0	-3.941579	-0.574591	0.702849
60	6	0	-5.274989	-0.301626	0.625854
61	6	0	-3.165296	-1.171615	-0.329335
62	8	0	-3.875708	0.216034	2.921568
63	6	0	-3.183909	0.557125	4.162507
64	6	0	-4.221357	1.082122	5.129852
65	7	0	-2.482368	-1.664172	-1.121767
66	6	0	-0.302774	3.807829	-0.483456
67	6	0	-0.145411	2.451809	-0.012170
68	6	0	-0.824325	4.800880	0.265780

69	6	0	-1.001095	6.201868	-0.140533
70	6	0	-0.224156	6.800959	-1.054060
71	6	0	-2.110236	6.949544	0.563613
72	1	0	-4.942325	-1.243790	-1.994548
73	1	0	-7.816419	0.249342	0.852255
74	1	0	-6.723670	-1.474443	-3.656304
75	1	0	-9.056128	-0.857904	-3.094901
76	1	0	-9.601752	0.006231	-0.833524
77	1	0	-5.680087	0.135202	1.532426
78	1	0	-2.689708	-0.343190	4.531765
79	1	0	-2.418571	1.299913	3.931021
80	1	0	-3.737221	1.346077	6.073056
81	1	0	-4.709474	1.975552	4.735815
82	1	0	-4.982818	0.327772	5.336899
83	1	0	0.003834	4.022570	-1.502318
84	1	0	-0.537606	2.240340	0.980698
85	1	0	-1.176270	4.554867	1.267470
86	1	0	0.607123	6.289266	-1.524809
87	1	0	-0.391036	7.831418	-1.345118
88	1	0	-1.948355	6.952434	1.647385
89	1	0	-3.080674	6.473382	0.387043
90	1	0	-2.171429	7.985607	0.228321
91	6	0	1.045394	1.552299	-2.029734
92	6	0	0.528202	0.863585	-3.137932
93	6	0	2.169675	2.368034	-2.211055
94	6	0	1.114031	0.996961	-4.393927
95	6	0	2.760838	2.493223	-3.467086
96	6	0	2.235576	1.809565	-4.560863
97	1	0	-0.362443	0.257267	-3.012922
98	1	0	2.582786	2.897558	-1.360582
99	1	0	0.687206	0.481136	-5.247088
100	1	0	3.633181	3.124776	-3.589240
101	1	0	2.691166	1.914083	-5.538699

3-3-TS1-endo

Energy + zep (gas) = -2188.37099 au
Gibbs free energy (gas) = -2188.45732 au
Gibbs free energy (in solvent) = -2187.67487 au
Zero-point correction = 0.84884 au
Thermal correction to Gibbs free energy = 0.76251 au

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	0.161989	1.175641	-0.406348
2	7	0	-0.589615	1.550563	-1.015024
3	6	0	-1.909908	1.682779	-0.261283
4	6	0	-0.731502	0.700441	-2.261015
5	6	0	-0.094363	2.933853	-1.397255
6	6	0	-2.353637	0.384651	0.476060
7	6	0	-2.967677	2.198596	-1.272719
8	6	0	-1.668133	1.420651	-3.256418
9	6	0	-1.144582	3.665416	-2.275256
10	6	0	-3.703508	0.633928	1.152023
11	6	0	-2.282392	2.654777	-2.572640
12	6	0	-3.806780	1.589489	2.139192
13	6	0	-4.876539	-0.110518	0.810292
14	6	0	-5.040543	1.816512	2.790311
15	6	0	-6.076595	0.207965	1.534155
16	7	0	-6.138385	1.158468	2.503829
17	1	0	-1.115170	-0.268178	-1.948293
18	1	0	0.274964	0.538151	-2.643127
19	1	0	0.853644	2.779864	-1.909444
20	1	0	0.117745	3.453225	-0.464322
21	1	0	-2.458912	-0.414258	-0.252953
22	1	0	-3.540833	3.005861	-0.817666
23	1	0	-3.682962	1.406152	-1.506757
24	1	0	-1.113877	1.718932	-4.148968
25	1	0	-2.457277	0.739717	-3.581850
26	1	0	-0.675113	3.915867	-3.230258
27	1	0	-3.016636	3.122958	-3.229568
28	1	0	-2.952835	2.187582	2.442982
29	6	0	-4.932715	-1.119909	-0.176555
30	1	0	-5.109088	2.570896	3.569451
31	6	0	-7.265434	-0.498906	1.231532
32	7	0	-1.375959	-0.063376	1.465738
33	1	0	-1.213868	0.587421	2.222722
34	6	0	-7.294021	-1.475464	0.268598
35	6	0	-6.110959	-1.794099	-0.446305
36	1	0	-8.153347	-0.236868	1.793035
37	1	0	-8.218663	-1.997075	0.063171
38	8	0	-6.042654	-2.747553	-1.407440
39	1	0	-4.062273	-1.420633	-0.743804
40	6	0	-7.217944	-3.484128	-1.749180
41	1	0	-6.911602	-4.172919	-2.533492
42	1	0	-7.594632	-4.053936	-0.894359

43	1	0	-8.003570	-2.826296	-2.132841
44	6	0	-1.550478	6.140369	-2.234504
45	1	0	-1.911804	7.037096	-1.745358
46	6	0	-1.618014	4.950436	-1.646278
47	1	0	-2.039149	4.881011	-0.644436
48	1	0	-1.132132	6.262229	-3.228933
49	1	0	-1.705005	2.443757	0.494886
50	6	0	-0.384239	-1.001283	1.286929
51	6	0	6.004423	-0.592782	-0.849855
52	6	0	5.721217	-1.385462	-1.971990
53	6	0	7.321074	-0.141893	-0.667054
54	6	0	6.721182	-1.696625	-2.887239
55	6	0	8.021070	-1.228742	-2.701682
56	6	0	8.318352	-0.448860	-1.586691
57	6	0	2.968718	1.216023	0.695369
58	8	0	1.808220	1.600618	0.496438
59	6	0	3.683227	0.265474	-0.131565
60	6	0	4.996523	-0.206518	0.175027
61	6	0	2.983940	-0.098516	-1.299744
62	8	0	3.701045	1.697998	1.721817
63	6	0	3.097357	2.712224	2.557934
64	6	0	4.160330	3.206534	3.517421
65	7	0	2.366976	-0.371408	-2.245697
66	6	0	1.962035	-1.599641	1.914852
67	6	0	0.749998	-0.894371	2.060001
68	6	0	3.052209	-1.359987	2.731527
69	6	0	4.395933	-1.679696	2.446283
70	6	0	4.830762	-2.017046	1.157316
71	6	0	5.423230	-1.472382	3.529426
72	1	0	4.721861	-1.765195	-2.137773
73	1	0	7.560535	0.466303	0.199031
74	1	0	6.484041	-2.309198	-3.749399
75	1	0	8.796107	-1.474200	-3.418198
76	1	0	9.325775	-0.080587	-1.431371
77	1	0	5.440300	0.350958	0.989536
78	1	0	2.721192	3.515072	1.920728
79	1	0	2.245945	2.275021	3.087027
80	1	0	3.742570	3.981642	4.164664
81	1	0	4.529188	2.396546	4.149996
82	1	0	5.005280	3.633610	2.973957
83	1	0	2.050549	-2.316604	1.106721
84	1	0	0.763216	-0.076703	2.777258
85	1	0	2.871757	-0.790556	3.640376
86	1	0	4.129470	-2.433413	0.444452

87	1	0	5.844427	-2.384043	1.049679
88	1	0	6.415070	-1.277561	3.117626
89	1	0	5.499081	-2.376711	4.144093
90	1	0	5.150774	-0.651870	4.197183
91	6	0	-0.683984	-2.143065	0.376670
92	6	0	0.102263	-2.472245	-0.734116
93	6	0	-1.791898	-2.948193	0.689844
94	6	0	-0.213632	-3.585831	-1.511280
95	6	0	-2.096307	-4.062073	-0.085048
96	6	0	-1.307685	-4.384202	-1.188627
97	1	0	0.942782	-1.853070	-1.018987
98	1	0	-2.400237	-2.708453	1.554010
99	1	0	0.399593	-3.821942	-2.373075
100	1	0	-2.949197	-4.677803	0.174481
101	1	0	-1.545918	-5.251732	-1.792708

3-3-IM1-endo

Energy + zep (gas) = -2188.38620 au
Gibbs free energy (gas) = -2188.47252 au
Gibbs free energy (in solvent) = -2187.70176 au
Zero-point correction = 0.85106 au
Thermal correction to Gibbs free energy = 0.76474 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.526023	1.686321	-0.206932
2	7	0	-0.294493	2.215896	-0.605793
3	6	0	-1.553925	1.900106	0.196811
4	6	0	-0.471043	1.941064	-2.079319
5	6	0	0.056821	3.672908	-0.396154
6	6	0	-1.800532	0.383059	0.391615
7	6	0	-2.735117	2.650466	-0.467385
8	6	0	-1.542750	2.899310	-2.645837
9	6	0	-1.118777	4.586648	-0.841277
10	6	0	-3.090258	0.164409	1.184687
11	6	0	-2.195214	3.671414	-1.484475
12	6	0	-3.117266	0.450806	2.531310
13	6	0	-4.286642	-0.318519	0.567346
14	6	0	-4.308455	0.277864	3.270867
15	6	0	-5.437233	-0.453566	1.417597
16	7	0	-5.429931	-0.153585	2.742702

17	1	0	-0.721870	0.889843	-2.189733
18	1	0	0.508350	2.064495	-2.537519
19	1	0	0.964804	3.853106	-0.971046
20	1	0	0.306909	3.782697	0.658116
21	1	0	-1.885651	-0.096926	-0.578695
22	1	0	-3.336818	3.132415	0.303087
23	1	0	-3.395337	1.949849	-0.982332
24	1	0	-1.092761	3.596538	-3.356036
25	1	0	-2.297870	2.330494	-3.191981
26	1	0	-0.753570	5.256592	-1.624202
27	1	0	-3.015331	4.287715	-1.854743
28	1	0	-2.228987	0.798795	3.047270
29	6	0	-4.410951	-0.667470	-0.795657
30	1	0	-4.322811	0.507415	4.332831
31	6	0	-6.649074	-0.925377	0.856569
32	7	0	-0.635074	-0.185278	1.092914
33	1	0	0.044266	0.483015	1.470737
34	6	0	-6.745192	-1.253883	-0.471469
35	6	0	-5.609536	-1.126857	-1.312663
36	1	0	-7.499020	-1.016566	1.521120
37	1	0	-7.685748	-1.611815	-0.866916
38	8	0	-5.608094	-1.434580	-2.632171
39	1	0	-3.577612	-0.611587	-1.483031
40	6	0	-6.806590	-1.918134	-3.241621
41	1	0	-6.552576	-2.091155	-4.285118
42	1	0	-7.133014	-2.858648	-2.787875
43	1	0	-7.610371	-1.178130	-3.183289
44	6	0	-1.723070	6.767265	0.241169
45	1	0	-2.110315	7.339809	1.075514
46	6	0	-1.636793	5.441715	0.286518
47	1	0	-1.955666	4.924633	1.190399
48	1	0	-1.409914	7.330233	-0.632792
49	1	0	-1.353438	2.323885	1.184182
50	6	0	-0.230295	-1.445690	1.192296
51	6	0	5.288374	-0.487985	-1.493377
52	6	0	4.927449	-1.239294	-2.617519
53	6	0	6.295077	0.473081	-1.632901
54	6	0	5.555259	-1.032939	-3.843983
55	6	0	6.556409	-0.072555	-3.968970
56	6	0	6.924707	0.681716	-2.857625
57	6	0	2.838992	0.851132	0.942934
58	8	0	1.693310	1.403402	1.031050
59	6	0	3.239580	-0.049911	-0.055030
60	6	0	4.620405	-0.679937	-0.135056

61	6	0	2.264056	-0.320211	-1.022533
62	8	0	3.768832	1.119903	1.891413
63	6	0	3.460449	2.123263	2.881992
64	6	0	4.662102	2.240779	3.797853
65	7	0	1.411941	-0.526604	-1.791509
66	6	0	1.982839	-2.347321	1.649536
67	6	0	0.878234	-1.668571	2.076156
68	6	0	3.228470	-2.377446	2.360603
69	6	0	4.447596	-2.372883	1.764132
70	6	0	4.632832	-2.207812	0.284715
71	6	0	5.700042	-2.377316	2.590424
72	1	0	4.148232	-1.989582	-2.546507
73	1	0	6.590583	1.063800	-0.771505
74	1	0	5.262470	-1.626445	-4.702844
75	1	0	7.047883	0.083220	-4.922398
76	1	0	7.706722	1.428146	-2.941139
77	1	0	5.233018	-0.148600	0.593256
78	1	0	3.246698	3.069177	2.377586
79	1	0	2.563801	1.826995	3.432039
80	1	0	4.472389	2.996121	4.564653
81	1	0	4.867775	1.291403	4.296765
82	1	0	5.551577	2.537072	3.238341
83	1	0	1.937143	-2.826144	0.676180
84	1	0	0.956378	-1.026335	2.948482
85	1	0	3.178375	-2.292640	3.443285
86	1	0	3.860967	-2.732071	-0.284198
87	1	0	5.596926	-2.627156	-0.012439
88	1	0	5.491516	-2.378860	3.660940
89	1	0	6.324263	-1.508437	2.356387
90	1	0	6.300778	-3.262682	2.353348
91	6	0	-0.852626	-2.561913	0.458537
92	6	0	-1.018674	-2.550470	-0.936222
93	6	0	-1.249942	-3.691209	1.193851
94	6	0	-1.588712	-3.646422	-1.572717
95	6	0	-1.848204	-4.768710	0.550931
96	6	0	-2.018075	-4.747546	-0.831798
97	1	0	-0.608450	-1.735157	-1.518893
98	1	0	-1.105638	-3.709590	2.266948
99	1	0	-1.684601	-3.647246	-2.651897
100	1	0	-2.169680	-5.627773	1.127244
101	1	0	-2.468760	-5.595385	-1.334369

3-3-TS2-endo

Energy + zep (gas) = -2188.37723 au
Gibbs free energy (gas) = -2188.46213 au
Gibbs free energy (in solvent) = -2187.69112 au
Zero-point correction = 0.85120 au
Thermal correction to Gibbs free energy = 0.76631 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.268079	1.215423	-0.196028
2	7	0	-0.482689	1.696681	-0.724293
3	6	0	-1.793919	1.699166	0.057673
4	6	0	-0.634020	1.071086	-2.094484
5	6	0	0.010940	3.123822	-0.867991
6	6	0	-2.236012	0.289965	0.554827
7	6	0	-2.858704	2.398315	-0.827772
8	6	0	-1.603168	1.930027	-2.936226
9	6	0	-1.033454	3.986489	-1.628133
10	6	0	-3.540299	0.439961	1.339629
11	6	0	-2.190666	3.045592	-2.053397
12	6	0	-3.544539	1.134961	2.528995
13	6	0	-4.774636	-0.122759	0.884485
14	6	0	-4.739262	1.280109	3.269866
15	6	0	-5.928809	0.099078	1.711375
16	7	0	-5.892263	0.789950	2.881428
17	1	0	-0.991402	0.054278	-1.949794
18	1	0	0.367462	0.998894	-2.514786
19	1	0	0.966815	3.061822	-1.385422
20	1	0	0.206111	3.485990	0.140335
21	1	0	-2.407278	-0.348576	-0.307265
22	1	0	-3.401035	3.134374	-0.234541
23	1	0	-3.598610	1.670696	-1.169168
24	1	0	-1.079344	2.361659	-3.791709
25	1	0	-2.404546	1.304182	-3.334051
26	1	0	-0.566783	4.359575	-2.543765
27	1	0	-2.930422	3.618295	-2.614266
28	1	0	-2.639972	1.584152	2.927474
29	6	0	-4.931972	-0.865213	-0.307401
30	1	0	-4.729124	1.825644	4.209659
31	6	0	-7.177337	-0.424545	1.297075
32	7	0	-1.216834	-0.367710	1.371282
33	1	0	-0.944086	0.149896	2.196174
34	6	0	-7.305504	-1.135988	0.131326

