

† *Electronic Supplementary Information*

**DFT Study of Ni-Catalyzed Intramolecular Asymmetric *anti*-Hydrometalative
Cyclization of Alkynone: Mechanism and Origins of Selectivity**

Jinxia Li^a, Dingyi Tang^a, Yu Zhang^a, Weichi Chen^a, Xiaoxi Su^a, Peiyuan Yu^{*b}, Shuanglin Qu^{*a}

^a*College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, P. R. China.*

^b*Department of Chemistry, Southern University of Science and Technology, Shenzhen 518055, P. R.*

China.

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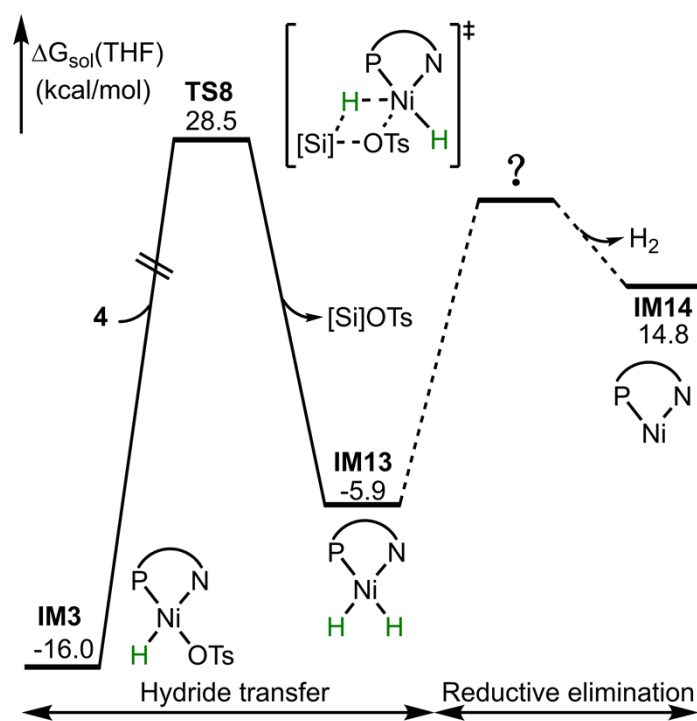


Fig. S1. Free energy profile of the formation of Ni(0) catalyst from the intermediate **IM3**.

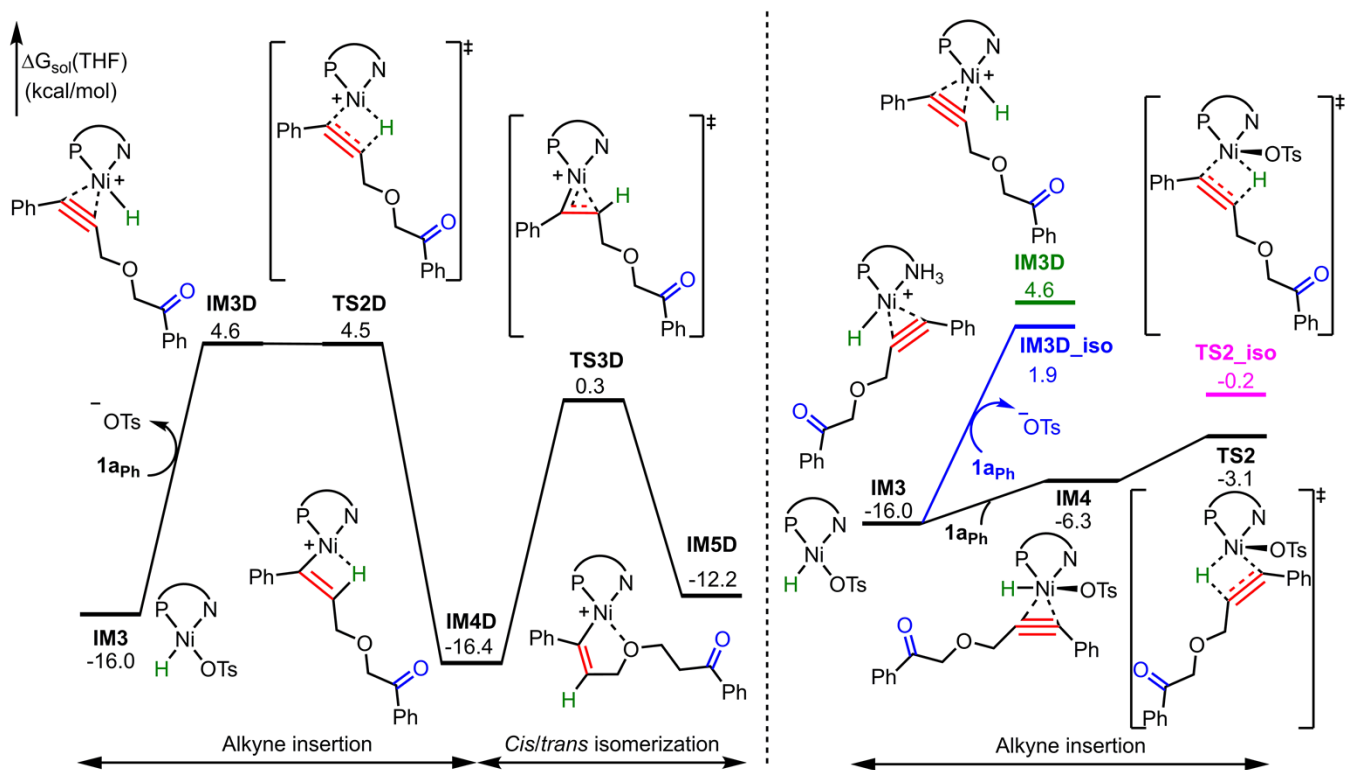


Fig. S2. Free energy profiles of the possible cationic alkyne insertion, *cis/trans* isomerization steps.

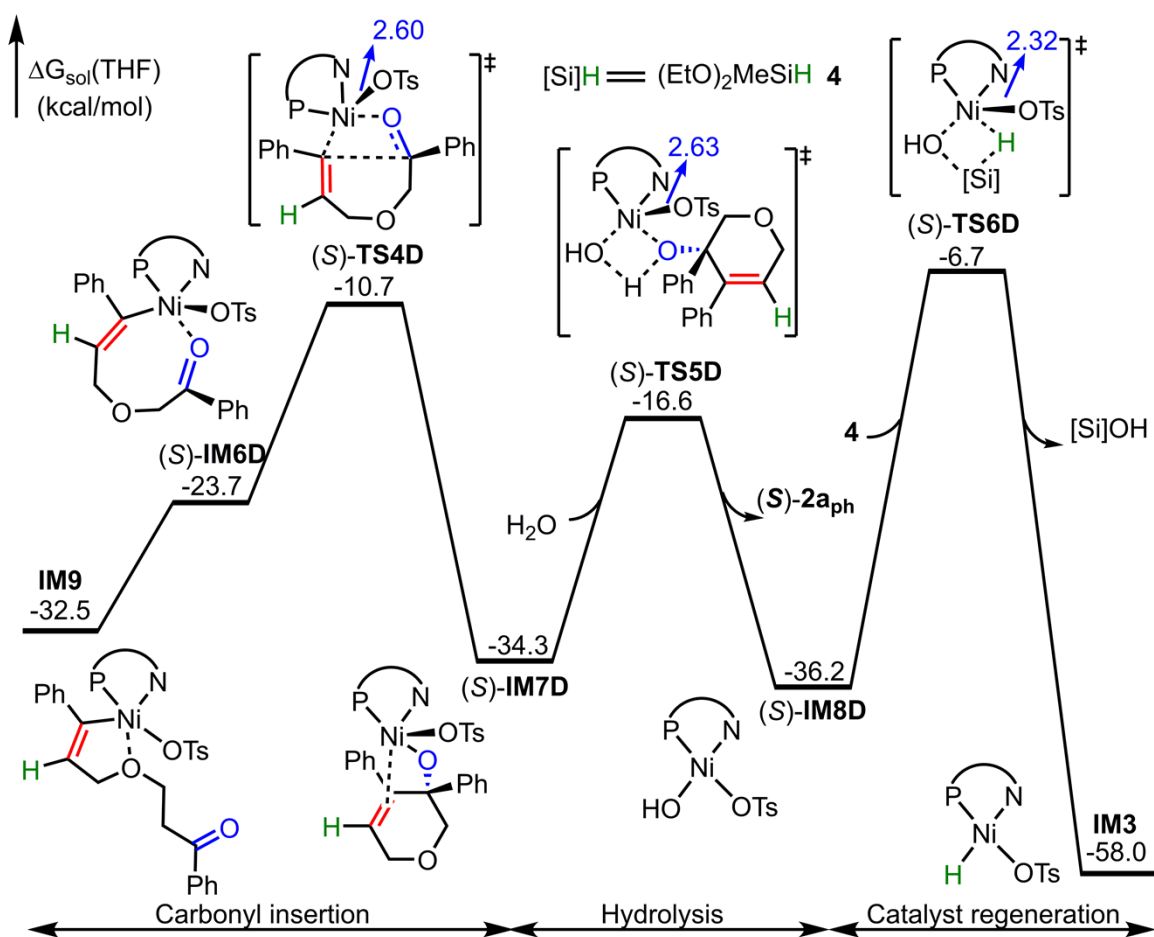


Fig. S3 Free energy profile of the possible neutral carbonyl insertion, hydrolysis, and catalyst regeneration steps to generate 6-endocyclic product (S)-2a_{ph}.

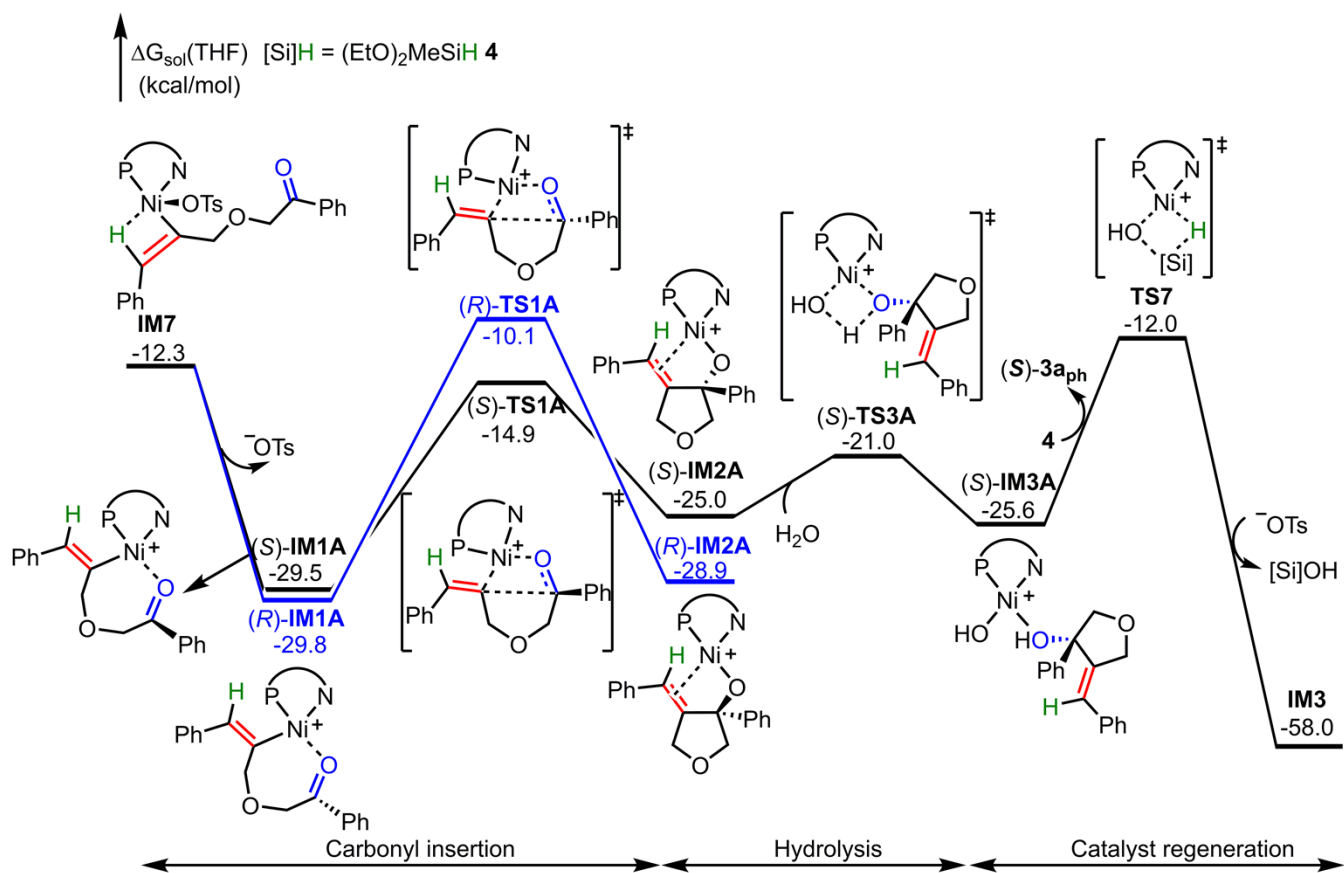


Fig. S4 Free energy profile of Ni(II)H-catalyzed asymmetric hydrometalative cyclization of Ph-alkynone to generate 5-exocyclic product (*S*)-3a_{ph}.

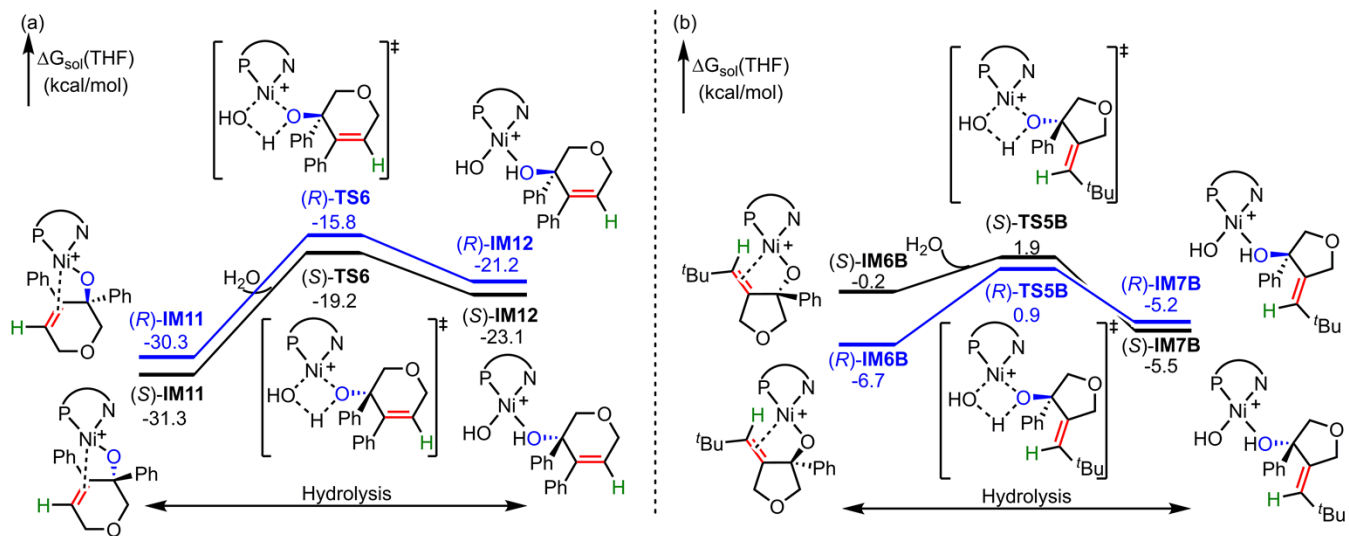


Fig. S5 Free energy profiles of the hydrolysis steps of (a) Ph-alkynone, (b) ^tBu-alkynone.

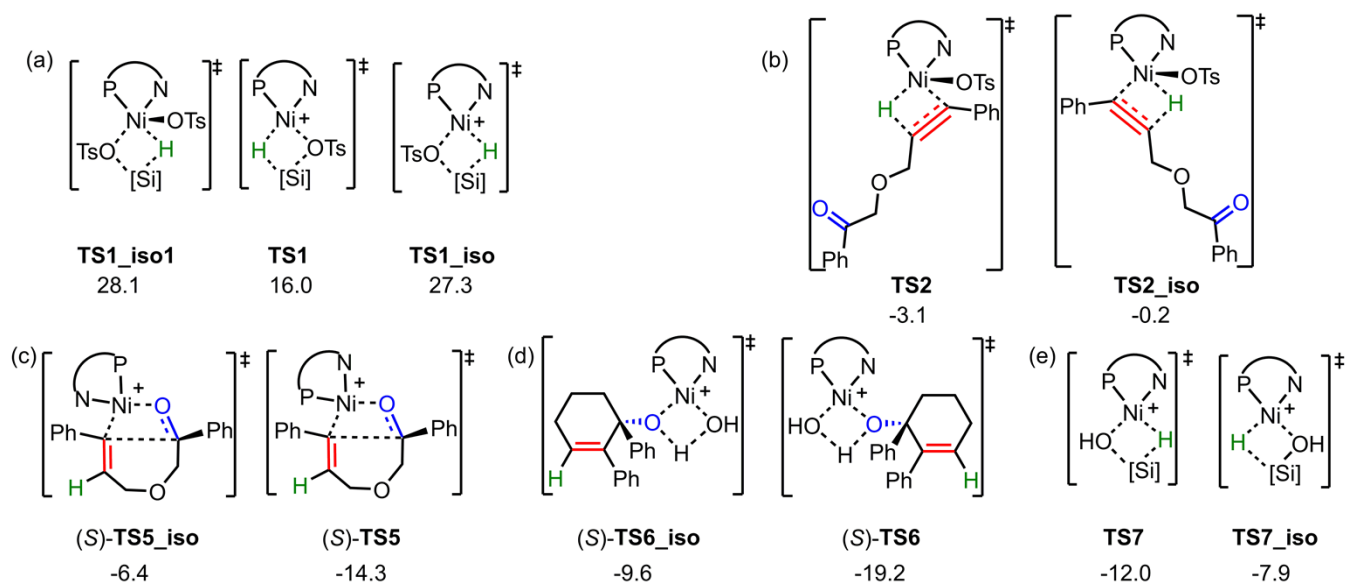


Fig. S6. Calculated relative energies of other possible scenarios of (a) hydride transfer **TS1/TS1_iso/TS1_iso1**, (b) alkyne insertion **TS2/TS2_iso**, (c) carbonyl insertion **(S)-TS5/(S)-TS5_iso**, (d) hydrolysis **(S)-TS6/(S)-TS6_iso**, (e) hydride transfer **TS7/TS7_iso**.

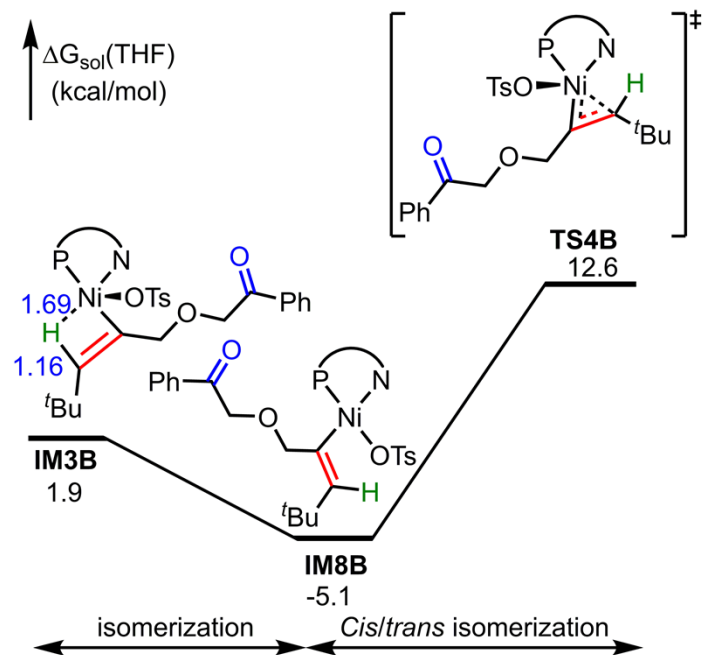


Fig. S7. Free energy profile for the possible *cis/trans* isomerization steps of **1a'**_{Bu}.

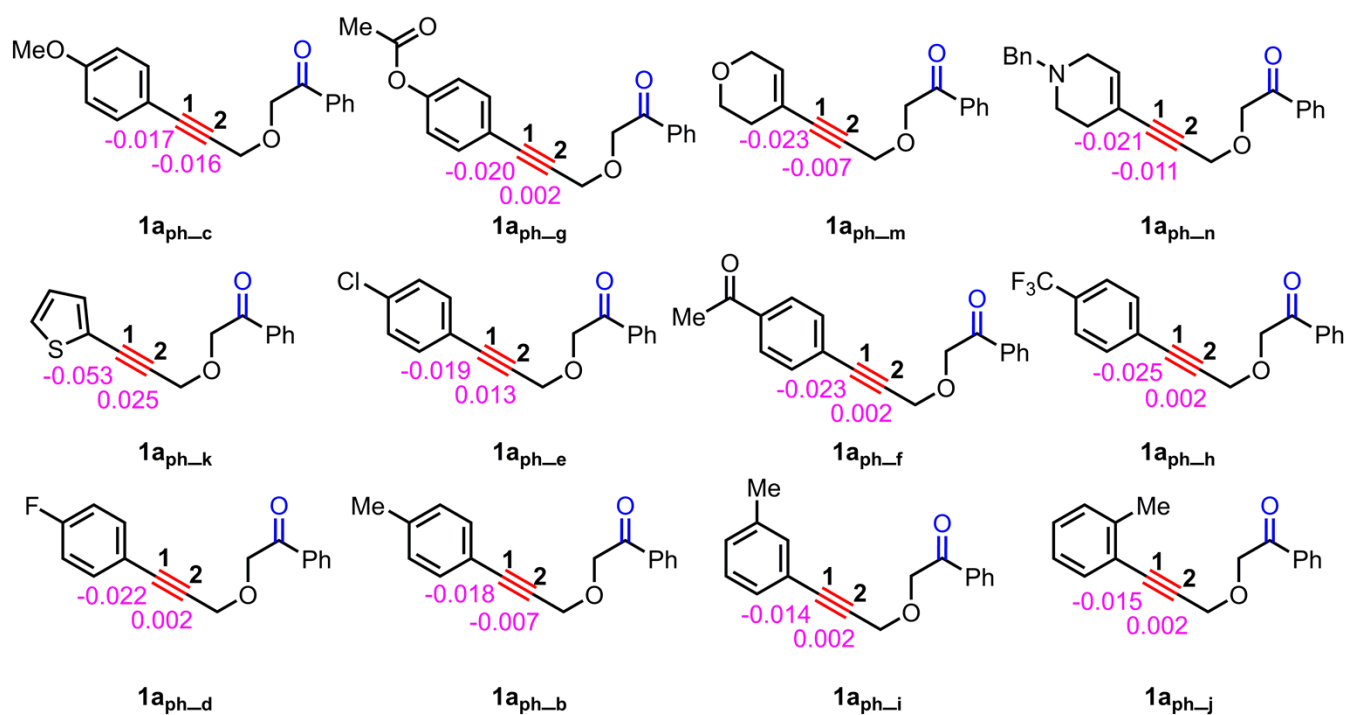


Fig. S8. The calculated NPA charges of various aryl-substituted alkynones and alkenyl-substituted alkynones.

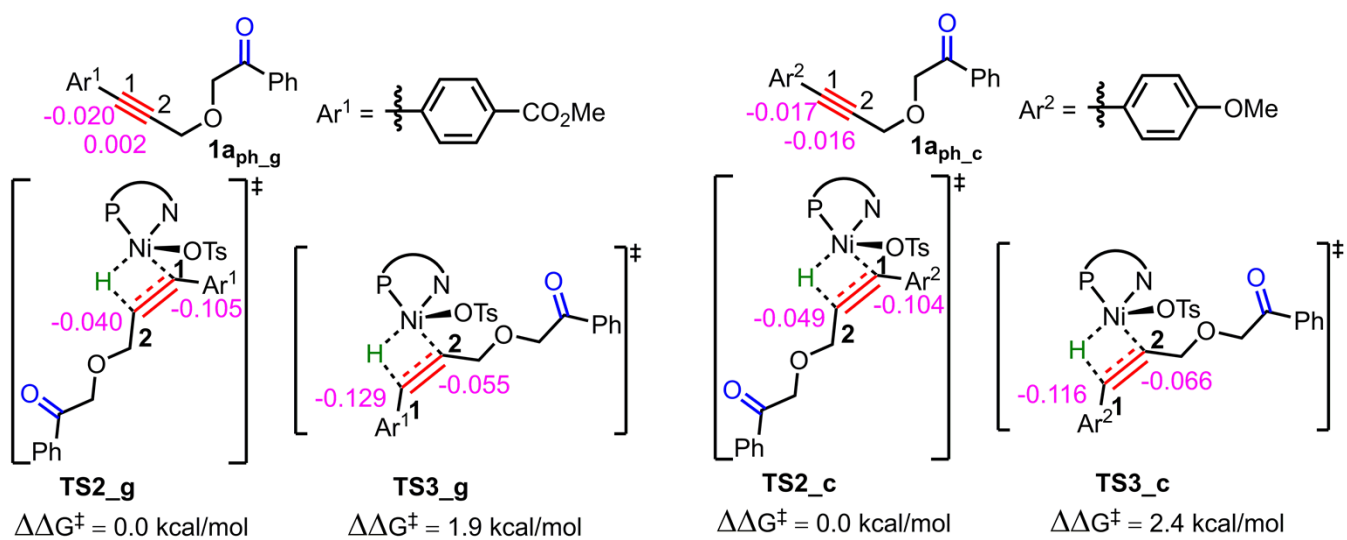


Fig. S9. The two insertion modes for substrates of **1a_{ph_g}** and **1a_{ph_c}**.

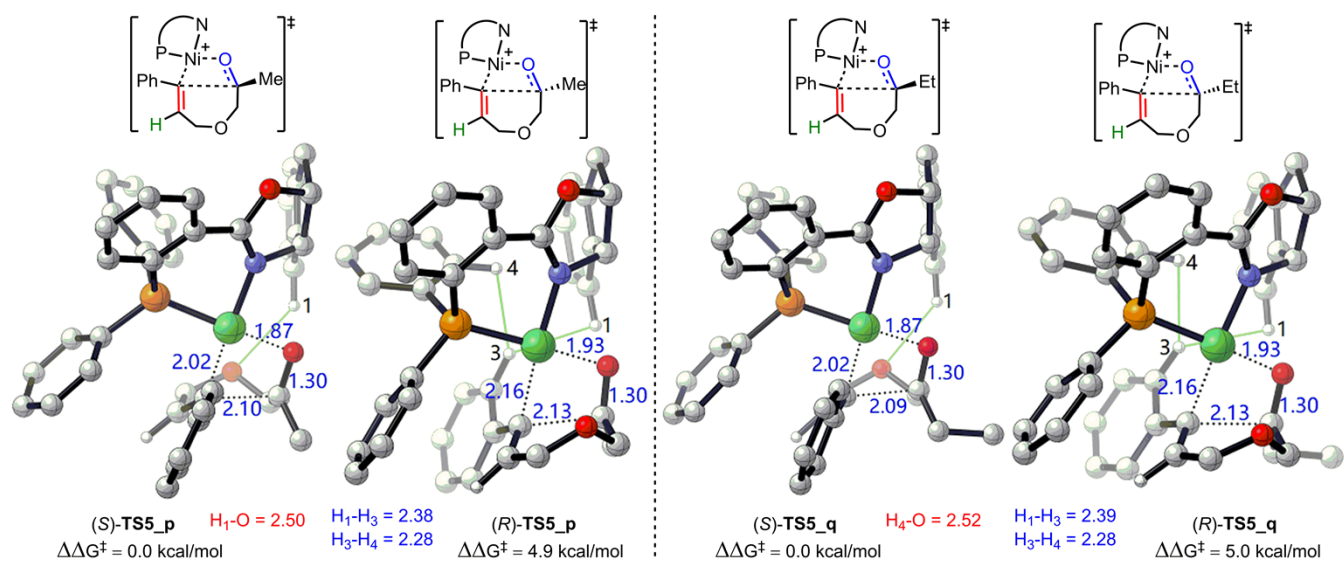


Fig. S10. The possible carbonyl insertion transition states for substrates of **1a_{ph_p}** and **1a_{ph_q}**. Selected bond distances given in angstroms.

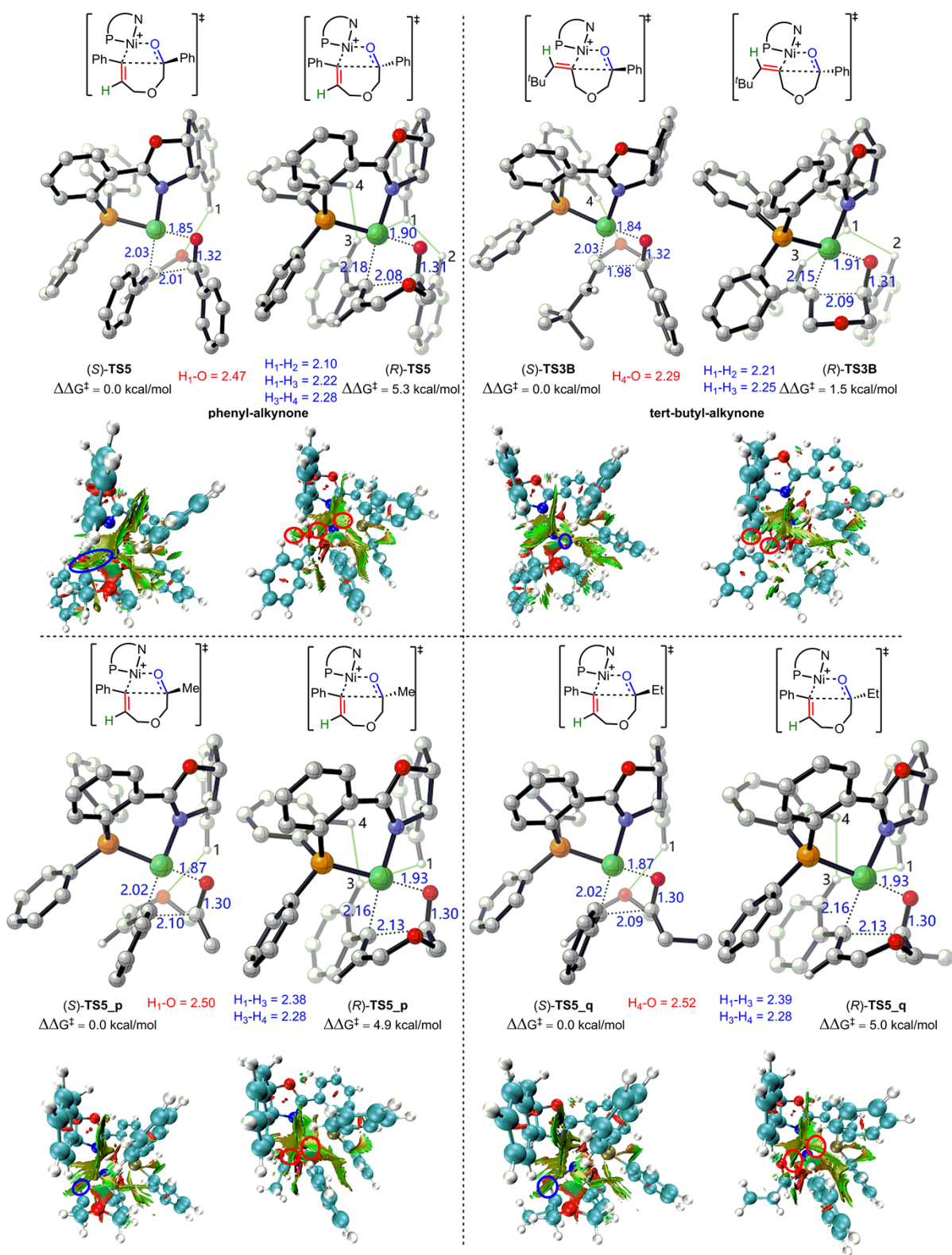


Fig. S11. NCI analysis of (S)-TS5, (R)-TS5, (S)-TS3B, (R)-TS3B, (S)-TS5_p, (R)-TS5_p, (S)-TS5_q, and (R)-TS5_q, with key steric repulsions highlighted by the red circles and hydrogen bonds labeled by the blue circle.

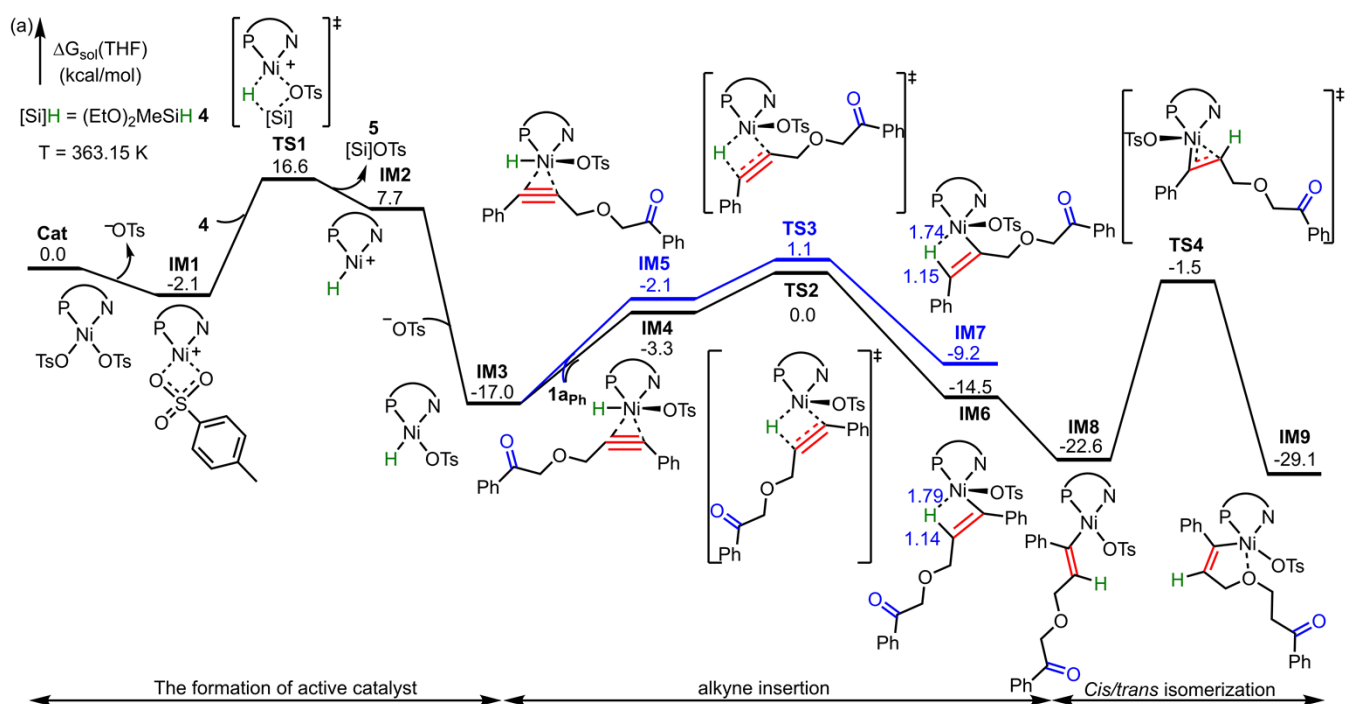


Fig. S12. Free energy profiles at 363.15 K for the initial steps of active catalyst formation, alkyne insertion, and *cis/trans* isomerization in the Ni(II)H-catalyzed asymmetric *anti*-hydrometalative cyclization .