35	6	0	-6.166850	-1.364221	-0.683445
36	1	0	-8.029039	-0.240195	1.939702
37	1	0	-8.273849	-1.522009	-0.155906
38	8	0	-6.196956	-2.063577	-1.844220
39	1	0	-4.099126	-1.090807	-0.959646
40	6	0	-7.434097	-2.614246	-2.298534
41	1	0	-7.201086	-3.122058	-3.231937
42	1	0	-7.835289	-3.338374	-1.583048
43	1	0	-8.173883	-1.830686	-2.488534
44	6	0	-1.403201	6.437726	-1.244452
45	1	0	-1.744250	7.263339	-0.631259
46	6	0	-1.477424	5.179770	-0.821767
47	1	0	-1.881640	4.980809	0.169710
48	1	0	-0.999914	6.689725	-2.220498
49	1	0	-1.572888	2.307841	0.937241
50	6	0	-0.246686	-1.233908	0.892999
51	6	0	5.803887	-0.379167	-0.829116
52	6	0	5.843300	-1.034700	-2.064108
53	6	0	6.639071	0.725906	-0.632801
54	6	0	6.696229	-0.595936	-3.074235
55	6	0	7.522655	0.505736	-2.867100
56	6	0	7.491686	1.166879	-1.641584
57	6	0	2.973767	0.810402	0.972377
58	8	0	1.921730	1.419268	0.758943
59	6	0	3.455306	-0.314425	0.170971
60	6	0	4.889087	-0.829635	0.306913
61	6	0	2.872659	-0.323654	-1.121900
62	8	0	3.744078	1.084406	2.034948
63	6	0	3.329255	2.170418	2.905639
64	6	0	4.377465	2.312373	3.988633
65	7	0	2.358484	-0.343194	-2.160969
66	6	0	2.174671	-1.906415	1.158639
67	6	0	0.964975	-1.254570	1.535623
68	6	0	3.110095	-2.363295	2.168069
69	6	0	4.387726	-2.696905	1.886060
70	6	0	4.935138	-2.386961	0.527094
71	6	0	5.334981	-3.206866	2.929843
72	1	0	5.207490	-1.892766	-2.249133
73	1	0	6.625188	1.241695	0.321969
74	1	0	6.715729	-1.118377	-4.023827
75	1	0	8.188662	0.843109	-3.652705
76	1	0	8.136133	2.021071	-1.467392
77	1	0	5.278911	-0.382678	1.220257
78	1	0	3.233359	3.077067	2.304804

79	1	0	2.346148	1.931796	3.317824
80	1	0	4.094803	3.119121	4.669242
81	1	0	4.470015	1.391723	4.568059
82	1	0	5.352309	2.553461	3.560670
83	1	0	2.168631	-2.455318	0.223679
84	1	0	1.042791	-0.609468	2.409147
85	1	0	2.753494	-2.402464	3.193693
86	1	0	4.367526	-2.882579	-0.266978
87	1	0	5.970545	-2.718678	0.437119
88	1	0	4.856997	-3.303908	3.905808
89	1	0	6.200866	-2.542039	3.028778
90	1	0	5.729874	-4.187071	2.640730
91	6	0	-0.704863	-2.229746	-0.122573
92	6	0	-0.070071	-2.469798	-1.347458
93	6	0	-1.819600	-3.013779	0.225592
94	6	0	-0.535732	-3.473697	-2.196118
95	6	0	-2.274084	-4.016940	-0.622421
96	6	0	-1.632856	-4.251279	-1.837777
97	1	0	0.771749	-1.866995	-1.659137
98	1	0	-2.313806	-2.845499	1.174946
99	1	0	-0.034969	-3.641201	-3.142608
100	1	0	-3.127812	-4.617192	-0.330992
101	1	0	-1.988012	-5.032386	-2.499583

3-3-IM2-endo

Energy + zep (gas) = -2188.39366 au
Gibbs free energy (gas) = -2188.48082 au
Gibbs free energy (in solvent) = -2187.72214 au
Zero-point correction = 0.85303 au
Thermal correction to Gibbs free energy = 0.76587 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.051268	0.881420	-0.576797
2	7	0	-0.612511	1.474498	-1.091560
3	6	0	-1.865157	1.687596	-0.235839
4	6	0	-0.926012	0.814380	-2.419059
5	6	0	0.061116	2.811530	-1.336378
6	6	0	-2.367043	0.378056	0.440148
7	6	0	-2.904628	2.401793	-1.131617
8	6	0	-1.772242	1.786251	-3.268676

9	6	0	-0.948375	3.788202	-2.003555
10	6	0	-3.670887	0.665929	1.180519
11	6	0	-2.211637	2.968009	-2.385913
12	6	0	-3.692367	1.603035	2.190133
13	6	0	-4.887001	-0.024975	0.878673
14	6	0	-4.887488	1.867025	2.897564
15	6	0	-6.042148	0.330017	1.655820
16	7	0	-6.023972	1.263458	2.644485
17	1	0	-1.442458	-0.118194	-2.201529
18	1	0	0.035619	0.570475	-2.866546
19	1	0	0.926117	2.603553	-1.964023
20	1	0	0.429251	3.162135	-0.373089
21	1	0	-2.554274	-0.361166	-0.336960
22	1	0	-3.397173	3.186234	-0.557952
23	1	0	-3.686642	1.700817	-1.436008
24	1	0	-1.195922	2.144965	-4.124366
25	1	0	-2.645848	1.264824	-3.664560
26	1	0	-0.501818	4.147871	-2.934259
27	1	0	-2.903093	3.610022	-2.932814
28	1	0	-2.801242	2.157680	2.467953
29	6	0	-5.023872	-1.017407	-0.117417
30	1	0	-4.891133	2.606456	3.694032
31	6	0	-7.271071	-0.320350	1.389871
32	7	0	-1.404312	-0.220248	1.370802
33	1	0	-1.219245	0.367824	2.173374
34	6	0	-7.379324	-1.278033	0.413521
35	6	0	-6.239596	-1.635491	-0.351435
36	1	0	-8.124151	-0.031302	1.990791
37	1	0	-8.333138	-1.755793	0.236704
38	8	0	-6.250867	-2.574189	-1.330198
39	1	0	-4.187660	-1.348422	-0.718481
40	6	0	-7.466882	-3.260638	-1.627708
41	1	0	-7.222997	-3.948347	-2.434652
42	1	0	-7.826164	-3.829286	-0.764556
43	1	0	-8.244003	-2.568347	-1.965790
44	6	0	-1.077684	6.249017	-1.536363
45	1	0	-1.311957	7.082485	-0.884900
46	6	0	-1.243135	4.990193	-1.143420
47	1	0	-1.615741	4.797434	-0.138780
48	1	0	-0.702355	6.493790	-2.525327
49	1	0	-1.523342	2.360039	0.553646
50	6	0	-0.254373	-0.900481	0.900820
51	6	0	5.516618	-0.811804	-0.937974
52	6	0	5.263003	-1.750733	-1.944413

53	6	0	6.460149	0.190716	-1.188144
54	6	0	5.931132	-1.685988	-3.164092
55	6	0	6.865425	-0.680087	-3.400498
56	6	0	7.128524	0.260084	-2.408006
57	6	0	3.335564	1.196418	1.121554
58	8	0	2.510466	2.042815	0.855270
59	6	0	3.373256	-0.187986	0.418238
60	6	0	4.817237	-0.853356	0.412874
61	6	0	2.849770	0.054863	-0.928803
62	8	0	4.252628	1.324842	2.071989
63	6	0	4.247985	2.573501	2.834597
64	6	0	5.405390	2.517995	3.806221
65	7	0	2.341313	0.238123	-1.947827
66	6	0	2.297643	-1.155053	1.146459
67	6	0	0.962939	-0.493073	1.326796
68	6	0	2.898580	-1.682279	2.429189
69	6	0	4.103069	-2.256930	2.389495
70	6	0	4.803938	-2.267378	1.051017
71	6	0	4.790314	-2.862599	3.576963
72	1	0	4.541567	-2.544252	-1.784299
73	1	0	6.681652	0.920028	-0.415308
74	1	0	5.724383	-2.425120	-3.929557
75	1	0	7.388186	-0.633562	-4.348660
76	1	0	7.859598	1.042019	-2.578526
77	1	0	5.405694	-0.236568	1.087905
78	1	0	4.332092	3.400149	2.127541
79	1	0	3.284213	2.654121	3.340858
80	1	0	5.424203	3.434809	4.400348
81	1	0	5.306645	1.670822	4.487438
82	1	0	6.358121	2.434669	3.279821
83	1	0	2.188450	-1.992699	0.452055
84	1	0	0.971446	0.397054	1.951216
85	1	0	2.320422	-1.608346	3.343856
86	1	0	4.311632	-2.984430	0.382854
87	1	0	5.839465	-2.600361	1.147497
88	1	0	4.177993	-2.793088	4.477761
89	1	0	5.747843	-2.365860	3.769653
90	1	0	5.016440	-3.919478	3.397789
91	6	0	-0.553730	-2.112459	0.080538
92	6	0	0.125325	-2.425520	-1.105616
93	6	0	-1.558756	-2.985159	0.529185
94	6	0	-0.182388	-3.586489	-1.813098
95	6	0	-1.857610	-4.145913	-0.176087
96	6	0	-1.169880	-4.451594	-1.349522

97	1	0	0.882319	-1.757030	-1.494215
98	1	0	-2.093423	-2.747906	1.440370
99	1	0	0.349149	-3.809901	-2.731011
100	1	0	-2.628348	-4.812796	0.192150
101	1	0	-1.405214	-5.355012	-1.899820

3-4-COM-exo

Energy + zep (gas) = -2188.40893 au
Gibbs free energy (gas) = -2188.50388 au
Gibbs free energy (in solvent) = -2187.71159 au
Zero-point correction = 0.84837 au
Thermal correction to Gibbs free energy = 0.75342 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.603307	-1.720429	0.851146
2	7	0	-0.078758	-2.487769	0.738188
3	6	0	-0.998763	-2.140144	-0.425705
4	6	0	-0.827205	-2.651806	2.038219
5	6	0	0.668583	-3.756511	0.409649
6	6	0	-1.482857	-0.679454	-0.334658
7	6	0	-2.116574	-3.206799	-0.479312
8	6	0	-1.797862	-3.847665	1.914035
9	6	0	-0.340964	-4.920586	0.181474
10	6	0	-2.281460	-0.341893	-1.596045
11	6	0	-1.765793	-4.370973	0.466478
12	6	0	-1.642421	-0.314064	-2.816510
13	6	0	-3.682641	-0.050868	-1.565566
14	6	0	-2.361885	-0.009878	-3.993946
15	6	0	-4.312891	0.236217	-2.824490
16	7	0	-3.647714	0.251605	-4.010323
17	1	0	-1.332676	-1.710757	2.242948
18	1	0	-0.069660	-2.792714	2.808449
19	1	0	1.347587	-3.945791	1.240041
20	1	0	1.265273	-3.546089	-0.476853
21	1	0	-2.128847	-0.572007	0.535146
22	1	0	-2.244948	-3.552007	-1.505143
23	1	0	-3.072571	-2.773074	-0.175803
24	1	0	-1.515689	-4.641234	2.609465
25	1	0	-2.809740	-3.534200	2.178096
26	1	0	-0.140963	-5.698329	0.923683

27	1	0	-2.489396	-5.178059	0.345209
28	1	0	-0.579828	-0.520713	-2.900708
29	6	0	-4.476468	-0.031381	-0.396053
30	1	0	-1.846101	0.010263	-4.950472
31	6	0	-5.700042	0.518298	-2.846401
32	6	0	-6.449764	0.524602	-1.697374
33	6	0	-5.830033	0.248624	-0.452033
34	1	0	-6.146526	0.729770	-3.809951
35	1	0	-7.507152	0.744659	-1.749972
36	8	0	-6.489441	0.240566	0.734817
37	1	0	-4.058286	-0.210605	0.585125
38	6	0	-7.884629	0.538369	0.759953
39	1	0	-8.176823	0.478693	1.806331
40	1	0	-8.085143	1.547215	0.386033
41	1	0	-8.460472	-0.191687	0.182598
42	6	0	0.046249	-6.830399	-1.396958
43	1	0	0.139235	-7.232135	-2.398912
44	6	0	-0.189227	-5.539774	-1.183798
45	1	0	-0.280524	-4.871025	-2.037878
46	1	0	0.153512	-7.534635	-0.577453
47	1	0	-0.348440	-2.222022	-1.298095
48	7	0	-0.316443	0.191902	-0.096942
49	1	0	0.296122	0.202756	-0.906571
50	6	0	-0.554071	1.516278	0.369782
51	6	0	-0.074886	3.958357	0.098954
52	6	0	-0.112021	2.582797	-0.339252
53	6	0	0.339376	4.977407	-0.681939
54	6	0	0.424467	6.391927	-0.292664
55	6	0	0.659120	6.786913	0.966799
56	6	0	0.255820	7.388783	-1.416067
57	1	0	-0.406461	4.172966	1.109925
58	1	0	0.298562	2.386515	-1.328338
59	1	0	0.609287	4.755621	-1.714060
60	1	0	0.835126	6.077034	1.766676
61	1	0	0.697448	7.837948	1.228513
62	1	0	1.011973	7.229595	-2.192964
63	1	0	0.348495	8.415012	-1.058428
64	1	0	-0.721661	7.278177	-1.896918
65	6	0	-1.210682	1.612563	1.700588
66	6	0	-0.678594	0.928675	2.805345
67	6	0	-2.364465	2.386506	1.883886
68	6	0	-1.279405	1.025805	4.057581
69	6	0	-2.967213	2.477994	3.136831
70	6	0	-2.427791	1.799231	4.226700

71	1	0	0.228827	0.348345	2.678880
72	1	0	-2.793039	2.908198	1.036579
73	1	0	-0.845889	0.509355	4.907249
74	1	0	-3.861604	3.077783	3.258938
75	1	0	-2.895088	1.874863	5.201644
76	6	0	3.463154	-0.870968	1.589696
77	8	0	2.352023	-1.331641	1.805215
78	6	0	3.993445	-0.638292	0.216935
79	6	0	5.255420	-0.165550	0.003205
80	6	0	3.056182	-0.958939	-0.804729
81	8	0	4.319407	-0.532759	2.546477
82	6	0	5.989309	0.129474	-1.207387
83	6	0	7.311442	0.596745	-1.044901
84	6	0	5.484904	-0.014794	-2.517511
85	6	0	8.101289	0.906221	-2.142106
86	6	0	7.585072	0.757110	-3.428172
87	6	0	6.278318	0.297509	-3.610134
88	6	0	3.894551	-0.713068	3.932311
89	6	0	5.048918	-0.298210	4.817143
90	7	0	2.247483	-1.229688	-1.586694
91	1	0	5.809605	0.020416	0.917018
92	1	0	7.711512	0.713646	-0.043744
93	1	0	4.477703	-0.368786	-2.684938
94	1	0	9.113839	1.262811	-1.998086
95	1	0	8.197574	0.998253	-4.289094
96	1	0	5.880632	0.183522	-4.611372
97	1	0	3.007276	-0.098522	4.094732
98	1	0	3.620910	-1.760657	4.069733
99	1	0	4.763711	-0.416755	5.865156
100	1	0	5.928764	-0.917105	4.631362
101	1	0	5.313283	0.747922	4.652281

3-4-TS1-exo

Energy + zep (gas) = -2188.37054 au
Gibbs free energy (gas) = -2188.45601 au
Gibbs free energy (in solvent) = -2187.67389 au
Zero-point correction = 0.84873 au
Thermal correction to Gibbs free energy = 0.76326 au

Standard orientation:

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

1	1	0	-0.034807	1.139862	1.068967
2	7	0	0.768743	1.777775	1.237221
3	6	0	1.763536	1.778415	0.078700
4	6	0	1.415983	1.346291	2.533854
5	6	0	0.204203	3.174607	1.386128
6	6	0	1.975546	0.363862	-0.515930
7	6	0	3.024400	2.529658	0.557688
8	6	0	2.431713	2.419970	2.976358
9	6	0	1.367481	4.193931	1.568375
10	6	0	3.063711	0.406468	-1.592842
11	6	0	2.670849	3.377734	1.795700
12	6	0	2.786746	0.945472	-2.828692
13	6	0	4.383122	-0.092075	-1.352041
14	6	0	3.793090	1.010348	-3.818966
15	6	0	5.324247	0.027224	-2.430445
16	7	0	5.017516	0.575447	-3.635961
17	1	0	1.886147	0.381397	2.350879
18	1	0	0.603188	1.190397	3.240352
19	1	0	-0.464446	3.145923	2.246078
20	1	0	-0.398664	3.363168	0.497936
21	1	0	2.276550	-0.333379	0.262930
22	1	0	3.403556	3.146764	-0.256575
23	1	0	3.821613	1.828264	0.814192
24	1	0	2.058659	2.970134	3.843369
25	1	0	3.365957	1.941513	3.276451
26	1	0	1.177840	4.759632	2.484490
27	1	0	3.487941	4.063142	2.022711
28	1	0	1.797153	1.316086	-3.072410
29	6	0	4.814162	-0.687276	-0.144672
30	1	0	3.565265	1.438690	-4.791293
31	6	0	6.644320	-0.448587	-2.241114
32	6	0	7.039690	-1.017826	-1.057238
33	6	0	6.111575	-1.143060	0.007982
34	1	0	7.331091	-0.345075	-3.071825
35	1	0	8.055680	-1.370819	-0.946532
36	8	0	6.410233	-1.697359	1.209501
37	1	0	4.149375	-0.830892	0.696934
38	6	0	7.720975	-2.218781	1.432476
39	1	0	7.708168	-2.615564	2.445398
40	1	0	7.953870	-3.025641	0.731164
41	1	0	8.480683	-1.434357	1.361660
42	6	0	1.427089	6.501857	0.592149
43	1	0	1.500534	7.176355	-0.252517
44	6	0	1.456017	5.182598	0.433810

45	1	0	1.546901	4.776303	-0.572031
46	1	0	1.327267	6.957586	1.572605
47	1	0	1.265505	2.368019	-0.694571
48	7	0	0.678898	-0.065497	-1.025859
49	1	0	0.126391	0.648901	-1.489442
50	6	0	0.086465	-1.291955	-1.041307
51	6	0	-2.187698	-2.123986	-1.446555
52	6	0	-1.034123	-1.429600	-1.850524
53	6	0	-3.398882	-2.026860	-2.113609
54	6	0	-4.673536	-2.194845	-1.533097
55	6	0	-4.874625	-2.196374	-0.148562
56	6	0	-5.877757	-2.198850	-2.438482
57	1	0	-2.147273	-2.668538	-0.507352
58	1	0	-1.161217	-0.693714	-2.639517
59	1	0	-3.374078	-1.669470	-3.140311
60	1	0	-4.066294	-2.452659	0.523173
61	1	0	-5.866445	-2.437929	0.219286
62	1	0	-6.732366	-1.700860	-1.977337
63	1	0	-6.173516	-3.234375	-2.644200
64	1	0	-5.669699	-1.721535	-3.397624
65	6	0	0.589619	-2.395177	-0.187905
66	6	0	0.740545	-2.272634	1.202151
67	6	0	0.911109	-3.614963	-0.800107
68	6	0	1.214564	-3.342950	1.954627
69	6	0	1.396239	-4.678926	-0.044419
70	6	0	1.552795	-4.544686	1.332531
71	1	0	0.413945	-1.366651	1.696092
72	1	0	0.792039	-3.716507	-1.871714
73	1	0	1.308620	-3.245734	3.030390
74	1	0	1.649921	-5.612248	-0.532824
75	1	0	1.926389	-5.374518	1.920874
76	6	0	-2.583631	-0.174962	1.688734
77	8	0	-1.409968	0.169581	1.896157
78	6	0	-3.374745	0.214843	0.538478
79	6	0	-4.754723	-0.131897	0.439945
80	6	0	-2.636475	1.005540	-0.366984
81	8	0	-3.241448	-0.967771	2.554128
82	6	0	-5.750201	0.569805	-0.394441
83	6	0	-7.077136	0.610651	0.068104
84	6	0	-5.454816	1.197280	-1.615226
85	6	0	-8.070781	1.262424	-0.652451
86	6	0	-7.760590	1.884520	-1.860663
87	6	0	-6.451428	1.847261	-2.336667
88	6	0	-2.557424	-1.364693	3.769687

89	6	0	-3.532220	-2.178832	4.594505
90	7	0	-1.913527	1.628158	-1.032822
91	1	0	-5.160169	-0.453614	1.390338
92	1	0	-7.326267	0.130943	1.009132
93	1	0	-4.447846	1.183993	-2.008944
94	1	0	-9.084808	1.287967	-0.270688
95	1	0	-8.532031	2.394913	-2.425258
96	1	0	-6.202879	2.329356	-3.275176
97	1	0	-1.672420	-1.944320	3.498068
98	1	0	-2.230232	-0.465201	4.295713
99	1	0	-3.050807	-2.499595	5.521638
100	1	0	-4.413592	-1.589189	4.854116
101	1	0	-3.856325	-3.069495	4.052605

3-4-IM1-exo

Energy + zep (gas) = -2188.38625 au
Gibbs free energy (gas) = -2188.47102 au
Gibbs free energy (in solvent) = -2187.69881 au
Zero-point correction = 0.85153 au
Thermal correction to Gibbs free energy = 0.76676 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.445123	-0.460481	1.599399
2	8	0	-1.260600	-0.110734	1.852278
3	6	0	-3.207341	-0.094077	0.463310
4	6	0	-4.654489	-0.536512	0.321642
5	6	0	-2.515007	0.744114	-0.410854
6	8	0	-3.093241	-1.282354	2.462537
7	6	0	-5.581640	0.448714	-0.376653
8	6	0	-6.764273	0.828400	0.269446
9	6	0	-5.324849	0.984476	-1.645179
10	6	0	-7.662834	1.711265	-0.324906
11	6	0	-7.391875	2.237850	-1.584906
12	6	0	-6.219045	1.871489	-2.241127
13	6	0	-2.424213	-1.650308	3.687979
14	6	0	-3.397735	-2.473953	4.506935
15	7	0	-1.818730	1.402291	-1.082631
16	1	0	-5.024317	-0.622410	1.343969
17	1	0	-6.983733	0.428890	1.254610
18	1	0	-4.421162	0.716459	-2.177588

19	1	0	-8.570517	1.989591	0.198515
20	1	0	-8.085891	2.928174	-2.050263
21	1	0	-5.996527	2.277844	-3.221442
22	1	0	-1.522378	-2.218613	3.445930
23	1	0	-2.120656	-0.742898	4.215409
24	1	0	-2.927452	-2.779080	5.445186
25	1	0	-4.293321	-1.896716	4.745127
26	1	0	-3.699910	-3.373967	3.967453
27	1	0	-0.204512	1.010489	1.222986
28	7	0	0.558739	1.739505	1.313903
29	6	0	1.496395	1.807364	0.117510
30	6	0	1.296482	1.409728	2.588939
31	6	0	-0.130762	3.079573	1.450755
32	6	0	1.856501	0.411586	-0.451462
33	6	0	2.696429	2.695333	0.522064
34	6	0	2.223846	2.582783	2.966148
35	6	0	0.930387	4.212076	1.574210
36	6	0	2.943461	0.533238	-1.521349
37	6	0	2.315757	3.533505	1.759045
38	6	0	2.643448	1.082877	-2.747756
39	6	0	4.284084	0.096791	-1.280341
40	6	0	3.648813	1.211744	-3.732545
41	6	0	5.221295	0.279622	-2.353817
42	7	0	4.891389	0.830386	-3.551385
43	1	0	1.847448	0.486481	2.412849
44	1	0	0.531866	1.195079	3.332876
45	1	0	-0.768765	3.008781	2.331490
46	1	0	-0.772814	3.186373	0.576584
47	1	0	2.203119	-0.247434	0.339072
48	1	0	2.973464	3.328048	-0.320677
49	1	0	3.572869	2.085795	0.755533
50	1	0	1.838568	3.113633	3.839663
51	1	0	3.212950	2.203518	3.230572
52	1	0	0.721945	4.773325	2.489080
53	1	0	3.071714	4.299676	1.934203
54	1	0	1.640231	1.419024	-2.986453
55	6	0	4.741150	-0.490093	-0.078969
56	1	0	3.404801	1.646481	-4.697922
57	6	0	6.563189	-0.132097	-2.166284
58	6	0	6.983167	-0.696409	-0.988798
59	6	0	6.059940	-0.881013	0.072411
60	1	0	7.246295	0.017838	-2.992881
61	1	0	8.015215	-0.999464	-0.878990
62	8	0	6.382732	-1.433069	1.267520

63	1	0	4.083974	-0.673408	0.760932
64	6	0	7.720451	-1.880799	1.494546
65	1	0	7.724574	-2.284201	2.504834
66	1	0	8.001981	-2.668553	0.789472
67	1	0	8.434189	-1.053811	1.433011
68	6	0	0.741038	6.499081	0.563624
69	1	0	0.713286	7.161292	-0.293423
70	6	0	0.877124	5.184506	0.423157
71	1	0	0.951419	4.769004	-0.580346
72	1	0	0.649181	6.962888	1.541078
73	1	0	0.910178	2.317250	-0.649852
74	7	0	0.627264	-0.160071	-1.020444
75	1	0	-0.022456	0.515975	-1.438054
76	6	0	0.168454	-1.405967	-1.047775
77	6	0	-2.086117	-2.266548	-1.457633
78	6	0	-0.960294	-1.625783	-1.897971
79	6	0	-3.308258	-2.279119	-2.206035
80	6	0	-4.559145	-2.235436	-1.674835
81	6	0	-4.814055	-2.032705	-0.213381
82	6	0	-5.762091	-2.305817	-2.569241
83	1	0	-2.074115	-2.724790	-0.473368
84	1	0	-1.036335	-0.998287	-2.780575
85	1	0	-3.208581	-2.231664	-3.288016
86	1	0	-4.140642	-2.637823	0.398652
87	1	0	-5.835163	-2.344899	0.020342
88	1	0	-5.492826	-2.337397	-3.625929
89	1	0	-6.430710	-1.458275	-2.397356
90	1	0	-6.336010	-3.210278	-2.333626
91	6	0	0.761297	-2.500662	-0.255599
92	6	0	0.970804	-2.398185	1.129544
93	6	0	1.096596	-3.692342	-0.916905
94	6	0	1.524362	-3.464805	1.828545
95	6	0	1.673364	-4.744838	-0.213675
96	6	0	1.889849	-4.632291	1.157605
97	1	0	0.613358	-1.524144	1.659070
98	1	0	0.921212	-3.780084	-1.981865
99	1	0	1.658702	-3.392577	2.901533
100	1	0	1.945246	-5.654346	-0.735526
101	1	0	2.328037	-5.457563	1.706442

3-4-TS2-exo

Energy + zep (gas) = -2188.37210 au
Gibbs free energy (gas) = -2188.45628 au
Gibbs free energy (in solvent) = -2187.68756 au

Zero-point correction = 0.85149 au
Thermal correction to Gibbs free energy = 0.76731 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.805290	-0.588959	1.451831
2	8	0	-1.717622	-0.148528	1.831491
3	6	0	-3.456347	-0.227576	0.192797
4	6	0	-4.926822	-0.596847	0.009832
5	6	0	-2.914980	0.980544	-0.321931
6	8	0	-3.482313	-1.515443	2.151958
7	6	0	-5.797086	0.437992	-0.690938
8	6	0	-6.971683	0.855229	-0.053696
9	6	0	-5.505353	0.971086	-1.952429
10	6	0	-7.832726	1.770478	-0.653661
11	6	0	-7.530347	2.290950	-1.908984
12	6	0	-6.363422	1.889004	-2.554160
13	6	0	-2.971833	-1.897917	3.457890
14	6	0	-4.017432	-2.771028	4.118656
15	7	0	-2.346473	1.910050	-0.719501
16	1	0	-5.332482	-0.702673	1.016677
17	1	0	-7.216937	0.457885	0.926285
18	1	0	-4.602281	0.678287	-2.472108
19	1	0	-8.735886	2.077622	-0.138940
20	1	0	-8.195439	3.006059	-2.378889
21	1	0	-6.115812	2.293355	-3.529031
22	1	0	-2.027744	-2.430375	3.323681
23	1	0	-2.772791	-0.989806	4.030029
24	1	0	-3.665631	-3.079955	5.106026
25	1	0	-4.956184	-2.228611	4.245321
26	1	0	-4.210858	-3.669137	3.528837
27	1	0	-0.139147	0.796555	0.910940
28	7	0	0.602314	1.405015	1.288885
29	6	0	1.680977	1.732802	0.256664
30	6	0	1.168661	0.718263	2.512972
31	6	0	-0.094152	2.690732	1.700072
32	6	0	2.178127	0.492545	-0.543309
33	6	0	2.802119	2.496849	1.005728
34	6	0	2.095878	1.700265	3.260372
35	6	0	0.943430	3.695881	2.272385
36	6	0	3.357311	0.899267	-1.426401

37	6	0	2.300873	2.951332	2.387856
38	6	0	3.183424	1.859047	-2.399120
39	6	0	4.649679	0.300174	-1.294152
40	6	0	4.259442	2.232008	-3.236566
41	6	0	5.669990	0.761376	-2.194521
42	7	0	5.460085	1.712217	-3.143163
43	1	0	1.685790	-0.176647	2.171580
44	1	0	0.308509	0.398054	3.095812
45	1	0	-0.849569	2.399375	2.427756
46	1	0	-0.612887	3.058443	0.815286
47	1	0	2.500996	-0.274165	0.157076
48	1	0	3.125913	3.343413	0.401215
49	1	0	3.677708	1.855058	1.134380
50	1	0	1.662297	1.976281	4.224260
51	1	0	3.055483	1.221158	3.464697
52	1	0	0.634312	3.963527	3.286385
53	1	0	3.035414	3.614110	2.846908
54	1	0	2.226424	2.349286	-2.549262
55	6	0	4.983673	-0.697467	-0.350982
56	1	0	4.109751	2.988018	-4.002635
57	6	0	6.967585	0.202961	-2.100579
58	6	0	7.267298	-0.764072	-1.174838
59	6	0	6.261443	-1.224805	-0.287231
60	1	0	7.715516	0.570419	-2.791912
61	1	0	8.268510	-1.170079	-1.130785
62	8	0	6.463467	-2.181700	0.652663
63	1	0	4.257149	-1.102715	0.340377
64	6	0	7.756123	-2.775407	0.779755
65	1	0	7.665203	-3.501601	1.584701
66	1	0	8.051467	-3.289856	-0.139737
67	1	0	8.512430	-2.031639	1.048329
68	6	0	0.862427	6.184948	1.975556
69	1	0	0.926933	7.071327	1.355913
70	6	0	1.013490	4.967072	1.465576
71	1	0	1.194846	4.862876	0.397161
72	1	0	0.665979	6.341978	3.031816
73	1	0	1.173450	2.398536	-0.444497
74	7	0	1.125969	-0.095487	-1.373957
75	1	0	0.765115	0.541489	-2.072939
76	6	0	0.194911	-1.028647	-0.937686
77	6	0	-2.267887	-1.649022	-1.142443
78	6	0	-1.073974	-0.928904	-1.444195
79	6	0	-3.240120	-1.853337	-2.200470
80	6	0	-4.546224	-2.131701	-1.995040

81	6	0	-5.094172	-2.046167	-0.608907
82	6	0	-5.494354	-2.392927	-3.126058
83	1	0	-2.242466	-2.385477	-0.346328
84	1	0	-1.222945	-0.108239	-2.143671
85	1	0	-2.875866	-1.728275	-3.217115
86	1	0	-4.579961	-2.734687	0.068592
87	1	0	-6.155794	-2.298758	-0.589443
88	1	0	-4.996777	-2.350812	-4.096312
89	1	0	-6.315509	-1.668918	-3.118766
90	1	0	-5.948325	-3.384302	-3.015912
91	6	0	0.751545	-2.179343	-0.165149
92	6	0	0.245430	-2.624860	1.061018
93	6	0	1.823944	-2.877899	-0.746495
94	6	0	0.790274	-3.746914	1.683737
95	6	0	2.359911	-3.999515	-0.123867
96	6	0	1.843559	-4.439782	1.093778
97	1	0	-0.548486	-2.072494	1.541571
98	1	0	2.220934	-2.545801	-1.697966
99	1	0	0.392099	-4.077421	2.636491
100	1	0	3.180515	-4.530324	-0.591675
101	1	0	2.261571	-5.313790	1.579072