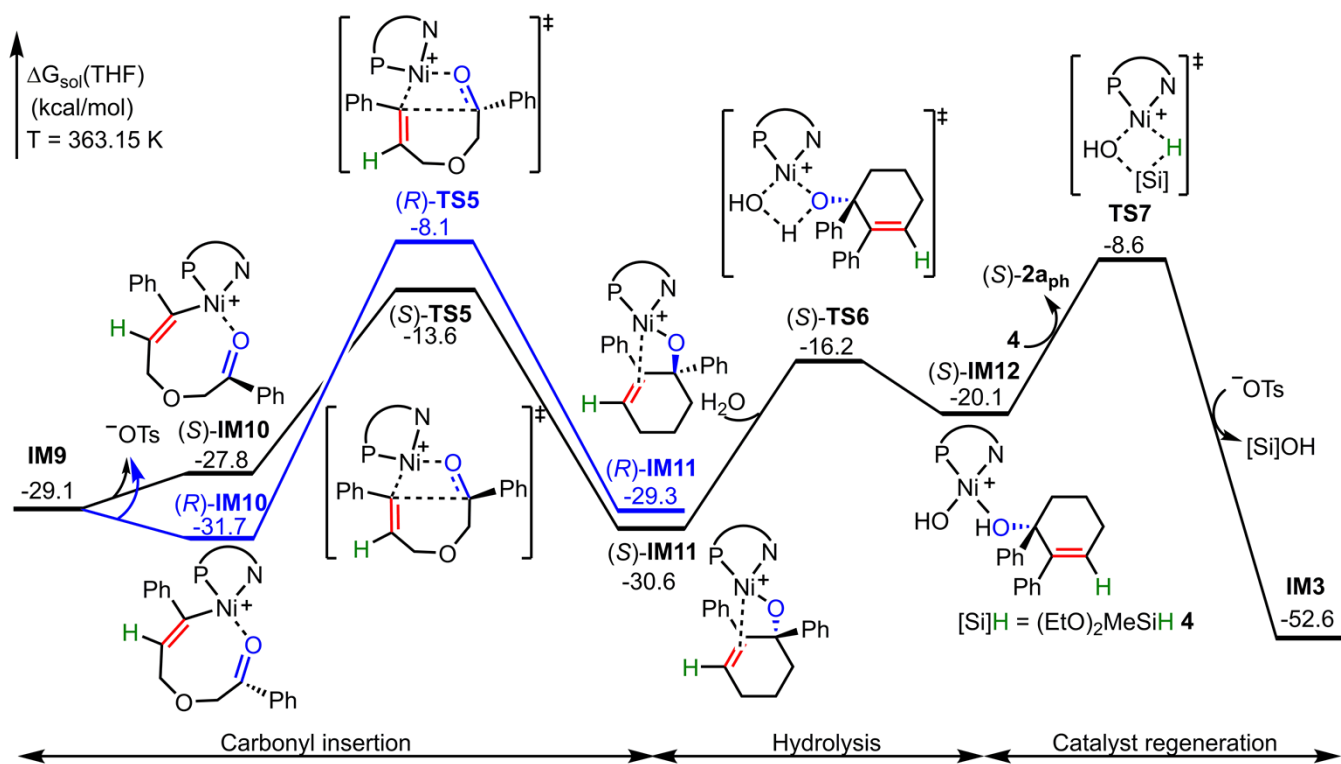


Fig. S13. Free energy profiles at 363.15 K for the final steps of carbonyl insertion, hydrolysis, and catalyst regeneration to produce 6-endocyclic product (S)-2a_{ph}.

Table S1. The calculated energies barrier differences ($\Delta\Delta G^\ddagger$) of regioselectivity-determining transition states by using various density functionals in THF. Values are given in kcal/mol.

Energy Functionals	$\Delta\Delta G^\ddagger$ (TS3- TS2)	$\Delta\Delta G^\ddagger$ (TS2B- TS1B)
M06	1.2	1.5
M06-L	3.0	2.5
M06-2X	6.0	3.0
MN15	4.4	2.7
ωb97X-D	2.0	2.6

Table S2. The calculated energies barrier differences ($\Delta\Delta G^\ddagger$) of enantioselectivity-determining transition states by using various density functionals in THF. Values are given in kcal/mol.

Energy Functionals	$\Delta\Delta G^\ddagger$ ((R)-TS5-(S)-TS5)	$\Delta\Delta G^\ddagger$ ((R)-TS3B-(S)-TS3B)	$\Delta\Delta G^\ddagger$ ((R)-TS1A-(S)-TS1A)
M06	5.3	1.5	4.7
M06-L	8.4	2.3	5.1
M06-2X	5.0	2.1	3.3
MN15	7.4	1.7	5.6
ωb97X-D	7.3	3.2	5.0

Cartesian coordinates of DFT-optimized structures for all intermediates and transition states

1a_{ph_b}				1	-6.109843	-0.649030	2.205288
SCF Energy = -846.012917				6	-2.103178	-0.829171	-0.089461
Gibbs Free Energy = -845.776948				6	-0.930794	-1.120012	-0.182564
6	2.577802	-0.720368	0.002731	6	0.468726	-1.500847	-0.303854
6	1.412135	-1.049234	0.003939	1	0.663758	-1.897403	-1.315643
6	0.020508	-1.477726	0.005566	1	0.696424	-2.317023	0.403705
1	-0.176996	-2.103731	0.893152	8	1.307623	-0.380378	-0.047704
1	-0.176929	-2.110572	-0.877165	6	2.661833	-0.717366	-0.154712
8	-0.840414	-0.345698	0.001191	1	2.942697	-1.510197	0.562252
6	-2.188064	-0.724678	0.002574	1	2.907207	-1.106677	-1.159665
1	-2.439020	-1.341082	-0.879727	6	3.521927	0.514919	0.115181
1	-2.439036	-1.334625	0.889350	8	3.016000	1.590379	0.372962
6	-3.072097	0.520334	-0.001946	6	5.008065	0.343521	0.048169
8	-2.586626	1.635344	-0.005914	6	5.805833	1.470077	0.294415
6	-4.554585	0.310200	-0.001249	6	5.624305	-0.881118	-0.247194
6	-5.374120	1.448007	-0.005282	6	7.192152	1.375512	0.246689
6	-5.146957	-0.960949	0.003224	1	5.308335	2.406570	0.520754
6	-6.758459	1.318868	-0.004852	6	7.013905	-0.975081	-0.294916
1	-4.894902	2.420676	-0.008704	1	5.029150	-1.767019	-0.441390
6	-6.534588	-1.089537	0.003644	6	7.798951	0.151861	-0.048295
1	-4.534710	-1.856434	0.006394	1	7.802493	2.252468	0.438661
6	-7.341416	0.048948	-0.000389	1	7.483593	-1.926425	-0.524151
1	-7.385778	2.204791	-0.007990	1	8.881467	0.076910	-0.085782
1	-6.985770	-2.076763	0.007116	8	-7.516170	0.489825	0.445303
1	-8.422367	-0.052997	-0.000050	6	-8.226708	1.140513	-0.596679
6	3.949905	-0.329782	0.001333	1	-9.243406	1.278031	-0.227392
6	4.638440	-0.120674	1.209564	1	-7.790592	2.119492	-0.831133
6	4.641781	-0.140992	-1.208410	1	-8.251808	0.531304	-1.508812
6	5.974735	0.262251	1.200987	1a_{ph_d}			
1	4.111368	-0.255851	2.147913	SCF Energy = -905.91877			
6	5.978000	0.241996	-1.202631	Gibbs Free Energy = -905.716369			
1	4.117245	-0.291933	-2.145780	6	-2.601765	-0.714480	0.000056
6	6.669261	0.447263	-0.001482	6	-1.438059	-1.049314	0.000140
1	6.489910	0.424005	2.143966	6	-0.047217	-1.481572	0.000206
1	6.495759	0.387864	-2.146797	1	0.147521	-2.111921	-0.884838
6	8.127260	0.831281	-0.002939	1	0.147505	-2.111655	0.885447
1	8.768903	-0.058602	-0.002555	8	0.814512	-0.351220	0.000046
1	8.385063	1.417418	-0.889645	6	2.162495	-0.731050	0.000058
1	8.386337	1.419407	0.882019	1	2.412761	-1.343998	0.884775
1a_{ph_c}				1	2.412725	-1.344172	-0.884545
SCF Energy = -921.219379				6	3.045972	0.514672	-0.000082
Gibbs Free Energy = -920.977701				8	2.558843	1.628964	-0.000191
6	-5.497958	0.494332	-0.934792	6	4.528225	0.305579	-0.000050
6	-4.151771	0.151602	-1.035199	6	5.347064	1.443937	-0.000119
6	-3.481462	-0.483182	0.021880	6	5.121254	-0.965307	0.000047
6	-4.206032	-0.769206	1.197623	6	6.731451	1.315512	-0.000092
6	-5.544768	-0.433780	1.305123	1	4.867429	2.416399	-0.000194
6	-6.201312	0.201049	0.239830	6	6.508922	-1.093117	0.000075
1	-5.983837	0.985272	-1.768495	1	4.509597	-1.861224	0.000095
1	-3.605554	0.380018	-1.943983	6	7.315061	0.045881	0.000005
1	-3.700011	-1.256639	2.023840	1	7.358294	2.201754	-0.000152
				1	6.960694	-2.080061	0.000153

1	8.396054	-0.055461	0.000035
6	-3.971372	-0.316041	0.000016
6	-4.658190	-0.116458	-1.212313
6	-4.658085	-0.115920	1.212317
6	-5.993809	0.270624	-1.217027
1	-4.131906	-0.266241	-2.148307
6	-5.993705	0.271166	1.216974
1	-4.131724	-0.265289	2.148334
6	-6.639807	0.457586	-0.000039
1	-6.537065	0.429608	-2.141450
1	-6.536881	0.430564	2.141374
9	-7.934717	0.832174	-0.000067

1a_{ph_e}

SCF Energy = -1266.284745

Gibbs Free Energy = -1266.084492

6	-2.111937	0.861001	-0.000001
6	-0.944550	1.181631	-0.000001
6	0.455108	1.587168	0.000028
1	0.662926	2.214042	0.885064
1	0.662955	2.214073	-0.884979
8	1.285960	0.436717	0.000020
6	2.644513	0.778787	0.000033
1	2.911255	1.384064	-0.884868
1	2.911249	1.384019	0.884965
6	3.490535	-0.493022	-0.000000
8	2.968900	-1.591654	-0.000028
6	4.977868	-0.328663	-0.000002
6	5.762375	-1.490995	-0.000073
6	5.608378	0.924080	0.000064
6	7.149942	-1.403750	-0.000079
1	5.254176	-2.448827	-0.000122
6	6.999186	1.010540	0.000059
1	5.023734	1.837867	0.000122
6	7.771003	-0.152006	-0.000013
1	7.750170	-2.308205	-0.000136
1	7.480162	1.983561	0.000112
1	8.854517	-0.082887	-0.000018
6	-3.480186	0.460193	-0.000005
6	-4.510479	1.417408	-0.000104
6	-3.820490	-0.904886	0.000094
6	-5.844601	1.024969	-0.000101
1	-4.256805	2.471723	-0.000181
6	-5.152520	-1.303731	0.000092
1	-3.030754	-1.647788	0.000170
6	-6.154611	-0.334232	-0.000003
1	-6.638612	1.762518	-0.000177
1	-5.414817	-2.355211	0.000166
17	-7.838015	-0.833906	0.000001

1a_{ph_f}

SCF Energy = -959.347935

Gibbs Free Energy = -959.102897

6	-1.753330	-0.946984	0.000073
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6	-0.580378	-1.247963	0.000126
6	0.825529	-1.629951	0.000162
1	1.041988	-2.254187	-0.884631
1	1.042072	-2.253742	0.885248
8	1.637783	-0.466765	-0.000157
6	3.001909	-0.787133	-0.000217
1	3.278100	-1.388080	0.884641
1	3.278077	-1.387806	-0.885275
6	3.827114	0.498377	-0.000032
8	3.287283	1.588202	0.000093
6	5.316769	0.358215	-0.000010
6	6.082364	1.533108	0.000301
6	5.967426	-0.884199	-0.000315
6	7.471151	1.468279	0.000336
1	5.558810	2.482630	0.000515
6	7.359434	-0.948166	-0.000304
1	5.397688	-1.807358	-0.000563
6	8.112340	0.226720	0.000032
1	8.056701	2.382297	0.000606
1	7.856072	-1.913275	-0.000557
1	9.196821	0.175120	0.000039
6	-3.127962	-0.572869	0.000043
6	-4.140384	-1.553309	0.000202
6	-3.491498	0.786453	-0.000145
6	-5.474497	-1.178681	0.000172
1	-3.861497	-2.601407	0.000348
6	-4.831921	1.151702	-0.000180
1	-2.713266	1.541406	-0.000263
6	-5.839582	0.176328	-0.000023
1	-6.266064	-1.919583	0.000296
1	-5.089477	2.205064	-0.000327
6	-7.296002	0.516215	-0.000043
6	-7.701598	1.978575	-0.000248
1	-8.789683	2.039317	-0.000287
1	-7.307012	2.493805	0.882030
1	-7.306943	2.493604	-0.882608
8	-8.141777	-0.365949	0.000215

1a_{ph_g}

SCF Energy = -1034.577405

Gibbs Free Energy = -1034.332358

6	-4.869921	-0.546154	-0.849214
6	-3.531719	-0.916942	-0.778268
6	-2.661878	-0.323618	0.154474
6	-3.167925	0.663004	1.020198
6	-4.503875	1.038065	0.954482
6	-5.346653	0.430542	0.025479
1	-5.534306	-1.013552	-1.562362
1	-3.146366	-1.674323	-1.451795
1	-2.503672	1.130079	1.738498
1	-4.907309	1.799890	1.612118
6	-1.291095	-0.711742	0.221139
6	-0.125172	-1.033158	0.281603
6	1.268233	-1.448927	0.364900
1	1.455502	-2.268878	-0.349886

1	1.479368	-1.852809	1.370638
8	2.121940	-0.346615	0.088953
6	3.472293	-0.710220	0.161397
1	3.734218	-1.106881	1.159024
1	3.719195	-1.505726	-0.564676
6	4.347478	0.507577	-0.126753
8	3.853364	1.592493	-0.367267
6	5.831019	0.309179	-0.099437
6	6.642454	1.421606	-0.364783
6	6.432201	-0.927214	0.177576
6	8.027548	1.301523	-0.353853
1	6.156556	2.367591	-0.576328
6	7.820579	-1.046645	0.188528
1	5.826362	-1.802588	0.386056
6	8.619308	0.066327	-0.076947
1	8.648622	2.167520	-0.560467
1	8.278656	-2.006834	0.403847
1	9.700862	-0.028472	-0.068137
8	-6.649634	0.920125	-0.017662
6	-7.721143	0.075680	-0.160644
8	-7.637835	-1.122810	-0.258764
6	-8.993709	0.881863	-0.170324
1	-9.844619	0.211614	-0.282428
1	-9.082677	1.450892	0.759287
1	-8.971198	1.602448	-0.992787

1a_{ph_h}

SCF Energy = -1143.729192

Gibbs Free Energy = -1143.518595

6	-1.294367	-0.980425	-0.007121
6	-0.120523	-1.276306	0.001163
6	1.287530	-1.651521	0.011505
1	1.510216	-2.286694	-0.863866
1	1.503817	-2.261885	0.905948
8	2.092942	-0.484041	-0.001883
6	3.459101	-0.796214	0.007519
1	3.735401	-1.383070	0.901700
1	3.742020	-1.407353	-0.868144
6	4.276201	0.494501	-0.007171
8	3.729156	1.580546	-0.023985
6	5.766614	0.363970	-0.000070
6	6.524637	1.543694	-0.013813
6	6.425186	-0.874115	0.019472
6	7.913797	1.487806	-0.008183
1	5.995047	2.489742	-0.028836
6	7.817560	-0.929101	0.025112
1	5.861372	-1.800852	0.030423
6	8.562904	0.250522	0.011288
1	8.493474	2.405490	-0.018908
1	8.320384	-1.890881	0.040254
1	9.647685	0.205934	0.015688
6	-2.670691	-0.609037	-0.016305
6	-3.678407	-1.590603	-0.036375
6	-3.037645	0.749576	-0.009712
6	-5.017676	-1.221614	-0.046718

1	-3.398900	-2.638106	-0.046662
6	-4.378227	1.113507	-0.020235
1	-2.262039	1.506857	0.000650
6	-5.370034	0.129935	-0.039048
1	-5.792498	-1.979354	-0.069163
1	-4.658820	2.160525	-0.022081
6	-6.818209	0.525113	0.011446
9	-7.608989	-0.381304	-0.605649
9	-7.034464	1.722398	-0.576901
9	-7.263265	0.628848	1.286264

1a_{ph_i}

SCF Energy = -846.012768

Gibbs Free Energy = -845.774773

6	-2.687281	-0.961207	-0.003414
6	-1.514767	-1.263334	-0.007073
6	-0.110721	-1.651100	-0.012051
1	0.105912	-2.266373	-0.903210
1	0.107260	-2.283576	0.866624
8	0.709472	-0.491442	-0.001551
6	2.070146	-0.821260	-0.005683
1	2.343663	-1.432318	0.873445
1	2.342093	-1.416767	-0.895915
6	2.906922	0.456131	0.004670
8	2.379105	1.551783	0.014187
6	4.395929	0.301962	0.002490
6	5.172359	1.469603	0.011939
6	5.035306	-0.946182	-0.008490
6	6.560539	1.392200	0.010466
1	4.657270	2.423721	0.020339
6	6.426736	-1.022871	-0.009965
1	4.456961	-1.863907	-0.015943
6	7.190457	0.144947	-0.000491
1	7.154373	2.300871	0.017835
1	6.914475	-1.992509	-0.018490
1	8.274450	0.083441	-0.001646
6	-4.063445	-0.583187	0.001189
6	-4.419079	0.778232	-0.014193
6	-5.074891	-1.557615	0.019340
6	-5.755907	1.175509	-0.010651
6	-6.410717	-1.165192	0.021147
1	-4.804315	-2.607759	0.030037
6	-6.749626	0.186331	0.005852
1	-7.192528	-1.918580	0.032979
1	-7.795721	0.480888	0.005881
1	-3.630737	1.524014	-0.029378
6	-6.129453	2.637586	-0.013347
1	-6.594007	2.928108	0.936000
1	-5.252991	3.272836	-0.163002
1	-6.849823	2.861872	-0.807065

1a_{ph_j}

SCF Energy = -846.014709

Gibbs Free Energy = -845.777002

1a_{ph_n}

SCF Energy = -1095.519545

Gibbs Free Energy = -1095.173102

6	-0.452640	0.149574	0.689534
6	0.672557	0.598587	0.661262
6	2.010021	1.174235	0.654854
1	2.244895	1.586953	1.651582
1	2.053330	2.020354	-0.053771
8	2.962155	0.182623	0.293476
6	4.263390	0.698646	0.276452
1	4.359671	1.538073	-0.435895
1	4.557592	1.094454	1.265341
6	5.245394	-0.399643	-0.125056
8	4.859136	-1.524546	-0.379289
6	6.695468	-0.033784	-0.192328
6	7.604659	-1.036760	-0.557979
6	7.173123	1.253875	0.091595
6	8.964638	-0.759216	-0.638319
1	7.213528	-2.024909	-0.773171
6	8.536387	1.531261	0.010674
1	6.489954	2.046899	0.376498
6	9.433075	0.526182	-0.353918
1	9.661936	-1.541330	-0.921957
1	8.898611	2.530279	0.231862
1	10.494917	0.743944	-0.416353
6	-1.752578	-0.433764	0.655076
6	-2.730544	-0.044185	1.494949
6	-1.992845	-1.513317	-0.386243
6	-4.120598	-0.628088	1.453290
1	-2.521343	0.710747	2.248680
6	-3.310477	-2.255952	-0.112240
1	-2.000249	-1.055137	-1.383955
1	-1.151740	-2.215407	-0.384752
1	-4.866669	0.164377	1.573290
1	-4.258369	-1.302338	2.312680
1	-3.593521	-2.863035	-0.978671
1	-3.171470	-2.940470	0.732958
7	-4.422932	-1.366287	0.224770
6	-4.794365	-0.480147	-0.880878
1	-4.837130	-1.101341	-1.785164
1	-4.044199	0.305094	-1.076507
6	-6.142788	0.172049	-0.660820
6	-7.216880	-0.573579	-0.159618
6	-6.343986	1.518395	-0.976427
6	-8.467210	0.015713	0.013387
1	-7.047839	-1.611880	0.106304
6	-7.596989	2.110528	-0.808843
1	-5.511889	2.107238	-1.354027
6	-8.662382	1.359832	-0.313566
1	-9.292078	-0.572892	0.404373
1	-7.737269	3.158308	-1.057550
1	-9.637061	1.818764	-0.177720

1a_{ph}

SCF Energy = -806.686724

Gibbs Free Energy = -806.475005

6	-6.832184	-0.631796	-0.000815
6	-5.515374	-1.082206	-0.000742
6	-4.451812	-0.161593	0.000081
6	-4.737954	1.216070	0.000821
6	-6.057951	1.656517	0.000734
6	-7.108365	0.736659	-0.000079
1	-7.645550	-1.350917	-0.001451
1	-5.295593	-2.144455	-0.001318
1	-3.917205	1.924983	0.001453
1	-6.267778	2.721672	0.001307
1	-8.136680	1.084440	-0.000142
6	-3.098533	-0.614285	0.000183
6	-1.944655	-0.981058	0.000251
6	-0.564278	-1.446596	0.000314
1	-0.382671	-2.081995	-0.884495
1	-0.382609	-2.081538	0.885442
8	0.318845	-0.334491	-0.000006
6	1.659334	-0.739270	0.000112
1	1.898075	-1.356390	0.885061
1	1.898066	-1.356945	-0.884459
6	2.565232	0.490203	-0.000280
8	2.098233	1.613145	-0.000694
6	4.043403	0.254401	-0.000122
6	4.882734	1.377728	-0.000381
6	4.613287	-1.027031	0.000270
6	6.264559	1.224240	-0.000246
1	4.420800	2.358718	-0.000689
6	5.998408	-1.179963	0.000403
1	3.985469	-1.911695	0.000463
6	6.825055	-0.055763	0.000147
1	6.907375	2.098968	-0.000447
1	6.432210	-2.174934	0.000705
1	7.904035	-0.176682	0.000255

1a'_{Bu}

SCF Energy = -732.890407

Gibbs Free Energy = -732.647208

6	-3.739735	-0.353647	0.000002
6	-2.604545	-0.768373	0.000016
6	-1.243607	-1.288934	0.000107
1	-1.084637	-1.929694	-0.884831
1	-1.084688	-1.929530	0.885170
8	-0.312958	-0.213332	0.000046
6	1.007929	-0.674942	0.000027
1	1.220798	-1.302691	0.884485
1	1.220773	-1.302682	-0.884442
6	1.967905	0.512285	0.000025
8	1.553351	1.655717	0.000056
6	3.434515	0.210119	-0.000005
6	4.323599	1.294434	0.000015
6	3.946299	-1.095569	-0.000041
6	5.697170	1.079026	-0.000009
1	3.906114	2.295162	0.000046

6	5.323181	-1.310663	-0.000061	1	0.385344	5.752971	0.921594
1	3.279139	-1.950927	-0.000051	14	2.754702	-0.511421	-0.132921
6	6.199620	-0.224848	-0.000048	8	2.941870	-2.123174	-0.438929
1	6.378662	1.924004	0.000001	8	3.301474	-0.191564	1.392717
1	5.711756	-2.324176	-0.000086	6	1.967900	-2.955753	-1.080539
1	7.272090	-0.394152	-0.000064	1	2.523390	-3.765810	-1.564917
6	-5.113615	0.172060	-0.000021	1	1.435723	-2.396838	-1.858048
6	-5.852096	-0.321380	-1.262738	6	0.979272	-3.518263	-0.068797
1	-6.875468	0.068483	-1.274304	1	0.410065	-2.708058	0.394614
1	-5.342288	0.017776	-2.168654	1	0.277620	-4.202778	-0.559101
1	-5.899116	-1.413901	-1.285474	1	1.503301	-4.070775	0.717034
6	-5.852375	-0.321971	1.262295	6	2.732600	-0.813881	2.551954
1	-5.342768	0.016757	2.168484	1	2.776291	-0.074600	3.359488
1	-6.875749	0.067886	1.273824	1	1.673313	-1.041776	2.376369
1	-5.899403	-1.414502	1.284512	6	3.501463	-2.070150	2.930488
6	-5.056355	1.715306	0.000326	1	3.080282	-2.518824	3.836832
1	-4.531968	2.084956	0.885493	1	3.456119	-2.800043	2.118842
1	-4.531801	2.085339	-0.884581	1	4.552023	-1.829926	3.117807
1	-6.071931	2.125393	0.000321	6	3.761707	0.560154	-1.273086
				1	4.815412	0.492960	-0.986379
				1	3.678418	0.236384	-2.314325
				1	3.458483	1.608931	-1.204930
				1	-1.776266	1.035442	0.908040

3a_{phOSi}
 SCF Energy = -1445.864474
 Gibbs Free Energy = -1445.464660

6	-5.111605	-2.001268	0.074965				
6	-3.822151	-1.530054	-0.159166				
6	-3.375649	-0.330702	0.426264				
6	-4.265438	0.360867	1.269708				
6	-5.554149	-0.108535	1.501139	14	0.115416	0.779309	0.635555
6	-5.985367	-1.292473	0.900251	1	-0.101704	1.582664	1.864002
1	-5.432660	-2.931404	-0.384161	8	-1.138961	-0.276499	0.361928
1	-3.154935	-2.117077	-0.776719	8	1.447456	-0.139594	0.960129
1	-3.932750	1.282302	1.739404	6	-2.391868	0.089136	-0.207362
1	-6.222113	0.447190	2.152185	1	-2.240374	0.587615	-1.175627
1	-6.989473	-1.663545	1.080226	1	-2.912484	0.801544	0.449406
6	-2.044955	0.242759	0.213046	6	-3.232706	-1.162492	-0.389156
6	-1.143463	-0.042420	-0.735519	1	-3.396564	-1.653329	0.574105
6	-1.228745	-1.007437	-1.893826	1	-4.205408	-0.913903	-0.825717
1	-2.163055	-0.867461	-2.458783	1	-2.723207	-1.869081	-1.050706
1	-1.173040	-2.057477	-1.584835	6	1.894898	-1.222949	0.142777
8	-0.092163	-0.749627	-2.725874	1	2.317028	-1.974915	0.818255
6	0.433666	0.521714	-2.368298	1	1.044622	-1.687972	-0.371867
1	1.482672	0.556971	-2.661160	6	2.948317	-0.764715	-0.856195
1	-0.102739	1.331744	-2.882221	1	3.337093	-1.618431	-1.421715
6	0.222510	0.635627	-0.844839	1	2.532139	-0.045122	-1.567568
8	1.120543	-0.222668	-0.152522	1	3.782014	-0.285181	-0.335460
6	0.274551	2.063413	-0.330225	6	0.335915	1.904599	-0.849173
6	-0.588311	3.030047	-0.868667	1	0.442505	1.331901	-1.776561
6	1.160548	2.444471	0.681094	1	-0.518735	2.579282	-0.970728
6	-0.548250	4.348482	-0.424274	1	1.231957	2.521871	-0.729390
1	-1.311009	2.744034	-1.626137				
6	1.200874	3.767938	1.125900				
1	1.817490	1.710882	1.130268				
6	0.352612	4.724924	0.574260				
1	-1.223999	5.081403	-0.854554				
1	1.898758	4.044565	1.910333	8	0.654910	0.353157	-0.384150

4 (EtO)₂MeSiH
 SCF Energy = -639.040385
 Gibbs Free Energy = -638.892058

5 (EtO)₂MeSiOTs
 SCF Energy = -1533.326285
 Gibbs Free Energy = -1533.068185

16	-0.378625	1.541070	-0.020186	6	-5.192137	-1.391476	2.130500
8	-0.345758	2.535298	-1.088652	1	-4.412031	0.345998	1.131078
8	-0.135906	1.947363	1.368078	6	-4.894882	-2.521651	2.896781
6	-1.900140	0.628226	-0.104575	1	-3.331897	-3.651003	3.862164
6	-2.555964	0.510091	-1.328895	1	-6.219523	-1.178068	1.848396
6	-2.401869	0.033068	1.051723	1	-5.688279	-3.191730	3.214648
6	-3.732728	-0.229990	-1.389564	8	-1.833781	3.517525	0.192330
1	-2.149093	0.996135	-2.208092	1	-0.398128	2.550559	-0.969557
6	-3.580102	-0.703184	0.969805	1	-1.447910	3.733417	-1.756300
1	-1.878350	0.156615	1.992257	8	-1.702792	1.033752	-2.406486
6	-4.261209	-0.846003	-0.246607	6	-3.704538	1.598992	-1.292209
1	-4.252029	-0.330151	-2.338155	6	-4.482920	2.597656	-0.686595
1	-3.980317	-1.171781	1.864086	6	-4.309427	0.388791	-1.667650
14	2.352673	0.350560	-0.096851	6	-5.840698	2.379101	-0.455078
8	3.023018	-0.360978	-1.407436	1	-4.017277	3.531518	-0.396028
8	2.584919	-0.611634	1.216332	6	-5.660891	0.170276	-1.425645
6	2.692929	-1.682803	-1.858063	1	-3.697643	-0.372950	-2.135941
1	2.801667	-1.673464	-2.947208	6	-6.430200	1.166400	-0.817496
1	1.641560	-1.905218	-1.635339	1	-6.438146	3.155447	0.013049
6	3.609510	-2.720491	-1.229992	1	-6.114582	-0.776572	-1.701280
1	3.490017	-2.725496	-0.143924	1	-7.485599	0.996816	-0.625328
1	3.376600	-3.718137	-1.617763	6	3.169884	0.268521	1.390047
1	4.654157	-2.493835	-1.461423	6	3.134254	-1.102393	1.746721
6	1.721182	-0.694237	2.359683	6	4.142355	-1.643809	2.553258
1	2.367699	-0.863876	3.226637	6	5.164999	-0.835109	3.046074
1	1.193432	0.253136	2.512874	6	5.190623	0.519420	2.720729
6	0.730343	-1.836956	2.198003	6	4.205669	1.060596	1.890270
1	0.108484	-1.932529	3.094893	1	4.109528	-2.699922	2.795587
1	0.076138	-1.660610	1.340333	1	5.934609	-1.263008	3.680487
1	1.258551	-2.782260	2.042197	1	5.982580	1.157578	3.101127
6	2.985018	2.079214	0.068218	1	4.248925	2.109345	1.618491
1	4.077204	2.078981	0.119847	15	1.877624	0.933436	0.248502
1	2.671812	2.682627	-0.787967	6	2.437565	0.230123	-1.356289
1	2.587646	2.544940	0.973743	6	1.500074	0.165751	-2.397596
6	-5.553905	-1.617848	-0.318504	6	3.730050	-0.274407	-1.560231
1	-5.597031	-2.397164	0.446976	6	1.858553	-0.388563	-3.625248
1	-6.411996	-0.953842	-0.159327	1	0.488256	0.530934	-2.252442
1	-5.683417	-2.089204	-1.296530	6	4.079746	-0.836544	-2.788558
				1	4.461158	-0.235835	-0.759599
				6	3.143935	-0.894819	-3.822347
				1	1.120139	-0.445153	-4.417725
				1	5.081595	-1.229963	-2.935431
				1	3.414371	-1.339078	-4.775924
28	-0.007321	0.146795	0.973687	6	2.268955	2.716458	0.120151
6	-1.989649	2.664757	1.348466	6	3.236578	3.227576	-0.756384
6	-1.425285	2.921854	-1.017254	6	1.533013	3.597790	0.924843
6	-2.256598	1.776181	-1.601220	6	3.468183	4.601336	-0.818455
6	-1.452222	1.285799	1.246642	1	3.797134	2.551007	-1.393390
1	-1.493931	3.195866	2.171090	6	1.768679	4.970337	0.862937
1	-3.063208	2.629943	1.582512	1	0.768636	3.196874	1.581614
6	-1.773045	0.072860	1.589535	6	2.735910	5.473172	-0.009056
6	-2.834620	-0.789823	2.059611	1	4.215838	4.992252	-1.502366
6	-2.550509	-1.929160	2.836522	1	1.186676	5.645830	1.482248
6	-4.177717	-0.529776	1.722992	1	2.913248	6.543143	-0.065224
6	-3.569654	-2.781204	3.255752	6	2.056993	-1.992096	1.284330
1	-1.518145	-2.116936	3.117159	8	2.368040	-3.305883	1.170570

Cat1

SCF Energy = -2529.466104

Gibbs Free Energy = -2528.851302

6	0.127527	-2.859229	0.537860	6	1.264141	2.604470	-0.302862
6	1.185718	-3.995042	0.670668	8	2.356558	3.316144	0.013590
7	0.847120	-1.653091	0.998941	6	2.754617	1.030294	0.258192
6	1.434933	-4.570746	-0.739973	6	3.293075	2.406779	0.684400
1	2.497829	-4.490389	-0.990852	7	1.342477	1.320619	-0.124499
1	1.173976	-5.634597	-0.779765	6	4.699008	2.557494	0.105437
6	0.554900	-3.742473	-1.650617	1	4.885591	3.582214	-0.231001
6	0.418303	-3.833994	-3.034925	1	5.436818	2.332181	0.885699
6	-0.194873	-2.805825	-0.935187	6	4.734444	1.527230	-0.999443
6	-0.471135	-2.974633	-3.684561	6	5.702055	1.361042	-1.986914
1	0.995977	-4.558506	-3.602376	6	3.638032	0.658941	-0.920722
6	-1.077904	-1.941849	-1.576973	6	5.556003	0.318159	-2.904874
6	-1.210456	-2.031481	-2.963204	1	6.554702	2.032047	-2.045243
1	-0.580753	-3.032695	-4.763785	6	3.484726	-0.377280	-1.839729
1	-1.623080	-1.195182	-1.010980	6	4.454450	-0.539629	-2.831233
1	-1.862525	-1.334761	-3.477966	1	6.300460	0.176490	-3.682996
1	0.934741	-4.759559	1.407771	1	2.646257	-1.056640	-1.755372
1	-0.761717	-2.989776	1.158555	1	4.354032	-1.350048	-3.546499
				1	3.216113	2.620027	1.753061
				1	2.744900	0.307192	1.067290
Cat				28	0.014417	-0.104910	-0.269115
SCF Energy = -3512.429075				8	1.334824	-1.561114	-0.056562
Gibbs Free Energy = -3511.819419				8	-1.299127	-1.335803	-0.812111
6	-1.184991	2.943570	-0.790598	16	1.847207	-2.104893	1.307320
6	0.149858	3.393580	-0.848857	16	-1.773545	-2.518842	0.112027
6	0.445378	4.628951	-1.440946	8	1.760676	-1.043942	2.344117
6	-0.569646	5.400025	-2.002048	8	1.313623	-3.426624	1.624407
6	-1.888333	4.949835	-1.960522	8	-1.681353	-2.095192	1.521954
6	-2.193827	3.731441	-1.351655	8	-1.193864	-3.787543	-0.322635
1	1.473663	4.968298	-1.466153	6	-3.518666	-2.588155	-0.294998
1	-0.328777	6.348823	-2.470121	6	-4.459068	-2.128920	0.622929
1	-2.683665	5.547218	-2.395030	6	-3.916070	-3.131325	-1.516545
1	-3.221814	3.391866	-1.306812	6	-5.813048	-2.205285	0.304818
15	-1.552068	1.374624	0.072825	1	-4.120612	-1.729212	1.571391
6	-3.290025	1.055125	-0.335848	6	-5.272641	-3.191405	-1.824381
6	-4.316351	1.504351	0.505257	1	-3.168523	-3.516017	-2.201535
6	-3.600378	0.453938	-1.564721	6	-6.239521	-2.726365	-0.922331
6	-5.646329	1.370037	0.107877	1	-6.550829	-1.849111	1.018640
1	-4.075539	1.956547	1.461193	1	-5.588964	-3.615341	-2.774005
6	-4.930275	0.328994	-1.955517	6	3.585276	-2.295773	0.899551
1	-2.805086	0.059951	-2.185791	6	4.548811	-1.510718	1.526206
6	-5.952126	0.789356	-1.123020	6	3.939582	-3.166934	-0.131480
1	-6.441135	1.713336	0.762824	6	5.865128	-1.545629	1.067538
1	-5.169836	-0.155337	-2.895714	1	4.255730	-0.871700	2.351893
1	-6.988469	0.679821	-1.427538	6	5.257006	-3.195421	-0.575503
6	-1.453513	1.804582	1.841391	1	3.180619	-3.790200	-0.591975
6	-1.103085	0.792785	2.749697	6	6.232051	-2.363517	-0.006456
6	-1.682829	3.113591	2.292679	1	6.616097	-0.918789	1.541753
6	-0.989785	1.101228	4.105243	1	5.532623	-3.855655	-1.393566
1	-0.924189	-0.222383	2.410203	6	7.627627	-2.314565	-0.573352
6	-1.571815	3.406995	3.650415	1	8.361573	-2.026312	0.184865
1	-1.939255	3.897880	1.587523	1	7.927713	-3.280019	-0.991184
6	-1.223094	2.401100	4.555666	1	7.680272	-1.574654	-1.382043
1	-0.705718	0.318925	4.801229	6	-7.704547	-2.752327	-1.278984
1	-1.750426	4.419421	3.999904	1	-7.931514	-3.552123	-1.989541
1	-1.128092	2.634770	5.611967	1	-8.330242	-2.894942	-0.393096

1 -8.011578 -1.806275 -1.744043

H₂O

SCF Energy = -76.420311

Gibbs Free Energy = -76.416598

8 0.000000 0.000000 0.119188
1 -0.000000 0.759272 -0.476753
1 -0.000000 -0.759272 -0.476753

H₂

SCF Energy = -1.17868

Gibbs Free Energy = -1.180004

1 0.000000 0.000000 0.371423
1 0.000000 0.000000 -0.371423

IM13

SCF Energy = -1723.88752

Gibbs Free Energy = -1723.505090

6 0.905012 -0.438280 -1.393505
6 -0.337735 -1.095152 -1.570654
6 -0.639962 -1.666883 -2.820213
6 0.246165 -1.572831 -3.887518
6 1.455254 -0.899109 -3.725544
6 1.773502 -0.342749 -2.487894
1 -1.588447 -2.172304 -2.946533
1 -0.014094 -2.015650 -4.843666
1 2.150025 -0.807454 -4.554868
1 2.716296 0.178413 -2.365098
15 1.395537 0.239007 0.251322
6 2.521682 1.612931 -0.195613
6 3.898894 1.444373 -0.389694
6 1.955677 2.887337 -0.341167
6 4.695480 2.534383 -0.743248
1 4.346896 0.464924 -0.255648
6 2.752281 3.972367 -0.702191
1 0.894776 3.021973 -0.150145
6 4.123041 3.796947 -0.905039
1 5.763093 2.397568 -0.888195
1 2.306796 4.956499 -0.812165
1 4.744924 4.644448 -1.177594
6 2.524569 -1.056136 0.905286
6 2.842975 -0.984262 2.271955
6 3.068645 -2.087577 0.128655
6 3.706173 -1.917916 2.841772
1 2.400016 -0.199582 2.877242
6 3.926220 -3.025554 0.706413
1 2.823609 -2.163175 -0.924857
6 4.249255 -2.940661 2.060840
1 3.947092 -1.852288 3.898546
1 4.340906 -3.822491 0.095985
1 4.916277 -3.671791 2.507934
6 -1.390158 -1.178683 -0.538903
8 -2.424096 -1.999493 -0.856921

6 -2.851937 -0.814601 1.115772
6 -3.363030 -1.996550 0.254237
7 -1.498876 -0.537497 0.578799
6 -4.773235 -1.644769 -0.238542
1 -4.900314 -1.924312 -1.289112
1 -5.521343 -2.204270 0.336885
6 -4.883002 -0.157798 0.013497
6 -5.877354 0.720152 -0.415097
6 -3.824201 0.306074 0.801077
6 -5.795254 2.064959 -0.047713
1 -6.701855 0.366749 -1.028321
6 -3.736317 1.647046 1.171311
6 -4.733067 2.524169 0.739299
1 -6.561465 2.760389 -0.377829
1 -2.898615 1.985012 1.772462
1 -4.681623 3.573318 1.014640
1 -3.294210 -2.976947 0.732112
1 -2.771081 -1.027472 2.181549
28 -0.266979 0.580583 1.585796
1 0.554204 1.399854 2.463758
1 -1.182049 0.858225 2.719099

IM14

SCF Energy = -1722.66494

Gibbs Free Energy = -1722.296320

28 0.059198 0.365019 -2.040700
6 1.287099 1.499994 0.432988
6 0.109831 2.303027 0.491306
6 0.099681 3.466358 1.278758
6 1.232097 3.881920 1.972691
6 2.391368 3.116021 1.902230
6 2.405118 1.939073 1.150949
1 -0.813470 4.047710 1.330597
1 1.204036 4.794435 2.559849
1 3.286501 3.422565 2.435509
1 3.311601 1.347486 1.125953
15 1.377157 -0.095868 -0.565737
6 0.572842 -1.322140 0.558726
6 -0.332138 -0.949579 1.561268
6 0.768742 -2.689462 0.302464
6 -1.021894 -1.918831 2.290513
1 -0.504495 0.098424 1.777314
6 0.090388 -3.655934 1.041123
1 1.461835 -2.993323 -0.476780
6 -0.811526 -3.273139 2.037151
1 -1.729108 -1.611014 3.054751
1 0.260855 -4.708970 0.835211
1 -1.349796 -4.025749 2.605549
6 3.166085 -0.535747 -0.389148
6 4.018282 -0.191269 -1.446965
6 3.701247 -1.198170 0.726116
6 5.379902 -0.486822 -1.388445
1 3.598317 0.302853 -2.319555
6 5.060368 -1.508041 0.778492
1 3.051904 -1.472464 1.551215

6	5.902727	-1.149963	-0.276406	1	2.034792	-0.324349	1.730962
1	6.030056	-0.211201	-2.213774	6	2.477119	-2.418588	1.929616
1	5.463046	-2.026307	1.644265	8	1.986113	-3.336956	2.575574
1	6.960642	-1.392094	-0.234082	6	3.046353	-2.665281	0.568157
6	-1.159539	1.980764	-0.188226	6	3.470949	-1.630094	-0.276677
8	-2.285093	2.376766	0.474712	6	3.146420	-3.996996	0.134089
6	-2.808874	1.105833	-1.419439	6	3.999546	-1.931441	-1.532408
6	-3.432755	2.040182	-0.350952	1	3.379188	-0.594366	0.021393
7	-1.351180	1.357615	-1.312456	6	3.662824	-4.292626	-1.122223
6	-4.436911	1.209211	0.459571	1	2.814115	-4.778499	0.809337
1	-4.387687	1.465732	1.522154	6	4.094758	-3.256774	-1.957284
1	-5.459033	1.421827	0.120803	1	4.323521	-1.120767	-2.174816
6	-4.039039	-0.219367	0.161588	1	3.738334	-5.324791	-1.451103
6	-4.433284	-1.386669	0.813759	1	4.504629	-3.485194	-2.937031
6	-3.154369	-0.282358	-0.918764	1	-2.089244	0.079878	1.371164
6	-3.919774	-2.609857	0.378818	6	-0.369905	0.854021	-2.121734
1	-5.116812	-1.345829	1.657416	6	0.327949	-0.375085	-2.150981
6	-2.634633	-1.500340	-1.351696	6	1.310046	-0.602452	-3.120485
6	-3.023414	-2.666918	-0.693537	6	1.643475	0.395761	-4.033791
1	-4.204920	-3.524962	0.889064	6	0.978014	1.619140	-3.991302
1	-1.909185	-1.532392	-2.160384	6	-0.027358	1.840481	-3.046526
1	-2.607901	-3.621448	-0.998792	1	1.815047	-1.559750	-3.136700
1	-3.843157	2.975847	-0.740532	1	2.416815	0.215374	-4.773870
1	-3.144877	1.302286	-2.440213	1	1.230487	2.404899	-4.696690
				1	-0.546324	2.790502	-3.029911
				15	-1.703564	1.101544	-0.875351
				6	-2.968927	-0.115417	-1.426136
				6	-2.958044	-0.677860	-2.709300
				6	-4.002667	-0.456948	-0.542714
				6	-3.953397	-1.578202	-3.093832
				1	-2.174023	-0.414884	-3.410177
				6	-5.008310	-1.335685	-0.936302
				1	-4.010829	-0.042427	0.459362
				6	-4.981100	-1.906230	-2.209813
				1	-3.928557	-2.013314	-4.088636
				1	-5.794477	-1.597763	-0.237405
				1	-5.755602	-2.605879	-2.509133
				6	-2.477177	2.708022	-1.305991
				6	-1.776308	3.896210	-1.037673
				6	-3.766123	2.777903	-1.856021
				6	-2.358992	5.128582	-1.329232
				1	-0.776166	3.850181	-0.619723
				6	-4.345369	4.016655	-2.131767
				1	-4.318606	1.870848	-2.069642
				6	-3.644077	5.193954	-1.870827
				1	-1.805226	6.039603	-1.123376
				1	-5.344649	4.058192	-2.555068
				1	-4.096870	6.157004	-2.087753
				6	0.016793	-1.466615	-1.211792
				8	0.168127	-2.717972	-1.704244
				6	-0.632820	-2.721584	0.524189
				6	-0.340844	-3.637479	-0.700332
				7	-0.399947	-1.359382	0.000265
				6	-1.684845	-4.263851	-1.136238
				1	-2.001632	-3.823897	-2.088649
				1	-1.601637	-5.344996	-1.287009

IM1B

SCF Energy = -3351.108032

Gibbs Free Energy = -3350.332484

28	-0.756373	0.426545	1.073809	6	-3.953397	-1.578202	-3.093832
8	1.856161	2.793776	2.067661	1	-2.174023	-0.414884	-3.410177
16	1.745785	2.381160	0.656754	6	-5.008310	-1.335685	-0.936302
8	1.157987	3.368622	-0.276564	1	-4.010829	-0.042427	0.459362
8	1.105299	1.001974	0.484068	6	-4.981100	-1.906230	-2.209813
6	3.399698	2.027847	0.068297	1	-3.928557	-2.013314	-4.088636
6	3.618521	1.902749	-1.303790	1	-5.794477	-1.597763	-0.237405
6	4.420391	1.775710	0.981914	1	-5.755602	-2.605879	-2.509133
6	4.870621	1.498090	-1.756878	6	-2.477177	2.708022	-1.305991
1	2.813967	2.118210	-1.996487	6	-1.776308	3.896210	-1.037673
6	5.667241	1.361734	0.512431	6	-3.766123	2.777903	-1.856021
1	4.224800	1.902964	2.040966	6	-2.358992	5.128582	-1.329232
6	5.906483	1.201793	-0.857981	1	-0.776166	3.850181	-0.619723
1	5.047702	1.401912	-2.825449	6	-4.345369	4.016655	-2.131767
1	6.465228	1.155261	1.220525	1	-4.318606	1.870848	-2.069642
6	7.230820	0.682724	-1.357902	6	-3.644077	5.193954	-1.870827
1	7.189014	-0.404697	-1.499672	1	-1.805226	6.039603	-1.123376
1	8.037060	0.889320	-0.648858	1	-5.344649	4.058192	-2.555068
1	7.499299	1.127542	-2.320806	1	-4.096870	6.157004	-2.087753
6	-0.802802	1.230081	2.880285	6	0.016793	-1.466615	-1.211792
6	-0.230175	0.121016	2.990654	8	0.168127	-2.717972	-1.704244
6	0.467981	-0.970710	3.717477	6	-0.632820	-2.721584	0.524189
1	0.175524	-0.918035	4.771526	6	-0.340844	-3.637479	-0.700332
1	0.161914	-1.951693	3.339409	7	-0.399947	-1.359382	0.000265
8	1.887123	-0.865141	3.730528	6	-1.684845	-4.263851	-1.136238
6	2.494862	-0.995930	2.466440	1	-2.001632	-3.823897	-2.088649
1	3.537773	-0.676810	2.577804	1	-1.601637	-5.344996	-1.287009

6	-2.641892	-3.905749	-0.021170	6	2.401956	0.309127	4.078616
6	-3.947695	-4.353528	0.168565	1	1.416330	1.332670	2.456916
6	-2.064617	-3.019315	0.892009	6	3.918832	-1.461973	3.438686
6	-4.667422	-3.897429	1.275298	1	4.124315	-1.810884	1.323595
1	-4.401764	-5.047567	-0.533057	6	3.297094	-0.703121	4.431844
6	-2.777771	-2.559437	1.996981	1	1.910535	0.896287	4.848519
6	-4.089380	-3.001729	2.181130	1	4.610113	-2.253793	3.711382
1	-5.684460	-4.243525	1.435437	1	3.504609	-0.904084	5.478484
1	-2.320959	-1.869227	2.698098	6	0.603633	-2.350127	0.331976
1	-4.659209	-2.657921	3.039135	8	0.254897	-3.402752	1.096647
1	0.442911	-4.372200	-0.521466	6	-0.866630	-1.414919	1.751161
1	0.043281	-2.896889	1.360164	6	-0.865699	-2.956842	1.919961
6	-1.414221	2.480269	3.412068	7	-0.027622	-1.245855	0.535947
6	-0.504727	2.972832	4.558075	6	-2.236443	-3.444514	1.406345
1	-0.925565	3.882308	5.001257	1	-2.153542	-3.738549	0.352936
1	-0.418708	2.214989	5.343185	1	-2.610000	-4.306470	1.966457
1	0.492218	3.190345	4.169794	6	-3.103511	-2.210607	1.534695
6	-1.531349	3.568185	2.335638	6	-4.492072	-2.116210	1.512322
1	-2.189036	3.243911	1.527186	6	-2.323799	-1.055790	1.656151
1	-1.953795	4.478004	2.775714	6	-5.081936	-0.851304	1.587128
1	-0.553105	3.805500	1.915472	1	-5.106975	-3.006761	1.421868
6	-2.818504	2.124102	3.943769	6	-2.903174	0.207362	1.728596
1	-3.448030	1.734329	3.137339	6	-4.295455	0.302343	1.683908
1	-2.760629	1.367782	4.732427	1	-6.164408	-0.763018	1.566738
1	-3.300301	3.017901	4.354473	1	-2.292901	1.099403	1.807067
				1	-4.760624	1.281577	1.730645
				1	-0.652481	-3.288276	2.935958
				1	-0.355654	-0.875009	2.556698
				28	0.108353	0.397298	-0.438916
				6	-2.018594	-3.323784	-2.539406
				6	-1.445355	-2.108311	-2.175101
				6	-2.230906	-1.042441	-1.693026
				6	-3.619720	-1.242728	-1.607991
				6	-4.195675	-2.460175	-1.966594
				6	-3.400264	-3.510990	-2.427623
				1	-1.388034	-4.126207	-2.914009
				1	-0.375421	-1.959902	-2.276263
				1	-4.238299	-0.447708	-1.207234
				1	-5.270133	-2.592730	-1.873465
				1	-3.849883	-4.460702	-2.702551
				6	-1.604152	0.216947	-1.282164
				6	-2.068214	1.437403	-1.581722
				6	-3.159471	1.958885	-2.473385
				1	-4.149530	1.985704	-1.998359
				1	-3.247802	1.366204	-3.396182
				8	-2.790854	3.321133	-2.768307
				6	-1.415276	3.517979	-2.412601
				1	-0.739848	3.205527	-3.222631
				1	-1.280035	4.583519	-2.209995
				6	-1.160306	2.591956	-1.201763
				8	0.155662	2.111446	-1.103902
				6	-1.615434	3.218690	0.124483
				6	-2.907272	3.739783	0.293066
				6	-0.753869	3.207992	1.227586
				6	-3.333887	4.194889	1.540918
				1	-3.573856	3.794926	-0.560508

IM1C

SCF Energy = -2529.482908

Gibbs Free Energy = -2528.864209

6	2.603651	-1.436628	-0.849312	6	-2.230906	-1.042441	-1.693026
6	1.720087	-2.518598	-0.607432	6	-3.619720	-1.242728	-1.607991
6	1.917961	-3.753125	-1.229903	6	-4.195675	-2.460175	-1.966594
6	2.970223	-3.922287	-2.129651	6	-3.400264	-3.510990	-2.427623
6	3.832429	-2.859137	-2.389319	1	-1.388034	-4.126207	-2.914009
6	3.655014	-1.629223	-1.747031	1	-0.375421	-1.959902	-2.276263
1	1.233346	-4.566000	-1.013979	1	-4.238299	-0.447708	-1.207234
1	3.111932	-4.877624	-2.624274	1	-5.270133	-2.592730	-1.873465
1	4.652690	-2.982738	-3.089807	1	-3.849883	-4.460702	-2.702551
1	4.341620	-0.814107	-1.945930	6	-1.604152	0.216947	-1.282164
15	2.304483	0.186144	-0.005045	6	-2.068214	1.437403	-1.581722
6	3.599362	1.292448	-0.643196	6	-3.159471	1.958885	-2.473385
6	4.935278	1.229739	-0.218866	1	-4.149530	1.985704	-1.998359
6	3.208218	2.236468	-1.606472	1	-3.247802	1.366204	-3.396182
6	5.880452	2.092789	-0.769521	8	-2.790854	3.321133	-2.768307
1	5.230884	0.515033	0.542914	6	-1.415276	3.517979	-2.412601
6	4.164467	3.093798	-2.153544	1	-0.739848	3.205527	-3.222631
1	2.159138	2.305149	-1.885562	1	-1.280035	4.583519	-2.209995
6	5.495484	3.021481	-1.740652	6	-1.160306	2.591956	-1.201763
1	6.914076	2.044974	-0.439917	8	0.155662	2.111446	-1.103902
1	3.864567	3.826750	-2.896393	6	-1.615434	3.218690	0.124483
1	6.233715	3.694558	-2.166805	6	-2.907272	3.739783	0.293066
6	2.757572	-0.191892	1.730777	6	-0.753869	3.207992	1.227586
6	2.128670	0.560904	2.734698	6	-3.333887	4.194889	1.540918
6	3.650503	-1.209089	2.092845	1	-3.573856	3.794926	-0.560508

6	-1.178354	3.666973	2.476259	1	-1.222933	5.006894	1.887318
1	0.252026	2.833566	1.078040	6	-2.319391	1.889437	-0.192089
6	-2.476866	4.149167	2.643595	6	-3.049052	2.284855	0.930713
1	-4.341087	4.587718	1.652738	1	-3.229468	3.703399	2.542351
1	-0.492055	3.649347	3.319577	1	-2.639100	1.048215	-0.792702
1	-2.814049	4.497673	3.615491	1	-3.937905	1.730119	1.211923

IM1

SCF Energy = -2617.417157

Gibbs Free Energy = -2616.927161

6	3.185872	-0.191365	-0.459264	8	-0.713261	-2.194638	-1.080552
6	3.175730	0.993333	-1.230273	8	-2.278054	-2.699370	-3.040721
6	4.369350	1.489502	-1.764734	6	-3.274203	-1.536093	-0.866907
6	5.564044	0.797064	-1.566545	6	-3.078068	-1.617852	0.511808
6	5.573261	-0.380581	-0.821186	6	-4.513178	-1.185244	-1.409516
6	4.388626	-0.869502	-0.261582	6	-4.146813	-1.332419	1.358478
1	4.353174	2.407317	-2.340871	1	-2.113266	-1.913539	0.905983
1	6.484002	1.179015	-1.995663	6	-5.563207	-0.896217	-0.545087
1	6.501832	-0.920175	-0.666781	1	-4.651632	-1.141098	-2.484388
1	4.401187	-1.777660	0.330809	6	-5.399209	-0.964335	0.848074
15	1.631044	-0.758449	0.307330	1	-4.007553	-1.401948	2.433153
6	1.344066	0.371413	1.700612	1	-6.528904	-0.618013	-0.956047
6	2.399517	1.058972	2.316015	6	-6.557172	-0.677853	1.768066
6	0.026919	0.564722	2.143815	1	-6.218937	-0.457228	2.783407
6	2.134976	1.929778	3.373141	1	-7.151332	0.167432	1.409344
1	3.418431	0.918801	1.970440	1	-7.226956	-1.543785	1.823759

IM2B

SCF Energy = -3351.105215

Gibbs Free Energy = -3350.330669

1	-1.248537	1.589004	3.532004	28	1.003232	1.009262	0.299804
1	0.621876	2.796266	4.636413	8	-2.172139	2.191033	-1.745350
6	1.916198	-2.421865	0.948107	16	-1.448763	0.895374	-1.747355
6	2.225011	-2.630162	2.300771	8	-0.465947	0.739952	-2.842320
6	1.849959	-3.508496	0.060397	8	-0.887380	0.573403	-0.366932
6	2.476355	-3.922716	2.758253	8	-0.887380	0.573403	-0.366932
1	2.266902	-1.790950	2.986815	6	-2.662995	-0.408184	-1.954097
6	2.106379	-4.794948	0.527993	6	-3.218113	-1.038532	-0.842059
1	1.583156	-3.350251	-0.978733	6	-3.072003	-0.752979	-3.241060
6	2.418811	-5.001886	1.873966	6	-4.198258	-2.008238	-1.022608
1	2.715253	-4.086516	3.803984	1	-2.877941	-0.774927	0.149228
1	2.052382	-5.635967	-0.155282	6	-4.054392	-1.727555	-3.408201
1	2.612139	-6.006920	2.235061	1	-2.609312	-0.271752	-4.095795
6	1.928895	1.734865	-1.460495	6	-4.637601	-2.362229	-2.303972
8	2.041231	3.040627	-1.706895	1	-4.634901	-2.490084	-0.152655
6	-0.242128	2.370779	-1.693081	1	-4.373554	-2.000515	-4.410732
6	0.694077	3.612762	-1.707522	6	-5.732338	-3.384563	-2.481463
7	0.721459	1.260101	-1.444884	1	-6.712934	-2.950948	-2.249245
6	0.435439	4.399551	-0.402212	1	-5.772205	-3.757710	-3.508534
1	1.311262	4.324092	0.251846	1	-5.594079	-4.240407	-1.812704
1	0.274149	5.463322	-0.600293	6	0.751033	3.002713	0.299657
6	-0.784604	3.736337	0.196499	6	0.327300	2.497376	1.370475
6	-1.516847	4.133140	1.313579	6	-0.479523	2.532735	2.617363
6	-1.182523	2.616249	-0.539178	1	0.112638	2.960549	3.433250
6	-2.647526	3.397180	1.678345	1	-0.786256	1.531093	2.923784

8	-1.610956	3.391790	2.480070	6	-1.789677	-1.335782	4.107616
6	-2.576567	2.933852	1.556571	1	-1.530213	-0.406120	2.188173
1	-3.219451	3.790208	1.324917	6	0.073130	-2.666827	4.893246
1	-2.121710	2.613182	0.610503	1	1.780138	-2.777424	3.580340
6	-3.444644	1.802564	2.098634	6	-1.209365	-2.149372	5.084222
8	-3.222097	1.309584	3.197971	1	-2.771662	-0.898459	4.247721
6	-4.565842	1.307107	1.244481	1	0.524546	-3.297705	5.653363
6	-4.770340	1.759143	-0.067624	1	-1.753255	-2.372932	5.997190
6	-5.424491	0.334581	1.781165	6	1.641984	-1.024000	-1.836852
6	-5.816742	1.239286	-0.828070	8	2.367396	-1.403510	-2.914476
1	-4.085298	2.459988	-0.527067	6	3.093903	0.664896	-2.034086
6	-6.470335	-0.176680	1.021536	6	3.468662	-0.467848	-3.029650
1	-5.247888	-0.001329	2.797221	7	1.965293	0.088075	-1.278222
6	-6.666902	0.275912	-0.287541	6	4.794714	-1.089349	-2.530215
1	-5.948724	1.572179	-1.852352	1	4.590855	-2.069297	-2.083188
1	-7.131991	-0.927927	1.442927	1	5.509711	-1.245071	-3.344289
1	-7.477063	-0.130700	-0.886059	6	5.293983	-0.108724	-1.493026
1	2.243974	1.199669	0.926591	6	6.524661	-0.097660	-0.840298
6	0.922825	4.194079	-0.588096	6	4.338327	0.871450	-1.208188
6	-0.458394	4.886723	-0.660670	6	6.783590	0.900005	0.102834
1	-0.373225	5.814373	-1.238354	1	7.273119	-0.854244	-1.058142
1	-0.816100	5.130482	0.343799	6	4.591532	1.868330	-0.268855
1	-1.183974	4.229939	-1.144863	6	5.823014	1.875187	0.390169
6	1.384036	3.817737	-2.003850	1	7.741128	0.920340	0.615183
1	2.423388	3.477078	-1.988857	1	3.841712	2.620471	-0.052225
1	1.336076	4.697167	-2.654460	1	6.038899	2.647942	1.121786
1	0.756546	3.031552	-2.430864	1	3.511001	-0.147819	-4.070579
6	1.947369	5.148156	0.060901	1	2.738591	1.574534	-2.518429
1	2.927366	4.670622	0.161521				
1	1.614574	5.458073	1.055472				
1	2.069407	6.043380	-0.559034				
6	0.259066	-2.151812	-0.066560				
6	0.594157	-1.969984	-1.425548				
6	-0.048849	-2.718370	-2.415629	28	0.118011	0.148962	-0.771571
6	-1.029491	-3.645920	-2.072322	6	0.288280	-2.092383	-2.703775
6	-1.348299	-3.845803	-0.732374	6	-1.983432	-1.637990	-3.140048
6	-0.704430	-3.106599	0.262599	6	-2.135267	-1.119141	-1.674310
1	0.212216	-2.547054	-3.452835	6	-1.127626	-1.872400	-0.736054
1	-1.548757	-4.196727	-2.848963	8	-0.907355	-2.529426	-3.346580
1	-2.110950	-4.566398	-0.454865	1	-1.871368	-0.736180	-3.766060
1	-0.969018	-3.261832	1.301795	1	-2.878337	-2.180101	-3.454764
15	1.056767	-1.087949	1.205388	8	-1.653328	0.206916	-1.562071
6	2.745664	-1.787029	1.327731	6	-3.591280	-1.207557	-1.247876
6	3.063854	-3.060707	0.836649	6	-4.181035	-2.452434	-0.991977
6	3.758438	-0.998881	1.893218	6	-4.380337	-0.058987	-1.149203
6	4.376043	-3.532189	0.902159	6	-5.518294	-2.543362	-0.613849
1	2.289072	-3.678534	0.395682	1	-3.581275	-3.353439	-1.078308
6	5.063577	-1.478015	1.972160	6	-5.721745	-0.146196	-0.770631
1	3.526308	-0.000269	2.247583	1	-3.928357	0.899243	-1.370744
6	5.376494	-2.742338	1.469896	6	-6.294463	-1.387327	-0.495157
1	4.613748	-4.517522	0.512118	1	-5.954818	-3.516184	-0.405665
1	5.840111	-0.851475	2.396702	1	-6.318813	0.758660	-0.694254
1	6.398044	-3.107701	1.515540	1	-7.336116	-1.456936	-0.195069
6	0.206907	-1.558575	2.746654	6	3.049309	1.060180	0.433783
6	-1.083585	-1.042357	2.944037	6	2.671437	2.387264	0.127722
6	0.783487	-2.374827	3.727425	6	3.566878	3.441621	0.399623

IM2C

SCF Energy = -2529.420251

Gibbs Free Energy = -2528.801607

6	4.559970	-1.143750	-0.730430	1	0.769318	-5.527286	-3.294987
6	3.043215	-0.290145	0.947870	1	3.106897	-4.680311	-3.215889
6	4.118308	-2.434611	-0.433898	1	-0.518252	1.078223	2.385685
1	5.318753	-0.984146	-1.490587	6	0.611851	0.727148	-1.689026
6	2.598627	-1.576230	1.246881	6	0.208003	-0.580472	-2.038021
6	3.143791	-2.651793	0.546637	6	0.996111	-1.355866	-2.889862
1	4.536076	-3.280732	-0.970106	6	2.211417	-0.859462	-3.359156
1	1.837851	-1.746364	2.005608	6	2.618213	0.425039	-3.010953
1	2.806985	-3.660482	0.759203	6	1.810968	1.221351	-2.193880
1	3.609821	2.979438	1.220911	1	0.674610	-2.358151	-3.142446
1	2.751467	1.116839	2.609026	1	2.840318	-1.485140	-3.983619
1	-1.247840	-0.680089	2.703344	1	3.573031	0.809542	-3.351850

IM3B

SCF Energy = -3351.12764

Gibbs Free Energy = -3350.349715

28	-0.959004	0.172401	1.031205	15	-0.432387	1.684286	-0.527632
8	3.083117	-1.452560	2.279924	6	-1.874189	2.158787	-1.554797
16	2.685536	-0.166605	1.656942	6	-1.898658	2.008807	-2.947233
8	2.585673	0.993726	2.583413	6	-3.008108	2.658604	-0.897805
8	1.462781	-0.312491	0.792596	6	-3.042269	2.354575	-3.670538
6	3.994289	0.243316	0.489588	1	-1.028616	1.619169	-3.464490
6	4.205751	1.565547	0.103497	6	-4.139436	3.020222	-1.623159
6	4.743288	-0.781044	-0.087550	1	-3.007475	2.744969	0.184454
6	5.149836	1.855617	-0.880251	6	-4.160601	2.863429	-3.010794
1	3.638268	2.358766	0.573013	1	-3.054142	2.230948	-4.749459
6	5.679959	-0.482241	-1.074218	1	-5.013710	3.396233	-1.103635
1	4.598285	-1.797084	0.259717	1	-5.049768	3.130728	-3.573720
6	5.895472	0.838831	-1.490142	6	0.451674	3.245867	-0.217916
1	5.312047	2.888844	-1.177844	6	1.247155	3.342273	0.932335
1	6.261604	-1.283867	-1.523199	6	0.353752	4.337424	-1.093842
6	6.934424	1.159071	-2.536865	6	1.943096	4.522595	1.196865
1	7.005354	0.365113	-3.286819	1	1.363630	2.493597	1.599388
1	7.928811	1.268158	-2.086694	6	1.051344	5.513204	-0.821726
1	6.707138	2.096548	-3.053023	1	-0.269193	4.267295	-1.979679
6	-0.841645	0.244723	3.132588	6	1.845932	5.607096	0.323812
6	-1.327038	-0.830865	2.562280	1	2.563078	4.584043	2.085952
6	-1.764246	-2.176495	3.043753	1	0.972403	6.356496	-1.501299
1	-2.201769	-2.092515	4.044921	1	2.385717	6.525563	0.534691
1	-2.525904	-2.600996	2.383284	6	-1.048362	-1.145215	-1.527738
8	-0.687484	-3.100621	3.194911	8	-1.723754	-1.952718	-2.363868
6	0.251845	-3.145220	2.140806	6	-2.894687	-1.635156	-0.327630
1	1.089740	-3.748517	2.503736	6	-3.004532	-2.265066	-1.741706
1	0.667399	-2.156009	1.914525	7	-1.596157	-0.929837	-0.374580
6	-0.280090	-3.749039	0.853319	6	-4.166632	-1.556181	-2.474374
8	-1.460006	-4.066587	0.729873	1	-3.768414	-0.959518	-3.302746
6	0.684391	-3.954158	-0.270494	1	-4.874033	-2.274474	-2.901330
6	2.001290	-3.470721	-0.230640	6	-4.802237	-0.682865	-1.413975
6	0.244810	-4.683899	-1.386084	6	-5.963306	0.081902	-1.509427
6	2.861812	-3.731013	-1.297400	6	-4.081876	-0.714577	-0.216879
1	2.353403	-2.887562	0.613849	6	-6.387493	0.812472	-0.397010
6	1.111159	-4.949407	-2.441347	1	-6.533279	0.110203	-2.433708
1	-0.777240	-5.046478	-1.390367	6	-4.494958	0.017591	0.894143
6	2.426099	-4.474384	-2.394620	6	-5.656807	0.785850	0.795593
1	3.873864	-3.341937	-1.275505	1	-7.294357	1.406964	-0.458903
				1	-3.918755	-0.010038	1.813548
				1	-5.999892	1.358469	1.652021
				1	-3.088247	-3.350675	-1.726157
				1	-2.847038	-2.382602	0.461577

6	-0.491738	0.688126	4.551063	6	-5.764338	-0.605174	-1.811884
6	0.538839	-0.317001	5.108752	1	-6.495144	0.177868	-1.586699
1	0.787901	-0.052792	6.143057	1	-6.086556	-1.087671	-2.743113
1	0.145012	-1.336582	5.091671	6	-5.592054	-1.613306	-0.697631
1	1.453049	-0.294713	4.511983	6	-6.580910	-2.316792	-0.011958
6	0.115880	2.098690	4.533703	6	-4.241449	-1.817496	-0.394408
1	-0.579263	2.825223	4.095237	6	-6.200100	-3.222723	0.980532
1	0.339347	2.423444	5.554871	1	-7.631567	-2.161247	-0.241391
1	1.045569	2.098278	3.960242	6	-3.855355	-2.716650	0.597894
6	-1.775616	0.675560	5.401941	6	-4.848356	-3.419193	1.283342
1	-2.521598	1.369958	5.001058	1	-6.960569	-3.774987	1.524941
1	-2.222185	-0.322189	5.438064	1	-2.808408	-2.841459	0.842614
1	-1.544929	0.977551	6.429339	1	-4.566637	-4.120156	2.063358
				1	-4.097917	0.215391	-3.025388
				1	-2.700002	-1.503799	-1.913146
				28	-0.818539	-0.316447	0.646806
				6	0.783004	2.559947	4.469213
				6	1.091470	1.499716	3.616353
				6	0.087449	0.657784	3.100306
				6	-1.243127	0.924588	3.482975
				6	-1.550436	1.974951	4.342385
				6	-0.540140	2.805632	4.835286
				1	1.579652	3.197976	4.842700
				1	2.121883	1.336284	3.319269
				1	-2.028289	0.295524	3.078246
				1	-2.585653	2.156824	4.617440
				1	-0.782808	3.634844	5.493692
				6	0.408759	-0.380013	2.086258
				6	1.486781	-1.172430	2.221565
				6	2.337490	-1.436317	3.444298
				1	1.809427	-1.285536	4.387800
				1	3.268793	-0.840539	3.466581
				8	2.677788	-2.826030	3.323784
				6	2.991492	-3.013873	1.955303
				1	4.020732	-2.685657	1.747109
				1	2.901357	-4.076412	1.720392
				6	2.021937	-2.105729	1.136656
				8	2.776616	-1.300741	0.214487
				6	0.920801	-2.882073	0.438079
				6	0.288126	-3.937026	1.107046
				6	0.474379	-2.535122	-0.839763
				6	-0.736024	-4.654105	0.493090
				1	0.589982	-4.177594	2.121889
				6	-0.546919	-3.258995	-1.461571
				1	0.941067	-1.709864	-1.358263
				6	-1.153700	-4.324609	-0.800196
				1	-1.213185	-5.472130	1.025035
				1	-0.857485	-2.985906	-2.466527
				1	-1.951750	-4.885657	-1.276561
				14	3.648960	-1.589827	-1.155367
				8	5.181332	-0.984469	-0.952592
				8	3.009122	-0.704238	-2.397916
				6	6.039714	-1.347949	0.123743
				1	7.061286	-1.378094	-0.272320
				1	5.810436	-2.361153	0.484919
				6	5.942269	-0.349357	1.267821