3-4-IM2-exo

Energy + zep (gas) = -2188.39926 au
Gibbs free energy (gas) = -2188.48470 au
Gibbs free energy (in solvent) = -2187.72926 au
Zero-point correction = 0.85385 au
Thermal correction to Gibbs free energy = 0.76841 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.552946	-1.778053	-0.743364
2	8	0	4.292171	-2.949982	-0.742924
3	6	0	3.675505	-0.682153	-0.042337
4	6	0	4.609408	0.282600	0.795176
5	6	0	3.022177	0.044755	-1.131725
6	8	0	5.595850	-1.224724	-1.365055
7	6	0	3.943809	1.578240	1.255330
8	6	0	3.949179	2.682474	0.392740
9	6	0	3.382250	1.741924	2.527965
10	6	0	3.393349	3.901570	0.775680

11	6	0	2.826185	4.044694	2.040345
12	6	0	2.828224	2.960836	2.915989
13	6	0	6.468858	-2.130895	-2.112186
14	6	0	7.545519	-1.292155	-2.763465
15	7	0	2.462382	0.582569	-1.986263
16	1	0	5.401234	0.580123	0.107803
17	1	0	4.411207	2.594497	-0.584646
18	1	0	3.377042	0.914881	3.226863
19	1	0	3.428769	4.745563	0.095801
20	1	0	2.412415	4.997618	2.349954
21	1	0	2.414889	3.067173	3.912824
22	1	0	6.874622	-2.862685	-1.411512
23	1	0	5.855318	-2.662974	-2.841309
24	1	0	8.212345	-1.939795	-3.337690
25	1	0	7.111914	-0.557616	-3.444900
26	1	0	8.142840	-0.766306	-2.015942
27	1	0	0.192625	0.876697	-0.852720
28	7	0	-0.538637	1.395025	-1.356256
29	6	0	-1.756963	1.578005	-0.448366
30	6	0	-0.862312	0.626999	-2.621548
31	6	0	0.014454	2.760571	-1.714755
32	6	0	-2.124098	0.288049	0.337398
33	6	0	-2.890436	2.158136	-1.327209
34	6	0	-1.833099	1.463784	-3.480168
35	6	0	-1.091192	3.605908	-2.412387
36	6	0	-3.354423	0.577655	1.196030
37	6	0	-2.309847	2.674171	-2.658375
38	6	0	-3.285592	1.536358	2.183126
39	6	0	-4.589373	-0.124420	1.025857
40	6	0	-4.408946	1.810039	2.996246
41	6	0	-5.667420	0.242712	1.901945
42	7	0	-5.560822	1.196893	2.864761
43	1	0	-1.277966	-0.331861	-2.318889
44	1	0	0.093596	0.440325	-3.107386
45	1	0	0.880891	2.581613	-2.348201
46	1	0	0.361585	3.214562	-0.786304
47	1	0	-2.363024	-0.497525	-0.377189
48	1	0	-3.402676	2.949450	-0.780685
49	1	0	-3.639536	1.388877	-1.533687
50	1	0	-1.340586	1.797527	-4.396024
51	1	0	-2.685027	0.849970	-3.778857
52	1	0	-0.712120	3.911656	-3.391010
53	1	0	-3.074740	3.224257	-3.207655
54	1	0	-2.374888	2.098799	2.364324

55	6	0	-4.814246	-1.138979	0.068672
56	1	0	-4.340975	2.565392	3.774679
57	6	0	-6.912108	-0.418290	1.768274
58	6	0	-7.106613	-1.398050	0.827961
59	6	0	-6.042531	-1.768134	-0.033925
60	1	0	-7.705733	-0.119767	2.441628
61	1	0	-8.069732	-1.883963	0.753922
62	8	0	-6.140886	-2.730200	-0.984648
63	1	0	-4.036747	-1.479283	-0.601959
64	6	0	-7.372278	-3.436293	-1.140039
65	1	0	-7.201091	-4.146174	-1.946435
66	1	0	-7.637541	-3.981006	-0.228863
67	1	0	-8.187084	-2.761570	-1.419831
68	6	0	-1.350393	6.085577	-2.138106
69	1	0	-1.615668	6.954470	-1.547676
70	6	0	-1.430680	4.855475	-1.641205
71	1	0	-1.764584	4.723041	-0.613370
72	1	0	-1.018738	6.270330	-3.155322
73	1	0	-1.425198	2.322659	0.278149
74	7	0	-1.041948	-0.219936	1.180718
75	1	0	-0.792676	0.396363	1.942591
76	6	0	0.047586	-0.962636	0.668949
77	6	0	2.575526	-1.401268	0.822289
78	6	0	1.308735	-0.593058	0.993498
79	6	0	3.138033	-1.817649	2.164333
80	6	0	4.320490	-1.459983	2.668956
81	6	0	5.257635	-0.535291	1.927117
82	6	0	4.825746	-1.986075	3.985004
83	1	0	2.335987	-2.319998	0.285483
84	1	0	1.417781	0.329623	1.556606
85	1	0	2.501392	-2.497339	2.723457
86	1	0	6.082564	-1.131755	1.515763
87	1	0	5.730122	0.156601	2.631517
88	1	0	4.116139	-2.674879	4.445686
89	1	0	5.020588	-1.168582	4.688343
90	1	0	5.775451	-2.516263	3.851302
91	6	0	-0.334250	-2.193329	-0.083022
92	6	0	0.298817	-2.570231	-1.276245
93	6	0	-1.352854	-3.015922	0.424636
94	6	0	-0.066374	-3.741747	-1.935710
95	6	0	-1.712727	-4.187036	-0.234067
96	6	0	-1.070927	-4.554163	-1.416075
97	1	0	1.076499	-1.945668	-1.697788
98	1	0	-1.847144	-2.735101	1.346605

99	1	0	0.437653	-4.019574	-2.854010
100	1	0	-2.492997	-4.815722	0.178639
101	1	0	-1.351387	-5.467596	-1.927199

T-n-TS

Energy + zep (gas) = -1519.25645 au
Gibbs free energy (gas) = -1519.32262 au
Gibbs free energy (in solvent) = -1518.75533 au
Zero-point correction = 0.63769 au
Thermal correction to Gibbs free energy = 0.57151 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.283988	1.592446	1.129382
2	6	0	-0.792383	1.176161	-0.250123
3	6	0	1.146767	2.035669	1.095155
4	6	0	-1.132067	2.750776	1.595198
5	6	0	-0.126903	-0.156436	-0.805271
6	6	0	-0.769290	2.432162	-1.170444
7	6	0	1.338550	3.111060	-0.001505
8	6	0	-0.843463	4.041381	0.784432
9	6	0	1.054748	-0.065967	-1.760420
10	6	0	-0.046628	3.597374	-0.466635
11	6	0	0.884719	0.312550	-3.075508
12	6	0	2.372948	-0.452462	-1.346970
13	6	0	1.987887	0.376777	-3.956226
14	6	0	3.420812	-0.337298	-2.322923
15	7	0	3.215310	0.083771	-3.598348
16	1	0	1.779051	1.165397	0.934067
17	1	0	1.371577	2.421528	2.090981
18	1	0	-0.929982	2.887212	2.657511
19	1	0	-2.174749	2.440705	1.499555
20	1	0	0.199736	-0.688710	0.077986
21	1	0	-1.788021	2.721441	-1.438180
22	1	0	-0.246532	2.215173	-2.099125
23	1	0	1.923403	3.945487	0.391245
24	1	0	1.894507	2.698618	-0.846237
25	1	0	-0.195173	4.694844	1.376356
26	1	0	0.057623	4.435477	-1.157270
27	1	0	-0.092703	0.565487	-3.471311
28	6	0	2.705196	-0.958691	-0.068249

29	1	0	1.837544	0.688623	-4.986113
30	6	0	4.741741	-0.697053	-1.958318
31	6	0	-1.335867	-2.286914	1.700384
32	6	0	-1.103848	-2.568804	0.357273
33	6	0	-1.880171	-1.904149	-0.621283
34	7	0	-1.202979	-1.004801	-1.388481
35	1	0	-2.293156	-1.836242	1.951711
36	1	0	-0.080276	-2.793187	0.073432
37	1	0	-1.652078	-0.664535	-2.227811
38	6	0	-0.307445	-2.214628	2.644250
39	6	0	-0.162357	-1.088765	3.477920
40	6	0	5.038613	-1.171762	-0.706539
41	6	0	4.003108	-1.315756	0.252235
42	1	0	5.508362	-0.591251	-2.715585
43	1	0	6.056811	-1.443282	-0.464347
44	8	0	4.194524	-1.797233	1.505824
45	1	0	1.960850	-1.117411	0.701019
46	6	0	5.498571	-2.237676	1.894442
47	1	0	6.218072	-1.413832	1.878151
48	1	0	5.391893	-2.601451	2.913947
49	1	0	5.849227	-3.052312	1.254396
50	6	0	-0.955018	0.075264	3.353500
51	6	0	-3.323726	-2.057097	-0.769858
52	6	0	-4.130677	-1.048607	-1.335209
53	6	0	-3.933061	-3.256365	-0.353317
54	6	0	-5.497791	-1.235865	-1.476454
55	1	0	-3.694490	-0.103493	-1.638688
56	6	0	-5.304315	-3.432738	-0.484610
57	1	0	-3.314474	-4.050198	0.045745
58	6	0	-6.087771	-2.427659	-1.050201
59	1	0	-6.109510	-0.452545	-1.907691
60	1	0	-5.761193	-4.360926	-0.163440
61	1	0	-7.155851	-2.571625	-1.162609
62	6	0	-2.343509	6.050542	0.876235
63	1	0	-3.269178	6.556808	0.629642
64	6	0	-2.106349	4.802600	0.484302
65	1	0	-2.867801	4.276470	-0.089997
66	6	0	1.020644	-1.059772	4.413310
67	1	0	1.282940	-0.043095	4.709138
68	1	0	0.770746	-1.616583	5.323303
69	1	0	0.556231	-2.862392	2.520071
70	1	0	-1.620007	6.613999	1.457429
71	1	0	1.898602	-1.537857	3.972410
72	1	0	-0.892724	0.789875	4.171456

73	1	0	-1.967485	-0.040587	2.962940
74	1	0	-1.826002	0.891890	-0.049719
75	1	0	-0.470361	0.783328	2.089752

T-H_2O-COM

Energy + zep (gas) = -1595.78311 au
Gibbs free energy (gas) = -1595.85439 au
Gibbs free energy (in solvent) = -1595.25150 au
Zero-point correction = 0.66803 au
Thermal correction to Gibbs free energy = 0.59675 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.216745	0.491829	2.706214
2	1	0	0.775914	0.378475	3.480765
3	1	0	-6.811975	0.289083	2.510991
4	7	0	1.057868	2.129247	0.570063
5	6	0	0.311312	1.439642	-0.515587
6	6	0	2.458395	2.430555	0.172065
7	6	0	0.359803	3.412045	0.840400
8	6	0	0.562405	-0.113484	-0.509128
9	6	0	0.482635	2.195243	-1.860057
10	6	0	2.502481	3.401214	-1.042063
11	6	0	0.252351	4.309770	-0.441219
12	6	0	1.834627	-0.665417	-1.139318
13	6	0	1.063922	3.593319	-1.554393
14	6	0	1.977975	-0.754925	-2.508456
15	6	0	2.901055	-1.169776	-0.323591
16	6	0	3.144966	-1.319091	-3.074896
17	6	0	4.036834	-1.722927	-1.007265
18	7	0	4.140253	-1.786974	-2.361669
19	1	0	2.963960	1.493149	-0.050763
20	1	0	2.957114	2.857858	1.044304
21	1	0	0.912642	3.927777	1.628550
22	1	0	-0.630425	3.182644	1.241719
23	1	0	0.545998	-0.404183	0.537093
24	1	0	-0.474339	2.269869	-2.383175
25	1	0	1.176081	1.682134	-2.528471
26	1	0	2.929115	4.366710	-0.757377
27	1	0	3.135026	2.994939	-1.835724
28	1	0	0.748842	5.264818	-0.245003

29	1	0	1.057975	4.203094	-2.459814
30	1	0	1.210733	-0.397581	-3.187362
31	6	0	2.904497	-1.153486	1.088384
32	1	0	3.243632	-1.377821	-4.155483
33	6	0	5.111245	-2.237126	-0.242164
34	6	0	-3.349120	-0.683317	1.250731
35	6	0	-2.077518	-0.705469	0.738147
36	6	0	-1.783408	-1.046119	-0.612505
37	7	0	-0.595039	-0.790214	-1.147824
38	1	0	-4.180059	-0.933797	0.601256
39	1	0	-1.264661	-0.403181	1.391279
40	1	0	-0.430146	-1.171819	-2.071012
41	6	0	-3.622517	-0.309715	2.598533
42	6	0	-4.856269	-0.252388	3.174566
43	6	0	5.090906	-2.212770	1.129453
44	6	0	3.972780	-1.661364	1.805800
45	1	0	5.952184	-2.650081	-0.784927
46	1	0	5.928883	-2.612940	1.683594
47	8	0	3.868070	-1.586476	3.156721
48	1	0	2.085412	-0.734504	1.656888
49	6	0	4.922196	-2.104452	3.969568
50	1	0	5.862787	-1.575351	3.788850
51	1	0	4.607627	-1.936492	4.997408
52	1	0	5.061432	-3.177212	3.805515
53	6	0	-6.144938	-0.579281	2.481568
54	6	0	-2.761217	-1.704517	-1.511497
55	6	0	-2.981022	-1.198357	-2.802354
56	6	0	-3.438528	-2.862697	-1.101076
57	6	0	-3.872340	-1.833076	-3.660221
58	1	0	-2.484480	-0.288157	-3.119980
59	6	0	-4.314677	-3.502158	-1.971699
60	1	0	-3.249492	-3.278202	-0.118949
61	6	0	-4.536329	-2.987354	-3.247951
62	1	0	-4.051878	-1.425318	-4.647675
63	1	0	-4.819050	-4.407436	-1.655907
64	1	0	-5.224212	-3.485329	-3.920805
65	6	0	-1.681002	5.830149	-0.957626
66	1	0	-2.717356	5.989152	-1.232469
67	6	0	-1.172061	4.608880	-0.821907
68	1	0	-1.825107	3.751770	-0.985629
69	6	0	-4.991166	0.162079	4.608642
70	1	0	-5.638260	1.042681	4.691450
71	1	0	-5.477305	-0.629494	5.190071
72	1	0	-2.760486	-0.043207	3.203628

73	1	0	-1.077751	6.718728	-0.798213
74	1	0	-4.029310	0.391115	5.066789
75	1	0	-6.662823	-1.379855	3.020651
76	1	0	-6.032265	-0.885905	1.443459
77	1	0	-0.735977	1.522308	-0.211676
78	1	0	0.672278	1.142553	2.121407

T-H_2O-TS

Energy + zep (gas) = -1595.72048 au
Gibbs free energy (gas) = -1595.789790 au
Gibbs free energy (in solvent) = -1595.18761 au
Zero-point correction = 0.66155 au
Thermal correction to Gibbs free energy = 0.59223 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.512915	-0.880942	2.414786
2	1	0	1.391567	-1.012155	2.789396
3	1	0	-0.157941	-1.927994	2.796828
4	7	0	0.133709	1.484915	1.530425
5	6	0	-0.617838	1.482494	0.211520
6	6	0	1.403479	2.287026	1.474171
7	6	0	-0.771039	2.071932	2.581613
8	6	0	-0.057452	0.445552	-0.832438
9	6	0	-0.801654	2.948643	-0.249125
10	6	0	1.072907	3.770049	1.177059
11	6	0	-1.196911	3.521735	2.206846
12	6	0	1.134282	0.839300	-1.692079
13	6	0	-0.437145	3.900929	0.907622
14	6	0	0.976286	1.612885	-2.821065
15	6	0	2.450666	0.354561	-1.392603
16	6	0	2.089591	1.939151	-3.629211
17	6	0	3.505461	0.746508	-2.284467
18	7	0	3.310999	1.533008	-3.376173
19	1	0	2.043778	1.843747	0.716470
20	1	0	1.895548	2.155249	2.438571
21	1	0	-0.222145	2.032942	3.522598
22	1	0	-1.626374	1.401952	2.676286
23	1	0	0.221014	-0.419218	-0.238957
24	1	0	-1.829812	3.112325	-0.579668
25	1	0	-0.151275	3.171635	-1.096405