IM3C

SCF Energy = -3168.569723

Gibbs Free Energy = -3167.775348

6	-1.267721	2.642177	0.260331	6	0.087449	0.657784	3.100306
6	-2.653794	2.362747	0.194264	6	-1.243127	0.924588	3.482975
6	-3.578452	3.209861	0.808327	6	-1.550436	1.974951	4.342385
6	-3.135992	4.303552	1.552766	6	-0.540140	2.805632	4.835286
6	-1.770531	4.558166	1.661462	1	1.579652	3.197976	4.842700
6	-0.844649	3.744729	1.004270	1	2.121883	1.336284	3.319269
1	-4.637152	2.989995	0.720366	1	-2.028289	0.295524	3.078246
1	-3.855422	4.944781	2.051701	1	-2.585653	2.156824	4.617440
1	-1.418218	5.395139	2.255951	1	-0.782808	3.634844	5.493692
1	0.214175	3.959557	1.086279	6	0.408759	-0.380013	2.086258
15	-0.075457	1.458140	-0.505260	6	1.486781	-1.172430	2.221565
6	1.521492	2.341071	-0.449270	6	2.337490	-1.436317	3.444298
6	1.772906	3.457778	-1.261498	1	1.809427	-1.285536	4.387800
6	2.513860	1.878453	0.422850	1	3.268793	-0.840539	3.466581
6	3.000853	4.111321	-1.191906	8	2.677788	-2.826030	3.323784
1	1.011097	3.806186	-1.951890	6	2.991492	-3.013873	1.955303
6	3.737952	2.545594	0.498196	1	4.020732	-2.685657	1.747109
1	2.331195	0.986240	1.007371	1	2.901357	-4.076412	1.720392
6	3.983284	3.658290	-0.306200	6	2.021937	-2.105729	1.136656
1	3.193128	4.971414	-1.826401	8	2.776616	-1.300741	0.214487
1	4.502191	2.184977	1.177314	6	0.920801	-2.882073	0.438079
1	4.940127	4.169106	-0.250936	6	0.288126	-3.937026	1.107046
6	-0.516317	1.505801	-2.294950	6	0.474379	-2.535122	-0.839763
6	0.035009	0.511017	-3.118127	6	-0.736024	-4.654105	0.493090
6	-1.405361	2.433814	-2.852729	1	0.589982	-4.177594	2.121889
6	-0.305156	0.443801	-4.468428	6	-0.546919	-3.258995	-1.461571
1	0.746430	-0.199091	-2.710925	1	0.941067	-1.709864	-1.358263
6	-1.754080	2.356086	-4.202884	6	-1.153700	-4.324609	-0.800196
1	-1.839805	3.210635	-2.233303	1	-1.213185	-5.472130	1.025035
6	-1.208869	1.359362	-5.012918	1	-0.857485	-2.985906	-2.466527
1	0.136168	-0.327239	-5.093029	1	-1.951750	-4.885657	-1.276561
1	-2.450128	3.078276	-4.619584	14	3.648960	-1.589827	-1.155367
1	-1.480962	1.300037	-6.062545	8	5.181332	-0.984469	-0.952592
6	-3.124426	1.152046	-0.499811	8	3.009122	-0.704238	-2.397916
8	-4.239620	1.250949	-1.254228	6	6.039714	-1.347949	0.123743
6	-3.356277	-0.935388	-1.250592	1	7.061286	-1.378094	-0.272320
6	-4.363762	-0.008813	-1.989784	1	5.810436	-2.361153	0.484919
7	-2.540178	0.005885	-0.460887	6	5.942269	-0.349357	1.267821

1	4.918299	-0.312464	1.648190	6	-2.140287	-1.563401	-1.064211
1	6.614027	-0.629651	2.086190	6	-3.164658	-2.439995	-1.432771
1	6.217737	0.648823	0.916129	6	-2.861781	-3.686886	-1.979703
6	3.513103	0.572001	-2.822366	6	-1.533437	-4.055968	-2.172823
1	2.652918	1.140513	-3.187690	6	-0.502036	-3.173113	-1.835068
1	3.933615	1.116361	-1.972676	1	-4.194242	-2.145597	-1.270850
6	4.553390	0.403920	-3.917512	1	-3.663928	-4.364921	-2.250908
1	4.883321	1.383178	-4.282151	1	-1.292202	-5.024854	-2.598401
1	5.423574	-0.134336	-3.532524	1	0.530125	-3.453497	-2.013130
1	4.137053	-0.156976	-4.760123	15	0.528575	-0.712301	-0.877799
6	3.689953	-3.395987	-1.615847	6	0.257383	0.569829	-2.155688
1	4.354965	-3.547082	-2.471476	6	-0.276327	0.227180	-3.408573
1	4.060890	-4.007820	-0.786798	6	0.544519	1.910999	-1.865799
1	2.694588	-3.761803	-1.877173	6	-0.509340	1.217178	-4.362313
1	-1.460661	-1.305106	1.544292	1	-0.519115	-0.805595	-3.636037
				6	0.309386	2.894828	-2.825829
				1	0.922459	2.183379	-0.889426
				6	-0.217618	2.551782	-4.071206
				1	-0.921562	0.946283	-5.329282
				1	0.516460	3.931218	-2.584950
				1	-0.406521	3.321563	-4.812967
				6	2.104430	-1.534403	-1.274011
				6	2.768824	-2.264429	-0.278464
				6	2.656329	-1.457666	-2.561156
				6	3.964632	-2.916484	-0.568347
				1	2.357785	-2.297386	0.724789
				6	3.857119	-2.107586	-2.844544
				1	2.156932	-0.884791	-3.334382
				6	4.510957	-2.837831	-1.850967
				1	4.477653	-3.471923	0.209920
				1	4.281802	-2.041056	-3.841233
				1	5.447756	-3.338934	-2.073589
				6	-2.503760	-0.275568	-0.450886
				8	-3.741011	0.178795	-0.706281
				6	-2.557796	1.634145	0.748961
				6	-3.838718	1.512830	-0.126518
				7	-1.769524	0.449937	0.328326
				6	-3.747571	2.604886	-1.215819
				1	-3.510932	2.138554	-2.179276
				1	-4.695046	3.137578	-1.339086
				6	-2.628136	3.502926	-0.741791
				6	-2.237084	4.734178	-1.261841
				6	-1.958148	2.961090	0.359489
				6	-1.167140	5.408091	-0.666864
				1	-2.755664	5.167721	-2.111781
				6	-0.900763	3.632354	0.967720
				6	-0.503403	4.861693	0.437125
				1	-0.855390	6.371550	-1.058799
				1	-0.378916	3.204040	1.815514
				1	0.319832	5.402404	0.893123
				1	-4.771544	1.542615	0.435628
				1	-2.734208	1.547091	1.826142

IM3D_iso

SCF Energy = -2529.87621

Gibbs Free Energy = -2529.253270

28	-0.048050	-0.156683	1.139871	1	-0.406521	3.321563	-4.812967
6	-2.335258	-4.261701	1.525549	6	2.104430	-1.534403	-1.274011
6	-1.502072	-3.223890	1.925766	6	2.768824	-2.264429	-0.278464
6	-2.057451	-2.006103	2.362043	6	2.656329	-1.457666	-2.561156
6	-3.455005	-1.844107	2.381292	6	3.964632	-2.916484	-0.568347
6	-4.280291	-2.891331	1.982021	1	2.357785	-2.297386	0.724789
6	-3.722874	-4.098586	1.554510	6	3.857119	-2.107586	-2.844544
1	-1.904542	-5.196624	1.183528	1	2.156932	-0.884791	-3.334382
1	-0.423626	-3.330734	1.894265	6	4.510957	-2.837831	-1.850967
1	-3.877414	-0.902294	2.715273	1	4.477653	-3.471923	0.209920
1	-5.358035	-2.766860	2.004892	1	4.281802	-2.041056	-3.841233
1	-4.369746	-4.911604	1.240955	1	5.447756	-3.338934	-2.073589
6	-1.209231	-0.923344	2.749229	6	-2.503760	-0.275568	-0.450886
6	-0.552121	0.047713	3.147490	8	-3.741011	0.178795	-0.706281
6	0.013209	0.953538	4.181502	6	-2.557796	1.634145	0.748961
1	-0.812748	1.505504	4.640340	6	-3.838718	1.512830	-0.126518
1	0.473399	0.331568	4.964322	7	-1.769524	0.449937	0.328326
8	0.925149	1.933918	3.732637	6	-3.747571	2.604886	-1.215819
6	2.203191	1.454213	3.379736	1	-3.510932	2.138554	-2.179276
1	2.389746	0.458073	3.801899	1	-4.695046	3.137578	-1.339086
1	2.950850	2.134932	3.807191	6	-2.628136	3.502926	-0.741791
6	2.403761	1.417036	1.865589	6	-2.237084	4.734178	-1.261841
8	1.507016	1.827442	1.132735	6	-1.958148	2.961090	0.359489
6	3.678169	0.902163	1.318413	6	-1.167140	5.408091	-0.666864
6	4.640655	0.271290	2.123687	1	-2.755664	5.167721	-2.111781
6	3.907587	1.022052	-0.062769	6	-0.900763	3.632354	0.967720
6	5.804388	-0.238624	1.553480	6	-0.503403	4.861693	0.437125
1	4.489158	0.168588	3.192739	1	-0.855390	6.371550	-1.058799
6	5.072723	0.519891	-0.627376	1	-0.378916	3.204040	1.815514
1	3.160876	1.510987	-0.676564	1	0.319832	5.402404	0.893123
6	6.020059	-0.115909	0.179372	1	-4.771544	1.542615	0.435628
1	6.542897	-0.728934	2.179235	1	-2.734208	1.547091	1.826142
1	5.238662	0.608680	-1.695278				
1	6.927415	-0.515087	-0.262828				
1	1.143648	-0.840775	1.573403				
6	-0.789662	-1.926631	-1.281771				

IM3D

SCF Energy = -2529.874249

Gibbs Free Energy = -2529.249669

6	0.891861	0.806226	3.669955	1	-3.518716	-3.308999	3.267885
1	2.433988	0.968504	2.176152	1	-4.505296	-1.858529	3.530917
6	-0.885289	-0.762421	3.195617	1	-5.215257	-3.292189	2.789025
1	-0.769871	-1.779474	1.307259				
6	-0.298949	0.183240	4.040856				
1	1.345091	1.547525	4.320902				
1	-1.821575	-1.237897	3.468389				
1	-0.775945	0.441858	4.981285				
6	2.133553	-2.590979	0.058840	28	0.637791	0.642812	-0.534130
6	2.582976	-3.141485	1.267586	8	-2.925821	1.787382	-1.985874
6	2.119333	-3.375787	-1.101763	16	-2.066482	0.616335	-1.732731
6	3.025258	-4.463169	1.309569	8	-1.164723	0.167460	-2.814748
1	2.574263	-2.540021	2.171233	8	-1.286444	0.801384	-0.408197
6	2.567798	-4.695219	-1.055608	6	-3.147443	-0.765900	-1.381298
1	1.735230	-2.955063	-2.025880	6	-4.292851	-0.571745	-0.615428
6	3.021193	-5.238617	0.147990	6	-2.795900	-2.036523	-1.832038
1	3.366792	-4.888767	2.248223	6	-5.073056	-1.671325	-0.269392
1	2.550883	-5.301403	-1.955895	1	-4.563528	0.423809	-0.292781
1	3.361634	-6.269056	0.183606	6	-3.582129	-3.127914	-1.472810
6	1.815476	2.170597	-0.930599	1	-1.920181	-2.148643	-2.458530
8	1.863920	3.519013	-0.905797	6	-4.721135	-2.965691	-0.673451
6	-0.323553	2.736019	-1.260582	1	-5.961560	-1.521017	0.337948
6	0.545708	4.017407	-1.309162	1	-3.308817	-4.122913	-1.815584
7	0.673619	1.641931	-1.208289	6	-5.520959	-4.161889	-0.226446
6	0.007818	4.985239	-0.246955	1	-6.538225	-3.881671	0.060646
1	0.827463	5.492153	0.271532	1	-5.583887	-4.921474	-1.011632
1	-0.600592	5.761387	-0.727730	1	-5.047101	-4.631520	0.644654
6	-0.831828	4.101493	0.649326	6	0.814461	2.511737	-0.966340
6	-1.377143	4.392291	1.898589	6	0.509755	3.153970	0.171789
6	-1.052955	2.852449	0.061065	6	0.290644	4.614871	0.480131
6	-2.139311	3.416502	2.546667	1	0.899929	5.270365	-0.144623
1	-1.210427	5.359293	2.365249	1	0.557742	4.792720	1.528034
6	-1.807506	1.875636	0.702883	8	-1.062859	5.084505	0.288376
6	-2.353503	2.168490	1.952526	6	-2.108361	4.144753	0.246568
1	-2.566385	3.629702	3.522327	1	-3.001531	4.726456	-0.002800
1	-1.958795	0.909042	0.241787	1	-1.988047	3.397508	-0.549754
1	-2.940110	1.413236	2.464725	6	-2.348573	3.368591	1.530802
1	0.665877	4.460637	-2.300028	8	-1.528442	3.347887	2.438231
1	-0.985451	2.572978	-2.111127	6	-3.618557	2.574432	1.648188
28	0.090559	-0.256677	-1.402074	6	-4.723909	2.768697	0.808440
8	-1.490700	0.314099	-2.302733	6	-3.706219	1.633716	2.685037
16	-2.704472	-0.587691	-2.677493	6	-5.905136	2.056608	1.024485
8	-3.786106	0.285981	-3.153438	1	-4.670529	3.463014	-0.020747
8	-2.306490	-1.740824	-3.496782	6	-4.876443	0.908381	2.886825
6	-3.232253	-1.240916	-1.084079	1	-2.841831	1.502455	3.326685
6	-4.039208	-0.461027	-0.256837	6	-5.984728	1.127196	2.062487
6	-2.790415	-2.494374	-0.661370	1	-6.758440	2.221314	0.373983
6	-4.371071	-0.925003	1.015629	1	-4.934245	0.186260	3.696307
1	-4.395924	0.498291	-0.614576	1	-6.905168	0.574872	2.228465
6	-3.133804	-2.950326	0.610320	1	0.252473	2.530539	1.029916
1	-2.186026	-3.092956	-1.332394	6	1.096924	3.120008	-2.344830
6	-3.919700	-2.170553	1.470882	6	-0.189849	3.821766	-2.841399
1	-4.995951	-0.314046	1.662237	1	-0.018948	4.251435	-3.836014
1	-2.788630	-3.926900	0.941080	1	-0.485339	4.626967	-2.164079
1	-0.240851	-1.656522	-1.491328	1	-1.020048	3.117028	-2.912458
6	-4.305523	-2.681355	2.837700	6	1.482725	2.036924	-3.372860

IM4B

SCF Energy = -3351.131522

Gibbs Free Energy = -3350.350930

1	2.455312	1.590442	-3.139641	1	2.367980	2.416572	1.684434
1	1.562100	2.485046	-4.369815	1	3.271336	2.410149	4.011125
1	0.731463	1.246621	-3.404697	1	5.389109	0.906426	-1.909404
6	2.240272	4.160804	-2.311849	1	3.464591	2.093720	-0.969753
1	3.178901	3.731133	-1.945716				
1	2.004433	5.022088	-1.685777				
1	2.426724	4.530892	-3.326609				
6	1.007627	-2.380844	-1.325908				
6	2.077010	-1.860042	-2.093190				
6	2.410230	-2.434541	-3.322416	28	-0.006220	-0.371221	-0.704706
6	1.664830	-3.502548	-3.821098	6	-3.420794	3.298942	-1.283792
6	0.605005	-4.013484	-3.075382	6	-2.386659	2.373186	-1.348905
6	0.287177	-3.463160	-1.830319	6	-2.661290	1.008092	-1.546486
1	3.244695	-2.031971	-3.885415	6	-3.999686	0.587063	-1.669656
1	1.914194	-3.931459	-4.785945	6	-5.031158	1.520226	-1.594016
1	0.022024	-4.845840	-3.457542	6	-4.747176	2.872819	-1.400432
1	-0.534385	-3.871187	-1.254004	1	-3.197396	4.349608	-1.128994
15	0.611313	-1.533657	0.254196	1	-1.357125	2.697864	-1.238659
6	2.032373	-1.996510	1.322253	1	-4.216598	-0.468492	-1.781949
6	2.982488	-2.963233	0.972374	1	-6.060937	1.187791	-1.679948
6	2.142457	-1.339861	2.556718	1	-5.555523	3.594587	-1.336349
6	4.028122	-3.268786	1.846724	6	-1.582950	0.037676	-1.557212
1	2.909609	-3.479676	0.021363	6	-1.391560	-1.065068	-2.289367
6	3.174149	-1.660402	3.433653	6	-2.259902	-1.672940	-3.370153
1	1.424405	-0.570298	2.823702	1	-2.705041	-0.879615	-3.974284
6	4.122561	-2.622012	3.078254	1	-1.663631	-2.329536	-4.019706
1	4.761411	-4.019416	1.566259	8	-3.366881	-2.397026	-2.833584
1	3.254376	-1.139857	4.381305	6	-2.998767	-3.453153	-1.968481
1	4.935131	-2.860295	3.757734	1	-2.186241	-4.046164	-2.403946
6	-0.767432	-2.425223	1.046719	1	-3.875651	-4.102885	-1.883133
6	-1.881270	-1.684550	1.463922	6	-2.685255	-2.957818	-0.541975
6	-0.690722	-3.796515	1.340429	8	-3.484180	-2.213428	0.007252
6	-2.916691	-2.318229	2.152171	6	-1.450056	-3.410205	0.171058
1	-1.939331	-0.627572	1.231717	6	-0.403186	-4.105908	-0.454275
6	-1.735242	-4.425352	2.012649	6	-1.335272	-3.090183	1.534314
1	0.190781	-4.363834	1.057534	6	0.734470	-4.466332	0.267922
6	-2.848478	-3.684230	2.421305	1	-0.461736	-4.371163	-1.503512
1	-3.777904	-1.737029	2.461658	6	-0.206982	-3.459573	2.255583
1	-1.675504	-5.486987	2.233212	1	-2.152851	-2.558885	2.007665
1	-3.656773	-4.173812	2.956861	6	0.832663	-4.146939	1.622499
6	2.886699	-0.737694	-1.587599	1	1.535090	-5.010545	-0.223544
8	4.199890	-0.769877	-1.879446	1	-0.129809	-3.207167	3.307547
6	3.637260	1.108780	-0.538512	1	1.713976	-4.436408	2.186395
6	4.832210	0.334312	-1.167171	1	-0.528246	-1.721215	-1.999228
7	2.474188	0.261872	-0.880682	6	0.664613	-0.084233	2.397287
6	5.713584	-0.180974	-0.008420	6	1.811181	-0.887644	2.206824
1	5.631123	-1.271814	0.055119	6	2.429390	-1.495697	3.306363
1	6.770157	0.058425	-0.165265	6	1.890495	-1.356652	4.584050
6	5.141654	0.489039	1.219816	6	0.734277	-0.600458	4.769531
6	5.656148	0.488001	2.514603	6	0.133406	0.041145	3.682747
6	3.963545	1.184214	0.933293	1	3.319205	-2.093150	3.147490
6	4.974643	1.184621	3.514899	1	2.370036	-1.841302	5.427778
1	6.574584	-0.044684	2.744143	1	0.303986	-0.494132	5.760093
6	3.275530	1.876787	1.927357	1	-0.749137	0.651308	3.837001
6	3.790166	1.869871	3.225184	15	-0.040662	0.879168	1.001494
1	5.369454	1.195058	4.526690	6	1.148652	2.247662	0.812594

IM4D

SCF Energy = -2529.911961

Gibbs Free Energy = -2529.282577

6	1.744301	2.856232	1.928374	6	4.072026	0.228753	3.742503
6	1.492244	2.673204	-0.478327	1	2.454572	1.664129	3.711912
6	2.658432	3.892705	1.749256	6	4.773031	-0.755715	3.034352
1	1.501007	2.516706	2.930083	1	4.897957	-1.813183	1.160905
6	2.411023	3.707388	-0.651255	1	4.362240	0.460124	4.764063
1	1.062879	2.180725	-1.343776	6	5.954594	-1.463862	3.648281
6	2.991000	4.319087	0.460737	1	5.971961	-1.350364	4.735700
1	3.115019	4.363723	2.613874	1	5.945794	-2.533855	3.416713
1	2.680026	4.020345	-1.653865	1	6.896717	-1.058674	3.258567
1	3.707813	5.122895	0.325847	6	-0.969684	2.317815	-1.738753
6	-1.606505	1.545955	1.617409	6	-0.323465	1.540980	-2.474899
6	-2.737532	0.715519	1.572239	6	0.612568	1.208920	-3.580952
6	-1.716444	2.861807	2.085592	1	0.060894	1.188572	-4.526857
6	-3.969362	1.205446	1.995526	1	1.052933	0.220571	-3.434437
1	-2.673894	-0.291219	1.171475	8	1.622074	2.197416	-3.746581
6	-2.954712	3.342633	2.509009	6	2.535121	2.283826	-2.671835
1	-0.848268	3.511041	2.103808	1	3.081044	3.224706	-2.803476
6	-4.079726	2.518173	2.460184	1	2.025905	2.345077	-1.700620
1	-4.844581	0.567353	1.937420	6	3.542220	1.136294	-2.642866
1	-3.041481	4.363720	2.866317	8	3.463022	0.213947	-3.445835
1	-5.044892	2.900913	2.776448	6	4.619800	1.163353	-1.608871
6	2.363825	-1.148069	0.872625	6	4.662600	2.124288	-0.588228
8	3.646470	-1.535993	0.819721	6	5.607789	0.166844	-1.659862
6	2.692246	-1.407337	-1.346111	6	5.673741	2.077689	0.370558
6	4.031345	-1.631215	-0.584761	1	3.881389	2.866993	-0.493101
7	1.738872	-1.073271	-0.257574	6	6.618663	0.128730	-0.706898
6	4.984346	-0.479744	-0.974709	1	5.558808	-0.564892	-2.458819
1	5.243053	0.104429	-0.085548	6	6.650561	1.085033	0.313671
1	5.921828	-0.866081	-1.387477	1	5.680919	2.805958	1.174883
6	4.211431	0.323634	-1.997265	1	7.380166	-0.644373	-0.752520
6	4.622989	1.465758	-2.682374	1	7.432959	1.049356	1.066340
6	2.952677	-0.227689	-2.250462	1	-2.053995	0.088628	-1.725181
6	3.761104	2.042461	-3.618569	6	-0.027908	-1.990227	1.004387
1	5.601043	1.899883	-2.498236	6	-0.559104	-1.232769	2.072325
6	2.094374	0.332995	-3.195301	6	-0.004391	-1.353164	3.351488
6	2.506095	1.479803	-3.877831	6	1.069825	-2.208249	3.583639
1	4.074447	2.928571	-4.161803	6	1.586516	-2.965583	2.536833
1	1.122611	-0.105508	-3.399984	6	1.036651	-2.857338	1.258202
1	1.854252	1.930003	-4.619560	1	-0.405791	-0.742963	4.150516
1	4.466831	-2.620496	-0.720331	1	1.508757	-2.267580	4.573838
1	2.319035	-2.292896	-1.870191	1	2.429761	-3.627900	2.704155
				1	1.454835	-3.438227	0.444453
				15	-0.716398	-1.795410	-0.690811
IM4				6	-2.260655	-2.774299	-0.573804
SCF Energy = -3424.903328				6	-2.336078	-3.908947	0.249784
Gibbs Free Energy = -3424.161942				6	-3.400262	-2.364374	-1.275842
				6	-3.529286	-4.620845	0.359552
28	-0.927294	0.431263	-0.950414	1	-1.464835	-4.224743	0.814185
8	1.877224	2.819924	0.574873	6	-4.595808	-3.072013	-1.157650
16	1.310162	1.548220	1.092273	1	-3.357619	-1.473000	-1.889788
8	0.271628	1.731134	2.128087	6	-4.661890	-4.201034	-0.341591
8	0.898540	0.629748	-0.053511	1	-3.577383	-5.496324	1.000259
6	2.638440	0.612977	1.848636	1	-5.477469	-2.723535	-1.684488
6	3.311007	-0.374233	1.131179	1	-5.595054	-4.747736	-0.243511
6	3.008268	0.913702	3.158317	6	0.429633	-2.752491	-1.736766
6	4.369789	-1.051195	1.726653	6	1.613150	-2.104245	-2.124838
1	3.001773	-0.611250	0.123372				

6	0.182109	-4.060190	-2.172102	1	5.728367	3.219491	-0.438515
6	2.541309	-2.755518	-2.933095	6	1.861194	-0.292171	-1.688394
1	1.797981	-1.087574	-1.796746	6	2.050158	-1.166084	-2.697149
6	1.114667	-4.710345	-2.982700	6	1.021013	-2.187455	-3.047114
1	-0.733040	-4.565288	-1.882082	1	0.438734	-1.911268	-3.934130
6	2.291355	-4.061766	-3.361714	1	1.436325	-3.185477	-3.228016
1	3.432033	-2.220222	-3.242005	8	0.049923	-2.261507	-1.963700
1	0.917775	-5.723311	-3.321437	6	0.252410	-3.331224	-1.009467
1	3.008336	-4.569944	-3.999761	1	0.684052	-4.189342	-1.527609
6	-1.661191	-0.271519	1.895302	1	-0.739263	-3.597007	-0.641420
8	-2.374035	0.000714	3.009676	6	1.067286	-2.865835	0.213279
6	-3.152587	1.217076	1.135986	8	0.438032	-2.325415	1.118873
6	-3.384871	0.983371	2.657934	6	2.533479	-3.038425	0.286919
7	-2.008577	0.341463	0.819695	6	3.286709	-3.634202	-0.736293
6	-4.801206	0.397073	2.833483	6	3.192405	-2.552316	1.430635
1	-4.747887	-0.557594	3.366883	6	4.672203	-3.724164	-0.627605
1	-5.430762	1.065318	3.432192	1	2.804112	-4.026410	-1.622955
6	-5.333537	0.257212	1.424116	6	4.574465	-2.641864	1.537541
6	-6.564659	-0.255870	1.017078	1	2.598123	-2.106424	2.219213
6	-4.433795	0.759628	0.479704	6	5.317695	-3.224943	0.505860
6	-6.888215	-0.248245	-0.341542	1	5.248211	-4.183631	-1.423839
1	-7.267320	-0.651096	1.745510	1	5.075885	-2.265005	2.423108
6	-4.757649	0.779373	-0.875106	1	6.397585	-3.296365	0.588247
6	-5.992933	0.272635	-1.282237	1	2.937883	-1.126500	-3.329992
1	-7.846076	-0.641824	-0.669095	6	-0.764014	2.573063	-0.571437
1	-4.053196	1.174738	-1.596724	6	-1.851515	2.318164	-1.446039
1	-6.260580	0.282327	-2.334833	6	-2.388299	3.357860	-2.216473
1	-3.197104	1.862336	3.275248	6	-1.833443	4.634711	-2.163107
1	-2.884190	2.244211	0.885416	6	-0.738167	4.877997	-1.337489
6	-1.688667	3.402074	-1.133560	6	-0.212036	3.855111	-0.544171
6	-2.966404	3.748828	-1.612898	1	-3.231970	3.150930	-2.863997
6	-1.160695	4.082174	-0.018956	1	-2.249472	5.429964	-2.772086
6	-3.715482	4.730459	-0.970495	1	-0.288699	5.865142	-1.304010
1	-3.361964	3.235099	-2.482587	1	0.644577	4.056984	0.086146
6	-1.917467	5.067815	0.609433	15	-0.088455	1.182034	0.411785
1	-0.170995	3.827831	0.341265	6	-1.361797	0.807742	1.681102
6	-3.197100	5.387817	0.147730	6	-2.665117	1.317445	1.640706
1	-4.704371	4.981438	-1.342183	6	-0.972254	-0.007627	2.754537
1	-1.504390	5.584363	1.470541	6	-3.567386	1.012358	2.658721
1	-3.784105	6.150422	0.650799	1	-2.982590	1.967807	0.834644
				6	-1.874778	-0.299749	3.772990
				1	0.031473	-0.413341	2.792142
				6	-3.174405	0.206870	3.726513
				1	-4.576269	1.409424	2.616515
				1	-1.562734	-0.928031	4.601243
28	0.058132	-0.392776	-1.071026	1	-3.878608	-0.026459	4.518460
6	5.200236	1.139324	-0.654809	6	1.281420	1.743094	1.465087
6	4.200673	0.229746	-0.995728	6	2.391796	0.906200	1.613988
6	2.927769	0.678607	-1.385152	6	1.166699	2.894013	2.260930
6	2.698605	2.060918	-1.461653	6	3.412144	1.247975	2.498636
6	3.700233	2.969123	-1.129220	1	2.461456	-0.000986	1.032479
6	4.951434	2.511930	-0.709864	6	2.192407	3.234731	3.139654
1	6.175194	0.775893	-0.343461	1	0.274395	3.509146	2.214138
1	4.387457	-0.836942	-0.933867	6	3.320870	2.418310	3.251568
1	1.729672	2.418442	-1.792160	1	4.278966	0.601568	2.588219
1	3.506092	4.035518	-1.197001	1	2.105572	4.130547	3.746061

IM5D

SCF Energy = -2529.916337

Gibbs Free Energy = -2529.283853

1	4.118796	2.689419	3.935533	6	-3.378336	-2.061524	-1.283468
6	-2.438117	0.976111	-1.586089	6	-3.648418	-1.051071	-0.350380
8	-3.682706	0.913955	-2.076477	6	-3.770531	-3.381092	-1.005627
6	-2.888785	-1.222441	-1.484663	6	-4.309596	-1.358008	0.839275
6	-4.027662	-0.501045	-2.255728	1	-3.317042	-0.037516	-0.521259
7	-1.879147	-0.155839	-1.288690	6	-4.424537	-3.685477	0.183264
6	-5.349715	-0.824621	-1.551299	1	-3.548344	-4.146290	-1.742023
1	-5.962794	0.075598	-1.445754	6	-4.696655	-2.671058	1.107887
1	-5.928014	-1.537045	-2.151203	1	-4.506321	-0.564310	1.551181
6	-4.922789	-1.428353	-0.232382	1	-4.728948	-4.707111	0.390842
6	-5.724456	-1.774263	0.853791	1	-5.210097	-2.907732	2.035610
6	-3.544979	-1.667324	-0.194743	1	1.914877	-0.513062	-1.199893
6	-5.128979	-2.361616	1.971565	6	0.216364	0.453943	2.204136
1	-6.795284	-1.594532	0.831532	6	-0.702145	-0.616461	2.111741
6	-2.941947	-2.238335	0.923801	6	-1.738628	-0.729059	3.045423
6	-3.749495	-2.588806	2.006449	6	-1.892758	0.227189	4.047318
1	-5.742078	-2.638928	2.823417	6	-1.003232	1.297905	4.125187
1	-1.867332	-2.374055	0.977152	6	0.044823	1.407458	3.208062
1	-3.297895	-3.027283	2.890009	1	-2.420003	-1.567261	2.970198
1	-4.040028	-0.679757	-3.332614	1	-2.704412	0.134428	4.762000
1	-2.427730	-2.040488	-2.041631	1	-1.119352	2.050498	4.899049
				1	0.735385	2.239888	3.270413
				15	1.618594	0.541601	1.021084
IM5				6	2.655300	-0.880230	1.563308
SCF Energy = -3424.904552				6	2.433081	-1.577982	2.757104
Gibbs Free Energy = -3424.161298				6	3.723996	-1.265441	0.740670
				6	3.257599	-2.647832	3.114208
28	0.682818	0.131324	-0.986435	6	3.257599	-2.647832	3.114208
8	-1.458375	3.072372	-1.874986	1	1.617931	-1.290387	3.411111
16	-1.385296	2.508918	-0.512290	6	4.554582	-2.320176	1.105631
8	-0.533204	3.219013	0.464421	1	3.894906	-0.742959	-0.194810
8	-1.087609	1.005584	-0.519499	6	4.319237	-3.019629	2.291116
6	-3.058383	2.493434	0.128708	1	3.070707	-3.183317	4.040545
6	-3.262372	2.312264	1.495096	1	5.368379	-2.614209	0.451764
6	-4.136236	2.557069	-0.752567	1	4.958005	-3.853092	2.567057
6	-4.561211	2.173338	1.977152	6	2.619237	1.985074	1.525048
1	-2.411795	2.283417	2.163450	6	2.465013	3.192843	0.831610
6	-5.430984	2.413166	-0.256115	6	3.557185	1.896474	2.566810
1	-3.947305	2.717886	-1.808216	6	3.237260	4.299326	1.183009
6	-5.662969	2.206849	1.110004	1	1.730422	3.273214	0.043211
1	-4.723456	2.032323	3.042913	6	4.324642	3.006646	2.912698
1	-6.275002	2.458794	-0.939150	1	3.690302	0.960893	3.099470
6	-7.061895	1.991566	1.630965	6	4.166422	4.209290	2.219156
1	-7.157061	2.316566	2.671051	1	3.113060	5.226441	0.633548
1	-7.331811	0.928627	1.593035	1	5.048183	2.931801	3.719175
1	-7.799923	2.535114	1.034240	1	4.769883	5.072109	2.486192
6	1.174756	1.177589	-2.604971	6	-0.552722	-1.686171	1.105670
6	0.420715	0.252004	-2.983341	8	-0.941494	-2.914966	1.517333
6	-0.297594	-0.559253	-4.002397	6	-0.030961	-2.953396	-0.669121
1	0.154741	-0.371388	-4.981814	6	-0.539770	-3.860665	0.489155
1	-0.191391	-1.626524	-3.777916	7	-0.066374	-1.595818	-0.082239
8	-1.669999	-0.223591	-4.165940	6	0.654735	-4.721504	0.960097
6	-2.453882	-0.357783	-3.002036	1	0.965796	-4.399334	1.960138
1	-3.432615	0.082837	-3.226861	1	0.391289	-5.782256	1.025710
1	-2.026583	0.211377	-2.168908	6	1.733912	-4.458527	-0.065797
6	-2.660905	-1.801683	-2.570028	6	2.970543	-5.088320	-0.192986
8	-2.231079	-2.732645	-3.242004	6	1.358185	-3.460439	-0.968577

6	3.824753	-4.703886	-1.228582	6	4.292389	1.899446	-0.209226
1	3.267760	-5.868092	0.502464	6	5.116702	1.735246	-2.485070
6	2.204083	-3.077023	-2.007262	6	5.414854	1.199715	0.236670
6	3.446192	-3.702918	-2.129276	1	3.546519	2.196564	0.519992
1	4.789555	-5.190410	-1.338862	6	6.235184	1.042365	-2.035027
1	1.899499	-2.308529	-2.709157	1	4.972427	1.959627	-3.536809
1	4.116085	-3.419939	-2.935655	6	6.382792	0.768990	-0.670100
1	-1.424754	-4.442346	0.235440	1	5.514735	0.981586	1.294663
1	-0.669501	-2.973517	-1.552040	1	6.992754	0.714547	-2.741091
6	2.061403	2.310982	-2.551910	1	7.252698	0.221883	-0.317717
6	1.555982	3.615766	-2.683978	1	-1.115262	1.450191	-2.079898
6	3.436256	2.116706	-2.326854	6	-0.113879	-2.333075	0.238155
6	2.425569	4.702262	-2.598228	6	-0.731945	-2.123173	1.489857
1	0.488414	3.753217	-2.807308	6	-0.329727	-2.880977	2.595249
6	4.293641	3.208399	-2.250043	6	0.685188	-3.826158	2.473992
1	3.812593	1.106697	-2.200731	6	1.297552	-4.033025	1.241155
6	3.791012	4.505388	-2.384955	6	0.894401	-3.291244	0.130027
1	2.029197	5.708804	-2.692738	1	-0.797402	-2.695956	3.553977
1	5.352964	3.050262	-2.071861	1	1.009546	-4.382958	3.346186
1	4.460814	5.357261	-2.315039	1	2.104241	-4.751661	1.144812
				1	1.384279	-3.441084	-0.825622
				15	-0.667990	-1.369576	-1.216343
IM6				6	-2.138437	-2.308780	-1.768410
SCF Energy = -3424.921086				6	-2.191236	-3.710504	-1.737097
Gibbs Free Energy = -3424.178751				6	-3.271501	-1.586973	-2.166841
				6	-3.354587	-4.376237	-2.119284
28	-1.124895	0.663076	-0.474258	1	-1.328853	-4.276009	-1.398174
8	2.267753	1.842081	2.194422	6	-4.437481	-2.254573	-2.540798
16	1.514141	0.601551	1.889895	1	-3.250194	-0.502708	-2.151050
8	0.351727	0.363688	2.788898	6	-4.478238	-3.648899	-2.520908
8	1.175787	0.486768	0.424580	1	-3.388694	-5.461311	-2.093923
6	2.628557	-0.779050	2.184743	1	-5.313420	-1.681510	-2.824759
6	3.400913	-1.297159	1.147568	1	-5.386901	-4.170341	-2.806831
6	2.741217	-1.302204	3.473252	6	0.633040	-1.602188	-2.471716
6	4.291954	-2.337823	1.405222	6	1.783745	-0.800011	-2.364595
1	3.293131	-0.898199	0.147668	6	0.517355	-2.518004	-3.525464
6	3.632072	-2.343780	3.718632	6	2.810733	-0.933470	-3.296302
1	2.113797	-0.902741	4.262285	1	1.867688	-0.091894	-1.545965
6	4.423623	-2.875515	2.690736	6	1.548072	-2.638702	-4.459020
1	4.890168	-2.741075	0.591971	1	-0.373304	-3.129668	-3.620142
1	3.713159	-2.755692	4.721657	6	2.693983	-1.851232	-4.343179
6	5.405767	-3.986350	2.970889	1	3.696000	-0.314345	-3.202565
1	5.010510	-4.695251	3.705386	1	1.452482	-3.347212	-5.276488
1	5.653094	-4.540853	2.060968	1	3.493469	-1.946822	-5.071894
1	6.344629	-3.590939	3.377855	6	-1.800693	-1.132304	1.688017
6	-1.223007	2.510147	-0.285184	8	-2.626963	-1.371952	2.725376
6	-0.888825	2.444812	-1.571790	6	-3.258036	0.586800	1.556199
6	-0.055082	3.346592	-2.463794	6	-3.691613	-0.384408	2.688512
1	-0.703495	4.059969	-2.984988	7	-2.067128	-0.078980	0.988481
1	0.451779	2.743102	-3.224025	6	-5.029386	-1.030455	2.257453
8	0.869280	4.138474	-1.743840	1	-4.892845	-2.110109	2.133776
6	1.910260	3.407553	-1.124480	1	-5.804494	-0.889609	3.018436
1	2.404887	4.097004	-0.433135	6	-5.384539	-0.339672	0.958924
1	1.530248	2.574739	-0.516683	6	-6.514463	-0.526660	0.164155
6	2.935111	2.868624	-2.121322	6	-4.417085	0.599425	0.591306
8	2.772968	2.993276	-3.327942	6	-6.662607	0.239495	-0.994829
6	4.133668	2.162060	-1.576565				

1	-7.272286	-1.254284	0.440605	6	-1.019974	-4.690357	-0.374699
6	-4.565713	1.377907	-0.554792	6	-2.646312	-3.730262	1.679910
6	-5.697906	1.188986	-1.350692	1	-2.918199	-1.987674	0.470283
1	-7.540878	0.104719	-1.619448	6	-1.217016	-5.458630	0.768344
1	-3.810233	2.109074	-0.822190	1	-0.396843	-5.041137	-1.190083
1	-5.833332	1.786330	-2.247254	6	-2.035367	-4.979133	1.797319
1	-3.731161	0.072499	3.677065	1	-3.267386	-3.343247	2.481070
1	-2.965200	1.580684	1.900349	1	-0.740461	-6.430261	0.859461
6	-1.290240	3.555070	0.707489	1	-2.190596	-5.578553	2.689951
6	-1.632660	4.872506	0.342096	1	-0.327335	2.158366	-0.840648
6	-1.009596	3.266933	2.057323	6	1.107252	-0.422494	2.252835
6	-1.694393	5.874939	1.302830	6	1.086422	-1.700291	1.650656
1	-1.841441	5.095525	-0.698791	6	0.662015	-2.814702	2.375592
6	-1.060085	4.280738	3.010987	6	0.208746	-2.660311	3.685027
1	-0.717840	2.261226	2.342529	6	0.205062	-1.399277	4.273934
6	-1.406859	5.581138	2.639936	6	0.664225	-0.285990	3.564442
1	-1.957725	6.887633	1.012325	1	0.649541	-3.785622	1.896918
1	-0.818167	4.053171	4.044504	1	-0.152733	-3.524726	4.232283
1	-1.448844	6.367727	3.387822	1	-0.164633	-1.269508	5.286036
				1	0.640940	0.694084	4.023495
				15	1.638227	1.016269	1.249638
IM7				6	3.434255	0.724739	1.009497
SCF Energy = -3424.916349				6	4.151689	-0.246941	1.718049
Gibbs Free Energy = -3424.171971				6	4.100846	1.512580	0.059995
28	0.516852	0.641496	-0.675933	6	5.515779	-0.427800	1.477650
8	-2.128800	2.372670	0.805342	1	3.647340	-0.861559	2.455502
16	-2.245055	1.016386	1.412310	6	5.463942	1.343827	-0.163658
8	-2.119652	0.968581	2.884777	1	3.545166	2.248757	-0.512982
8	-1.354928	0.017038	0.711881	6	6.173250	0.368539	0.540681
6	-3.891230	0.432743	1.001246	1	6.063046	-1.185957	2.030218
6	-4.563584	-0.411919	1.882781	1	5.966260	1.952447	-0.907219
6	-4.427827	0.720787	-0.254825	1	7.233412	0.227187	0.353739
6	-5.772467	-0.988129	1.493376	6	1.579227	2.455963	2.368323
1	-4.128934	-0.605681	2.857652	6	0.450595	3.287682	2.361879
6	-5.635389	0.138091	-0.631028	6	2.640440	2.723258	3.248705
1	-3.900824	1.393607	-0.922429	6	0.388178	4.371852	3.238656
6	-6.322753	-0.728319	0.231762	1	-0.389110	3.080920	1.705042
1	-6.297340	-1.650595	2.177114	6	2.570011	3.810841	4.115931
1	-6.052410	0.357638	-1.610722	1	3.517711	2.085137	3.251766
6	-7.641090	-1.336673	-0.178367	6	1.442677	4.636482	4.111981
1	-7.839162	-2.265014	0.365057	1	-0.494639	5.003406	3.236838
1	-7.662791	-1.557621	-1.249873	1	3.393958	4.014068	4.793547
1	-8.472897	-0.652001	0.028667	1	1.388937	5.483099	4.790257
6	-0.782333	1.848258	-1.853278	6	1.511953	-1.885799	0.258478
6	-0.437750	0.645956	-2.274222	8	2.139292	-3.039340	-0.030511
6	-0.865405	-0.172351	-3.446416	6	1.999151	-1.628265	-1.928536
1	-1.016050	0.480235	-4.315175	6	2.605451	-2.958284	-1.409078
1	-0.115219	-0.919767	-3.713174	7	1.371188	-1.051473	-0.722194
8	-2.129312	-0.818026	-3.248152	6	4.143524	-2.820592	-1.476402
6	-2.303836	-1.444652	-1.992615	1	4.552017	-2.772013	-0.460715
1	-3.358969	-1.732134	-1.937905	1	4.606967	-3.678187	-1.974498
1	-2.115202	-0.752837	-1.159843	6	4.370062	-1.523711	-2.223345
6	-1.441088	-2.677322	-1.772435	6	5.573665	-0.989453	-2.678895
8	-0.608983	-3.038863	-2.599245	6	3.171699	-0.841925	-2.451531
6	-1.646113	-3.441161	-0.505833	6	5.560341	0.232849	-3.354989
6	-2.457692	-2.962816	0.532680	1	6.510412	-1.513494	-2.512018

6	3.151789	0.381954	-3.116398	6	3.426164	-3.111964	1.199476
6	4.359632	0.918579	-3.567045	1	3.525499	-1.395843	2.502515
1	6.492345	0.655551	-3.718757	1	3.056171	-4.700492	-0.210859
1	2.213380	0.904060	-3.275811	1	4.426636	-3.454900	1.442038
1	4.365762	1.868292	-4.093341	6	-3.605274	-0.727713	1.582558
1	2.218411	-3.837444	-1.922175	8	-4.936417	-0.611301	1.775832
1	1.221645	-1.789755	-2.671582	6	-4.074518	1.141125	0.425765
6	-1.706359	2.888879	-2.305744	6	-5.386549	0.558136	1.028980
6	-2.752894	2.563085	-3.187453	7	-3.039799	0.185141	0.880991
6	-1.582460	4.207380	-1.844891	6	-6.294891	0.135353	-0.146574
6	-3.633086	3.553195	-3.618445	1	-6.560925	-0.922405	-0.051375
1	-2.897092	1.530593	-3.487655	1	-7.231994	0.703670	-0.138721
6	-2.463138	5.191611	-2.282669	6	-5.480151	0.434402	-1.386334
1	-0.800807	4.448914	-1.131015	6	-5.811042	0.186635	-2.718192
6	-3.488244	4.869453	-3.175141	6	-4.272658	1.062558	-1.070015
1	-4.443553	3.292412	-4.292796	6	-4.922432	0.580153	-3.722401
1	-2.358423	6.209113	-1.918326	1	-6.746496	-0.302670	-2.974993
1	-4.180104	5.636515	-3.509674	6	-3.392519	1.478397	-2.067324

IM8B

SCF Energy = -3351.135113

Gibbs Free Energy = -3350.358214

28	-1.180501	0.521560	0.198817	1	-3.788664	2.131003	0.786003
6	0.201998	1.040166	-1.034187	6	1.228280	0.126586	-1.648164
6	0.128669	2.332994	-1.407813	1	0.919603	-0.927367	-1.634116
1	-0.581584	2.948746	-0.862787	1	1.413923	0.373139	-2.704875
6	-1.684312	-2.335076	1.769343	8	2.442082	0.265456	-0.907477
6	-2.944542	-1.875667	2.209799	6	3.441814	-0.599555	-1.353371
6	-3.595096	-2.507600	3.276886	1	3.096922	-1.643404	-1.343759
6	-3.000077	-3.582442	3.931062	1	3.747879	-0.372274	-2.392808
6	-1.750535	-4.033422	3.513638	6	4.668010	-0.471915	-0.462407
6	-1.103217	-3.415537	2.442107	8	4.772658	0.425647	0.356365
1	-4.562521	-2.135891	3.592489	6	5.746627	-1.497823	-0.619815
1	-3.507231	-4.057247	4.764603	6	6.841237	-1.434376	0.253974
1	-1.271248	-4.865787	4.019546	6	5.690634	-2.522580	-1.575614
1	-0.130899	-3.777799	2.132734	6	7.857198	-2.381970	0.181395
15	-0.837399	-1.601859	0.293086	1	6.863392	-0.633006	0.984395
6	-1.578011	-2.532307	-1.096578	6	6.711694	-3.468044	-1.652320
6	-1.878949	-3.900651	-1.026769	1	4.852463	-2.591694	-2.260074
6	-1.917473	-1.806948	-2.247707	6	7.793660	-3.401760	-0.772391
6	-2.491623	-4.536266	-2.105420	1	8.698904	-2.328829	0.865172
1	-1.652746	-4.461119	-0.125209	1	6.662609	-4.257502	-2.396025
6	-2.541276	-2.443892	-3.319589	1	8.585715	-4.142425	-0.829997
1	-1.715800	-0.741800	-2.285577	8	-1.439578	2.399417	1.000134
6	-2.823576	-3.808631	-3.251486	16	-0.652947	2.453078	2.334582
1	-2.722311	-5.595743	-2.047260	8	-0.275888	1.074899	2.751104
1	-2.821582	-1.866159	-4.194256	8	-1.368501	3.286987	3.311201
1	-3.313387	-4.304766	-4.084064	6	0.862799	3.298423	1.900297
6	0.865313	-2.207601	0.548587	6	1.955760	2.573761	1.425534
6	1.642389	-1.498863	1.477672	6	0.907424	4.689966	1.970747
6	1.377264	-3.359572	-0.062640	6	3.100697	3.251436	1.017433
6	2.919149	-1.956719	1.799546	1	1.916205	1.496425	1.351939
1	1.240445	-0.603094	1.944623	6	2.056848	5.357572	1.549506
6	2.656905	-3.810839	0.266672	1	0.053078	5.231447	2.361469
1	0.780711	-3.900162	-0.789928	6	3.163716	4.650673	1.061223

1	3.941862	2.669486	0.654771	1	7.593432	-4.235234	1.489867
1	2.096076	6.442555	1.602724	1	9.679544	-2.885783	1.498061
6	4.389039	5.373916	0.560143	1	1.622830	-0.282079	0.297765
1	5.307323	4.878355	0.890700	6	-3.851045	-0.905820	0.786577
1	4.415095	6.410811	0.907056	6	-4.182638	-1.494554	-0.454992
1	4.408918	5.390737	-0.536698	6	-5.514697	-1.822671	-0.739938
6	0.859832	3.134556	-2.494725	6	-6.524003	-1.559685	0.182364
6	0.196467	2.842639	-3.858328	6	-6.203603	-0.981863	1.408334
1	0.649977	3.450200	-4.651024	6	-4.877252	-0.665059	1.706159
1	0.304472	1.788365	-4.133543	1	-5.746837	-2.280500	-1.693806
1	-0.874223	3.074261	-3.828015	1	-7.552872	-1.807849	-0.057206
6	2.379478	2.882317	-2.583598	1	-6.980857	-0.777310	2.138158
1	2.837498	3.649208	-3.219509	1	-4.639199	-0.218374	2.663882
1	2.837557	2.926892	-1.594838	15	-2.090254	-0.545341	1.213013
1	2.623216	1.912628	-3.021667	6	-1.500748	-2.159643	1.839727
6	0.660064	4.626273	-2.151448	6	-2.269411	-2.924678	2.729947
1	1.111412	4.862627	-1.183096	6	-0.267118	-2.647367	1.392657
1	1.119655	5.265592	-2.913419	6	-1.801510	-4.160734	3.169230
1	-0.404843	4.877182	-2.094651	1	-3.232313	-2.557475	3.070782

IM8

SCF Energy = -3424.946561

Gibbs Free Energy = -3424.201305

28	-1.018375	0.074613	-0.522187	1	0.195228	-3.888990	1.829226
6	-0.221545	4.358545	2.581864	1	0.323138	-2.068165	0.694975
6	0.170179	3.084712	2.176712	6	-0.569737	-4.644296	2.717249
6	-0.296893	2.528537	0.970694	1	-2.399187	-4.750358	3.857916
6	-1.222990	3.274138	0.217171	1	1.143963	-4.260172	1.457985
6	-1.606291	4.551237	0.618066	1	-0.212499	-5.612585	3.055317
6	-1.102989	5.104927	1.797564	6	-2.207760	0.545874	2.665353
1	0.149085	4.762068	3.520233	6	-2.914197	1.753620	2.549293
1	0.808234	2.489129	2.820508	6	-1.522870	0.256454	3.850012
1	-1.628746	2.852845	-0.696082	6	-2.952598	2.646329	3.615363
1	-2.299623	5.116709	0.002316	1	-3.417570	2.001136	1.621456
1	-1.406715	6.099973	2.110485	6	-1.557625	1.159847	4.913945
6	0.131325	1.195868	0.516606	1	-0.964009	-0.668296	3.940730
6	1.384829	0.719987	0.644373	6	-2.274290	2.350184	4.799804
6	2.623034	1.474301	1.036232	1	-3.486666	3.584276	3.509544
1	2.416615	2.534139	1.208851	1	-1.023675	0.929783	5.831002
1	3.080653	1.054749	1.943335	1	-2.295881	3.053035	5.627114
8	3.566345	1.387044	-0.056256	6	-3.167010	-1.818399	-1.470811
6	4.843225	0.935815	0.272241	8	-3.515501	-2.770910	-2.359997
1	5.257794	1.450920	1.156530	6	-1.310673	-1.970876	-2.739069
1	5.498471	1.182516	-0.572359	6	-2.353203	-3.027846	-3.203095
6	4.922025	-0.575462	0.517692	7	-1.997226	-1.302146	-1.601079
8	3.914317	-1.266089	0.497744	6	-1.767348	-4.426554	-2.908431
6	6.263302	-1.176830	0.787922	6	-2.429641	-4.970583	-2.226504
6	7.445661	-0.421272	0.795508	1	-1.692569	-5.022139	-3.825206
6	6.328876	-2.555274	1.040955	6	-0.403745	-4.149347	-2.314273
6	8.670180	-1.036317	1.050628	6	0.541988	-5.071782	-1.868935
1	7.420683	0.645633	0.602382	6	-0.120434	-2.780763	-2.279063
6	7.550829	-3.167911	1.295444	6	1.769779	-4.605151	-1.392432
1	5.403377	-3.120487	1.032954	1	0.330992	-6.137492	-1.894139
6	8.724443	-2.408498	1.300258	6	1.114380	-2.310436	-1.831640
1	9.581064	-0.445899	1.053421	6	2.058671	-3.235617	-1.378781
				1	2.512638	-5.315405	-1.039667
				1	1.326613	-1.247614	-1.840047
				1	3.010155	-2.880128	-0.999077
				1	-2.683922	-2.904185	-4.234254
				1	-1.055503	-1.215547	-3.481796

8	-2.019026	1.878593	-2.806472	1	8.127620	-2.278802	-1.464881
16	-0.596911	1.606793	-3.132842	1	-2.252580	-0.595409	-3.551511
8	-0.295304	1.254974	-4.530888	6	-0.827012	2.360863	1.870909
8	-0.004334	0.541046	-2.189871	6	-0.427169	1.473409	2.900716
6	0.302994	3.082737	-2.660349	6	-0.737324	1.766020	4.234607
6	-0.290119	4.330847	-2.848826	6	-1.425790	2.930573	4.566138
6	1.531485	2.967958	-2.013607	6	-1.792613	3.822588	3.562246
6	0.340745	5.467045	-2.350428	6	-1.492298	3.537018	2.228453
1	-1.256164	4.398226	-3.337067	1	-0.426077	1.070049	5.003749
6	2.145685	4.112657	-1.511832	1	-1.665666	3.139832	5.603574
1	1.974814	1.994813	-1.853651	1	-2.316397	4.741067	3.808420
6	1.552889	5.372613	-1.652985	1	-1.791286	4.234790	1.456202
1	-0.128273	6.439638	-2.475874	15	-0.495556	1.967328	0.097735
1	3.086617	4.008403	-0.978670	6	1.200059	2.592309	-0.202910
6	2.169551	6.591971	-1.015300	6	1.883739	3.383030	0.728115
1	3.255682	6.494035	-0.927854	6	1.831414	2.232265	-1.403787
1	1.769816	6.736617	-0.003589	6	3.185116	3.808596	0.460415
1	1.952212	7.499990	-1.586027	1	1.407002	3.658970	1.662459
				6	3.125203	2.677116	-1.674719
				1	1.336569	1.571308	-2.105307
				6	3.804462	3.462548	-0.741376
				1	3.714646	4.409942	1.193139
				1	3.599325	2.375814	-2.602694
28	-0.543912	-0.168764	-0.121735	1	4.817602	3.796509	-0.944885
6	-5.529395	0.747963	-1.699642	6	-1.585107	3.107465	-0.831441
6	-4.207204	0.529480	-2.076734	6	-2.964412	3.123422	-0.568258
6	-3.248466	0.082538	-1.149171	6	-1.073874	3.927802	-1.846580
6	-3.668484	-0.118057	0.178903	6	-3.810765	3.948636	-1.304500
6	-4.991827	0.097566	0.558068	1	-3.381648	2.487745	0.202675
6	-5.931254	0.534470	-0.377931	6	-1.927929	4.744442	-2.587802
1	-6.246152	1.103737	-2.435032	1	-0.011562	3.932768	-2.059166
1	-3.900364	0.743334	-3.095306	6	-3.296605	4.757766	-2.318512
1	-2.950956	-0.469310	0.913428	1	-4.875036	3.938231	-1.093748
1	-5.288936	-0.085138	1.586385	1	-1.518940	5.373560	-3.372576
1	-6.961635	0.710025	-0.082290	1	-3.959482	5.394829	-2.896431
6	-1.837791	-0.163479	-1.516365	6	0.381656	0.276521	2.630131
6	-1.492311	-0.489646	-2.773448	8	0.900466	-0.354792	3.695153
6	-0.114523	-0.845440	-3.244096	6	1.690643	-1.259616	1.698978
1	-0.099906	-1.900254	-3.566780	6	1.533688	-1.588595	3.198015
1	0.188560	-0.241333	-4.112442	7	0.692902	-0.195030	1.469503
8	0.823556	-0.668075	-2.189701	6	2.940420	-1.735294	3.783298
6	1.944623	-1.505381	-2.177727	1	3.002170	-1.310716	4.790026
1	1.739315	-2.473283	-2.660843	1	3.188810	-2.800707	3.865978
1	2.171983	-1.720041	-1.131611	6	3.822890	-1.030830	2.774890
6	3.143855	-0.839975	-2.856080	6	5.160268	-0.658679	2.891587
8	2.968249	0.089587	-3.631892	6	3.112619	-0.743061	1.602933
6	4.512873	-1.310175	-2.499659	6	5.772835	0.015676	1.830539
6	4.737545	-2.410067	-1.658427	1	5.718874	-0.878865	3.797300
6	5.607633	-0.574864	-2.977823	6	3.709291	-0.039207	0.562336
6	6.035474	-2.759943	-1.294249	6	5.048955	0.334698	0.678667
1	3.906824	-2.991641	-1.274690	1	6.815711	0.308433	1.910022
6	6.902588	-0.920080	-2.606913	1	3.137556	0.245554	-0.310267
1	5.411349	0.268617	-3.630637	1	5.524880	0.871887	-0.134603
6	7.117389	-2.011956	-1.760504	1	0.841058	-2.401461	3.411334
1	6.201275	-3.607374	-0.637008	1	1.477757	-2.102127	1.041237
1	7.745490	-0.341748	-2.972987	8	-1.392047	-2.229956	2.220646

IM9

SCF Energy = -3424.958686

Gibbs Free Energy = -3424.210783

16	-1.204881	-3.019310	0.975276
8	-0.538217	-4.323879	1.135183
8	-0.490084	-2.207955	-0.119037
6	-2.850121	-3.249188	0.307462
6	-3.930309	-3.344021	1.183518
6	-3.050261	-3.244944	-1.071448
6	-5.222822	-3.390781	0.669065
1	-3.753443	-3.329240	2.253019
6	-4.348689	-3.283427	-1.570889
1	-2.199474	-3.144129	-1.732722
6	-5.452764	-3.332343	-0.711515
1	-6.069573	-3.438585	1.348788
1	-4.510331	-3.238019	-2.644531
6	-6.854671	-3.248420	-1.257831
1	-6.937092	-3.733609	-2.235077
1	-7.143160	-2.197643	-1.386448
1	-7.580101	-3.711237	-0.582373

(S,R)-L1

SCF Energy = -1551.730222

Gibbs Free Energy = -1551.364194

6	0.997896	-1.509980	-0.040291
6	-0.188390	-2.151777	0.400694
6	-0.224640	-3.542269	0.575535
6	0.905506	-4.317334	0.341382
6	2.082632	-3.698554	-0.075698
6	2.121610	-2.317897	-0.267353
1	-1.150982	-3.999659	0.902769
1	0.867577	-5.392452	0.485171
1	2.976275	-4.288659	-0.256152
1	3.043717	-1.860378	-0.603169
15	1.017084	0.304875	-0.458710
6	2.716561	0.457377	-1.186559
6	3.871557	0.776410	-0.457992
6	2.830105	0.264028	-2.572348
6	5.106333	0.889034	-1.097916
1	3.803395	0.935154	0.612643
6	4.065004	0.363588	-3.210967
1	1.939678	0.033327	-3.151554
6	5.207589	0.678984	-2.473687
1	5.991473	1.138504	-0.519775
1	4.134626	0.205202	-4.283163
1	6.169741	0.766301	-2.969529
6	1.298244	1.098062	1.181044
6	1.123531	2.486213	1.259433
6	1.680227	0.399592	2.332221
6	1.332590	3.163699	2.459520
1	0.819211	3.037097	0.373276
6	1.881446	1.075271	3.536118
1	1.816299	-0.675868	2.286875
6	1.710401	2.458420	3.603217
1	1.195227	4.240199	2.503856
1	2.174484	0.520108	4.422656
1	1.868454	2.983181	4.540637
6	-1.398370	-1.379895	0.696828

8	-2.579124	-2.074765	0.742662
6	-2.847180	0.245799	1.062804
6	-3.614071	-1.115609	1.086787
7	-1.434515	-0.120933	0.910946
6	-4.702535	-1.056660	-0.001069
1	-4.675621	-1.960108	-0.618272
1	-5.698390	-1.008924	0.456368
6	-4.392352	0.204258	-0.777872
6	-4.985602	0.665745	-1.952178
6	-3.377940	0.946314	-0.167948
6	-4.546637	1.869960	-2.505881
1	-5.774389	0.095625	-2.435143
6	-2.929587	2.142976	-0.720256
6	-3.523472	2.603884	-1.895634
1	-4.999169	2.237282	-3.422088
1	-2.119542	2.691538	-0.249860
1	-3.185861	3.533146	-2.344183
1	-4.003446	-1.398709	2.067661
1	-2.977151	0.841781	1.972105

-OTS

SCF Energy = -894.880104

Gibbs Free Energy = -894.787066

8	-2.356089	1.254428	-0.705066
16	-1.986430	-0.000003	0.004889
8	-2.356050	-1.253736	-0.706320
8	-2.310052	-0.000735	1.456751
6	-0.169144	0.000032	-0.035590
6	0.535043	-1.204202	-0.026138
6	0.535050	1.204240	-0.026142
6	1.928724	-1.201495	0.001762
1	-0.029087	-2.130330	-0.056015
6	1.928750	1.201513	0.001753
1	-0.029096	2.130358	-0.055995
6	2.648347	0.000013	0.016575
1	2.471081	-2.145720	0.008758
1	2.471117	2.145732	0.008740
6	4.158624	-0.000023	0.008524
1	4.562028	-0.885043	0.512310
1	4.559950	-0.000916	-1.014227
1	4.562044	0.885843	0.510798

(R)-IM10

SCF Energy = -2529.94357

Gibbs Free Energy = -2529.314589

28	0.337879	0.500562	-0.494141
6	0.568177	1.647864	3.956006
6	0.820333	1.612335	2.586657
6	0.040162	2.360209	1.685571
6	-0.998001	3.152616	2.204698
6	-1.257552	3.178589	3.574536
6	-0.481577	2.423609	4.455073
1	1.189023	1.070499	4.634986
1	1.635587	1.012899	2.199047

1	-1.614098	3.728241	1.523687	1	-3.716273	4.754007	-1.044533
1	-2.072787	3.787763	3.953179	1	-5.264878	2.555711	2.312926
1	-0.687594	2.443701	5.520604	1	-5.218446	4.619133	0.931040
6	0.265340	2.250984	0.230834	6	-0.394035	-1.939746	-2.046583
6	0.429790	3.314518	-0.569236	8	-0.122735	-3.220333	-2.345784
6	0.607921	3.195829	-2.059745	6	1.410655	-2.344490	-0.760856
1	1.123139	4.076683	-2.466861	6	0.941497	-3.658820	-1.451213
1	-0.350614	3.115936	-2.586354	7	0.397777	-1.355118	-1.210463
8	1.317682	2.005827	-2.459621	6	0.387817	-4.587169	-0.346220
6	2.697237	2.050112	-2.214425	1	-0.700962	-4.662017	-0.444955
1	3.219339	1.686063	-3.109758	1	0.791038	-5.600916	-0.427868
1	3.045505	3.075533	-2.032388	6	0.783705	-3.906688	0.943862
6	3.151165	1.178095	-1.051967	6	0.658767	-4.391809	2.244301
8	2.335718	0.521173	-0.388059	6	1.352195	-2.650531	0.716268
6	4.587136	1.071067	-0.751349	6	1.104685	-3.604626	3.308384
6	5.544733	1.848020	-1.428868	1	0.225442	-5.369907	2.430295
6	5.009017	0.167514	0.242040	6	1.798177	-1.862282	1.774253
6	6.894254	1.723834	-1.114805	6	1.668323	-2.345930	3.076750
1	5.246378	2.553724	-2.195842	1	1.016103	-3.975993	4.324644
6	6.357862	0.044967	0.549253	1	2.235920	-0.891762	1.581370
1	4.269059	-0.432806	0.757569	1	2.011874	-1.744668	3.912678
6	7.301822	0.823686	-0.127532	1	1.699377	-4.133504	-2.073490
1	7.627974	2.328156	-1.637346	1	2.394954	-1.993221	-1.080353
1	6.677854	-0.654332	1.314576				
1	8.355525	0.728867	0.114788				
1	0.435636	4.326397	-0.159063				
6	-2.335889	-0.351245	-2.039209				
6	-1.585821	-1.362261	-2.683220				
6	-2.007682	-1.877538	-3.913500	28	-0.111413	-0.268388	-0.974826
6	-3.152817	-1.375033	-4.529305	6	-1.361756	-2.694423	2.995105
6	-3.894790	-0.377327	-3.900851	6	-1.267747	-2.703113	1.606306
6	-3.494444	0.122318	-2.658493	6	-1.852251	-1.681607	0.833295
1	-1.432585	-2.668611	-4.380621	6	-2.565551	-0.671872	1.505255
1	-3.466411	-1.769143	-5.490010	6	-2.661288	-0.667478	2.894053
1	-4.794787	0.009277	-4.367971	6	-2.053466	-1.672879	3.647675
1	-4.092678	0.880757	-2.168382	1	-0.898090	-3.492979	3.564762
15	-1.798343	0.257533	-0.391601	1	-0.743336	-3.521464	1.127539
6	-2.188799	-1.106178	0.756652	1	-3.041864	0.112963	0.940464
6	-1.645514	-1.051293	2.049892	1	-3.212786	0.126863	3.386527
6	-2.982283	-2.196243	0.377190	1	-2.129598	-1.668585	4.730239
6	-1.909249	-2.075800	2.954941	6	-1.672541	-1.663700	-0.642053
1	-1.019229	-0.216224	2.345266	6	-0.634492	-2.346818	-1.247311
6	-3.224846	-3.228313	1.284907	6	-0.558278	-2.622981	-2.726693
1	-3.410540	-2.241844	-0.618075	1	-0.952039	-3.647216	-2.881894
6	-2.691076	-3.167710	2.572629	1	0.481969	-2.623639	-3.066366
1	-1.485339	-2.029654	3.951779	8	-1.251443	-1.693896	-3.517485
1	-3.839018	-4.072590	0.987537	6	-2.552110	-1.445130	-3.009754
1	-2.883210	-3.970457	3.277458	1	-3.025686	-0.742155	-3.696465
6	-2.936794	1.613539	0.019101	1	-3.144823	-2.373218	-2.980455
6	-2.912431	2.781556	-0.759285	6	-2.509421	-0.792802	-1.608856
6	-3.792058	1.536647	1.124318	8	-1.702281	0.359952	-1.656969
6	-3.737298	3.855133	-0.436670	6	-3.939923	-0.515648	-1.196716
1	-2.250275	2.848438	-1.614489	6	-4.768387	-1.548327	-0.743805
6	-4.609294	2.619663	1.450565	6	-4.460947	0.774108	-1.332439
1	-3.811235	0.642626	1.736068	6	-6.095095	-1.288612	-0.404771
6	-4.582520	3.777822	0.674610	1	-4.371294	-2.553972	-0.633960

(R)-IM11

SCF Energy = -2529.943866

Gibbs Free Energy = -2529.308565

6	-5.788915	1.034383	-0.990676	1	-2.372390	1.861408	0.138450
1	-3.816802	1.564952	-1.699707	1	-3.028842	2.802705	2.369713
6	-6.607146	0.005459	-0.522892	1	0.769008	4.412000	-2.485853
1	-6.727669	-2.093913	-0.044757	1	-0.847113	2.564418	-2.109983
1	-6.184595	2.040152	-1.093587				
1	-7.639251	0.208262	-0.255276				
1	0.006594	-2.973892	-0.641361				
6	3.151952	-0.377894	-1.006467				
6	3.070976	0.783733	-1.807726				
6	4.131823	1.126692	-2.653454	28	-0.179907	-0.011618	-0.483621
6	5.262823	0.314985	-2.726623	6	-1.304015	2.877448	2.358191
6	5.351896	-0.823854	-1.929265	6	-1.640011	1.529955	2.269176
6	4.305753	-1.162148	-1.066365	6	-2.522044	1.051978	1.281089
1	4.062949	2.029680	-3.248256	6	-3.018696	1.980392	0.347784
1	6.074352	0.580650	-3.395405	6	-2.685513	3.331419	0.438485
1	6.237717	-1.449380	-1.967650	6	-1.836077	3.790581	1.447039
1	4.395161	-2.038092	-0.435485	1	-0.618005	3.207919	3.130963
15	1.759244	-0.766380	0.112126	1	-1.197816	0.828420	2.966187
6	1.889679	0.429948	1.478425	1	-3.688809	1.659814	-0.436431
6	0.750630	0.659408	2.264520	1	-3.104035	4.029486	-0.280327
6	3.069330	1.144120	1.725113	1	-1.584229	4.844338	1.515294
6	0.798985	1.590439	3.298326	6	-2.884121	-0.392308	1.286358
1	-0.170396	0.124467	2.066336	6	-2.942884	-1.076269	2.442881
6	3.103656	2.087245	2.752654	6	-3.064330	-2.568782	2.519463
1	3.952203	0.970645	1.119068	1	-4.091429	-2.876812	2.782352
6	1.970757	2.310448	3.537533	1	-2.401945	-2.960330	3.298540
1	-0.087731	1.771161	3.894702	8	-2.668885	-3.185084	1.302543
1	4.016348	2.643405	2.941733	6	-3.406179	-2.636787	0.228241
1	2.000383	3.048245	4.332871	1	-3.143857	-3.191718	-0.673922
6	2.108435	-2.409941	0.814384	1	-4.480594	-2.758906	0.421064
6	2.283557	-3.514402	-0.038654	6	-3.115775	-1.136470	-0.025250
6	2.116065	-2.602957	2.201511	8	-1.902411	-1.057876	-0.829440
6	2.459420	-4.790012	0.491726	6	-4.308941	-0.621847	-0.829610
1	2.293517	-3.376256	-1.116028	6	-5.466646	-0.204598	-0.158636
6	2.289769	-3.884036	2.727171	6	-4.310367	-0.660385	-2.227718
1	1.977070	-1.759596	2.867376	6	-6.589242	0.204245	-0.873254
6	2.456643	-4.977074	1.877280	1	-5.475778	-0.179546	0.926542
1	2.599854	-5.636105	-0.173142	6	-5.436211	-0.245429	-2.943264
1	2.295663	-4.024774	3.803236	1	-3.442630	-1.017860	-2.771794
1	2.589939	-5.971889	2.289716	6	-6.575402	0.191201	-2.270282
6	1.924817	1.699870	-1.711466	1	-7.473874	0.537109	-0.339742
8	2.170474	2.971564	-2.046934	1	-5.419356	-0.272375	-4.028100
6	-0.080260	2.689086	-1.344202	1	-7.448823	0.513984	-2.827491
6	1.006384	3.756513	-1.649320	1	-2.863659	-0.548254	3.389129
7	0.722602	1.431950	-1.312227	6	1.838893	1.640670	1.388438
6	1.284538	4.515417	-0.330169	6	1.627164	0.653228	2.374855
1	2.250683	4.196041	0.077723	6	1.847430	0.949718	3.723376
1	1.341720	5.596494	-0.486098	6	2.242404	2.233619	4.100132
6	0.136786	4.115346	0.567768	6	2.444826	3.213530	3.128708
6	-0.218084	4.649415	1.804629	6	2.252597	2.915180	1.776998
6	-0.634331	3.098830	-0.003499	1	1.701943	0.175619	4.468309
6	-1.354642	4.158309	2.452951	1	2.398647	2.463102	5.148769
1	0.368808	5.444775	2.254273	1	2.761040	4.210278	3.418577
6	-1.777673	2.619624	0.627786	1	2.422621	3.676531	1.024396
6	-2.132868	3.154200	1.867110	15	1.589967	1.198550	-0.365525
1	-1.645959	4.574558	3.412529	6	3.033871	0.202019	-0.833862