26	1	0	1.359858	4.403937	2.019092
27	1	0	1.641531	4.112473	0.310176
28	1	0	-0.850177	4.197942	2.993090
29	1	0	-0.682718	4.927418	0.631896
30	1	0	0.000340	1.971763	-3.127800
31	6	0	2.768983	-0.480507	-0.295036
32	1	0	1.950996	2.555807	-4.513091
33	6	0	4.821591	0.288993	-2.031195
34	6	0	-1.312787	-3.049398	0.138445
35	6	0	-1.013909	-2.278675	-0.988188
36	6	0	-1.817401	-1.206860	-1.401342
37	7	0	-1.207757	-0.010898	-1.644085
38	1	0	-2.257341	-2.849062	0.638316
39	1	0	0.018211	-2.273955	-1.323281
40	1	0	-1.748963	0.694712	-2.123076
41	6	0	-0.395700	-3.870974	0.783474
42	6	0	-0.299466	-3.949136	2.184430
43	6	0	5.107694	-0.516155	-0.957952
44	6	0	4.067477	-0.906026	-0.076024
45	1	0	5.594543	0.599197	-2.723101
46	1	0	6.123555	-0.848977	-0.795425
47	8	0	4.257818	-1.693026	1.014627
48	1	0	2.023077	-0.809784	0.418600
49	6	0	5.564005	-2.204063	1.287748
50	1	0	6.277881	-1.396685	1.476942
51	1	0	5.459236	-2.808076	2.186551
52	1	0	5.924284	-2.834166	0.469270
53	6	0	-0.932462	-3.014729	3.044403
54	6	0	-3.276823	-1.293133	-1.528414
55	6	0	-4.106649	-0.173315	-1.327019
56	6	0	-3.872952	-2.519015	-1.876353
57	6	0	-5.484142	-0.279701	-1.460763
58	1	0	-3.677557	0.778129	-1.033318
59	6	0	-5.252879	-2.622226	-2.003550
60	1	0	-3.242357	-3.376354	-2.073336
61	6	0	-6.060541	-1.504990	-1.798779
62	1	0	-6.112458	0.587006	-1.293482
63	1	0	-5.697991	-3.570907	-2.278187
64	1	0	-7.135830	-1.585570	-1.905562
65	6	0	-3.407240	4.556159	2.793434
66	1	0	-4.482695	4.628133	2.682779
67	6	0	-2.692567	3.670795	2.106254
68	1	0	-3.207956	2.996429	1.423459
69	6	0	0.694358	-4.907845	2.780708

70	1	0	1.196812	-4.479550	3.650579
71	1	0	0.159676	-5.800103	3.127301
72	1	0	0.424836	-4.282717	0.202338
73	1	0	-2.942893	5.243039	3.494310
74	1	0	1.442869	-5.232301	2.056259
75	1	0	-0.930756	-3.247757	4.106694
76	1	0	-1.865117	-2.565263	2.699910
77	1	0	-1.586888	1.064636	0.490049
78	1	0	0.339788	0.424893	1.887722

T-TFA-COM

Energy + zep (gas) = -2046.26868 au
Gibbs free energy (gas) = -2046.34988 au
Gibbs free energy (in solvent) = -2046.63231 au
Zero-point correction = 0.68213 au
Thermal correction to Gibbs free energy = 0.60094 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.548907	1.873943	-0.509565
2	7	0	-0.491961	2.201922	-0.618650
3	6	0	-1.381946	1.646949	0.479208
4	6	0	-0.948353	1.768680	-1.989256
5	6	0	-0.507453	3.706077	-0.537612
6	6	0	-1.049327	0.161500	0.817393
7	6	0	-2.850230	1.945862	0.082896
8	6	0	-2.322637	2.398577	-2.304902
9	6	0	-1.968628	4.236519	-0.640480
10	6	0	-2.223677	-0.570275	1.465349
11	6	0	-2.872141	3.029736	-1.013539
12	6	0	-2.556208	-0.322361	2.777944
13	6	0	-3.001991	-1.524238	0.737563
14	6	0	-3.643076	-0.998388	3.377127
15	6	0	-4.079544	-2.153328	1.448993
16	7	0	-4.380637	-1.881019	2.745422
17	1	0	-0.976052	0.679587	-1.994769
18	1	0	-0.168191	2.069281	-2.685303
19	1	0	0.128155	4.067173	-1.344990
20	1	0	-0.031867	3.982146	0.404221
21	1	0	-0.770997	-0.347508	-0.101755
22	1	0	-3.407197	2.253800	0.967689

23	1	0	-3.342478	1.048555	-0.297088
24	1	0	-2.227899	3.153626	-3.088562
25	1	0	-3.007731	1.633859	-2.676281
26	1	0	-2.013666	4.944488	-1.472182
27	1	0	-3.894148	3.378975	-1.165069
28	1	0	-1.994090	0.382294	3.381535
29	6	0	-2.785539	-1.882476	-0.612681
30	1	0	-3.899345	-0.795902	4.413296
31	6	0	-4.877761	-3.108956	0.773780
32	6	0	2.407945	-2.203727	0.093433
33	6	0	1.227956	-1.763651	0.638276
34	6	0	1.201383	-0.682614	1.561469
35	7	0	0.138233	0.110822	1.685185
36	1	0	3.312921	-1.676960	0.369232
37	1	0	0.288856	-2.180487	0.290963
38	1	0	0.176600	0.777371	2.445146
39	6	0	2.503916	-3.248610	-0.867820
40	6	0	3.648665	-3.590286	-1.525380
41	6	0	-4.646731	-3.440882	-0.536779
42	6	0	-3.584709	-2.820404	-1.244360
43	1	0	-5.681258	-3.567605	1.336296
44	1	0	-5.275836	-4.174556	-1.021669
45	8	0	-3.281077	-3.084777	-2.536919
46	1	0	-1.991833	-1.448407	-1.206916
47	6	0	-4.057346	-4.043627	-3.259996
48	1	0	-5.105019	-3.736759	-3.328916
49	1	0	-3.624838	-4.074232	-4.257520
50	1	0	-3.988145	-5.035669	-2.804250
51	6	0	4.959796	-2.877165	-1.364624
52	6	0	2.323793	-0.412149	2.480076
53	6	0	2.777011	0.899724	2.693531
54	6	0	2.915033	-1.472229	3.185738
55	6	0	3.799709	1.141457	3.601476
56	1	0	2.385550	1.699648	2.078774
57	6	0	3.928365	-1.218636	4.103364
58	1	0	2.558795	-2.483701	3.035877
59	6	0	4.371135	0.085956	4.312409
60	1	0	4.167908	2.150818	3.740461
61	1	0	4.370189	-2.038767	4.656274
62	1	0	5.167941	0.279827	5.020797
63	6	0	-2.848305	6.221266	0.616680
64	1	0	-3.161231	6.703306	1.535191
65	6	0	-2.410112	4.966480	0.602000
66	1	0	-2.361394	4.418021	1.542019

67	6	0	3.647260	-4.742329	-2.482476
68	1	0	4.444130	-5.448843	-2.224633
69	1	0	2.696122	-5.274956	-2.499006
70	1	0	1.598985	-3.809434	-1.087189
71	1	0	-2.910710	6.814205	-0.290597
72	1	0	3.870873	-4.389093	-3.495719
73	1	0	5.487704	-2.850238	-2.321393
74	1	0	5.602346	-3.438017	-0.674345
75	1	0	-1.130023	2.242743	1.360945
76	8	0	1.905030	1.361416	-0.305322
77	8	0	3.870325	0.405288	-0.835337
78	6	0	2.926273	1.149360	-1.042308
79	6	0	2.900567	1.922656	-2.396030
80	9	0	2.068691	1.278549	-3.267850
81	9	0	4.090269	2.029276	-2.974325
82	9	0	2.390572	3.177390	-2.254508
83	1	0	4.859972	-1.853759	-1.006707

T-TFA-TS

Energy + zep (gas) = -2046.23073 au
Gibbs free energy (gas) = -2046.31030 au
Gibbs free energy (in solvent) = -2046.632318552 au
Zero-point correction = 0.67865 au
Thermal correction to Gibbs free energy = 0.5991 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.572644	-0.621461	1.338988
2	7	0	-0.388770	-1.648502	1.303544
3	6	0	0.726332	-1.901925	0.292417
4	6	0	-1.653577	-2.420717	1.005287
5	6	0	0.119098	-2.029564	2.678445
6	6	0	0.574129	-1.025332	-1.003745
7	6	0	0.891238	-3.430189	0.155041
8	6	0	-1.355245	-3.932059	1.123804
9	6	0	0.558310	-3.522840	2.688901
10	6	0	-0.348525	-1.530679	-2.106261
11	6	0	0.158992	-4.133220	1.317354
12	6	0	0.073913	-2.489697	-3.000717
13	6	0	-1.660586	-0.980386	-2.286166
14	6	0	-0.782329	-2.933338	-4.034477

15	6	0	-2.444518	-1.509137	-3.366962
16	7	0	-1.998652	-2.474445	-4.213341
17	1	0	-1.983945	-2.133370	0.011299
18	1	0	-2.399318	-2.072679	1.717945
19	1	0	-0.691423	-1.826138	3.377291
20	1	0	0.938660	-1.349701	2.910509
21	1	0	0.192545	-0.072828	-0.644963
22	1	0	1.952544	-3.686315	0.148677
23	1	0	0.467063	-3.782067	-0.786691
24	1	0	-1.901747	-4.365222	1.964279
25	1	0	-1.692745	-4.445802	0.221869
26	1	0	-0.023470	-4.041798	3.455000
27	1	0	0.399794	-5.196829	1.314984
28	1	0	1.072460	-2.908656	-2.946589
29	6	0	-2.223153	0.038925	-1.482168
30	1	0	-0.437976	-3.693573	-4.730255
31	6	0	-3.749717	-1.000396	-3.578382
32	6	0	1.685451	2.848592	-0.853582
33	6	0	1.553853	1.640757	-1.572464
34	6	0	2.426191	0.570045	-1.460282
35	7	0	1.922833	-0.707698	-1.485754
36	1	0	2.545594	2.943971	-0.197143
37	1	0	0.588298	1.452499	-2.029874
38	1	0	2.565157	-1.463929	-1.668191
39	6	0	0.728342	3.833414	-0.819358
40	6	0	0.597723	4.783498	0.235384
41	6	0	-4.275843	-0.016475	-2.780291
42	6	0	-3.501230	0.516080	-1.717546
43	1	0	-4.315639	-1.418734	-4.401297
44	1	0	-5.274471	0.351200	-2.971971
45	8	0	-3.930517	1.494753	-0.884668
46	1	0	-1.683604	0.493516	-0.661745
47	6	0	-5.249373	2.022882	-1.041429
48	1	0	-6.007505	1.244679	-0.912884
49	1	0	-5.359968	2.765512	-0.254346
50	1	0	-5.372251	2.505458	-2.015532
51	6	0	1.147450	4.586083	1.502012
52	6	0	3.879970	0.716113	-1.266231
53	6	0	4.611334	-0.189094	-0.476916
54	6	0	4.567823	1.766909	-1.896717
55	6	0	5.982736	-0.039585	-0.312661
56	1	0	4.099493	-0.994562	0.037675
57	6	0	5.939963	1.914518	-1.728879
58	1	0	4.022108	2.445550	-2.539925

59	6	0	6.650454	1.013005	-0.938517
60	1	0	6.532210	-0.736700	0.308943
61	1	0	6.458124	2.725147	-2.227157
62	1	0	7.720759	1.126576	-0.813123
63	6	0	2.470047	-4.440164	4.029389
64	1	0	3.529984	-4.534055	4.233305
65	6	0	2.016513	-3.688528	3.031515
66	1	0	2.731824	-3.148422	2.412799
67	6	0	-0.329600	5.946631	0.010390
68	1	0	0.158738	6.672717	-0.649060
69	1	0	-1.247227	5.629534	-0.492291
70	1	0	-0.050113	3.826816	-1.577680
71	1	0	1.798330	-4.989801	4.681554
72	1	0	-0.590282	6.452168	0.939975
73	1	0	1.162915	5.422209	2.195261
74	1	0	1.944420	3.857164	1.632225
75	1	0	1.600016	-1.478254	0.789013
76	8	0	-0.309269	1.130097	1.581751
77	8	0	-0.831958	3.134878	2.501947
78	6	0	-0.983122	1.899081	2.275005
79	6	0	-2.192264	1.275560	3.032459
80	9	0	-2.827178	0.378760	2.233498
81	9	0	-3.083954	2.159128	3.453429
82	9	0	-1.732813	0.580772	4.101735
83	1	0	0.080178	3.762315	1.985849

T-SA-COM

Energy + zep (gas) = -2015.41633 au
Gibbs free energy (gas) = -2015.50002 au
Gibbs free energy (in solvent) = -2014.75561 au
Zero-point correction = 0.76335 au
Thermal correction to Gibbs free energy = 0.67966 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.495517	-1.147277	-2.597373
2	8	0	-0.349169	-0.181004	-2.564841
3	8	0	1.347223	1.238775	-2.526513
4	6	0	0.970097	0.093321	-2.625912
5	6	0	1.915254	-1.059246	-2.781167
6	6	0	1.556583	-2.409607	-2.605881

7	6	0	3.255891	-0.754731	-3.055804
8	6	0	2.523790	-3.411419	-2.683150
9	6	0	3.846100	-3.081820	-2.954500
10	6	0	4.215913	-1.750298	-3.151703
11	8	0	0.235734	-2.718772	-2.394189
12	1	0	2.227511	-4.446013	-2.554096
13	1	0	3.513875	0.288250	-3.188553
14	1	0	5.243369	-1.497163	-3.382217
15	1	0	4.586750	-3.869843	-3.026964
16	1	0	0.118369	-3.467551	-1.776299
17	1	0	6.662011	1.540096	-0.081906
18	7	0	-3.191711	-0.546317	-0.577657
19	6	0	-2.544247	0.719808	-0.191528
20	6	0	-4.066743	-1.086083	0.490904
21	6	0	-4.036796	-0.246597	-1.754623
22	6	0	-1.193281	0.503250	0.559415
23	6	0	-3.566598	1.688224	0.468246
24	6	0	-5.240978	-0.118180	0.817734
25	6	0	-5.067002	0.905681	-1.454312
26	6	0	-1.204998	-0.224029	1.895997
27	6	0	-4.980360	1.200298	0.071096
28	6	0	-1.410424	0.431325	3.087768
29	6	0	-0.931046	-1.631384	1.945864
30	6	0	-1.354136	-0.281360	4.310595
31	6	0	-0.865913	-2.242608	3.238679
32	7	0	-1.084119	-1.561928	4.398307
33	1	0	-3.465023	-1.278116	1.376341
34	1	0	-4.434046	-2.054721	0.145616
35	1	0	-4.558182	-1.164244	-2.035305
36	1	0	-3.384948	0.024736	-2.588100
37	1	0	-0.576564	-0.063400	-0.134431
38	1	0	-3.409427	2.719239	0.134475
39	1	0	-3.492844	1.684883	1.560615
40	1	0	-6.200099	-0.539785	0.504591
41	1	0	-5.307532	0.061221	1.894613
42	1	0	-6.078806	0.536529	-1.648095
43	1	0	-5.723759	1.952914	0.339987
44	1	0	-1.593458	1.499003	3.113860
45	6	0	-0.721416	-2.434610	0.801435
46	1	0	-1.529370	0.244971	5.245263
47	6	0	-0.563684	-3.623225	3.325046
48	6	0	3.030847	1.341067	1.021612
49	6	0	1.681669	1.128307	1.113706
50	6	0	0.724670	2.126595	0.780697