(R)-IM12

SCF Energy = -2606.402922

Gibbs Free Energy = -2605.746434

6	2.960210	-0.527927	-2.030678	6	-2.203821	-1.954587	-2.467453
6	4.180110	0.127343	-0.032045	1	-2.623245	-1.799536	-3.469345
6	4.039412	-1.312566	-2.426859	1	-2.522741	-2.955824	-2.135482
1	2.059601	-0.488275	-2.635152	6	-2.847139	-0.925471	-1.546185
6	5.249755	-0.676033	-0.429201	8	-2.161589	-0.093231	-0.930945
1	4.239756	0.691320	0.892506	6	-4.310414	-0.897311	-1.399295
6	5.180737	-1.391293	-1.625385	6	-5.144458	-1.761352	-2.132586
1	3.980118	-1.879526	-3.348698	6	-4.885387	0.014421	-0.493309
1	6.137903	-0.735325	0.191847	6	-6.524467	-1.708529	-1.964923
1	6.015233	-2.013615	-1.932484	1	-4.726514	-2.473663	-2.834783
6	1.650920	2.746875	-1.302761	6	-6.263568	0.060598	-0.328165
6	0.571292	3.638250	-1.188532	1	-4.238825	0.668384	0.079873
6	2.734133	3.058580	-2.133632	6	-7.084637	-0.799167	-1.064630
6	0.583305	4.835676	-1.899233	1	-7.163360	-2.375254	-2.534036
1	-0.263820	3.401997	-0.537354	1	-6.701824	0.761666	0.374468
6	2.734905	4.258840	-2.845637	1	-8.161614	-0.762009	-0.934979
1	3.566357	2.369751	-2.226126	1	-0.006723	-1.465493	1.798200
6	1.663444	5.145319	-2.730494	6	2.626397	1.717379	-1.204442
1	-0.250887	5.524155	-1.808192	6	1.866641	2.883543	-1.450115
1	3.573359	4.499252	-3.491178	6	2.480202	4.003578	-2.034011
1	1.668262	6.075957	-3.288767	6	3.826944	3.976759	-2.381349
6	1.209836	-0.703131	1.992866	6	4.581883	2.832209	-2.132098
8	1.635673	-1.705430	2.770554	6	3.983905	1.717830	-1.544455
6	0.405036	-2.517402	0.904418	1	1.888566	4.892767	-2.212294
6	1.317642	-2.958987	2.082640	1	4.283486	4.847509	-2.839575
7	0.493318	-1.031223	0.967597	1	5.635255	2.802946	-2.391324
6	2.589455	-3.591265	1.473335	1	4.581262	0.833467	-1.357170
1	3.450997	-2.941646	1.664973	15	1.906406	0.253574	-0.348303
1	2.811943	-4.562918	1.924451	6	2.361975	0.526401	1.395226
6	2.279999	-3.697986	-0.003452	6	3.688228	0.420248	1.838939
6	3.033981	-4.321966	-0.995127	6	1.361182	0.930233	2.288291
6	1.058723	-3.098661	-0.324548	6	4.000009	0.701600	3.167290
6	2.550914	-4.333424	-2.305824	1	4.472011	0.111721	1.155195
1	3.978933	-4.799871	-0.754700	6	1.679013	1.218159	3.614728
6	0.569389	-3.108113	-1.630115	1	0.336931	1.022147	1.949112
6	1.329842	-3.729302	-2.623010	6	2.997325	1.100697	4.055763
1	3.126043	-4.824357	-3.084906	1	5.025890	0.611363	3.509802
1	-0.387676	-2.654152	-1.862469	1	0.893213	1.531728	4.294485
1	0.963888	-3.755722	-3.644577	1	3.247170	1.319626	5.089083
1	0.823692	-3.596640	2.814672	6	2.892792	-1.150075	-0.961139
1	-0.642528	-2.803418	1.011411	6	3.135817	-1.270912	-2.338595
8	-0.772353	0.701196	-2.043101	6	3.256326	-2.194946	-0.101160
1	-0.766906	1.664627	-2.086609	6	3.757531	-2.412140	-2.842696
1	-1.977815	-0.360060	-1.540727	1	2.837343	-0.477918	-3.016735
				6	3.876258	-3.335403	-0.611392
				1	3.039222	-2.129472	0.958180
				6	4.129145	-3.445692	-1.979874
				1	3.945369	-2.495793	-3.908228
				1	4.151588	-4.139915	0.062694
				1	4.610506	-4.335043	-2.373795
				6	0.446881	3.010183	-1.084811
				8	-0.008825	4.270328	-0.991513
				6	-1.680312	2.710230	-0.408957
				6	-1.423353	4.225304	-0.639782
				7	-0.408545	2.071070	-0.841670
				6	-1.665954	4.954495	0.691790
28	-0.200378	0.127417	-0.663230				
6	-0.002214	-2.190484	0.983936				
6	-0.045098	-1.719238	-0.277653				
6	-0.096277	-2.549863	-1.525260				
1	-0.556029	-3.535081	-1.358495				
1	0.901983	-2.709296	-1.941658				
8	-0.815601	-1.865942	-2.575897				

(R)-IM1A

SCF Energy = -2529.936592

Gibbs Free Energy = -2529.307210

1	-0.835142	5.630475	0.914870	6	3.126598	2.690819	-2.798250
1	-2.571798	5.568374	0.630815	6	4.363734	2.183327	-3.188786
6	-1.828711	3.841783	1.702348	6	4.782915	0.943304	-2.712617
6	-1.940893	3.950876	3.087758	6	3.967548	0.208977	-1.847643
6	-1.903209	2.588427	1.085286	1	2.791880	3.658305	-3.152840
6	-2.135849	2.794595	3.846914	1	4.995832	2.757090	-3.857835
1	-1.880434	4.920719	3.572471	1	5.747904	0.543206	-3.006420
6	-2.115418	1.432116	1.838536	1	4.313172	-0.747656	-1.475639
6	-2.229826	1.544151	3.226427	15	1.674266	-0.206434	-0.236631
1	-2.225146	2.868727	4.926203	6	2.072902	0.646304	1.324537
1	-2.175986	0.461897	1.359473	6	3.407697	0.812496	1.727804
1	-2.390449	0.653759	3.826143	6	1.040275	1.178346	2.106694
1	-1.967490	4.655737	-1.481743	6	3.698676	1.479364	2.914928
1	-2.498761	2.300044	-1.001125	1	4.214788	0.424259	1.114751
6	0.046874	-3.592184	1.434492	6	1.336985	1.850444	3.293061
6	-0.526223	-3.929135	2.674482	1	0.009755	1.087813	1.785970
6	0.676831	-4.611582	0.697546	6	2.663101	1.995838	3.699606
6	-0.508880	-5.239321	3.142518	1	4.731269	1.601979	3.225539
1	-0.995742	-3.148244	3.267259	1	0.528807	2.264331	3.885075
6	0.697599	-5.924017	1.168757	1	2.893868	2.518299	4.622637
1	1.193592	-4.371033	-0.223584	6	2.432795	-1.857958	-0.168055
6	0.098938	-6.245565	2.386958	6	2.454174	-2.624931	-1.346667
1	-0.965194	-5.477804	4.098449	6	2.983681	-2.379184	1.006541
1	1.193397	-6.695349	0.586823	6	3.020020	-3.897002	-1.343520
1	0.117149	-7.267412	2.752378	1	2.050537	-2.217051	-2.269368
				6	3.553935	-3.652655	1.001522
				1	2.954561	-1.805594	1.924453
				6	3.573071	-4.411958	-0.167192
				1	3.037895	-4.481145	-2.257988
				1	3.976096	-4.051701	1.917909
28	-0.442936	0.053167	-0.861324	1	4.018665	-5.401542	-0.166059
6	-1.315735	-1.621632	0.453398	6	1.005315	2.532272	-1.561469
6	-1.556077	-1.796837	-0.883374	8	0.893466	3.861740	-1.674381
6	-1.019973	-2.786887	-1.882446	6	-1.129803	2.897628	-0.893258
1	-1.592099	-3.730966	-1.811247	6	-0.387743	4.246839	-1.088659
1	0.038721	-3.017361	-1.778494	7	-0.040836	1.906607	-1.129268
8	-1.243364	-2.156960	-3.135624	6	-0.191198	4.868500	0.313944
6	-2.543595	-1.569073	-3.035270	1	0.869072	4.828974	0.588230
1	-2.645588	-0.808309	-3.808855	1	-0.488263	5.921198	0.334638
1	-3.315846	-2.341612	-3.157965	6	-1.045107	4.011743	1.221532
6	-2.621963	-0.944744	-1.615095	6	-1.320182	4.199823	2.575315
8	-2.086286	0.349232	-1.585336	6	-1.601199	2.926467	0.538211
6	-4.012658	-1.001750	-1.009619	6	-2.152224	3.287946	3.230856
6	-4.545147	-2.205521	-0.532285	1	-0.900249	5.043884	3.114359
6	-4.789159	0.158662	-0.948595	6	-2.456028	2.029461	1.177798
6	-5.829505	-2.245979	0.007486	6	-2.721074	2.212872	2.537038
1	-3.953761	-3.116749	-0.574645	1	-2.377082	3.427579	4.283817
6	-6.076650	0.118808	-0.410391	1	-2.914712	1.223757	0.617905
1	-4.373390	1.087758	-1.321284	1	-3.391123	1.531531	3.052172
6	-6.598830	-1.081736	0.070757	1	-0.863308	4.921580	-1.798867
1	-6.229670	-3.184066	0.379457	1	-1.922902	2.687661	-1.611186
1	-6.670985	1.026437	-0.368035	6	-0.526697	-2.450207	1.367477
1	-7.598823	-1.112677	0.491563	6	-0.243000	-1.945260	2.649642
1	-1.914857	-0.855098	0.944659	6	-0.123082	-3.760269	1.052929
6	2.715543	0.693428	-1.460453	6	0.446004	-2.714506	3.581814
6	2.295810	1.951050	-1.947447	1	-0.572454	-0.945271	2.910519

(R)-IM2A

SCF Energy = -2529.941100

Gibbs Free Energy = -2529.307703

6	0.546538	-4.535093	1.993835	1	5.666434	1.362026	-3.176726
1	-0.356154	-4.188908	0.087077	1	4.496021	-0.215465	-1.691973
6	0.837730	-4.014898	3.256943	15	1.883297	-0.219443	-0.384252
1	0.660098	-2.308226	4.565006	6	2.523198	0.343075	1.228124
1	0.842175	-5.547766	1.741465	6	3.859619	0.143242	1.604285
1	1.359235	-4.624278	3.988209	6	1.663678	1.056166	2.074376

(R)-IM5B

SCF Energy = -2456.136579

Gibbs Free Energy = -2455.476128

28	-0.236844	-0.154561	-0.573058	1	5.351407	0.468914	3.116494
6	-0.283056	-1.919816	1.599575	1	1.451036	2.097265	3.938548
6	-0.303342	-1.862790	0.260881	1	3.817749	1.711510	4.621690
6	-0.477412	-2.960038	-0.750345	6	2.645991	-1.831430	-0.751111
1	-1.097349	-3.793261	-0.403851	6	2.710351	-2.268348	-2.083434
1	0.490485	-3.365392	-1.053343	6	2.987615	-2.713685	0.282029
8	-1.051935	-2.445027	-1.974912	6	3.130593	-3.564656	-2.375975
6	-2.442326	-2.335353	-1.950198	1	2.424358	-1.600944	-2.890000
1	-2.790902	-2.321762	-2.990706	6	3.401640	-4.011831	-0.015445
1	-2.909765	-3.208024	-1.466148	1	2.919508	-2.391210	1.313527
6	-2.983612	-1.077768	-1.279077	6	3.474383	-4.439177	-1.342648
8	-2.221533	-0.213696	-0.819363	1	3.180750	-3.893354	-3.408949
6	-4.437775	-0.872045	-1.188842	1	3.666411	-4.688476	0.790858
6	-5.350412	-1.748737	-1.803402	1	3.796307	-5.450066	-1.571240
6	-4.921841	0.229772	-0.458275	6	0.692730	2.503594	-1.560858
6	-6.718580	-1.521283	-1.693486	8	0.406988	3.814379	-1.632558
1	-5.002427	-2.603771	-2.371916	6	-1.391866	2.588106	-0.709262
6	-6.288866	0.448582	-0.347194	6	-0.952091	4.015954	-1.143370
1	-4.214129	0.892852	0.025700	7	-0.246418	1.732725	-1.120652
6	-7.188457	-0.425010	-0.966368	6	-0.941299	4.908481	0.110513
1	-7.418579	-2.197276	-2.172728	1	0.010630	5.442110	0.189163
1	-6.657901	1.295298	0.222141	1	-1.729900	5.666846	0.048583
1	-8.256561	-0.252574	-0.879931	6	-1.193558	3.952750	1.254653
1	-0.101055	-0.973998	2.113691	6	-1.166534	4.225211	2.621947
6	-0.443362	-3.043560	2.617056	6	-1.521853	2.671944	0.798195
6	-0.602642	-4.447703	2.019113	6	-1.479299	3.205684	3.524672
1	0.221622	-4.691776	1.341696	1	-0.909363	5.216567	2.982939
1	-1.546526	-4.554754	1.476769	6	-1.855783	1.655688	1.695817
1	-0.605067	-5.193586	2.820443	6	-1.829219	1.931344	3.064897
6	0.814138	-3.027714	3.514976	1	-1.461736	3.407895	4.591118
1	1.700932	-3.328230	2.948857	1	-2.111360	0.664019	1.343277
1	0.698545	-3.723773	4.352560	1	-2.079006	1.148953	3.774670
1	0.997764	-2.029172	3.925356	1	-1.522851	4.433883	-1.973457
6	-1.677560	-2.712186	3.483407	1	-2.294444	2.225174	-1.202386
1	-1.577641	-1.724498	3.947114				
1	-1.799701	-3.448107	4.285377				
1	-2.590006	-2.710985	2.878114				
6	2.684112	0.937482	-1.575680				
6	2.047192	2.127542	-1.994613				
6	2.727770	3.026028	-2.831167	28	-0.363543	-0.097661	-0.676504
6	4.020884	2.751798	-3.265053	6	-1.844578	-1.183453	0.891601
6	4.655073	1.582014	-2.850464	6	-1.939199	-1.598215	-0.400984
6	3.991381	0.689646	-2.008798	6	-1.607643	-2.892806	-1.096610
1	2.230274	3.937930	-3.137699	1	-2.441385	-3.608724	-0.993106
1	4.530467	3.450956	-3.919375	1	-0.693996	-3.375833	-0.762983

(R)-IM6B

SCF Energy = -2456.135283

Gibbs Free Energy = -2455.469372

8	-1.452080	-2.495333	-2.455691	6	1.937217	-4.804139	-0.179096
6	-2.541134	-1.601833	-2.710764	1	1.420480	-3.182936	-1.494101
1	-2.310627	-1.011780	-3.597452	6	2.625239	-4.182913	2.055062
1	-3.464926	-2.175169	-2.866824	1	2.647664	-2.075746	2.488292
6	-2.659263	-0.696629	-1.450811	6	2.368327	-5.166808	1.100438
8	-1.862482	0.445349	-1.545381	1	1.745744	-5.566079	-0.927701
6	-4.091054	-0.362441	-1.066354	1	2.967318	-4.461568	3.046449
6	-4.977734	-1.367750	-0.657758	1	2.508281	-6.213929	1.348307
6	-4.534565	0.961316	-1.101988	6	1.627093	1.756331	-1.824326
6	-6.281160	-1.051902	-0.280738	8	1.849619	3.026961	-2.183793
1	-4.650326	-2.403829	-0.627182	6	-0.315187	2.771435	-1.249069
6	-5.842796	1.278516	-0.729152	6	0.743706	3.826033	-1.662546
1	-3.847689	1.734297	-1.425464	7	0.482052	1.511638	-1.274998
6	-6.717430	0.275198	-0.314388	6	1.154608	4.581466	-0.376177
1	-6.957198	-1.839455	0.037591	1	2.158670	4.266138	-0.069410
1	-6.176930	2.311015	-0.764441	1	1.191988	5.663141	-0.533911
1	-7.733151	0.521712	-0.021998	6	0.106696	4.176949	0.636685
1	-2.230380	-0.180480	1.078346	6	-0.085496	4.671994	1.925569
6	-1.618774	-1.962600	2.169101	6	-0.735790	3.179089	0.137968
6	-1.151205	-3.409073	1.962494	6	-1.121719	4.149096	2.704581
1	-0.185347	-3.462356	1.462884	1	0.556120	5.453913	2.320897
1	-1.879518	-3.985166	1.384874	6	-1.790769	2.674863	0.896739
1	-1.046378	-3.899007	2.934701	6	-1.972139	3.161013	2.193731
6	-0.652602	-1.207519	3.098401	1	-1.281918	4.528622	3.709003
1	0.366693	-1.219222	2.711209	1	-2.460555	1.936926	0.471448
1	-0.640910	-1.677523	4.086224	1	-2.791207	2.788259	2.800888
1	-0.955930	-0.163402	3.224541	1	0.428760	4.485502	-2.469718
6	-3.024463	-1.981125	2.832308	1	-1.147983	2.641927	-1.940973
1	-3.376534	-0.969259	3.054930				
1	-2.972287	-2.538456	3.772525				
1	-3.764175	-2.461519	2.185654				
6	2.804080	-0.416546	-1.388061				
6	2.696921	0.794367	-2.106965				
6	3.631499	1.111603	-3.099856	28	0.057485	-0.112635	-0.148274
6	4.660997	0.223374	-3.404060	6	-4.012634	1.062133	-0.629451
6	4.770138	-0.974039	-2.701108	6	-3.222549	0.648000	0.362919
6	3.853483	-1.285983	-1.693217	6	-2.541542	1.448757	1.456340
1	3.539036	2.051039	-3.631763	1	-3.258535	1.758712	2.230905
1	5.374226	0.469745	-4.183128	1	-2.012737	2.335815	1.102392
1	5.572564	-1.668681	-2.927304	8	-1.570747	0.559427	2.028175
1	3.963088	-2.213044	-1.144109	6	-2.171028	-0.735852	1.950490
15	1.657246	-0.736927	0.018100	1	-1.407821	-1.485989	2.150210
6	2.364252	0.317241	1.328054	1	-2.979111	-0.830324	2.688652
6	3.733887	0.249637	1.632502	6	-2.747026	-0.805908	0.522170
6	1.546459	1.233509	2.001386	8	-1.687482	-1.063272	-0.415641
6	4.269871	1.075407	2.616784	1	-4.380480	0.287641	-1.302526
1	4.377389	-0.442528	1.098676	6	2.376533	1.258553	1.683076
6	2.089935	2.061623	2.984321	6	2.378062	0.064183	2.439150
1	0.494156	1.309752	1.756315	6	2.970164	0.044545	3.709109
6	3.447212	1.980553	3.294304	6	3.537224	1.200193	4.240955
1	5.327619	1.017738	2.852464	6	3.532407	2.381144	3.500639
1	1.448265	2.769528	3.495974	6	2.960560	2.405911	2.227414
1	3.868497	2.624773	4.059592	1	2.975434	-0.879308	4.274939
6	1.998083	-2.466959	0.466269	1	3.981777	1.175723	5.229989
6	1.750434	-3.461022	-0.496971	1	3.974637	3.283984	3.908923
6	2.444312	-2.834729	1.741750	1	2.959047	3.329329	1.659071

(R)-TS5B

SCF Energy = -2532.584329

Gibbs Free Energy = -2531.901907

15	1.700592	1.274146	-0.015102	1	-6.508940	-4.675734	0.176840
6	3.090559	0.926294	-1.126904	6	-4.430631	2.482541	-0.985992
6	4.256167	1.708411	-1.101491	6	-4.855626	3.297122	0.250572
6	2.993699	-0.164611	-2.002009	1	-4.020219	3.494996	0.926825
6	5.314146	1.397768	-1.951076	1	-5.255815	4.267179	-0.061033
1	4.337134	2.551570	-0.422740	1	-5.635534	2.776479	0.814215
6	4.061252	-0.473333	-2.844869	6	-3.249780	3.190076	-1.689966
1	2.094916	-0.769583	-2.025757	1	-2.933199	2.636594	-2.580461
6	5.217696	0.306094	-2.820339	1	-3.538755	4.196508	-2.011060
1	6.214941	2.002673	-1.934611	1	-2.391392	3.302818	-1.017224
1	3.982120	-1.323698	-3.513527	6	-5.621180	2.405409	-1.960168
1	6.047741	0.065988	-3.477215	1	-5.938514	3.406931	-2.265648
6	1.115434	2.965397	-0.318247	1	-5.355889	1.844374	-2.862377
6	0.333290	3.607899	0.657229	1	-6.476295	1.906717	-1.492871
6	1.295624	3.561909	-1.573359				
6	-0.248526	4.842689	0.378453				
1	0.185961	3.144462	1.627663				
6	0.704990	4.796794	-1.845581				
1	1.891854	3.064609	-2.330788				
6	-0.065241	5.436725	-0.873770	28	0.234870	0.276455	-1.072243
1	-0.845054	5.340436	1.136288	6	-2.396658	0.075019	0.199504
1	0.848939	5.257660	-2.817312	6	-1.853691	-0.061102	-1.038857
1	-0.522247	6.396971	-1.089598	6	-2.323811	-0.901761	-2.187733
6	1.805613	-1.189764	1.927305	1	-3.426639	-0.949684	-2.224518
8	2.278426	-2.318427	2.465462	1	-1.937295	-1.921033	-2.166699
6	0.696041	-2.788621	0.755100	8	-1.822543	-0.292896	-3.377744
6	1.711676	-3.450023	1.730438	6	-2.156399	1.077435	-3.305459
7	0.901317	-1.333590	1.011728	1	-1.668269	1.587280	-4.139776
6	2.798897	-4.137006	0.875802	1	-3.243643	1.215764	-3.379040
1	3.782578	-3.723209	1.120013	6	-1.632703	1.714978	-2.002541
1	2.842426	-5.210038	1.089635	8	-0.330972	1.902368	-1.920460
6	2.380066	-3.874338	-0.554173	6	-2.496337	2.761851	-1.368428
6	3.026164	-4.264394	-1.726395	6	-3.864721	2.558316	-1.128179
6	1.165197	-3.187022	-0.622547	6	-1.923228	3.996367	-1.036617
6	2.435548	-3.964194	-2.956916	6	-4.634807	3.561624	-0.550296
1	3.969318	-4.801116	-1.687800	1	-4.321596	1.602361	-1.362387
6	0.554345	-2.907762	-1.845190	6	-2.698949	5.005405	-0.464738
6	1.204760	-3.299857	-3.017698	1	-0.873585	4.158475	-1.248144
1	2.927923	-4.267731	-3.875656	6	-4.053432	4.789403	-0.215589
1	-0.403412	-2.399993	-1.877677	1	-5.688996	3.388431	-0.358653
1	0.749409	-3.093025	-3.980816	1	-2.244203	5.959980	-0.219291
1	1.261537	-4.104791	2.475536	1	-4.657501	5.571915	0.232596
1	-0.352108	-3.029417	0.941298	1	-2.005837	0.889961	0.810615
8	-0.819812	0.687701	-1.642173	6	2.364134	-2.216881	-0.789310
1	-1.181371	1.573572	-1.496882	6	3.367063	-1.324046	-1.234552
1	-1.582813	-0.137620	-1.272608	6	4.576282	-1.826520	-1.733922
6	-3.816313	-1.873078	0.381642	6	4.794928	-3.199909	-1.811628
6	-3.541634	-3.071564	-0.283635	6	3.811123	-4.082146	-1.372154
6	-5.074230	-1.696329	0.973332	6	2.608439	-3.591238	-0.858808
6	-4.508277	-4.076143	-0.357111	1	5.338709	-1.131153	-2.063056
1	-2.573998	-3.204666	-0.751935	1	5.731300	-3.575218	-2.210138
6	-6.037319	-2.700443	0.902936	1	3.975186	-5.153713	-1.421515
1	-5.304685	-0.762519	1.477084	1	1.855673	-4.288164	-0.510729
6	-5.756929	-3.895281	0.236299	15	0.822876	-1.560042	-0.035514
1	-4.284608	-4.999679	-0.882645	6	1.318395	-1.220973	1.687401
1	-7.008819	-2.548159	1.362929	6	2.081921	-2.148412	2.413430

(R)-TS1A

SCF Energy = -2529.912102

Gibbs Free Energy = -2529.282109

6	0.948553	-0.008810	2.281538	28	-0.281535	0.293867	0.440614
6	2.462521	-1.861011	3.721683	6	-2.191681	2.969571	0.780495
1	2.382976	-3.085445	1.956156	6	-1.370732	3.003080	-1.427625
6	1.339888	0.279420	3.588613	6	-1.827748	1.531416	-1.308867
1	0.380008	0.719474	1.717331	6	-1.854944	1.549710	0.441572
6	2.093860	-0.646697	4.308882	1	-1.612239	3.318847	1.645670
1	3.052864	-2.579404	4.281387	1	-3.258039	3.085470	1.023678
1	1.068111	1.232217	4.029246	6	-1.978725	0.401871	1.115267
1	2.401478	-0.423270	5.325547	6	-2.892347	-0.227521	2.022434
6	-0.316862	-2.979789	0.043025	6	-2.442262	-1.154473	2.985907
6	-0.622776	-3.691200	-1.130053	6	-4.278901	0.009994	1.896133
6	-0.936763	-3.336295	1.247075	6	-3.348734	-1.802308	3.817822
6	-1.525855	-4.751668	-1.090808	1	-1.375107	-1.336610	3.067279
1	-0.143482	-3.426798	-2.068299	6	-5.181156	-0.664412	2.712042
6	-1.843528	-4.396726	1.279619	1	-4.625346	0.701699	1.134695
1	-0.712798	-2.790216	2.156111	6	-4.720043	-1.563713	3.678598
6	-2.136731	-5.106249	0.115753	1	-2.993504	-2.501030	4.569778
1	-1.749497	-5.301880	-1.999130	1	-6.246633	-0.487090	2.600293
1	-2.322266	-4.662584	2.216154	1	-5.427811	-2.080686	4.319807
1	-2.837987	-5.934060	0.145090	8	-1.896044	3.787484	-0.357843
6	3.210442	0.137506	-1.168766	1	-0.274855	3.002125	-1.418771
8	4.346298	0.845936	-1.197793	1	-1.724552	3.446092	-2.364707
6	2.454042	2.263957	-1.005600	8	-1.024102	0.636609	-1.826471
6	4.007643	2.264335	-1.098356	6	-3.318263	1.304799	-1.593477
7	2.112935	0.818552	-1.094859	6	-4.281564	2.321832	-1.544846
6	4.560354	2.860411	0.211227	6	-3.735347	-0.006018	-1.859344
1	5.255609	2.157229	0.680635	6	-5.631862	2.029098	-1.752568
1	5.121391	3.779750	0.012127	1	-3.975714	3.341567	-1.334464
6	3.332239	3.136286	1.049498	6	-5.081401	-0.298859	-2.060982
6	3.274180	3.660099	2.340840	1	-2.979163	-0.781554	-1.903890
6	2.153796	2.853689	0.353625	6	-6.038464	0.718739	-2.005676
6	2.026327	3.910454	2.916187	1	-6.366309	2.829304	-1.716828
1	4.184606	3.883657	2.888919	1	-5.387614	-1.321752	-2.263484
6	0.905978	3.114179	0.917798	1	-7.089257	0.491977	-2.162168
6	0.848785	3.647775	2.206376	6	2.752894	0.290554	1.584939
1	1.970830	4.327944	3.916830	6	2.480472	-1.020975	2.050927
1	0.001979	2.910771	0.357625	6	3.244331	-1.560396	3.096196
1	-0.114896	3.867938	2.655684	6	4.250546	-0.812727	3.702663
1	4.406074	2.738002	-1.995586	6	4.507282	0.483968	3.262228
1	1.944398	2.779997	-1.820361	6	3.767136	1.023039	2.207993
6	-3.486342	-0.660430	0.816310	1	3.032815	-2.568823	3.430864
6	-4.133600	-0.083967	1.929313	1	4.826564	-1.241965	4.516114
6	-3.928256	-1.915572	0.350989	1	5.287183	1.076919	3.730323
6	-5.209179	-0.722165	2.534940	1	3.983391	2.026313	1.858365
1	-3.791995	0.879267	2.297499	15	1.803943	0.980325	0.163754
6	-4.998072	-2.555520	0.966325	6	2.665957	0.238804	-1.272835
1	-3.406441	-2.409803	-0.457648	6	1.961253	0.182716	-2.485286
6	-5.645820	-1.959439	2.051888	6	3.970385	-0.270755	-1.197326
1	-5.706247	-0.262526	3.382965	6	2.572092	-0.369487	-3.610832
1	-5.322594	-3.526299	0.605922	1	0.933818	0.540888	-2.518183
1	-6.481981	-2.462290	2.527358	6	4.569204	-0.826636	-2.327710
				1	4.515272	-0.237934	-0.259362
				6	3.870796	-0.874594	-3.535894
				1	2.021814	-0.420664	-4.545392
				1	5.578157	-1.223766	-2.263899
				1	4.336541	-1.312845	-4.413870

(R)-TS1C

SCF Energy = -2529.420822

Gibbs Free Energy = -2528.807630

6	2.263201	2.748597	0.121070	1	6.794103	1.326438	-0.518825
6	3.374118	3.230948	-0.584917	1	5.736358	-2.832466	-0.795427
6	1.431835	3.651522	0.799402	1	7.409826	-1.069052	-0.278183
6	3.651556	4.597787	-0.601323	1	1.991043	0.047187	1.103683
1	4.010041	2.539050	-1.127303	6	2.401132	1.964461	2.036355
6	1.712694	5.016122	0.783000	6	2.358888	3.472011	1.756537
1	0.558286	3.277820	1.321988	1	1.358289	3.799138	1.462211
6	2.822957	5.490473	0.081911	1	3.063156	3.755203	0.969830
1	4.510692	4.966592	-1.153784	1	2.639136	4.023781	2.658757
1	1.054976	5.707824	1.299801	6	1.485041	1.628920	3.234205
1	3.036344	6.554943	0.058674	1	0.450982	1.922686	3.038287
6	1.408970	-1.856573	1.488190	1	1.830436	2.159630	4.126960
8	1.486906	-3.182204	1.751683	1	1.489011	0.556867	3.452899
6	-0.379284	-2.677264	0.407726	6	3.846094	1.531173	2.376153
6	0.270124	-3.810953	1.245997	1	3.896436	0.461291	2.603364
7	0.380788	-1.472502	0.807119	1	4.201747	2.081123	3.253255
6	0.616684	-4.960868	0.289978	1	4.527475	1.728199	1.545023
1	1.618435	-5.348750	0.499857	6	-3.170195	0.373177	-0.863452
1	-0.086695	-5.790798	0.431868	6	-3.299764	-0.905048	-1.451992
6	0.478074	-4.347247	-1.085569	6	-4.518268	-1.287464	-2.031750
6	0.833258	-4.897272	-2.315699	6	-5.600886	-0.412650	-2.046484
6	-0.111030	-3.079897	-1.026837	6	-5.478608	0.847823	-1.465535
6	0.590246	-4.160786	-3.477763	6	-4.273875	1.231880	-0.874853
1	1.293854	-5.879849	-2.372063	1	-4.604686	-2.272934	-2.472725
6	-0.355770	-2.334613	-2.178603	1	-6.534399	-0.717112	-2.507285
6	0.001181	-2.894165	-3.407823	1	-6.318428	1.535068	-1.467186
1	0.865296	-4.575728	-4.443271	1	-4.192357	2.214889	-0.426549
1	-0.777593	-1.332327	-2.117549	15	-1.622125	0.861921	0.003246
1	-0.174202	-2.330321	-4.319055	6	-1.888215	0.275030	1.708290
1	-0.310394	-4.120677	2.118500	6	-2.957325	0.747053	2.486398
1	-1.436119	-2.507766	0.624078	6	-1.038342	-0.712492	2.222282
				6	-3.154123	0.248519	3.771511
				1	-3.631263	1.500279	2.091089
				6	-1.246417	-1.217306	3.505848
				1	-0.221355	-1.092795	1.622925
				6	-2.299094	-0.733487	4.282050
28	0.098998	-0.054166	-0.985163	1	-3.977286	0.619839	4.373459
6	1.952262	1.113152	0.866715	1	-0.584679	-1.987412	3.887550
6	1.547958	1.420680	-0.379479	1	-2.460306	-1.121973	5.282665
6	1.467406	2.699593	-1.153393	6	-1.692169	2.679807	0.030034
1	2.397439	3.284505	-1.093384	6	-1.850495	3.358044	-1.191143
1	0.638842	3.338970	-0.858038	6	-1.474142	3.411005	1.203764
8	1.233753	2.312979	-2.512103	6	-1.800297	4.748569	-1.229804
6	2.273279	1.424927	-2.875906	1	-1.995129	2.798757	-2.109916
1	2.009139	0.979853	-3.838034	6	-1.415130	4.805559	1.157372
1	3.219890	1.969831	-2.976540	1	-1.354732	2.898233	2.150647
6	2.440819	0.257791	-1.870713	6	-1.577196	5.474554	-0.055839
8	1.594000	-0.736131	-1.963307	1	-1.923094	5.264871	-2.176165
6	3.826451	-0.081407	-1.427431	1	-1.244872	5.365764	2.071115
6	4.785021	0.907495	-1.151380	1	-1.531234	6.558254	-0.088799
6	4.185050	-1.430230	-1.296154	6	-2.205668	-1.886807	-1.459272
6	6.064240	0.553083	-0.736091	8	-2.571721	-3.163012	-1.639730
1	4.525561	1.957416	-1.234444	6	-0.225904	-2.977835	-1.338254
6	5.469407	-1.784254	-0.885396	6	-1.380342	-4.001299	-1.545021
1	3.453004	-2.190469	-1.538490	7	-0.938613	-1.669939	-1.317124
6	6.409951	-0.795005	-0.599146	6	-1.451869	-4.893426	-0.288573

(R)-TS3B

SCF Energy = -2456.112094

Gibbs Free Energy = -2455.448813

1	-2.455204	-4.849199	0.146567	6	0.183268	3.544249	0.949662
1	-1.259896	-5.941054	-0.543871	6	1.117603	3.780567	-1.279253
6	-0.378686	-4.346909	0.625782	6	-0.430823	4.788014	0.823024
6	-0.049483	-4.767943	1.914064	1	0.062800	2.968531	1.862214
6	0.356460	-3.329336	0.011714	6	0.494047	5.023985	-1.400341
6	1.027497	-4.167138	2.571004	1	1.718093	3.391031	-2.093932
1	-0.614612	-5.557993	2.399473	6	-0.279705	5.526984	-0.354345
6	1.449918	-2.746563	0.651116	1	-1.027220	5.180465	1.640577
6	1.780297	-3.169569	1.940200	1	0.616811	5.598694	-2.312557
1	1.295061	-4.492333	3.571649	1	-0.762488	6.493850	-0.452731
1	2.032504	-1.985746	0.148215	6	1.802376	-1.206657	1.876364
1	2.631377	-2.729146	2.450600	8	2.290949	-2.350072	2.372223
1	-1.323780	-4.563564	-2.476818	6	0.754310	-2.765371	0.630221
1	0.514408	-2.946942	-2.138696	6	1.603459	-3.469866	1.722687

(R)_IM7B

SCF Energy = -2532.592197

Gibbs Free Energy = -2531.908185

28	0.034254	-0.087172	-0.177900	6	1.475038	-3.075779	-0.662917
6	-4.039224	0.928844	-0.637828	6	3.142970	-3.773937	-2.761940
6	-3.264473	0.499901	0.360458	1	4.248372	-4.942624	-1.321326
6	-2.612565	1.275506	1.487940	6	1.202590	-2.576736	-1.935578
1	-3.348063	1.556762	2.255980	6	2.050072	-2.930108	-2.986555
1	-2.087209	2.174451	1.163062	1	3.794979	-4.039736	-3.587942
8	-1.642948	0.381273	2.051875	1	0.358146	-1.917620	-2.109298
6	-2.200926	-0.921737	1.912621	1	1.859779	-2.546507	-3.983544
1	-1.415457	-1.658336	2.074594	1	1.028331	-3.973533	2.500995
1	-3.009557	-1.084997	2.638004	1	-0.299652	-3.047193	0.621696
6	-2.787254	-0.945053	0.492940	8	-0.639371	0.788591	-1.628341
8	-1.668948	-1.153113	-0.438972	1	-0.910551	1.699455	-1.459728
1	-4.391413	0.168735	-1.335512	1	-1.812695	-0.552733	-1.213787
6	2.385452	1.241083	1.671033	6	-3.819224	-2.030558	0.277422
6	2.401110	0.029611	2.398859	6	-3.507700	-3.193928	-0.433161
6	3.042748	-0.025763	3.643986	6	-5.091632	-1.899890	0.850376
6	3.650717	1.108331	4.176431	6	-4.455465	-4.209871	-0.570464
6	3.635688	2.305792	3.462598	1	-2.530199	-3.295716	-0.889473
6	3.008627	2.368178	2.217188	6	-6.033650	-2.917020	0.717359
1	3.056476	-0.962182	4.188449	1	-5.348411	-0.992691	1.388365
1	4.135482	1.054713	5.145294	6	-5.718071	-4.076244	0.005065
1	4.111501	3.191657	3.870287	1	-4.204688	-5.104946	-1.131253
1	2.998461	3.302720	1.667150	1	-7.016489	-2.801853	1.163375
15	1.605910	1.338997	0.024074	1	-6.454289	-4.866208	-0.103572
6	2.911507	1.103853	-1.213951	6	-4.458167	2.354833	-0.965332
6	4.271141	1.225647	-0.896890	6	-4.956063	3.113653	0.279947
6	2.515480	0.757182	-2.517087	1	-4.158778	3.290088	1.006270
6	5.231526	1.006964	-1.883757	1	-5.347965	4.092556	-0.013571
1	4.579656	1.481653	0.110853	1	-5.760118	2.565486	0.780270
6	3.484553	0.550893	-3.496521	6	-3.253811	3.103200	-1.581874
1	1.457731	0.655005	-2.741030	1	-2.874805	2.577860	-2.463721
6	4.839715	0.672137	-3.181273	1	-3.550980	4.111229	-1.889612
1	6.284854	1.097693	-1.638807	1	-2.436561	3.209688	-0.860883
1	3.181573	0.286694	-4.504681	6	-5.598137	2.297796	-1.999477
1	5.591316	0.502342	-3.945716	1	-5.914750	3.306007	-2.282159
6	0.963361	3.036474	-0.103458	1	-5.279164	1.776687	-2.908258