51	7	0	-0.561995	1.842015	0.650261
52	1	0	3.368989	2.305936	0.663618
53	1	0	1.320747	0.155217	1.422181
54	1	0	-1.168529	2.632702	0.468537
55	6	0	4.007610	0.357098	1.349708
56	6	0	5.357360	0.516686	1.261440
57	6	0	-0.335370	-4.380088	2.200861
58	6	0	-0.419485	-3.774198	0.925061
59	1	0	-0.518996	-4.061764	4.314015
60	1	0	-0.101314	-5.430875	2.303210
61	8	0	-0.208092	-4.463021	-0.250568
62	1	0	-0.854608	-2.026361	-0.188692
63	6	0	-0.133039	-5.895121	-0.214932
64	1	0	-1.023575	-6.319260	0.254618
65	1	0	-0.086799	-6.216585	-1.253726
66	1	0	0.765486	-6.230224	0.309624
67	6	0	6.045266	1.764514	0.795050
68	6	0	1.094736	3.544208	0.549875
69	6	0	0.800937	4.131345	-0.689926
70	6	0	1.708541	4.301255	1.557491
71	6	0	1.118505	5.467944	-0.911031
72	1	0	0.393544	3.521019	-1.488019
73	6	0	2.003377	5.641751	1.331459
74	1	0	1.925603	3.849864	2.518606
75	6	0	1.709612	6.224827	0.099197
76	1	0	0.911708	5.914826	-1.876008
77	1	0	2.458810	6.231948	2.117643
78	1	0	1.947159	7.267684	-0.074762
79	6	0	-5.788651	2.683146	-3.079065
80	1	0	-5.578528	3.555330	-3.687371
81	6	0	-4.854769	2.118692	-2.318425
82	1	0	-3.853114	2.547789	-2.322724
83	6	0	6.270283	-0.608335	1.646204
84	1	0	6.942994	-0.294454	2.452238
85	1	0	5.725024	-1.493777	1.972584
86	1	0	3.633085	-0.600369	1.700887
87	1	0	-6.799878	2.290025	-3.123919
88	1	0	6.912328	-0.882757	0.801677
89	1	0	6.733043	2.120506	1.569460
90	1	0	5.371834	2.578833	0.535893
91	1	0	-2.216725	1.158395	-1.138158

T-SA-TS

Energy + zep (gas) = -2015.37684 au

Gibbs free energy (gas) = -2015.45569 au
Gibbs free energy (in solvent) = -2014.71301 au
Zero-point correction = 0.75923 au
Thermal correction to Gibbs free energy = 0.68038 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.441590	0.616077	0.951140
2	8	0	-0.013651	2.052012	0.311285
3	8	0	-0.114519	4.288549	0.140445
4	6	0	-0.629454	3.144589	0.358404
5	6	0	-2.093155	3.184046	0.724638
6	6	0	-3.014503	2.241910	0.233689
7	6	0	-2.566855	4.220179	1.538231
8	6	0	-4.365370	2.337989	0.580312
9	6	0	-4.807176	3.361568	1.411905
10	6	0	-3.906306	4.306711	1.898882
11	8	0	-2.566522	1.248635	-0.592243
12	1	0	-5.067582	1.609125	0.187125
13	1	0	-1.857797	4.967502	1.871747
14	1	0	-4.247889	5.111807	2.537620
15	1	0	-5.857820	3.422901	1.671226
16	1	0	-3.303114	0.826380	-1.063331
17	1	0	1.074494	4.390759	-0.429322
18	7	0	-0.370419	-0.195644	1.645248
19	6	0	0.764729	-1.119272	1.227881
20	6	0	-1.681068	-0.905775	1.848472
21	6	0	0.023557	0.489353	2.937598
22	6	0	0.695540	-1.588720	-0.285507
23	6	0	0.923323	-2.207023	2.320669
24	6	0	-1.496483	-2.017531	2.908315
25	6	0	0.152047	-0.542159	4.089738
26	6	0	-0.045714	-2.882115	-0.611663
27	6	0	-0.065652	-1.948073	3.473384
28	6	0	0.538494	-4.110703	-0.386769
29	6	0	-1.347129	-2.875512	-1.212650
30	6	0	-0.142690	-5.306391	-0.711403
31	6	0	-1.953295	-4.147457	-1.485363
32	7	0	-1.346334	-5.336799	-1.230718
33	1	0	-2.010008	-1.288652	0.887548
34	1	0	-2.393473	-0.142223	2.159634
35	1	0	-0.739986	1.241547	3.132871

36	1	0	0.956197	1.015100	2.736337
37	1	0	0.221686	-0.771328	-0.819506
38	1	0	1.951168	-2.219033	2.688880
39	1	0	0.718149	-3.196560	1.913782
40	1	0	-2.226137	-1.895753	3.711456
41	1	0	-1.672227	-2.997810	2.460143
42	1	0	-0.658333	-0.373005	4.804600
43	1	0	0.068487	-2.706501	4.246038
44	1	0	1.531984	-4.200266	0.037994
45	6	0	-2.065043	-1.704580	-1.549101
46	1	0	0.335701	-6.264107	-0.525366
47	6	0	-3.249884	-4.182613	-2.054909
48	6	0	2.431521	1.774208	-2.003140
49	6	0	2.076954	0.412186	-1.984822
50	6	0	2.754559	-0.566507	-1.277639
51	7	0	2.077380	-1.653735	-0.785317
52	1	0	3.264937	2.077560	-1.376871
53	1	0	1.104180	0.158413	-2.391577
54	1	0	2.640993	-2.428943	-0.471531
55	6	0	1.726118	2.753739	-2.666474
56	6	0	1.774543	4.127463	-2.329838
57	6	0	-3.941572	-3.031697	-2.337869
58	6	0	-3.340494	-1.777576	-2.073485
59	1	0	-3.676884	-5.157776	-2.252147
60	1	0	-4.934898	-3.092895	-2.760828
61	8	0	-3.970447	-0.580152	-2.291044
62	1	0	-1.647541	-0.719284	-1.398135
63	6	0	-5.193894	-0.556085	-3.038802
64	1	0	-6.001989	-1.052884	-2.495116
65	1	0	-5.438337	0.496173	-3.168337
66	1	0	-5.059319	-1.020391	-4.018681
67	6	0	2.219713	4.586760	-1.073762
68	6	0	4.205688	-0.513792	-1.011168
69	6	0	4.742298	-0.981492	0.201710
70	6	0	5.084673	-0.012414	-1.986035
71	6	0	6.110408	-0.931392	0.438504
72	1	0	4.084232	-1.356527	0.977678
73	6	0	6.453426	0.033774	-1.746691
74	1	0	4.689241	0.311450	-2.940321
75	6	0	6.969530	-0.423633	-0.535732
76	1	0	6.508569	-1.281893	1.383419
77	1	0	7.119725	0.414328	-2.511604
78	1	0	8.036998	-0.390128	-0.352670
79	6	0	1.552905	-0.185893	6.141104

80	1	0	2.515138	-0.089258	6.629711
81	6	0	1.454167	-0.391347	4.831634
82	1	0	2.364430	-0.451460	4.236770
83	6	0	1.131831	5.111946	-3.265500
84	1	0	1.900147	5.515488	-3.936096
85	1	0	0.366984	4.645172	-3.888522
86	1	0	1.008223	2.451454	-3.423680
87	1	0	0.674763	-0.104841	6.774320
88	1	0	0.693223	5.952651	-2.726197
89	1	0	2.420735	5.651209	-0.976353
90	1	0	2.876135	3.945898	-0.488278
91	1	0	1.623417	-0.448583	1.241905

T-SA-COM-1

Energy + zep (gas) = -2015.41888 au
Gibbs free energy (gas) = -2015.50059 au
Gibbs free energy (in solvent) = -2014.75077 au
Zero-point correction = 0.76366 au
Thermal correction to Gibbs free energy = 0.68193 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-5.195916	-3.717549	-0.929858
2	7	0	0.710072	0.820979	1.960949
3	6	0	-0.643094	1.081720	1.429419
4	6	0	1.374215	2.058072	2.439035
5	6	0	0.545059	-0.085670	3.119688
6	6	0	-0.619667	1.450163	-0.093636
7	6	0	-1.445671	2.008933	2.378807
8	6	0	0.595716	2.708904	3.619291
9	6	0	-0.439301	0.508852	4.193771
10	6	0	-0.042128	2.801189	-0.499533
11	6	0	-0.746171	1.970255	3.758042
12	6	0	-0.795629	3.953735	-0.425811
13	6	0	1.295886	2.920508	-1.001968
14	6	0	-0.266295	5.192843	-0.857985
15	6	0	1.726991	4.224761	-1.414541
16	7	0	0.941714	5.334014	-1.343916
17	1	0	1.467511	2.751089	1.605982
18	1	0	2.389220	1.783382	2.733414
19	1	0	1.532855	-0.252290	3.555079

20	1	0	0.187878	-1.050577	2.753538
21	1	0	-0.035615	0.666050	-0.572739
22	1	0	-2.485636	1.679368	2.451196
23	1	0	-1.457413	3.045803	2.031289
24	1	0	1.159923	2.636043	4.553186
25	1	0	0.426081	3.772898	3.431309
26	1	0	0.077422	0.563766	5.156851
27	1	0	-1.376047	2.450529	4.509338
28	1	0	-1.806930	3.951979	-0.033474
29	6	0	2.214192	1.849006	-1.087360
30	1	0	-0.878597	6.088443	-0.795196
31	6	0	3.041592	4.388468	-1.912509
32	6	0	-2.991394	-2.164030	-0.794276
33	6	0	-2.197416	-1.040089	-0.755743
34	6	0	-2.711728	0.271139	-0.917221
35	7	0	-1.994125	1.357828	-0.643795
36	1	0	-4.058600	-2.031941	-0.932465
37	1	0	-1.141151	-1.167824	-0.545085
38	1	0	-2.418336	2.236460	-0.910465
39	6	0	-2.479154	-3.478389	-0.636559
40	6	0	-3.225998	-4.622317	-0.639519
41	6	0	3.919388	3.335689	-1.975061
42	6	0	3.499484	2.055806	-1.543866
43	1	0	3.333003	5.383199	-2.224820
44	1	0	4.923614	3.496967	-2.341757
45	8	0	4.337195	0.964080	-1.524365
46	1	0	1.942657	0.855516	-0.762321
47	6	0	5.599915	1.042118	-2.201925
48	1	0	6.276597	1.738794	-1.700287
49	1	0	6.017057	0.038036	-2.164095
50	1	0	5.460971	1.335774	-3.244839
51	6	0	-4.714543	-4.685366	-0.801362
52	6	0	-4.086212	0.539633	-1.411694
53	6	0	-4.928382	1.408805	-0.701205
54	6	0	-4.539138	-0.031717	-2.609889
55	6	0	-6.205524	1.688529	-1.175483
56	1	0	-4.598359	1.834377	0.239966
57	6	0	-5.811204	0.267183	-3.087060
58	1	0	-3.884473	-0.680465	-3.178840
59	6	0	-6.646674	1.122031	-2.370141
60	1	0	-6.857283	2.344393	-0.610926
61	1	0	-6.147549	-0.163218	-4.022659
62	1	0	-7.639103	1.347278	-2.741977
63	6	0	-2.078244	-0.828326	5.553114

64	1	0	-2.973050	-1.434786	5.634250
65	6	0	-1.669647	-0.334472	4.387521
66	1	0	-2.254032	-0.557766	3.495178
67	6	0	-2.539857	-5.943157	-0.467815
68	1	0	-2.755420	-6.596918	-1.320926
69	1	0	-1.404755	-3.577383	-0.507868
70	1	0	-1.529303	-0.645017	6.471875
71	1	0	-2.930383	-6.459911	0.416790
72	1	0	-5.160594	-5.175616	0.070860
73	1	0	-4.966739	-5.311912	-1.663766
74	1	0	-1.130285	0.103647	1.435249
75	1	0	-1.460720	-5.834113	-0.367791
76	1	0	1.807733	-1.279672	0.462264
77	8	0	1.071953	-1.892178	0.250642
78	8	0	0.759872	-3.986433	-0.386615
79	6	0	1.542808	-3.101024	-0.126412
80	6	0	3.023860	-3.287086	-0.219463
81	6	0	3.965063	-2.253200	-0.071436
82	6	0	3.487640	-4.573181	-0.533762
83	6	0	5.326002	-2.509767	-0.235169
84	6	0	5.759469	-3.791187	-0.554286
85	6	0	4.839325	-4.830298	-0.700133
86	8	0	3.526304	-0.999616	0.283989
87	1	0	6.038106	-1.706413	-0.082868
88	1	0	2.750630	-5.356765	-0.652878
89	1	0	5.177868	-5.830121	-0.941274
90	1	0	6.819646	-3.981138	-0.675323
91	1	0	3.990090	-0.303386	-0.220197

T-SA-TS-1

Energy + zep (gas) = -2015.37862 au
Gibbs free energy (gas) = -2015.45657 au
Gibbs free energy (in solvent) = -2014.71390 au
Zero-point correction = 0.75985 au
Thermal correction to Gibbs free energy = 0.68190 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.993831	4.247222	-0.733116
2	7	0	-0.524644	0.251368	1.397678
3	6	0	0.745061	-0.576391	1.249863

4	6	0	-1.743934	-0.566072	1.733518
5	6	0	-0.300784	1.266486	2.500934
6	6	0	0.817305	-1.456290	-0.065032
7	6	0	1.009956	-1.287881	2.602011
8	6	0	-1.454634	-1.409773	2.995143
9	6	0	-0.183457	0.561843	3.877681
10	6	0	0.239669	-2.868092	-0.030840
11	6	0	-0.113113	-0.962542	3.604948
12	6	0	0.927899	-3.908035	0.560228
13	6	0	-1.013069	-3.181415	-0.655533
14	6	0	0.392888	-5.217339	0.568363
15	6	0	-1.468405	-4.539950	-0.571387
16	7	0	-0.763853	-5.530682	0.037138
17	1	0	-1.996755	-1.169498	0.867653
18	1	0	-2.552750	0.149051	1.882553
19	1	0	-1.138395	1.961131	2.457973
20	1	0	0.598767	1.820441	2.234056
21	1	0	0.286406	-0.902176	-0.837501
22	1	0	1.980457	-0.982531	2.996639
23	1	0	1.046314	-2.367427	2.469785
24	1	0	-2.262397	-1.285840	3.719287
25	1	0	-1.411525	-2.470945	2.740157
26	1	0	-1.097828	0.749805	4.448111
27	1	0	0.068796	-1.491637	4.541497
28	1	0	1.890831	-3.754446	1.033981
29	6	0	-1.822828	-2.245729	-1.339640
30	1	0	0.950226	-6.021624	1.040804
31	6	0	-2.712804	-4.885769	-1.153570
32	6	0	2.832985	1.943986	-1.587057
33	6	0	2.323423	0.632112	-1.449226
34	6	0	2.966222	-0.481474	-0.951898
35	7	0	2.239469	-1.524186	-0.430542
36	1	0	3.829060	2.165237	-1.216706
37	1	0	1.258141	0.557257	-1.629239
38	1	0	2.668840	-2.436264	-0.440379
39	6	0	2.015739	2.939612	-2.067151
40	6	0	2.138805	4.331935	-1.879330
41	6	0	-3.496120	-3.951118	-1.782458
42	6	0	-3.044999	-2.611981	-1.867788
43	1	0	-3.023971	-5.919851	-1.076233
44	1	0	-4.446384	-4.244612	-2.207086
45	8	0	-3.776364	-1.606006	-2.441042
46	1	0	-1.520166	-1.216080	-1.464830
47	6	0	-4.925815	-1.937187	-3.233255

48	1	0	-5.725540	-2.356404	-2.616831
49	1	0	-5.260151	-0.999468	-3.671962
50	1	0	-4.658698	-2.635931	-4.029450
51	6	0	3.328987	4.961444	-1.216818
52	6	0	4.435033	-0.638828	-0.907466
53	6	0	5.061413	-1.247714	0.192943
54	6	0	5.227817	-0.200348	-1.980153
55	6	0	6.442934	-1.397575	0.225828
56	1	0	4.465450	-1.575191	1.037011
57	6	0	6.609350	-0.355908	-1.944568
58	1	0	4.752870	0.231675	-2.852186
59	6	0	7.219996	-0.952339	-0.842894
60	1	0	6.915603	-1.855669	1.086674
61	1	0	7.208968	-0.023157	-2.783488
62	1	0	8.296460	-1.074051	-0.818514
63	6	0	0.863030	1.634741	5.889740
64	1	0	1.728210	2.002681	6.428282
65	6	0	0.973061	1.099929	4.677864
66	1	0	1.955984	1.042233	4.212728
67	6	0	1.020641	5.133461	-2.196565
68	1	0	0.434209	4.820401	-3.061051
69	1	0	1.061617	2.618291	-2.470197
70	1	0	-0.096718	1.725367	6.389093
71	1	0	1.127877	6.211298	-2.103754
72	1	0	3.004440	5.695285	-0.474721
73	1	0	3.904580	5.511868	-1.969131
74	1	0	1.502783	0.187274	1.079984
75	1	0	0.098553	4.725698	-1.325015
76	1	0	-0.677212	0.857551	0.534439
77	8	0	-0.530723	2.232598	-0.381888
78	8	0	-1.043289	4.391901	-0.744925
79	6	0	-1.343987	3.184969	-0.462372
80	6	0	-2.809217	2.958547	-0.183351
81	6	0	-3.475180	1.777825	-0.564070
82	6	0	-3.551920	3.974592	0.431736
83	6	0	-4.841143	1.632460	-0.301329
84	6	0	-5.549740	2.645802	0.334498
85	6	0	-4.905071	3.823555	0.708045
86	8	0	-2.775423	0.792282	-1.201390
87	1	0	-5.345181	0.720977	-0.607608
88	1	0	-3.039563	4.896487	0.676281
89	1	0	-5.455288	4.620552	1.192650
90	1	0	-6.608163	2.515930	0.528986
91	1	0	-3.378972	0.146083	-1.603137

T-SA-COM-2

Energy + zep (gas) = -1976.11695 au
Gibbs free energy (gas) = -1976.19703 au
Gibbs free energy (in solvent) = -1975.46749 au
Zero-point correction = 0.73567 au
Thermal correction to Gibbs free energy = 0.65559 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.465849	-0.768001	1.977547
2	6	0	0.899402	-0.781038	1.416450
3	6	0	-0.865548	-2.093180	2.511134
4	6	0	-0.455126	0.192791	3.104269
5	6	0	0.909121	-1.191649	-0.096708
6	6	0	1.884580	-1.511153	2.365223
7	6	0	0.047117	-2.536467	3.691718
8	6	0	0.653581	-0.161534	4.163601
9	6	0	0.553117	-2.630956	-0.451226
10	6	0	1.226439	-1.552126	3.764514
11	6	0	1.487984	-3.640768	-0.360458
12	6	0	-0.756806	-2.984768	-0.915482
13	6	0	1.161128	-4.964560	-0.738248
14	6	0	-0.976545	-4.357138	-1.270589
15	7	0	-0.017957	-5.319391	-1.184662
16	1	0	-0.835497	-2.821383	1.703597
17	1	0	-1.909328	-2.012679	2.821402
18	1	0	-1.445259	0.175886	3.564915
19	1	0	-0.304501	1.196149	2.700445
20	1	0	0.197492	-0.525950	-0.582050
21	1	0	2.848203	-0.995090	2.393281
22	1	0	2.077374	-2.540043	2.048771
23	1	0	-0.500906	-2.533582	4.637989
24	1	0	0.410941	-3.556301	3.537726
25	1	0	0.180754	-0.281849	5.143205
26	1	0	1.955084	-1.874273	4.510849
27	1	0	2.491609	-3.458818	0.008791
28	6	0	-1.839838	-2.081525	-1.014115
29	1	0	1.913700	-5.744939	-0.663652
30	6	0	-2.257231	-4.752912	-1.724703
31	6	0	2.690119	2.725591	-0.886736

32	6	0	2.070763	1.502178	-0.842083
33	6	0	2.779826	0.277825	-0.988519
34	7	0	2.241063	-0.896293	-0.681276
35	1	0	3.767798	2.764868	-1.019553
36	1	0	1.006157	1.471732	-0.636252
37	1	0	2.792299	-1.705983	-0.935168
38	6	0	2.008607	3.970277	-0.740865
39	6	0	2.681048	5.145030	-0.761084
40	6	0	-3.296741	-3.860523	-1.800375
41	6	0	-3.083006	-2.512814	-1.428396
42	1	0	-2.388335	-5.793437	-1.993060
43	1	0	-4.268852	-4.197335	-2.132939
44	8	0	-4.087748	-1.572290	-1.427395
45	1	0	-1.728512	-1.045186	-0.732328
46	6	0	-5.330098	-1.879704	-2.076860
47	1	0	-5.880982	-2.651553	-1.533064
48	1	0	-5.901093	-0.953593	-2.073960
49	1	0	-5.158057	-2.194656	-3.108492
50	6	0	4.169403	0.214209	-1.505426
51	6	0	5.142041	-0.523108	-0.811933
52	6	0	4.512414	0.845766	-2.710329
53	6	0	6.437190	-0.614150	-1.309879
54	1	0	4.895665	-0.989901	0.135337
55	6	0	5.805270	0.734591	-3.210838
56	1	0	3.760917	1.392316	-3.266659
57	6	0	6.768852	0.010211	-2.511192
58	1	0	7.187960	-1.167122	-0.758415
59	1	0	6.058792	1.209444	-4.150959
60	1	0	7.776609	-0.067892	-2.901360
61	6	0	2.031116	1.514457	5.433786
62	1	0	2.791539	2.286108	5.470566
63	6	0	1.699866	0.910893	4.295614
64	1	0	2.208072	1.214914	3.380680
65	6	0	2.052151	6.484563	-0.622379
66	1	0	2.281676	7.105040	-1.496658
67	1	0	0.928047	3.959385	-0.619276
68	1	0	1.550678	1.259330	6.373502
69	1	0	2.473048	7.014292	0.240466
70	1	0	3.763240	5.125200	-0.886980
71	1	0	1.192502	0.271134	1.385299
72	1	0	0.970191	6.418719	-0.506859
73	1	0	-1.914830	1.071310	0.432895
74	8	0	-1.269834	1.763980	0.174850
75	8	0	-1.253763	3.845918	-0.570821

76	6	0	-1.905842	2.878652	-0.249720
77	6	0	-3.399398	2.859437	-0.316184
78	6	0	-4.188882	1.716829	-0.098113
79	6	0	-4.038158	4.054872	-0.677580
80	6	0	-5.574350	1.778777	-0.241520
81	6	0	-6.182967	2.973523	-0.608104
82	6	0	-5.415011	4.118986	-0.822574
83	8	0	-3.577304	0.552942	0.307027
84	1	0	-6.167722	0.894774	-0.036554
85	1	0	-3.416216	4.923760	-0.849732
86	1	0	-5.890380	5.051426	-1.100012
87	1	0	-7.261034	3.013032	-0.712408
88	1	0	-3.933983	-0.222153	-0.168425

T-SA-TS-2

Energy + zep (gas) = -1976.07572 au
Gibbs free energy (gas) = -1976.15155 au
Gibbs free energy (in solvent) = -1975.42803 au
Zero-point correction = 0.73210 au
Thermal correction to Gibbs free energy = 0.65626 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.468479	-0.388511	1.351860
2	6	0	-0.901046	0.261502	1.229000
3	6	0	1.550759	0.565362	1.784061
4	6	0	0.372970	-1.511805	2.366139
5	6	0	-1.071261	1.205727	-0.031558
6	6	0	-1.281117	0.841427	2.615865
7	6	0	1.135772	1.233132	3.116145
8	6	0	0.099542	-0.949176	3.785290
9	6	0	-0.698567	2.679353	0.099223
10	6	0	-0.155093	0.571987	3.632005
11	6	0	-1.533408	3.574287	0.736645
12	6	0	0.503648	3.202478	-0.482711
13	6	0	-1.192200	4.943949	0.826397
14	6	0	0.757221	4.605539	-0.317277
15	7	0	-0.088708	5.449167	0.331308
16	1	0	1.711085	1.280642	0.983582
17	1	0	2.457897	-0.031095	1.877844
18	1	0	1.312515	-2.059530	2.308314

19	1	0	-0.416376	-2.176353	2.016745
20	1	0	-0.453150	0.778763	-0.818342
21	1	0	-2.220484	0.402183	2.955814
22	1	0	-1.435298	1.917420	2.557636
23	1	0	1.935815	1.127975	3.851698
24	1	0	0.973458	2.303137	2.968815
25	1	0	1.002401	-1.068717	4.391117
26	1	0	-0.429801	0.993142	4.600200
27	1	0	-2.469119	3.260075	1.185404
28	6	0	1.448747	2.431128	-1.197475
29	1	0	-1.863253	5.631982	1.333260
30	6	0	1.945003	5.158074	-0.856298
31	6	0	-2.510865	-2.296189	-1.884899
32	6	0	-2.225936	-0.936772	-1.660935
33	6	0	-3.036038	0.009363	-1.059399
34	7	0	-2.478890	1.097110	-0.444127
35	1	0	-3.439722	-2.719789	-1.510778
36	1	0	-1.194262	-0.665965	-1.848569
37	1	0	-3.062563	1.909327	-0.319021
38	6	0	-1.555907	-3.125977	-2.437444
39	6	0	-1.509550	-4.505466	-2.242077
40	6	0	2.862690	4.381339	-1.517431
41	6	0	2.612023	2.997613	-1.680742
42	1	0	2.102905	6.220231	-0.718509
43	1	0	3.765726	4.831169	-1.906493
44	8	0	3.489147	2.140406	-2.289446
45	1	0	1.302046	1.375927	-1.378450
46	6	0	4.596529	2.675561	-3.028659
47	1	0	5.310951	3.173800	-2.367950
48	1	0	5.074852	1.820056	-3.500717
49	1	0	4.249282	3.368245	-3.798839
50	6	0	-4.509460	-0.075481	-1.014483
51	6	0	-5.220772	0.336162	0.125796
52	6	0	-5.225753	-0.548338	-2.125913
53	6	0	-6.608082	0.262208	0.157275
54	1	0	-4.682795	0.682928	1.000797
55	6	0	-6.614130	-0.616697	-2.090930
56	1	0	-4.691062	-0.828831	-3.024712
57	6	0	-7.307762	-0.213364	-0.951364
58	1	0	-7.144882	0.568615	1.047305
59	1	0	-7.156209	-0.972791	-2.958806
60	1	0	-8.389822	-0.265495	-0.927709
61	6	0	-0.895256	-2.298933	5.651362
62	1	0	-1.729202	-2.816531	6.110257

63	6	0	-1.014193	-1.693085	4.474291
64	1	0	-1.971283	-1.729378	3.955928
65	6	0	-0.346005	-5.260258	-2.481636
66	1	0	0.262924	-4.951312	-3.333069
67	1	0	-0.670611	-2.660123	-2.858068
68	1	0	0.041504	-2.301454	6.200086
69	1	0	-0.405437	-6.336388	-2.349190
70	1	0	-2.343403	-4.971720	-1.718757
71	1	0	-1.543068	-0.586830	0.995037
72	1	0	0.490730	-4.760185	-1.596428
73	1	0	0.719403	-0.902440	0.449431
74	8	0	0.767949	-2.210243	-0.556314
75	8	0	1.583981	-4.262871	-0.984859
76	6	0	1.705783	-3.042147	-0.644450
77	6	0	3.117291	-2.631443	-0.300194
78	6	0	3.626846	-1.353584	-0.599555
79	6	0	3.973689	-3.568283	0.292733
80	6	0	4.951939	-1.038844	-0.281047
81	6	0	5.773542	-1.979051	0.330750
82	6	0	5.284817	-3.250633	0.624803
83	8	0	2.818011	-0.438561	-1.212495
84	1	0	5.335485	-0.052981	-0.525506
85	1	0	3.584726	-4.562369	0.473474
86	1	0	5.924244	-3.990352	1.090372
87	1	0	6.798339	-1.718122	0.568840
88	1	0	3.338170	0.304953	-1.558242

T-SA-TS-I

Energy + zep (gas) = -2015.39725 au
Gibbs free energy (gas) = -2015.47788 au
Gibbs free energy (in solvent) = -2014.74060 au
Zero-point correction = 0.76496 au
Thermal correction to Gibbs free energy = 0.68433 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.781366	4.044125	-2.713990
2	7	0	-0.774590	-0.395692	1.804483
3	6	0	0.556834	-1.014327	1.375050
4	6	0	-1.836403	-1.422007	2.116396
5	6	0	-0.527152	0.456953	3.034591

6	6	0	0.626799	-1.456607	-0.133179
7	6	0	0.945505	-2.059435	2.442999
8	6	0	-1.381718	-2.261831	3.331568
9	6	0	0.073242	-0.407317	4.178586
10	6	0	0.007000	-2.804704	-0.496466
11	6	0	0.065348	-1.880918	3.694784
12	6	0	0.699657	-3.979661	-0.285671
13	6	0	-1.287599	-2.908906	-1.105352
14	6	0	0.140573	-5.225533	-0.654396
15	6	0	-1.761810	-4.224816	-1.425914
16	7	0	-1.044361	-5.357422	-1.199389
17	1	0	-1.981445	-2.022499	1.223642
18	1	0	-2.755720	-0.866232	2.298240
19	1	0	-1.487803	0.895208	3.305181
20	1	0	0.134410	1.261907	2.721864
21	1	0	0.122377	-0.680532	-0.718503
22	1	0	2.002401	-1.950022	2.685054
23	1	0	0.806690	-3.072774	2.065457
24	1	0	-2.042319	-2.090124	4.184397
25	1	0	-1.441305	-3.324052	3.087269
26	1	0	-0.595118	-0.343564	5.041635
27	1	0	0.430112	-2.523602	4.497039
28	1	0	1.687931	-3.974128	0.157777
29	6	0	-2.128200	-1.807447	-1.392091
30	1	0	0.705578	-6.137794	-0.483191
31	6	0	-3.044833	-4.372884	-2.007757
32	6	0	3.057859	2.148349	-0.918276
33	6	0	2.289282	0.924012	-0.793672
34	6	0	2.803194	-0.332666	-0.770675
35	7	0	2.051280	-1.480014	-0.461847
36	1	0	4.135605	2.072528	-0.801590
37	1	0	1.218712	1.060666	-0.683501
38	1	0	2.334865	-2.288739	-0.995480
39	6	0	2.524462	3.362912	-1.140471
40	6	0	3.307097	4.627391	-1.253306
41	6	0	-3.854210	-3.290975	-2.245973
42	6	0	-3.388791	-1.995708	-1.920687
43	1	0	-3.366353	-5.379082	-2.245062
44	1	0	-4.836001	-3.437397	-2.674951
45	8	0	-4.154914	-0.864000	-2.071238
46	1	0	-1.814076	-0.790868	-1.200970
47	6	0	-5.330695	-0.920691	-2.892833
48	1	0	-6.113674	-1.523419	-2.424977
49	1	0	-5.671830	0.107894	-2.990657