1 -6.468438 1.770589 -1.595364

(R)-TS5

SCF Energy = -2529.915624

Gibbs Free Energy = -2529.282551

28 0.041715 -0.097717 -0.967309
6 3.919428 1.416486 2.550288
6 3.523235 1.513791 1.219897
6 2.445844 0.753542 0.731020
6 1.826023 -0.148779 1.608751
6 2.215199 -0.245838 2.942881
6 3.260455 0.543785 3.421650
1 4.749229 2.017476 2.909547
1 4.051033 2.187056 0.552214
1 1.017720 -0.771092 1.245159
1 1.697219 -0.934328 3.603298
1 3.570773 0.471868 4.459150
6 1.954272 0.907325 -0.650600
6 2.099595 2.048684 -1.357404
6 1.711906 2.196425 -2.793384
1 2.532963 2.698006 -3.334968
1 0.831802 2.842790 -2.885472
8 1.384907 0.973691 -3.421411
6 2.416590 0.016223 -3.239010
1 2.289386 -0.738859 -4.020678
1 3.403968 0.478237 -3.351035
6 2.279789 -0.720390 -1.906494
8 1.160168 -1.402052 -1.791573
6 3.509052 -1.298743 -1.297583
6 4.704913 -0.569483 -1.213262
6 3.471073 -2.610316 -0.805631
6 5.837440 -1.139891 -0.643315
1 4.737190 0.458479 -1.558731
6 4.607763 -3.181772 -0.237927
1 2.554169 -3.178171 -0.900922
6 5.791136 -2.447478 -0.151534
1 6.754850 -0.564477 -0.573394
1 4.571591 -4.201850 0.131190
1 6.675599 -2.890585 0.294976
1 2.532444 2.940991 -0.901175
6 -2.760675 1.613560 -0.600179
6 -3.389395 0.559436 -1.302990
6 -4.673470 0.751138 -1.836178
6 -5.333068 1.966954 -1.682843
6 -4.725926 2.998349 -0.969401
6 -3.453783 2.815551 -0.426511
1 -5.148271 -0.063471 -2.368487
1 -6.321109 2.101570 -2.109578
1 -5.239371 3.943980 -0.828997
1 -2.995579 3.620996 0.135116
15 -1.122581 1.364873 0.190579
6 -1.574553 0.826328 1.877127
6 -1.564329 -0.540691 2.182911
6 -2.001678 1.750274 2.842372
6 -1.958263 -0.979714 3.445938

1 -1.247203 -1.264765 1.444825
6 -2.389436 1.306925 4.105137
1 -2.020316 2.810854 2.615548
6 -2.366145 -0.056595 4.409435
1 -1.938819 -2.041667 3.667478
1 -2.710458 2.026250 4.851734
1 -2.667714 -0.395882 5.395359
6 -0.366662 3.011479 0.353972
6 -0.474859 3.952928 -0.682048
6 0.501666 3.261173 1.427107
6 0.267620 5.131029 -0.638463
1 -1.133132 3.765017 -1.523890
6 1.247234 4.438409 1.461148
1 0.614826 2.531864 2.220611
6 1.134312 5.373180 0.430619
1 0.171994 5.857784 -1.438913
1 1.921985 4.618071 2.291584
1 1.715163 6.289482 0.461236
6 -2.787817 -0.776073 -1.458487
8 -3.641518 -1.752105 -1.792437
6 -1.451521 -2.606116 -1.496687
6 -2.903028 -3.010334 -1.879881
7 -1.551896 -1.132091 -1.305100
6 -3.414276 -4.002978 -0.818611
1 -4.379822 -3.672619 -0.423499
1 -3.571640 -4.991889 -1.263111
6 -2.316410 -4.040867 0.220582
6 -2.308743 -4.709971 1.444300
6 -1.189066 -3.325792 -0.193591
6 -1.160363 -4.658384 2.239098
1 -3.179032 -5.268678 1.775458
6 -0.031340 -3.292799 0.582641
6 -0.025549 -3.960703 1.808673
1 -1.144132 -5.177279 3.192540
1 0.837281 -2.746848 0.237946
1 0.865537 -3.940290 2.428317
1 -3.020122 -3.364227 -2.904288
1 -0.699641 -2.798026 -2.262326

(R)-TS5_p

SCF Energy = -2338.153451

Gibbs Free Energy = -2337.569338

28 0.070827 -0.300788 -1.141140
6 3.676543 -3.154245 1.768629
6 3.500113 -2.469654 0.569808
6 2.232514 -1.986820 0.194362
6 1.145058 -2.275941 1.035168
6 1.317998 -2.957764 2.238030
6 2.588697 -3.392119 2.614810
1 4.664748 -3.510244 2.043392
1 4.352508 -2.303786 -0.081131
1 0.151783 -1.952938 0.748024
1 0.459561 -3.142633 2.876335
1 2.731345 -3.924902 3.549458
6 2.035895 -1.181634 -1.026809

6	3.029525	-0.466089	-1.595930	1	-5.662097	-1.766044	1.713366
6	2.896285	0.263009	-2.894393	6	-2.359460	-2.674197	-0.161473
1	3.802534	0.086261	-3.498575	6	-2.765457	-3.407271	0.955284
1	2.835212	1.343583	-2.723518	1	-4.250226	-3.650124	2.498539
8	1.741779	-0.093176	-3.630799	1	-1.458349	-2.924550	-0.707767
6	1.647293	-1.500467	-3.779160	1	-2.168630	-4.248487	1.293611
1	1.005858	-1.682811	-4.648039	1	-4.570283	0.393220	-2.690869
1	2.633829	-1.946183	-3.961828	1	-2.576196	-1.064736	-2.621241
6	0.962771	-2.157444	-2.582818	6	1.299523	-3.596727	-2.287899
8	-0.258600	-1.763029	-2.359837	1	0.826704	-4.212443	-3.063826
1	4.012065	-0.393366	-1.125741	1	2.375518	-3.777232	-2.304852
6	-0.342842	2.777538	-0.044264	1	0.895434	-3.896524	-1.320669
6	-1.569298	2.769199	-0.748369				
6	-2.224151	3.980738	-1.016783				
6	-1.676935	5.191206	-0.601462				
6	-0.481895	5.200436	0.114856				
6	0.171550	4.000419	0.397623				
1	-3.166152	3.962228	-1.550583	28	0.089907	-0.425761	-0.993764
1	-2.189913	6.120055	-0.826224	6	3.762885	-2.360827	2.526034
1	-0.057231	6.137474	0.460055	6	3.580087	-1.978812	1.200255
1	1.093669	4.019706	0.966113	6	2.300068	-1.656129	0.712166
15	0.484960	1.200659	0.404572	6	1.210108	-1.797257	1.586894
6	-0.224474	0.833654	2.048364	6	1.389035	-2.175963	2.915848
6	-1.270327	-0.092223	2.159242	6	2.670123	-2.450286	3.394289
6	0.214887	1.524617	3.187747	1	4.760348	-2.596314	2.884378
6	-1.858802	-0.337874	3.399214	1	4.436971	-1.926211	0.536378
1	-1.626870	-0.625236	1.288065	1	0.209346	-1.598415	1.223364
6	-0.372845	1.270997	4.425113	1	0.526882	-2.251076	3.571287
1	1.019565	2.248204	3.112908	1	2.817749	-2.746882	4.427746
6	-1.407959	0.338766	4.532963	6	2.092557	-1.160456	-0.662601
1	-2.664174	-1.061098	3.468581	6	3.065577	-0.544284	-1.367200
1	-0.023238	1.801648	5.304905	6	2.928976	-0.131513	-2.797445
1	-1.861558	0.143614	5.499535	1	3.854850	-0.396195	-3.336348
6	2.241720	1.589663	0.670276	1	2.817807	0.955937	-2.873633
6	2.914773	2.475332	-0.186439	8	1.806977	-0.696400	-3.447698
6	2.973503	0.841036	1.603886	6	1.776096	-2.104989	-3.279730
6	4.298138	2.616618	-0.101905	1	1.161448	-2.502387	-4.093716
1	2.361111	3.049979	-0.921583	1	2.784488	-2.534005	-3.348893
6	4.358393	0.980825	1.677997	6	1.097580	-2.509986	-1.972643
1	2.469928	0.136003	2.254843	8	-0.145638	-2.132942	-1.861529
6	5.023066	1.865018	0.826695	1	4.033349	-0.321097	-0.914175
1	4.810007	3.310067	-0.761554	6	-0.493295	2.794088	-0.622652
1	4.916046	0.391387	2.398260	6	-1.703926	2.565080	-1.316997
1	6.101242	1.972777	0.888518	6	-2.410477	3.650008	-1.857640
6	-2.246201	1.528862	-1.163553	6	-1.929791	4.949158	-1.722189
8	-3.553942	1.650166	-1.423914	6	-0.750745	5.180232	-1.016668
6	-2.842768	-0.600382	-1.671356	6	-0.046542	4.109620	-0.464466
6	-4.092882	0.324354	-1.713865	1	-3.339875	3.463709	-2.381283
7	-1.748251	0.340644	-1.294231	1	-2.481928	5.776176	-2.155332
6	-5.049198	-0.122535	-0.588178	1	-0.377999	6.191295	-0.888753
1	-5.254147	0.716026	0.084927	1	0.862230	4.303396	0.092705
1	-6.011725	-0.444203	-0.999834	15	0.399037	1.402883	0.178760
6	-4.329910	-1.268935	0.086037	6	-0.328681	1.379778	1.855223
6	-4.737330	-2.006592	1.197397	6	-1.330864	0.449584	2.161591
6	-3.138801	-1.592111	-0.570519	6	0.051123	2.331781	2.813379
6	-3.941973	-3.069380	1.634634	6	-1.934478	0.459701	3.418475

(R)-TS5_q

SCF Energy = -2377.474985

Gibbs Free Energy = -2376.863987

1	-1.641448	-0.284265	1.430011	6	-1.998921	3.871232	1.243495
6	-0.551095	2.333444	4.069648	1	-0.634711	3.410464	2.850717
1	0.821257	3.060963	2.585475	1	-1.112278	0.998992	2.815499
6	-1.542180	1.397020	4.374522	1	-3.910304	1.587144	-0.391927
1	-2.705430	-0.270091	3.641058	1	-3.411242	3.987348	-0.382071
1	-0.247198	3.066285	4.810218	1	-1.793595	4.937094	1.254696
1	-2.007289	1.401499	5.355213	6	-2.857813	-0.361252	1.314175
6	2.129083	1.930722	0.368755	6	-2.862750	-0.977525	2.508666
6	2.778883	2.632872	-0.658906	6	-2.921627	-2.467939	2.668383
6	2.874222	1.450046	1.455633	1	-3.932661	-2.799421	2.963857
6	4.151903	2.859459	-0.593191	1	-2.235073	-2.789168	3.459024
1	2.215728	2.997731	-1.511511	8	-2.518538	-3.136171	1.483174
6	4.249058	1.672743	1.511463	6	-3.285704	-2.674686	0.384257
1	2.389812	0.885221	2.243468	1	-3.008438	-3.272083	-0.485651
6	4.890383	2.374522	0.489471	1	-4.352038	-2.829571	0.598323
1	4.645312	3.410985	-1.387159	6	-3.040787	-1.182665	0.035553
1	4.817512	1.289822	2.352547	8	-1.863124	-1.088749	-0.772095
1	5.960707	2.547827	0.537182	6	-4.271359	-0.757722	-0.774802
6	-2.312151	1.230221	-1.447330	6	-5.464887	-0.426335	-0.117835
8	-3.619503	1.221701	-1.737213	6	-4.253371	-0.784351	-2.172153
6	-2.792846	-0.986940	-1.469862	6	-6.604391	-0.089355	-0.844044
6	-4.086979	-0.161599	-1.722036	1	-5.490331	-0.409285	0.967778
7	-1.754020	0.070690	-1.304426	6	-5.396657	-0.446285	-2.900788
6	-5.035077	-0.393901	-0.526552	1	-3.349767	-1.076783	-2.694319
1	-5.285020	0.561950	-0.055165	6	-6.572244	-0.092598	-2.241013
1	-5.977544	-0.842593	-0.857848	1	-7.516833	0.178346	-0.320401
6	-4.272086	-1.328087	0.385284	1	-5.365599	-0.466511	-3.985790
6	-4.660276	-1.823655	1.629901	1	-7.459030	0.172361	-2.807782
6	-3.056704	-1.726529	-0.178942	1	-2.790639	-0.393484	3.422692
6	-3.820811	-2.722427	2.293850	6	1.860720	1.674220	1.378477
1	-5.603522	-1.523041	2.076233	6	1.701241	0.681355	2.369827
6	-2.231618	-2.650842	0.461877	6	1.944616	0.984969	3.712390
6	-2.618620	-3.140388	1.710833	6	2.311087	2.280859	4.078396
1	-4.113622	-3.114144	3.263094	6	2.463177	3.264878	3.102157
1	-1.310125	-2.967395	-0.011145	6	2.248066	2.960005	1.754852
1	-1.986278	-3.854557	2.228939	1	1.839414	0.207997	4.461122
1	-4.553812	-0.339208	-2.690365	1	2.484460	2.516362	5.122947
1	-2.486840	-1.634242	-2.292279	1	2.757525	4.270456	3.384418
6	1.484888	-3.834975	-1.354235	1	2.377855	3.724470	0.997194
1	2.574390	-3.926601	-1.323957	15	1.571478	1.220981	-0.365684
1	1.122154	-3.859435	-0.324187	6	3.008459	0.228822	-0.864656
6	0.863501	-4.994823	-2.155931	6	2.918726	-0.492063	-2.065893
1	1.237910	-5.025848	-3.183649	6	4.166118	0.147305	-0.080199
1	1.111575	-5.948070	-1.682414	6	3.990526	-1.275418	-2.483170
1	-0.224770	-4.898813	-2.190044	1	2.012759	-0.447248	-2.662067
				6	5.229393	-0.654011	-0.498497
				1	4.240324	0.704723	0.847159
				6	5.142798	-1.361112	-1.698208
				1	3.917048	-1.836199	-3.407649
				1	6.126509	-0.717427	0.109067
28	-0.213061	-0.013473	-0.390801	1	5.971982	-1.982289	-2.021328
6	-1.358003	3.019058	2.142994	6	1.589598	2.754545	-1.325027
6	-1.633986	1.653404	2.127477	6	0.489887	3.620527	-1.220828
6	-2.567668	1.097865	1.231626	6	2.665407	3.082294	-2.160387
6	-3.181998	1.968516	0.309915	6	0.473308	4.810448	-1.942631
6	-2.901860	3.335450	0.321403	1	-0.337836	3.375184	-0.564712

(R)-TS6

SCF Energy = -2606.397198

Gibbs Free Energy = -2605.741884

Gibbs Free Energy = -733.877236

				6	-1.596863	1.240916	-0.743947
				6	-1.856348	1.221058	-2.060711
1	1.351455	2.296173	1.760935	6	-1.145616	0.258993	-2.967900
6	-1.217539	-0.511726	0.283635	1	-1.632446	0.202803	-3.950221
6	-0.812193	0.734509	0.040050	1	-0.097624	0.535355	-3.128519
6	-1.544352	1.938550	-0.529814	8	-1.071835	-1.077106	-2.406793
1	-1.954950	1.714783	-1.526111	6	-2.331905	-1.618873	-2.103092
1	-2.362452	2.295276	0.101419	1	-2.282216	-2.700921	-2.296028
8	-0.582844	2.991355	-0.625936	1	-3.115197	-1.212816	-2.752419
6	0.700504	2.394412	-0.659853	6	-2.764227	-1.472852	-0.642318
1	1.441013	3.140938	-0.353694	8	-1.949026	-1.202192	0.257950
1	0.960678	2.046935	-1.671507	6	-4.167803	-1.709574	-0.287985
6	0.617193	1.202370	0.313451	6	-5.070223	-2.340305	-1.164653
8	0.610823	1.680815	1.664849	6	-4.622104	-1.236593	0.957831
6	1.692538	0.153901	0.084195	6	-6.399158	-2.507564	-0.791584
6	1.845259	-0.450160	-1.172369	1	-4.737687	-2.718249	-2.125398
6	2.541159	-0.236361	1.122568	6	-5.955326	-1.391921	1.316754
6	2.837660	-1.402008	-1.388395	1	-3.921786	-0.728598	1.609894
1	1.168745	-0.188773	-1.980055	6	-6.842603	-2.030606	0.445654
6	3.536728	-1.191863	0.908234	1	-7.090886	-3.005909	-1.462320
1	2.401452	0.200459	2.104236	1	-6.306754	-1.013357	2.270813
6	3.692431	-1.773828	-0.347857	1	-7.883268	-2.154211	0.728461
1	2.941092	-1.859114	-2.367963	1	-2.606934	1.874215	-2.507181
1	4.186188	-1.483702	1.728219	6	1.945988	1.815584	1.309664
1	4.465723	-2.517193	-0.515571	6	2.005638	0.885311	2.375334
1	-0.449886	-1.191338	0.653464	6	2.515210	1.284732	3.617117
6	-2.564095	-1.183769	0.103264	6	2.936991	2.598068	3.818893
6	-2.453847	-2.132836	-1.110402	6	2.869410	3.516911	2.774175
1	-3.379696	-2.704964	-1.238317	6	2.384189	3.123300	1.523953
1	-2.269212	-1.568612	-2.029977	1	2.571532	0.561102	4.421370
1	-1.631140	-2.843537	-0.981057	1	3.318990	2.897801	4.788882
6	-3.731479	-0.209111	-0.112521	1	3.200512	4.539554	2.923321
1	-4.673320	-0.764612	-0.168322	1	2.348618	3.838401	0.710406
1	-3.812423	0.502019	0.714730	15	1.333052	1.254680	-0.323460
1	-3.629962	0.352526	-1.044442	6	2.690857	0.204287	-0.943487
6	-2.844566	-2.018072	1.371012	6	4.022439	0.464179	-0.587190
1	-2.923003	-1.374608	2.252855	6	2.390196	-0.872875	-1.787871
1	-3.783413	-2.572311	1.266221	6	5.043635	-0.349534	-1.074654
1	-2.043126	-2.741756	1.552432	1	4.259375	1.295244	0.068936

(S)-IM10

SCF Energy = -2529.936845

Gibbs Free Energy = -2529.308693

28	-0.387422	0.042084	0.077743	1	3.178890	-2.520159	-2.915693
6	-4.570059	2.792701	1.015064	1	5.538062	-2.055100	-2.294394
6	-3.794222	2.132480	0.066242	6	1.301382	2.719498	-1.401200
6	-2.404592	1.978191	0.243811	6	0.395697	3.760951	-1.138544
6	-1.834107	2.480053	1.431012	6	2.145358	2.801074	-2.517570
6	-2.610558	3.144871	2.378310	6	0.350506	4.872688	-1.974799
6	-3.981891	3.305559	2.173948	1	-0.272760	3.705247	-0.287465
1	-5.638750	2.899585	0.855127	6	2.084028	3.912464	-3.359497
1	-4.262345	1.709604	-0.816450	1	2.846708	2.002357	-2.729362
1	-0.771294	2.350532	1.609451	6	1.190724	4.948386	-3.088976
1	-2.144868	3.533085	3.279087	1	-0.347874	5.675734	-1.762072
1	-4.588826	3.816428	2.914636	1	2.738765	3.967485	-4.223265
				1	1.146990	5.813023	-3.743605

6	1.560639	-0.510732	2.224236	1	-6.914715	-2.070723	-0.552580
8	2.059067	-1.379134	3.117297	1	-4.664638	-4.070785	2.516126
6	0.596775	-2.448180	1.586152	1	-6.850724	-3.457629	1.508847
6	1.558892	-2.707521	2.783675	1	-1.166589	1.173042	-2.216207
7	0.737506	-0.989267	1.347074	6	1.135047	2.021617	1.596126
6	2.701778	-3.615628	2.282601	6	1.452173	1.041355	2.562576
1	3.657490	-3.087251	2.364415	6	1.732785	1.422565	3.880720
1	2.783830	-4.521467	2.891832	6	1.684586	2.764844	4.251641
6	2.330837	-3.933026	0.851724	6	1.376494	3.734869	3.300816
6	2.997470	-4.770809	-0.041355	6	1.111401	3.364594	1.979871
6	1.142456	-3.305042	0.469965	1	1.985843	0.660403	4.607712
6	2.452470	-4.980604	-1.309931	1	1.893373	3.048546	5.277504
1	3.919982	-5.265691	0.247288	1	1.345920	4.783217	3.579365
6	0.594172	-3.514109	-0.792231	1	0.882593	4.129044	1.247399
6	1.255414	-4.359607	-1.683231	15	0.867994	1.516737	-0.146423
1	2.958359	-5.638846	-2.009467	6	2.549169	1.308603	-0.810151
1	-0.317588	-3.010452	-1.080759	6	3.546854	2.263230	-0.557094
1	0.840623	-4.534839	-2.671049	6	2.847982	0.170630	-1.569619
1	1.067403	-3.086881	3.679480	6	4.828344	2.077103	-1.069060
1	-0.455452	-2.651086	1.800649	1	3.323628	3.141666	0.040182
				6	4.134787	-0.014203	-2.074749
				1	2.092659	-0.586740	-1.740941
				6	5.122465	0.938720	-1.826316
				1	5.599486	2.815280	-0.873581
				1	4.360050	-0.909981	-2.642036
28	-0.231827	-0.404037	-0.126161	1	6.125141	0.794606	-2.216144
6	-4.359475	2.635887	-0.117656	6	0.158555	2.979519	-0.961521
6	-3.608809	1.721212	-0.855795	6	-1.020281	3.547032	-0.450708
6	-2.924120	0.682343	-0.211770	6	0.729808	3.496968	-2.133515
6	-3.008468	0.566302	1.186525	6	-1.604726	4.633395	-1.097369
6	-3.733617	1.499089	1.922216	1	-1.479623	3.145452	0.446047
6	-4.411986	2.535598	1.272589	6	0.130767	4.577761	-2.780881
1	-4.900374	3.425515	-0.629423	1	1.640821	3.064358	-2.531924
1	-3.564034	1.802679	-1.937013	6	-1.032392	5.149114	-2.262215
1	-2.507331	-0.256559	1.683397	1	-2.513125	5.067714	-0.693860
1	-3.784557	1.409263	3.002547	1	0.578176	4.976867	-3.685405
1	-4.990566	3.250699	1.848601	1	-1.492356	5.993918	-2.764769
6	-2.146341	-0.286022	-1.017070	6	1.537822	-0.385649	2.220807
6	-1.274302	0.112355	-2.006286	8	2.254843	-1.142650	3.056795
6	-0.780307	-0.816189	-3.086679	6	1.366595	-2.439953	1.275199
1	-1.389077	-0.600753	-3.985630	6	2.299731	-2.501613	2.517164
1	0.259884	-0.599374	-3.346997	7	0.999312	-0.995729	1.214270
8	-0.846112	-2.182192	-2.755957	6	3.720681	-2.846905	2.022166
6	-2.065227	-2.547675	-2.119635	1	4.405588	-2.024858	2.256260
1	-1.997734	-3.618819	-1.921935	1	4.107889	-3.737892	2.526718
1	-2.922446	-2.360093	-2.783316	6	3.556021	-3.069934	0.535370
6	-2.247182	-1.806164	-0.780441	6	4.526353	-3.459827	-0.386617
8	-1.115322	-2.007305	0.030798	6	2.233596	-2.883024	0.123469
6	-3.540632	-2.251791	-0.129676	6	4.150806	-3.666582	-1.716447
6	-4.774878	-1.913329	-0.697083	1	5.555894	-3.613583	-0.077165
6	-3.508481	-3.031557	1.027820	6	1.845807	-3.102909	-1.197101
6	-5.962357	-2.344180	-0.109226	6	2.820731	-3.493874	-2.118129
1	-4.812412	-1.294663	-1.589799	1	4.896034	-3.980256	-2.441213
6	-4.697761	-3.465206	1.615499	1	0.815721	-2.961446	-1.504209
1	-2.547593	-3.283175	1.461703	1	2.539614	-3.675828	-3.150863
6	-5.926024	-3.122294	1.049933	1	1.946044	-3.156986	3.312460

(S)-IM11

SCF Energy = -2529.946627

Gibbs Free Energy = -2529.313522

1 0.440370 -3.007809 1.359811
(S)-IM12
 SCF Energy = -2606.402369
 Gibbs Free Energy = -2605.745834

28 -0.152474 -0.499942 -0.548913
 6 -0.106697 -2.248089 2.865024
 6 0.487853 -2.609338 1.658328
 6 1.769044 -2.144619 1.299061
 6 2.426293 -1.282940 2.192958
 6 1.831005 -0.922160 3.402093
 6 0.566031 -1.400493 3.745229
 1 -1.096973 -2.617715 3.113324
 1 -0.035977 -3.262751 0.968802
 1 3.414522 -0.911486 1.961051
 1 2.369858 -0.276632 4.089425
 1 0.108865 -1.116518 4.687319
 6 2.328670 -2.597131 -0.005175
 6 2.204127 -3.883167 -0.375692
 6 2.460748 -4.376542 -1.769762
 1 3.412705 -4.934074 -1.823638
 1 1.665382 -5.064419 -2.073169
 8 2.461519 -3.314869 -2.712153
 6 3.352760 -2.308262 -2.291099
 1 3.442515 -1.578763 -3.099145
 1 4.347664 -2.726416 -2.080831
 6 2.839607 -1.581547 -1.026084
 8 1.713779 -0.750124 -1.432728
 6 3.982774 -0.690992 -0.573950
 6 5.021113 -1.227499 0.199097
 6 4.095821 0.620197 -1.047792
 6 6.125170 -0.448398 0.539755
 1 4.953991 -2.254865 0.545775
 6 5.199205 1.402662 -0.700736
 1 3.316337 1.029927 -1.678555
 6 6.212705 0.874257 0.098166
 1 6.917177 -0.873978 1.147764
 1 5.266813 2.422949 -1.065595
 1 7.071450 1.481783 0.365236
 1 1.853942 -4.618694 0.344637
 6 -2.635077 0.061288 1.536947
 6 -1.699401 0.701992 2.375845
 6 -2.029165 0.962829 3.712378
 6 -3.263976 0.570707 4.223201
 6 -4.186464 -0.073343 3.398946
 6 -3.873583 -0.321462 2.061555
 1 -1.306284 1.464337 4.343847
 1 -3.504256 0.768687 5.262381
 1 -5.150717 -0.378984 3.791536
 1 -4.595418 -0.816276 1.421690
 15 -2.243436 -0.247892 -0.214691
 6 -2.736744 1.225286 -1.151897
 6 -3.339295 2.329816 -0.537945
 6 -2.413136 1.261899 -2.519439
 6 -3.618437 3.470190 -1.291849

1 -3.586473 2.303751 0.517902
 6 -2.713348 2.398554 -3.264874
 1 -1.918028 0.408815 -2.974161
 6 -3.308768 3.504247 -2.651755
 1 -4.080917 4.329080 -0.816373
 1 -2.470834 2.426947 -4.322446
 1 -3.529408 4.393014 -3.234305
 6 -3.311329 -1.632808 -0.699094
 6 -3.048802 -2.897523 -0.146275
 6 -4.370712 -1.469737 -1.598636
 6 -3.841900 -3.987595 -0.493724
 1 -2.233076 -3.019438 0.559671
 6 -5.160491 -2.567961 -1.944136
 1 -4.573444 -0.495495 -2.029029
 6 -4.897486 -3.823223 -1.395734
 1 -3.638805 -4.963339 -0.064095
 1 -5.980424 -2.440180 -2.643334
 1 -5.512975 -4.674101 -1.669188
 6 -0.385106 1.136231 1.884874
 8 0.214584 2.088058 2.610947
 6 1.432303 1.618628 0.658087
 6 1.509079 2.390728 1.996454
 7 0.249543 0.739684 0.827824
 6 1.605693 3.886123 1.666995
 1 0.958326 4.472817 2.325413
 1 2.631985 4.236655 1.828496
 6 1.221269 3.962130 0.205620
 6 0.951716 5.093720 -0.561839
 6 1.173143 2.691054 -0.376313
 6 0.628282 4.934124 -1.911521
 1 0.986765 6.084919 -0.119514
 6 0.858376 2.526604 -1.724356
 6 0.582738 3.661198 -2.489186
 1 0.410079 5.807616 -2.517855
 1 0.818868 1.537906 -2.168957
 1 0.325385 3.553095 -3.537548
 1 2.272067 2.030828 2.687344
 1 2.308364 1.009039 0.455447
 8 -0.535378 -1.443798 -2.062641
 1 -0.997142 -2.277978 -1.910874
 1 1.142447 -1.293035 -2.051199

(S)-IM1A
 SCF Energy = -2529.93428
 Gibbs Free Energy = -2529.306659

28 -0.106977 -0.245480 0.408694
 6 -2.851221 0.498286 0.616385
 6 -1.832710 0.195256 -0.206435
 6 -1.940410 -0.012518 -1.683900
 1 -2.976326 -0.114466 -2.035583
 1 -1.463867 0.790760 -2.255833
 8 -1.203351 -1.207371 -2.056992
 6 -1.798898 -2.388688 -1.599245
 1 -1.487190 -3.191129 -2.278729
 1 -2.897290 -2.333106 -1.646030

6	-1.410085	-2.826199	-0.187468	6	2.803050	-2.186422	-0.532253
8	-0.665248	-2.142250	0.535127	6	4.099543	-2.487213	-2.967288
6	-1.905736	-4.116048	0.315264	1	5.940425	-2.433785	-1.840919
6	-2.677174	-4.981360	-0.482896	6	2.043806	-2.287857	-1.696031
6	-1.606756	-4.482821	1.641092	6	2.702275	-2.442173	-2.916595
6	-3.133250	-6.188579	0.036077	1	4.600605	-2.606152	-3.922897
1	-2.924672	-4.723083	-1.506052	1	0.964369	-2.212815	-1.664298
6	-2.064887	-5.689150	2.154292	1	2.125259	-2.522275	-3.832824
1	-1.023816	-3.803024	2.251630	1	3.607145	-2.617985	2.612727
6	-2.827563	-6.543801	1.352106	1	1.607927	-2.787317	1.192087
1	-3.726339	-6.852698	-0.583424	1	-2.662263	0.502919	1.691526
1	-1.834666	-5.965927	3.177793	6	-4.226264	0.862615	0.228111
1	-3.186156	-7.486208	1.753785	6	-5.314498	0.438659	1.009998
6	1.432379	2.306833	1.683980	6	-4.483588	1.671612	-0.892391
6	2.307160	1.398172	2.325630	6	-6.619416	0.774911	0.659600
6	3.056094	1.819198	3.432465	1	-5.128355	-0.167484	1.892847
6	2.931327	3.118730	3.919592	6	-5.790250	2.009310	-1.242443
6	2.067716	4.013465	3.292461	1	-3.651940	2.074996	-1.460341
6	1.329720	3.609798	2.176787	6	-6.862638	1.556769	-0.472868
1	3.731526	1.118641	3.908116	1	-7.448509	0.430958	1.270506
1	3.509948	3.428229	4.783312	1	-5.969809	2.639364	-2.108496
1	1.969119	5.029083	3.661813	1	-7.879593	1.823024	-0.743229
1	0.671990	4.316712	1.685217				
15	0.535511	1.786877	0.172832				
6	1.807686	1.879501	-1.132042				
6	2.830174	2.838419	-1.076871				
6	1.747691	0.983546	-2.207855				
6	3.782168	2.897690	-2.092285	28	-0.085193	-0.594238	0.310016
1	2.884416	3.530624	-0.243194	6	-2.467603	-0.838560	0.329556
6	2.703258	1.049478	-3.221054	6	-1.787580	-1.372681	-0.732618
1	0.970540	0.228347	-2.245352	6	-1.736576	-1.016934	-2.194959
6	3.719236	2.003515	-3.164068	1	-2.653932	-1.355551	-2.707786
1	4.573762	3.638782	-2.046176	1	-1.596910	0.045984	-2.405315
1	2.662089	0.342947	-4.042519	8	-0.602963	-1.734768	-2.677151
1	4.465478	2.048909	-3.950961	6	-0.650578	-3.012764	-2.028263
6	-0.658874	3.107944	-0.197269	1	0.336111	-3.471740	-2.087475
6	-0.666372	3.732556	-1.450455	1	-1.388523	-3.654474	-2.525647
6	-1.650689	3.428591	0.744442	6	-1.056704	-2.732342	-0.557374
6	-1.656029	4.670369	-1.756221	8	0.044797	-2.410698	0.238760
1	0.095365	3.491559	-2.183456	6	-1.921767	-3.818317	0.058277
6	-2.627510	4.369843	0.437933	6	-3.129990	-4.201390	-0.540361
1	-1.663362	2.934170	1.709776	6	-1.531714	-4.424911	1.254022
6	-2.633316	4.990006	-0.815286	6	-3.930215	-5.179384	0.045184
1	-1.656488	5.151273	-2.729138	1	-3.456645	-3.729715	-1.463688
1	-3.393763	4.607999	1.167968	6	-2.330891	-5.410202	1.838111
1	-3.402533	5.716827	-1.055607	1	-0.600585	-4.116521	1.714229
6	2.484455	0.012172	1.862016	6	-3.530176	-5.789494	1.236955
8	3.611614	-0.593643	2.264855	1	-4.864483	-5.466682	-0.427107
6	2.313063	-2.011534	0.887172	1	-2.014941	-5.880332	2.764468
6	3.610610	-1.957733	1.744515	1	-4.151818	-6.554154	1.691845
7	1.680823	-0.689948	1.130279	6	0.809424	2.432229	1.440932
6	4.809234	-2.183833	0.805546	6	1.697542	1.738443	2.293880
1	5.538868	-1.376406	0.922319	6	2.259351	2.393747	3.399337
1	5.323473	-3.118216	1.055909	6	1.955672	3.726224	3.664338
6	4.199127	-2.243968	-0.576687	6	1.105872	4.422775	2.808685
6	4.856268	-2.388684	-1.797904	6	0.543543	3.779922	1.704051