50	1	0	-5.090323	-1.317373	-3.881618
51	6	0	4.049129	4.841990	-2.551150
52	6	0	4.230555	-0.654553	-1.044743
53	6	0	4.952598	-1.492967	-0.182266
54	6	0	4.866886	-0.161715	-2.192720
55	6	0	6.281181	-1.809274	-0.448071
56	1	0	4.472737	-1.880561	0.708817
57	6	0	6.194032	-0.485161	-2.460146
58	1	0	4.310973	0.460723	-2.883351
59	6	0	6.905625	-1.306179	-1.587989
60	1	0	6.831051	-2.445808	0.235662
61	1	0	6.670147	-0.102042	-3.355270
62	1	0	7.939218	-1.555996	-1.797095
63	6	0	1.738320	0.415629	5.863149
64	1	0	2.730076	0.760527	6.130310
65	6	0	1.429222	0.087946	4.612635
66	1	0	2.190300	0.179689	3.839546
67	6	0	3.320568	5.526540	-0.267525
68	1	0	2.796179	5.358814	0.667597
69	1	0	1.451264	3.438370	-1.318530
70	1	0	1.011710	0.350738	6.667388
71	1	0	3.869934	6.457614	-0.355866
72	1	0	4.573074	5.799465	-2.560412
73	1	0	3.360631	4.813296	-3.402511
74	1	0	1.243703	-0.169396	1.423423
75	1	0	0.253650	4.020815	0.325388
76	1	0	-1.104161	0.264286	1.078418
77	8	0	-0.814569	2.026440	0.473778
78	8	0	-0.685391	4.234393	0.201148
79	6	0	-1.383931	3.090739	0.265270
80	6	0	-2.830986	3.285124	0.061294
81	6	0	-3.702853	2.194307	-0.147440
82	6	0	-3.359389	4.589643	0.025768
83	6	0	-5.059126	2.434837	-0.387790
84	6	0	-5.554729	3.730932	-0.417954
85	6	0	-4.704763	4.817541	-0.205336
86	8	0	-3.227661	0.919567	-0.109569
87	1	0	-5.724646	1.590685	-0.532598
88	1	0	-2.685799	5.421438	0.178393
89	1	0	-5.090601	5.828670	-0.224344
90	1	0	-6.610557	3.893413	-0.601133
91	1	0	-3.785659	0.344453	-0.666012

SA-CH_3-COM
Energy + zep (gas) = -1823.67813 au
Gibbs free energy (gas) = -1823.75563 au
Gibbs free energy (in solvent) = -1823.08304 au
Zero-point correction = 0.71025 au
Thermal correction to Gibbs free energy = 0.63275 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.581708	-1.615580	-0.342979
2	6	0	0.797500	-1.790707	0.256024
3	6	0	-0.532285	-1.024314	-1.728434
4	6	0	-1.253392	-2.967758	-0.390201
5	6	0	1.446359	-0.466920	0.731097
6	6	0	1.665089	-2.556201	-0.779270
7	6	0	0.159175	-2.014414	-2.691212
8	6	0	-0.407950	-3.968955	-1.229611
9	6	0	2.880191	-0.697612	1.204905
10	6	0	0.759074	-3.166416	-1.864858
11	6	0	3.123076	-1.542891	2.265207
12	6	0	3.991760	-0.035392	0.596470
13	6	0	4.441510	-1.735424	2.736077
14	6	0	5.286196	-0.305338	1.159131
15	7	0	5.486924	-1.142420	2.210007
16	1	0	-0.007921	-0.071926	-1.656982
17	1	0	-1.565844	-0.804616	-1.987560
18	1	0	-2.245318	-2.790440	-0.800519
19	1	0	-1.376204	-3.292333	0.643773
20	1	0	1.444306	0.236495	-0.094041
21	1	0	2.253031	-3.319336	-0.270066
22	1	0	2.381828	-1.878764	-1.251280
23	1	0	-0.555769	-2.405403	-3.418978
24	1	0	0.943119	-1.505949	-3.256663
25	1	0	-1.029920	-4.339362	-2.049409
26	1	0	1.345679	-3.826986	-2.504749
27	1	0	2.319001	-2.076791	2.762575
28	6	0	3.906246	0.847391	-0.502927
29	1	0	4.624116	-2.402106	3.574206
30	6	0	6.421238	0.328171	0.596941
31	6	0	-0.876227	3.184892	0.592760
32	6	0	0.092176	2.237950	0.793343
33	6	0	-0.008952	1.280333	1.841104

34	7	0	0.658231	0.133418	1.818856
35	1	0	-1.759403	3.137046	1.217101
36	1	0	0.937654	2.189832	0.116476
37	1	0	0.573099	-0.436107	2.650830
38	6	0	-0.840257	4.169216	-0.436115
39	6	0	-1.864845	5.020793	-0.722176
40	6	0	6.310899	1.184314	-0.468651
41	6	0	5.035361	1.449171	-1.031048
42	1	0	7.382553	0.107420	1.043489
43	1	0	7.198047	1.651456	-0.873399
44	8	0	4.830102	2.276069	-2.083259
45	1	0	2.965164	1.090465	-0.978760
46	6	0	5.945366	2.939809	-2.683409
47	1	0	6.661545	2.222138	-3.094039
48	1	0	5.527920	3.534513	-3.492843
49	1	0	6.445938	3.600517	-1.969622
50	6	0	-3.197072	5.008086	-0.030698
51	6	0	-0.841721	1.537041	3.051758
52	6	0	-0.211098	-6.425286	-0.753724
53	1	0	0.138259	-7.250673	-0.144959
54	6	0	0.041354	-5.162034	-0.426406
55	1	0	0.606647	-4.959552	0.482441
56	6	0	-1.701732	6.057220	-1.792651
57	1	0	-0.696117	6.070980	-2.213722
58	1	0	-2.419614	5.882119	-2.602083
59	1	0	0.070868	4.246955	-1.024367
60	1	0	-0.778197	-6.681959	-1.643267
61	1	0	-1.929729	7.052059	-1.394111
62	1	0	-3.995030	5.134857	-0.768443
63	1	0	-3.268282	5.869018	0.645272
64	1	0	-0.515143	2.452080	3.549841
65	1	0	-0.798957	0.705599	3.756801
66	1	0	-1.258569	-0.984799	0.221926
67	1	0	-3.400579	4.098212	0.531964
68	1	0	0.636165	-2.416609	1.137162
69	1	0	-1.883725	1.661877	2.721651
70	6	0	-4.720883	-0.044239	0.435988
71	6	0	-5.861289	0.307550	1.171608
72	6	0	-7.124715	-0.175108	0.856664
73	6	0	-7.278756	-1.016188	-0.242267
74	6	0	-4.900438	-0.886445	-0.670130
75	6	0	-6.169386	-1.363271	-1.003794
76	6	0	-3.398690	0.538085	0.899811
77	1	0	-5.722543	0.986316	2.003196

78	8	0	-3.820720	-1.233327	-1.467370
79	1	0	-6.286663	-2.009406	-1.870090
80	1	0	-8.255898	-1.398561	-0.513086
81	1	0	-7.981657	0.108300	1.455506
82	8	0	-3.439649	1.674471	1.408942
83	8	0	-2.340364	-0.173405	0.813698
84	1	0	-4.180236	-1.635619	-2.266305

SA-CH_3-TSA

Energy + zep (gas) = -1823.64533 au
Gibbs free energy (gas) = -1823.71993 au
Gibbs free energy (in solvent) = -1823.07042 au
Zero-point correction = 0.70590 au
Thermal correction to Gibbs free energy = 0.63130 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.526968	-0.605877	-1.154977
2	7	0	-0.166639	-1.042454	1.238814
3	6	0	-0.994560	-1.908655	0.299597
4	6	0	-1.001930	-0.106871	2.071127
5	6	0	0.622011	-1.953461	2.157473
6	6	0	-1.461726	-1.163045	-1.022149
7	6	0	-2.071602	-2.630385	1.144315
8	6	0	-1.948682	-0.936775	2.971165
9	6	0	-0.329484	-2.852014	2.994076
10	6	0	-2.849608	-0.529314	-1.031967
11	6	0	-1.780455	-2.431922	2.644521
12	6	0	-3.977416	-1.297825	-1.224308
13	6	0	-3.034360	0.883760	-0.883881
14	6	0	-5.260866	-0.705017	-1.242486
15	6	0	-4.382121	1.376302	-0.899308
16	7	0	-5.468672	0.579160	-1.075658
17	1	0	-1.536766	0.552108	1.393411
18	1	0	-0.303259	0.503475	2.641821
19	1	0	1.234169	-1.301909	2.780387
20	1	0	1.296109	-2.524105	1.520257
21	1	0	-0.721718	-0.388869	-1.195954
22	1	0	-2.094803	-3.691217	0.886925
23	1	0	-3.061742	-2.226624	0.932173
24	1	0	-1.727370	-0.755556	4.025206

25	1	0	-2.983834	-0.632119	2.803699
26	1	0	-0.172970	-2.629272	4.052982
27	1	0	-2.480531	-3.025005	3.234548
28	1	0	-3.916565	-2.371005	-1.366893
29	6	0	-1.981397	1.814200	-0.725265
30	1	0	-6.138014	-1.327835	-1.395246
31	6	0	-4.607748	2.764403	-0.728918
32	6	0	2.067972	-1.282942	-3.278876
33	6	0	0.675571	-1.187076	-3.080428
34	6	0	-0.149905	-2.261636	-2.842216
35	7	0	-1.315941	-2.113749	-2.136314
36	1	0	2.522567	-2.265913	-3.199740
37	1	0	0.281036	-0.190796	-2.915712
38	1	0	-1.915014	-2.925594	-2.101872
39	6	0	2.904066	-0.202074	-3.434902
40	6	0	4.289274	-0.225061	-3.140942
41	6	0	-3.570522	3.643086	-0.540909
42	6	0	-2.240836	3.157109	-0.534305
43	1	0	-5.635471	3.104420	-0.748422
44	1	0	-3.777211	4.695468	-0.403387
45	8	0	-1.148348	3.957474	-0.323046
46	1	0	-0.945685	1.506649	-0.740500
47	6	0	-1.308721	5.382669	-0.339678
48	1	0	-1.910203	5.724319	0.506984
49	1	0	-0.304105	5.792625	-0.259016
50	1	0	-1.760144	5.711668	-1.278660
51	6	0	4.863135	-1.192337	-2.290531
52	6	0	0.225407	-5.174042	3.767684
53	1	0	0.412529	-6.222731	3.569742
54	6	0	-0.052437	-4.318684	2.789099
55	1	0	-0.081867	-4.683203	1.763320
56	6	0	5.130549	0.942704	-3.568904
57	1	0	5.622380	0.692310	-4.516742
58	1	0	4.533106	1.840085	-3.737443
59	1	0	2.464195	0.759427	-3.684053
60	1	0	0.277348	-4.857091	4.804803
61	1	0	5.914153	1.161458	-2.842079
62	1	0	5.948423	-1.260776	-2.275282
63	1	0	4.347500	-2.142481	-2.162507
64	6	0	0.135305	-3.658697	-3.317858
65	1	0	0.989412	-3.691856	-3.990382
66	1	0	0.310884	-4.340811	-2.478923
67	1	0	-0.728385	-4.040190	-3.873193
68	1	0	-0.260521	-2.629928	-0.058808

69	1	0	0.598510	-0.535865	0.688529
70	8	0	2.063848	-0.401334	-0.035640
71	8	0	4.259631	0.076488	-0.041856
72	6	0	3.065196	0.241468	0.365439
73	6	0	2.917795	1.291457	1.440537
74	6	0	1.852865	2.209717	1.448478
75	6	0	3.895944	1.393994	2.436570
76	6	0	1.773651	3.180838	2.450827
77	6	0	2.743798	3.245277	3.445735
78	6	0	3.809013	2.346924	3.444917
79	8	0	0.914936	2.138311	0.456379
80	1	0	0.951835	3.890321	2.440118
81	1	0	4.737334	0.713663	2.393523
82	1	0	4.572600	2.400851	4.210981
83	1	0	2.669303	4.004495	4.215709
84	1	0	0.380971	2.948633	0.417717

SA-CH_3-TSB

Energy + zep (gas) = -1823.67221 au
Gibbs free energy (gas) = -1823.74977 au
Gibbs free energy (in solvent) = -1823.04827 au
Zero-point correction = 0.70614 au
Thermal correction to Gibbs free energy = 0.62858 au

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.660104	-1.808209	-0.180514
2	6	0	0.747731	-1.912427	0.367194
3	6	0	-0.710117	-1.194632	-1.557915
4	6	0	-1.273772	-3.187955	-0.223017
5	6	0	1.302655	-0.548259	0.841694
6	6	0	1.613500	-2.630151	-0.700084
7	6	0	0.026936	-2.116129	-2.554897
8	6	0	-0.414446	-4.125774	-1.120192
9	6	0	2.752462	-0.696651	1.304964
10	6	0	0.698264	-3.257508	-1.769904
11	6	0	3.035027	-1.399073	2.455038
12	6	0	3.841711	-0.115018	0.583190
13	6	0	4.369623	-1.534114	2.899372
14	6	0	5.155188	-0.311825	1.130280
15	7	0	5.395771	-1.014262	2.268120

16	1	0	-0.265870	-0.202319	-1.489199
17	1	0	-1.768560	-1.066852	-1.779908
18	1	0	-2.292920	-3.050992	-0.580398
19	1	0	-1.330184	-3.539170	0.807874
20	1	0	1.258995	0.152460	0.012564
21	1	0	2.240087	-3.379670	-0.217237
22	1	0	2.293261	-1.923275	-1.181793
23	1	0	-0.673210	-2.522289	-3.288404
24	1	0	0.777016	-1.548765	-3.109820
25	1	0	-1.047110	-4.500805	-1.929436
26	1	0	1.291688	-3.878941	-2.441752
27	1	0	2.248850	-1.853049	3.049683
28	6	0	3.714510	0.629594	-0.611751
29	1	0	4.582458	-2.090344	3.808089
30	6	0	6.267108	0.251419	0.457751
31	6	0	-0.465347	3.288505	0.685003
32	6	0	0.335282	2.257307	1.059844
33	6	0	-0.091504	1.230757	1.990968
34	7	0	0.443237	-0.006228	1.897482
35	1	0	-1.483741	3.300848	1.056738
36	1	0	1.343643	2.196036	0.663823
37	1	0	0.215937	-0.634107	2.656299
38	6	0	-0.056438	4.346669	-0.194136
39	6	0	-0.834066	5.373806	-0.617344
40	6	0	6.116757	0.974219	-0.698102
41	6	0	4.821720	1.168287	-1.244021
42	1	0	7.243991	0.087953	0.895176
43	1	0	6.987276	1.391881	-1.184717
44	8	0	4.576453	1.866797	-2.379080
45	1	0	2.755817	0.812475	-1.079463
46	6	0	5.668740	2.450028	-3.093206
47	1	0	6.371362	1.686264	-3.439262
48	1	0	5.222705	2.944526	-3.953341
49	1	0	6.194042	3.190039	-2.482247
50	6	0	-2.279195	5.562870	-0.253577
51	6	0	-1.115116	1.458315	2.943643
52	6	0	-0.107088	-6.582201	-0.708773
53	1	0	0.299336	-7.406326	-0.134772
54	6	0	0.112851	-5.317669	-0.363790
55	1	0	0.710911	-5.111269	0.522809
56	6	0	-0.260858	6.436907	-1.510065
57	1	0	0.790012	6.260787	-1.742087
58	1	0	-0.821352	6.494115	-2.449952
59	1	0	0.976878	4.320643	-0.531861

60	1	0	-0.702626	-6.841299	-1.578834
61	1	0	-0.350978	7.421873	-1.038259
62	1	0	-2.881152	5.665579	-1.162677
63	1	0	-2.404011	6.497715	0.304161
64	1	0	-1.157060	2.462196	3.354226
65	1	0	-1.247439	0.681128	3.695069
66	1	0	-1.303893	-1.227465	0.424627
67	1	0	-2.701560	4.753347	0.338859
68	1	0	0.649907	-2.550764	1.249670
69	1	0	-2.240721	1.372457	2.222750
70	6	0	-4.905629	0.097776	0.339762
71	6	0	-5.967325	0.855386	0.856240
72	6	0	-7.258747	0.744457	0.361627
73	6	0	-7.510217	-0.131818	-0.691586
74	6	0	-5.175892	-0.777018	-0.728803
75	6	0	-6.473412	-0.879965	-1.234908
76	6	0	-3.552648	0.252344	0.968525
77	1	0	-5.744957	1.535757	1.667464
78	8	0	-4.164449	-1.509013	-1.309702
79	1	0	-6.669335	-1.554863	-2.063869
80	1	0	-8.510431	-0.233426	-1.096117
81	1	0	-8.060177	1.333103	0.790212
82	8	0	-3.358013	1.359702	1.584648
83	8	0	-2.712676	-0.670851	0.902071
84	1	0	-4.549231	-1.980138	-2.057933