(S)-IM2A

SCF Energy = -2529.933024

Gibbs Free Energy = -2529.299911

1	2.940992	1.849824	4.040995	1	-5.486393	1.720975	2.677442
1	2.392344	4.218147	4.526792	1	-5.684411	1.904273	-1.615559
1	0.879552	5.468101	2.992124	1	-6.572847	2.563351	0.606557
1	-0.107178	4.337528	1.042769				
15	0.113582	1.592917	-0.033350				
6	1.400916	1.799294	-1.312926				
6	2.310597	2.865729	-1.261266				
6	1.445897	0.894833	-2.383695				
6	3.253354	3.024662	-2.274675	28	-0.093557	0.251533	-1.091209
1	2.286323	3.566786	-0.434350	6	-2.070826	-1.098634	1.071388
6	2.382907	1.071221	-3.401402	6	-1.043432	-0.942100	2.028350
1	0.773219	0.044607	-2.424938	6	-1.054426	-1.708739	3.197111
6	3.287703	2.130897	-3.347463	6	-2.058705	-2.652079	3.404980
1	3.959380	3.847574	-2.227773	6	-3.066809	-2.818934	2.457976
1	2.412594	0.368099	-4.227068	6	-3.076643	-2.039866	1.298183
1	4.022659	2.258643	-4.135754	1	-0.260815	-1.580829	3.921984
6	-1.264434	2.657298	-0.575852	1	-2.047206	-3.257996	4.304090
6	-1.395629	3.002654	-1.928373	1	-3.851484	-3.550876	2.619353
6	-2.199625	3.139173	0.354392	1	-3.871594	-2.161558	0.571188
6	-2.438264	3.834222	-2.339612	15	-2.100362	-0.007138	-0.390171
1	-0.672232	2.646804	-2.653722	6	-2.768798	1.575753	0.193911
6	-3.217860	3.992677	-0.057987	6	-3.558181	1.661545	1.349280
1	-2.123151	2.863518	1.399789	6	-2.445134	2.734349	-0.528407
6	-3.339798	4.341676	-1.404968	6	-4.023093	2.904786	1.776332
1	-2.528693	4.102089	-3.387410	1	-3.802613	0.767036	1.912504
1	-3.925125	4.372869	0.670605	6	-2.917308	3.971215	-0.095865
1	-4.136888	5.005833	-1.723426	1	-1.817440	2.664736	-1.410442
6	2.128858	0.358075	2.031203	6	-3.702702	4.057075	1.055450
8	3.234689	-0.022003	2.679686	1	-4.633470	2.973280	2.671090
6	2.497180	-1.714027	1.217732	1	-2.656877	4.866875	-0.648168
6	3.494130	-1.430557	2.368300	1	-4.062832	5.023450	1.393875
7	1.598153	-0.524784	1.243866	6	-3.285592	-0.745828	-1.545715
6	4.915078	-1.595881	1.813853	6	-2.941820	-1.952976	-2.178965
1	5.558906	-0.776309	2.147266	6	-4.511037	-0.131545	-1.830114
1	5.357265	-2.525249	2.191202	6	-3.822110	-2.539563	-3.084132
6	4.718407	-1.650611	0.315623	1	-1.991468	-2.430826	-1.957354
6	5.691230	-1.655532	-0.682225	6	-5.386844	-0.723947	-2.741311
6	3.364551	-1.756066	-0.020197	1	-4.775873	0.801877	-1.345725
6	5.290889	-1.772650	-2.015266	6	-5.044632	-1.922963	-3.366985
1	6.744477	-1.574959	-0.430159	1	-3.554578	-3.470918	-3.572520
6	2.961061	-1.881501	-1.346868	1	-6.335338	-0.245713	-2.962807
6	3.936583	-1.888553	-2.344622	1	-5.727342	-2.377496	-4.077508
1	6.038968	-1.779502	-2.801838	6	0.032817	0.036119	1.830598
1	1.910047	-1.958102	-1.591796	8	0.630255	0.503034	2.934063
1	3.641878	-1.985461	-3.384739	6	1.509760	1.523312	0.980082
1	3.307048	-1.986844	3.288480	6	1.542648	1.573805	2.532864
1	1.889446	-2.607262	1.346627	7	0.465841	0.503140	0.704096
1	-2.351903	-1.385432	1.266044	6	1.000825	2.954384	2.964732
6	-3.500760	0.188340	0.358889	1	0.079907	2.826148	3.543512
6	-4.009488	0.578158	1.613291	1	1.714719	3.474991	3.610912
6	-4.114559	0.688661	-0.805240	6	0.771526	3.693980	1.664444
6	-5.099348	1.437037	1.704288	6	0.334095	5.005683	1.488000
1	-3.552012	0.181036	2.515253	6	1.087234	2.906907	0.553643
6	-5.212033	1.535512	-0.711452	6	0.223482	5.513992	0.191443
1	-3.755818	0.397850	-1.783588	1	0.090881	5.628810	2.343404
6	-5.709202	1.909320	0.539933	6	0.979938	3.407881	-0.743271

(S)-IM3A

SCF Energy = -2606.397476

Gibbs Free Energy = -2605.743498

6	0.545239	4.723237	-0.916996	1	-3.591762	-0.048351	-2.282407
1	-0.107990	6.537127	0.043478	1	-3.407517	1.661792	-1.876344
1	1.226648	2.788875	-1.599007	6	-3.183761	0.310839	-0.229193
1	0.461317	5.135180	-1.917682	8	-2.232018	-0.022270	0.495216
1	2.511705	1.331743	2.967710	6	-4.541362	0.335354	0.333281
1	2.444395	1.198034	0.521392	6	-5.671837	0.602409	-0.461201
8	-0.538178	0.309009	-2.837640	6	-4.705006	0.098404	1.711114
1	-1.256071	-0.260336	-3.137298	6	-6.938360	0.625677	0.113328
1	1.200285	0.215417	-2.822234	1	-5.573454	0.789330	-1.524437
6	2.184838	-2.004901	0.215781	6	-5.971709	0.124638	2.279858
6	2.118453	-1.827577	-1.111342	1	-3.825771	-0.092450	2.315580
6	1.457246	-2.673945	-2.179659	6	-7.089540	0.387058	1.481540
1	1.777253	-3.724164	-2.105493	1	-7.807295	0.829748	-0.503035
1	0.362455	-2.647254	-2.140237	1	-6.093092	-0.054218	3.343077
8	1.838458	-2.105673	-3.434808	1	-8.079224	0.408253	1.926661
6	2.994043	-1.306293	-3.221218	6	2.728816	-0.258221	1.566139
1	3.074062	-0.577220	-4.030988	6	2.230072	-1.403366	2.229465
1	3.912196	-1.909748	-3.185967	6	2.961704	-1.969688	3.284109
6	2.762495	-0.661356	-1.847094	6	4.169564	-1.411228	3.693049
8	1.738334	0.377413	-2.000950	6	4.664727	-0.284657	3.041168
6	4.003465	-0.043052	-1.248983	6	3.949536	0.281668	1.984357
6	5.010100	-0.861776	-0.717033	1	2.571808	-2.849764	3.779848
6	4.203583	1.342397	-1.280750	1	4.719150	-1.857208	4.515039
6	6.181800	-0.303661	-0.209165	1	5.607662	0.156336	3.347908
1	4.873664	-1.937909	-0.695491	1	4.346491	1.155872	1.483010
6	5.374354	1.899908	-0.764427	15	1.846390	0.449999	0.117051
1	3.440933	1.981389	-1.706971	6	2.468415	-0.543629	-1.283110
6	6.365304	1.080319	-0.224997	6	3.829940	-0.868371	-1.388708
1	6.951184	-0.951100	0.199501	6	1.568390	-0.993980	-2.257295
1	5.511769	2.976376	-0.792481	6	4.281489	-1.630680	-2.462780
1	7.276730	1.514264	0.173592	1	4.531720	-0.533019	-0.632189
1	2.808813	-1.301291	0.762475	6	2.025432	-1.763666	-3.327057
6	1.549522	-3.021989	1.052523	1	0.514584	-0.758324	-2.173409
6	2.023604	-3.186242	2.367565	6	3.379308	-2.080153	-3.431695
6	0.478693	-3.830499	0.627337	1	5.334756	-1.880316	-2.541620
6	1.475336	-4.143615	3.216159	1	1.319119	-2.124149	-4.067225
1	2.842526	-2.561523	2.713896	1	3.734099	-2.680969	-4.263133
6	-0.076052	-4.780699	1.479666	6	2.568919	2.110160	-0.081419
1	0.061084	-3.704793	-0.363231	6	3.112013	2.519516	-1.303932
6	0.424341	-4.948514	2.772690	6	2.519903	3.012971	0.993176
1	1.868659	-4.264337	4.220735	6	3.611183	3.816446	-1.447147
1	-0.904010	-5.391962	1.134749	1	3.154958	1.829030	-2.138885
1	-0.004583	-5.697976	3.430218	6	3.030724	4.299036	0.849825
				1	2.091207	2.706128	1.942037
				6	3.576638	4.703834	-0.372806
				1	4.032556	4.127081	-2.397755
				1	3.000466	4.987822	1.688011
				1	3.971411	5.708544	-0.484142
28	-0.269430	0.192744	0.315609	6	0.968289	-2.059505	1.852401
6	-0.680576	2.999648	0.285883	8	0.807210	-3.304462	2.328633
6	-0.588451	1.892952	-0.459252	6	-1.014918	-2.663481	0.979856
6	-0.885873	1.755855	-1.921465	6	-0.515880	-3.779584	1.938060
1	-1.419102	2.610719	-2.353635	7	-0.000592	-1.587165	1.136117
1	0.029130	1.602547	-2.502780	6	-0.403672	-5.082561	1.131570
8	-1.672941	0.563500	-2.171088	1	0.561531	-5.564577	1.314174
6	-2.987929	0.660097	-1.702139	1	-1.179812	-5.790421	1.444210

(S)-IM5B

SCF Energy = -2456.134903

Gibbs Free Energy = -2455.474575

6	-0.602871	-4.649462	-0.303055	6	3.269689	0.846632	3.318495
6	-0.488540	-5.422355	-1.457733	6	3.866697	2.084269	3.541992
6	-0.987835	-3.307735	-0.389142	6	3.621755	3.137057	2.663841
6	-0.771223	-4.838897	-2.694550	6	2.752795	2.959577	1.585528
1	-0.188557	-6.464367	-1.398575	1	3.485594	0.010403	3.971304
6	-1.280645	-2.724115	-1.619811	1	4.534074	2.216491	4.386724
6	-1.168995	-3.500136	-2.774776	1	4.106064	4.097103	2.809412
1	-0.686736	-5.431505	-3.600075	1	2.581463	3.783103	0.903973
1	-1.557616	-1.679729	-1.690070	15	0.975762	1.500221	-0.046352
1	-1.391710	-3.059471	-3.741852	6	2.046611	0.879933	-1.392273
1	-1.092707	-3.881360	2.858966	6	3.442272	0.988617	-1.328266
1	-1.992267	-2.256551	1.243286	6	1.442121	0.283057	-2.510207
1	-0.420506	2.896921	1.340874	6	4.224831	0.509574	-2.378054
6	-1.081162	4.428324	-0.103046	1	3.918900	1.441325	-0.466092
6	-0.223822	4.958228	-1.270575	6	2.232598	-0.170766	-3.564622
1	-0.390170	4.400989	-2.195747	1	0.365078	0.150423	-2.559102
1	-0.467571	6.007231	-1.471809	6	3.622081	-0.063973	-3.498677
1	0.839908	4.894826	-1.029950	1	5.305657	0.589374	-2.321293
6	-2.579394	4.491375	-0.468281	1	1.758969	-0.624204	-4.429506
1	-3.196817	4.094232	0.343996	1	4.235192	-0.431952	-4.315050
1	-2.886722	5.526531	-0.652592	6	0.457857	3.176269	-0.565559
1	-2.802260	3.918888	-1.373536	6	0.291341	3.448694	-1.932389
6	-0.839213	5.333293	1.120560	6	0.136138	4.170230	0.373473
1	0.216156	5.317049	1.411281	6	-0.199335	4.686965	-2.347215
1	-1.113024	6.369284	0.898792	1	0.555733	2.702959	-2.673327
1	-1.433620	5.002904	1.979297	6	-0.335133	5.411593	-0.047922
				1	0.259124	3.984362	1.433450
				6	-0.512176	5.670445	-1.408219
				1	-0.323945	4.884891	-3.406876
				1	-0.569863	6.173559	0.688257
				1	-0.886285	6.635342	-1.734406
28	-0.452904	-0.184579	0.289056	6	1.907815	-0.708943	1.993569
6	-2.775310	0.739913	0.606112	8	2.568379	-1.668497	2.650034
6	-2.541248	0.157359	-0.599309	6	1.015419	-2.602726	1.153310
6	-2.423415	0.674556	-2.010978	6	1.948154	-2.960064	2.334544
1	-3.421135	0.851512	-2.445269	7	0.966216	-1.113153	1.197538
1	-1.831602	1.582804	-2.122884	6	3.010533	-3.935784	1.814985
8	-1.759976	-0.386172	-2.699831	1	3.998558	-3.683153	2.211281
6	-2.329399	-1.601543	-2.198528	1	2.778272	-4.952162	2.154312
1	-1.648114	-2.423183	-2.419099	6	2.902037	-3.819460	0.311160
1	-3.297940	-1.784967	-2.680225	6	3.746970	-4.350379	-0.661283
6	-2.495279	-1.400843	-0.668554	6	1.758379	-3.106333	-0.063697
8	-1.342198	-1.762936	0.036384	6	3.431013	-4.156660	-2.008118
6	-3.745674	-2.046266	-0.093159	1	4.636127	-4.906824	-0.380066
6	-5.012994	-1.733440	-0.604973	6	1.433892	-2.918266	-1.404281
6	-3.647843	-2.922615	0.989103	6	2.282939	-3.447850	-2.376713
6	-6.160000	-2.291511	-0.045708	1	4.081623	-4.563754	-2.775807
1	-5.110768	-1.043436	-1.439170	1	0.546009	-2.360915	-1.673774
6	-4.797312	-3.487338	1.546587	1	2.052214	-3.306769	-3.427549
1	-2.666388	-3.153186	1.385414	1	1.441905	-3.288627	3.244059
6	-6.054610	-3.173643	1.032794	1	0.000716	-2.987308	1.231887
1	-7.135337	-2.040164	-0.450760	1	-2.853613	0.032647	1.434685
1	-4.708365	-4.172471	2.384260	6	-3.207313	2.132921	0.982487
1	-6.947754	-3.611261	1.467274	6	-3.136223	3.141998	-0.170264
6	2.106359	1.737594	1.372261	1	-3.807091	2.853128	-0.984744
6	2.396341	0.656801	2.237305	1	-3.454797	4.127406	0.180408

(S)-IM6B

SCF Energy = -2456.128167

Gibbs Free Energy = -2455.461877

1	-2.128867	3.245049	-0.568329	6	-4.540353	-0.721266	-2.749518
6	-4.689163	1.977395	1.420137	6	-2.176982	-1.028703	-3.238412
1	-4.791181	1.278193	2.255302	6	-4.806486	-1.974690	-3.286851
1	-5.076230	2.949851	1.739812	1	-5.352454	-0.143961	-2.323501
1	-5.308901	1.613814	0.595517	6	-2.448870	-2.282309	-3.772959
6	-2.382278	2.593655	2.200246	1	-1.155434	-0.666828	-3.198184
1	-1.316939	2.625018	1.966445	6	-3.762573	-2.755168	-3.794322
1	-2.695209	3.592669	2.517716	1	-5.823103	-2.354767	-3.291826
1	-2.520821	1.910504	3.044318	1	-1.622214	-2.894023	-4.114019

(S)-IM6D

SCF Energy = -3424.953181

Gibbs Free Energy = -3424.203516

28	-0.781330	0.580297	-0.104347	6	4.495202	-1.037808	1.765044
8	1.162350	-0.869602	-2.845007	6	3.666164	-1.407019	2.820660
16	0.975229	-2.035868	-1.932476	6	2.325601	-1.022323	2.818869
8	0.300310	-3.199293	-2.552777	1	4.611410	-0.015161	-0.120311
8	0.371935	-1.652560	-0.609107	1	5.535657	-1.343480	1.746932
6	2.635376	-2.564586	-1.486781	1	4.053953	-1.999883	3.643468
6	3.738713	-2.096227	-2.193440	1	1.683935	-1.322528	3.638659
6	2.806538	-3.442617	-0.414130	15	0.044815	0.292518	1.843977
6	5.020614	-2.505360	-1.820281	6	0.240132	1.856479	2.778605
1	3.581485	-1.406888	-3.014696	6	0.587110	1.884252	4.137856
6	4.086648	-3.844181	-0.052257	6	0.168336	3.060649	2.065887
1	1.939278	-3.786771	0.138330	6	0.819090	3.101525	4.775375
6	5.214491	-3.381410	-0.747778	1	0.679561	0.958721	4.695823
1	5.883228	-2.134007	-2.368051	6	0.413539	4.276738	2.702443
1	4.219970	-4.517191	0.791176	1	-0.053645	3.046700	1.006753
6	6.598093	-3.826386	-0.342402	6	0.730283	4.299330	4.060490
1	7.370808	-3.241445	-0.848778	1	1.077868	3.115112	5.829891
1	6.765437	-4.881317	-0.590408	1	0.359964	5.195773	2.126883
1	6.749771	-3.724811	0.738149	1	0.917201	5.244351	4.561668
6	-4.421307	-2.933470	1.821152	6	-0.745619	-0.932317	2.927074
6	-3.952865	-1.628281	1.703653	6	-0.646870	-2.279515	2.537671
6	-3.000106	-1.285114	0.725762	6	-1.527144	-0.581320	4.032446
6	-2.521189	-2.303314	-0.114261	6	-1.290086	-3.262879	3.281951
6	-3.001471	-3.606177	-0.007177	1	-0.096736	-2.536674	1.637852
6	-3.953922	-3.929436	0.959702	6	-2.169315	-1.575165	4.773234
1	-5.142988	-3.177407	2.596122	1	-1.640666	0.459638	4.312736
1	-4.295556	-0.869432	2.399099	6	-2.044848	-2.913666	4.404181
1	-1.745629	-2.082800	-0.830381	1	-1.227576	-4.298903	2.966675
1	-2.612447	-4.365347	-0.679150	1	-2.771542	-1.299202	5.633601
1	-4.320313	-4.948139	1.052590	1	-2.552264	-3.683849	4.977122
6	-2.545443	0.115223	0.557684	6	2.166175	0.886371	-0.451845
6	-3.453182	1.105182	0.729072	8	3.142431	1.286021	-1.285777
6	-3.183970	2.559284	0.507388	6	1.034347	2.054177	-2.003215
1	-3.787863	3.178269	1.180269	6	2.526647	1.968584	-2.412197
1	-2.131738	2.785378	0.688006	7	0.964669	1.238471	-0.762664
8	-3.483907	3.049880	-0.840100	6	3.073423	3.402439	-2.513443
6	-3.896184	2.098448	-1.782059	1	4.025270	3.489572	-1.980259
1	-4.064979	2.647723	-2.718148	1	3.265867	3.665169	-3.560680
1	-4.848010	1.627813	-1.510461	6	1.971594	4.263105	-1.936098
6	-2.856433	1.025035	-2.070205	6	1.999246	5.629477	-1.660657
8	-1.667761	1.278404	-1.789666	6	0.800489	3.524796	-1.730222
6	-3.218086	-0.239442	-2.715146	6	0.840423	6.249922	-1.186879

8	0.144337	-1.093140	-2.873014	6	2.718681	-3.512198	1.931659
16	-0.653625	-1.890463	-1.906061	6	1.881110	-2.440346	2.239751
8	-2.006733	-2.274526	-2.362560	1	3.757130	-2.500059	-1.133550
8	-0.676082	-1.298574	-0.512563	1	4.037429	-4.371691	0.459026
6	0.281167	-3.411808	-1.671329	1	2.823944	-4.332507	2.634910
6	1.270975	-3.765316	-2.583900	1	1.335350	-2.438260	3.176221
6	0.008399	-4.234518	-0.576607	15	0.649738	0.035955	1.783681
6	1.994817	-4.943933	-2.394984	6	1.819395	1.145035	2.645884
1	1.471685	-3.105214	-3.419923	6	2.421925	0.812587	3.868779
6	0.737167	-5.404320	-0.396542	6	2.206646	2.319606	1.985442
1	-0.762767	-3.948837	0.129916	6	3.369979	1.663257	4.433814
6	1.744073	-5.776640	-1.300230	1	2.155782	-0.110016	4.374287
1	2.770330	-5.217239	-3.106201	6	3.166668	3.161859	2.546077
1	0.531219	-6.038202	0.462640	1	1.782758	2.559262	1.018443
6	2.542419	-7.037116	-1.076108	6	3.742201	2.838901	3.774857
1	3.243702	-7.217186	-1.895250	1	3.827315	1.404259	5.383944
1	1.890750	-7.913880	-0.992780	1	3.463430	4.057649	2.009277
1	3.121728	-6.980820	-0.146216	1	4.487791	3.493340	4.216284
6	-4.786984	-0.258649	2.534652	6	-0.522832	-0.637693	3.000048
6	-3.831671	0.653921	2.094635	6	-1.328115	-1.709414	2.575125
6	-3.183187	0.480374	0.859738	6	-0.713349	-0.082910	4.271388
6	-3.517953	-0.632594	0.070445	6	-2.276663	-2.244330	3.439997
6	-4.462418	-1.549383	0.521142	1	-1.222833	-2.082129	1.561628
6	-5.104451	-1.366220	1.747852	6	-1.678195	-0.619284	5.126986
1	-5.280718	-0.102847	3.489091	1	-0.111300	0.758264	4.597226
1	-3.604308	1.524297	2.701932	6	-2.450188	-1.705094	4.717199
1	-3.029300	-0.805874	-0.875258	1	-2.903752	-3.062410	3.103335
1	-4.693557	-2.407853	-0.101535	1	-1.820451	-0.188300	6.113424
1	-5.850670	-2.079373	2.086993	1	-3.198951	-2.121008	5.384491
6	-2.241446	1.529420	0.412554	6	2.282776	-0.333518	-0.888975
6	-1.416877	2.204016	1.302770	8	3.143604	-0.429786	-1.914009
6	-1.070905	3.666263	1.159352	6	1.717625	1.435630	-2.161873
1	-1.744011	4.191876	1.865871	6	2.824766	0.618724	-2.875116
1	-0.047128	3.874614	1.481848	7	1.461898	0.661903	-0.921630
8	-1.210367	4.203487	-0.132721	6	4.043049	1.541071	-3.067359
6	-2.316020	3.688388	-0.865741	1	4.955914	1.048644	-2.717362
1	-2.251413	4.140331	-1.857309	1	4.187327	1.766912	-4.130644
1	-3.264760	3.989507	-0.395623	6	3.692263	2.792552	-2.291963
6	-2.230247	2.152064	-1.006615	6	4.491636	3.904569	-2.030465
8	-0.946133	1.813733	-1.452944	6	2.362676	2.766499	-1.858980
6	-3.321788	1.645159	-1.929572	6	3.940427	4.988142	-1.340843
6	-4.670784	1.927700	-1.679880	1	5.526766	3.933447	-2.359953
6	-2.977499	0.851183	-3.026002	6	1.792832	3.858184	-1.206755
6	-5.662953	1.423628	-2.518396	6	2.598389	4.969902	-0.943121
1	-4.954311	2.512158	-0.809101	1	4.554533	5.858898	-1.129347
6	-3.972843	0.338631	-3.857960	1	0.743799	3.844295	-0.928905
1	-1.935940	0.603408	-3.187761	1	2.173302	5.831753	-0.436448
6	-5.315021	0.625721	-3.610777	1	2.486643	0.113851	-3.778718
1	-6.706876	1.641117	-2.311051	1	0.778805	1.498920	-2.708261
1	-3.693417	-0.305629	-4.685455				
1	-6.088944	0.220746	-4.256553				
1	-1.394059	1.854651	2.332700				
6	1.711854	-1.383935	1.342401				
6	2.409046	-1.399290	0.118359				
6	3.248090	-2.481488	-0.179991	28	-0.098306	-0.525439	-1.190861
6	3.400363	-3.533236	0.718136	8	0.205924	-3.969266	-0.095686

(S)-IM8D

SCF Energy = -2693.441427

Gibbs Free Energy = -2692.935385

16	-0.649667	-3.519378	-1.217492	1	4.368543	-1.576158	2.574951
8	-1.144721	-4.533457	-2.154191	1	4.829875	-2.815776	1.410068
8	0.028203	-2.361191	-2.001728	6	4.442907	-0.892776	0.487162
6	-2.067199	-2.702044	-0.470912	6	5.545796	-0.055829	0.325410
6	-2.064420	-2.421733	0.892484	6	3.390640	-0.849970	-0.432722
6	-3.109977	-2.252579	-1.284645	6	5.575329	0.819931	-0.762577
6	-3.075181	-1.627591	1.433914	1	6.369825	-0.080533	1.033232
1	-1.261724	-2.812422	1.505993	6	3.414161	0.020205	-1.519966
6	-4.115598	-1.467926	-0.731022	6	4.519006	0.857295	-1.679152
1	-3.111909	-2.499548	-2.340142	1	6.426409	1.481065	-0.896888
6	-4.096682	-1.116057	0.628184	1	2.582551	0.054034	-2.217774
1	-3.055730	-1.384132	2.492076	1	4.552117	1.551342	-2.512327
1	-4.919609	-1.102589	-1.364972	1	2.483981	-3.372217	1.531084
6	-5.129966	-0.172601	1.189449	1	2.062139	-2.581851	-0.753714
1	-4.928914	0.854057	0.858765	8	-1.035588	0.043582	-2.617159
1	-5.124370	-0.177898	2.282766	1	-1.010903	-0.739651	-3.188679
1	-6.138735	-0.430386	0.851065				
6	-0.762606	0.924571	1.619060				
6	-0.057098	-0.121962	2.256261				
6	-0.315644	-0.432563	3.596491				
6	-1.293506	0.262983	4.304291				
6	-2.007048	1.281802	3.675717	8	-0.150082	2.169217	-0.956680
6	-1.737081	1.612388	2.346154	14	0.226778	0.830804	-0.058860
1	0.245533	-1.232063	4.065708	8	1.621115	0.184549	-0.659263
1	-1.498072	0.005617	5.338385	8	-0.901256	-0.377197	-0.214374
1	-2.775461	1.825008	4.216818	6	1.914159	-1.211947	-0.727974
1	-2.297259	2.407336	1.869250	1	1.093546	-1.739184	-1.227864
15	-0.438167	1.331372	-0.148587	1	2.808851	-1.308750	-1.351901
6	1.054450	2.382495	-0.148721	6	2.162148	-1.814899	0.647887
6	1.948309	2.428087	0.926764	1	1.250051	-1.785571	1.251943
6	1.359112	3.067187	-1.336072	1	2.472588	-2.861243	0.556829
6	3.132813	3.156500	0.818806	1	2.948025	-1.264163	1.173107
1	1.724954	1.899579	1.846844	6	-2.256819	-0.237081	0.207502
6	2.534527	3.807495	-1.430445	1	-2.294951	-0.029524	1.286515
1	0.677491	3.012468	-2.179592	1	-2.722949	0.613712	-0.307743
6	3.424807	3.849827	-0.354931	6	-3.004545	-1.520895	-0.105732
1	3.827856	3.177693	1.652061	1	-2.978157	-1.724236	-1.180063
1	2.761600	4.341058	-2.348332	1	-2.543846	-2.366173	0.413679
1	4.347909	4.415299	-0.435781	1	-4.050089	-1.445271	0.209751
6	-1.815157	2.414121	-0.624532	6	0.367703	1.414538	1.701635
6	-2.936952	1.840011	-1.239079	1	-0.553058	1.903054	2.035248
6	-1.806328	3.781734	-0.310472	1	0.573452	0.577425	2.375220
6	-4.051239	2.633241	-1.512859	1	1.182123	2.138017	1.797961
1	-2.902592	0.796539	-1.525414	1	-0.014574	2.069803	-1.906022
6	-2.922862	4.566889	-0.593386				
1	-0.931277	4.227596	0.151437				
6	-4.047900	3.991131	-1.188751				
1	-4.918433	2.190032	-1.992778				
1	-2.914513	5.625053	-0.350536				
1	-4.916922	4.604257	-1.408286	28	0.142558	-0.663244	0.306787
6	0.949946	-0.912011	1.537463	6	-2.725316	-0.299655	0.151485
8	1.874271	-1.542912	2.276991	6	-1.628175	-0.615337	-0.591180
6	2.285972	-1.799613	-0.031624	6	-1.486618	-0.494923	-2.084180
6	2.720183	-2.322948	1.357413	1	-2.455923	-0.580456	-2.601057
7	1.039488	-1.055577	0.260484	1	-1.005867	0.434934	-2.402018
6	4.191862	-1.935703	1.556558	8	-0.632100	-1.569560	-2.492926

[Si]OH/(EtO)₂MeSiOH

SCF Energy = -714.326782

Gibbs Free Energy = -714.173432

(S)-TS1A

SCF Energy = -2529.916978

Gibbs Free Energy = -2529.287398

6	-1.142166	-2.739040	-1.875708	1	5.726668	-2.905090	1.321647
1	-0.437163	-3.553250	-2.061187	6	4.690421	-2.036528	-0.368689
1	-2.116516	-3.002134	-2.303548	6	5.464255	-2.035928	-1.528549
6	-1.242710	-2.543169	-0.349045	6	3.298499	-2.138955	-0.452119
8	-0.092239	-2.500901	0.289323	6	4.828596	-2.152302	-2.766586
6	-2.375090	-3.205875	0.374495	1	6.545895	-1.956714	-1.472467
6	-3.659867	-3.318329	-0.181642	6	2.660761	-2.271616	-1.683671
6	-2.146046	-3.694719	1.666647	6	3.437114	-2.277305	-2.843508
6	-4.688566	-3.914892	0.540051	1	5.421491	-2.157939	-3.675974
1	-3.871723	-2.910387	-1.164029	1	1.582927	-2.347603	-1.738816
6	-3.177750	-4.296595	2.386903	1	2.955767	-2.381325	-3.811184
1	-1.152604	-3.598842	2.088307	1	3.856619	-2.595477	2.751874
6	-4.450151	-4.408099	1.826776	1	2.028950	-2.946558	1.131147
1	-5.678108	-3.993504	0.101254	1	-2.720515	-0.653225	1.182969
1	-2.986913	-4.678985	3.384717	6	-3.963918	0.337455	-0.250808
1	-5.253960	-4.875338	2.386849	6	-5.109249	0.108443	0.540515
6	1.248005	2.082762	1.747732	6	-4.079805	1.159904	-1.389407
6	2.180153	1.263900	2.424519	6	-6.337431	0.653303	0.185025
6	2.823349	1.743627	3.573913	1	-5.024217	-0.521235	1.421361
6	2.541940	3.016673	4.063893	6	-5.307256	1.712074	-1.735024
6	1.624543	3.826787	3.398858	1	-3.198239	1.418874	-1.961216
6	0.987366	3.362540	2.246045	6	-6.439171	1.454447	-0.956084
1	3.541723	1.109041	4.078011	1	-7.214141	0.459802	0.794483
1	3.040885	3.372233	4.958991	1	-5.382152	2.355985	-2.605289
1	1.403824	4.822491	3.769679	1	-7.396030	1.886904	-1.230932
1	0.280356	4.003346	1.733067				
15	0.475061	1.494260	0.192109				
6	1.708856	1.889026	-1.089597				
6	2.445919	3.082902	-1.044812				
6	1.923904	0.973624	-2.128625				
6	3.383204	3.357058	-2.037370	28	0.037624	-0.022749	-0.390993
1	2.293106	3.788864	-0.234971	6	-0.163594	-3.138661	0.196936
6	2.868800	1.252069	-3.116057	6	-0.044566	-2.772357	-2.158517
1	1.372586	0.040967	-2.160106	6	-1.166620	-1.777130	-1.811394
6	3.595647	2.441308	-3.072329	6	-0.759935	-1.789538	0.002931
1	3.953007	4.280041	-2.000986	1	0.701160	-3.095901	0.869188
1	3.045080	0.529330	-3.905006	1	-0.895603	-3.838272	0.624769
1	4.333592	2.654681	-3.839172	6	-1.323209	-0.828524	0.714447
6	-0.926908	2.625771	-0.074878	6	-2.112372	-0.686498	1.901301
6	-1.045741	3.375712	-1.251847	6	-3.046767	-1.682642	2.262765
6	-1.923233	2.720612	0.910907	6	-2.033316	0.483956	2.684764
6	-2.144963	4.218299	-1.433824	6	-3.861841	-1.512093	3.376264
1	-0.277457	3.314085	-2.014855	1	-3.132799	-2.569151	1.641746
6	-3.010091	3.570031	0.729039	6	-2.822527	0.629909	3.820269
1	-1.841294	2.137262	1.823115	1	-1.353651	1.269315	2.369526
6	-3.122884	4.319373	-0.444776	6	-3.743754	-0.363570	4.166666
1	-2.229338	4.800181	-2.346112	1	-4.585704	-2.278455	3.638135
1	-3.776309	3.636745	1.494265	1	-2.742004	1.529879	4.422922
1	-3.974507	4.976414	-0.587662	1	-4.374643	-0.239049	5.041773
6	2.534139	-0.083972	1.952761	8	0.262949	-3.656616	-1.076041
8	3.686248	-0.573524	2.426850	1	0.829110	-2.172189	-2.435133
6	2.667928	-2.089025	0.921418	1	-0.334163	-3.399744	-3.008781
6	3.869791	-1.922808	1.893352	8	-1.023520	-0.556722	-2.232571
7	1.871130	-0.851599	1.148682	6	-2.571478	-2.345155	-1.812219
6	5.164537	-1.999805	1.066549	6	-2.835522	-3.707154	-1.606328
1	5.812076	-1.147051	1.293048	6	-3.645756	-1.462216	-1.973539

(S)-TS1C

SCF Energy = -2529.416395

Gibbs Free Energy = -2528.804439

6	-4.150877	-4.169178	-1.548864	1	-5.233911	4.137781	1.106149
1	-2.010901	-4.402726	-1.484414	1	-2.910099	0.782828	-0.273915
6	-4.958375	-1.924249	-1.915657	1	-4.837420	1.688643	1.018958
1	-3.420235	-0.416941	-2.148597	1	-0.141750	3.841238	-3.160459
6	-5.217093	-3.279941	-1.697507	1	-1.182842	1.687120	-2.489911
1	-4.343148	-5.226629	-1.389074				
1	-5.782341	-1.227139	-2.042042				
1	-6.240349	-3.641062	-1.648420				
6	2.826909	1.476732	0.544693				
6	2.224097	2.683096	0.118567				
6	2.818863	3.911163	0.460754	28	-0.143968	0.097546	-1.070659
6	3.976638	3.955794	1.228116	6	-2.132937	-1.102281	1.207958
6	4.569031	2.768373	1.659295	6	-1.093625	-0.865705	2.137524
6	3.997165	1.547111	1.312590	6	-1.092558	-1.529364	3.368512
1	2.352448	4.827650	0.121600	6	-2.095903	-2.448036	3.670156
1	4.412640	4.914484	1.490585	6	-3.115418	-2.692995	2.753149
1	5.471895	2.791720	2.261760	6	-3.136472	-2.018394	1.529425
1	4.460593	0.625261	1.647157	1	-0.287277	-1.342890	4.066644
15	2.152356	-0.179318	0.091760	1	-2.075172	-2.972939	4.619006
6	2.441324	-1.130421	1.639840	1	-3.899599	-3.406163	2.985224
6	3.522918	-1.999862	1.830465	1	-3.936751	-2.207259	0.823002
6	1.503936	-0.968447	2.672101	15	-2.164843	-0.217194	-0.388769
6	3.657008	-2.702084	3.030058	6	-2.896459	1.420306	-0.112080
1	4.251570	-2.139649	1.039753	6	-3.055347	1.951489	1.173232
6	1.642494	-1.666298	3.868721	6	-3.169268	2.210955	-1.241122
1	0.656228	-0.308839	2.525021	6	-3.491810	3.266965	1.327904
6	2.718717	-2.539023	4.049384	1	-2.843920	1.345614	2.047697
1	4.495361	-3.379302	3.164318	6	-3.622586	3.516435	-1.075592
1	0.903062	-1.536443	4.653229	1	-3.021444	1.806151	-2.237830
1	2.822381	-3.091693	4.978322	6	-3.778007	4.046837	0.207451
6	3.407810	-0.848645	-1.066678	1	-3.610946	3.679844	2.324178
6	3.288338	-2.195409	-1.456043	1	-3.842436	4.123901	-1.947558
6	4.403645	-0.054677	-1.650460	1	-4.119168	5.069285	0.332807
6	4.166533	-2.734117	-2.393127	6	-3.268674	-1.162109	-1.469727
1	2.506810	-2.822924	-1.035981	6	-2.753960	-2.281350	-2.142242
6	5.273082	-0.598084	-2.597901	6	-4.621282	-0.823455	-1.612162
1	4.504552	0.986882	-1.365740	6	-3.584545	-3.054445	-2.948794
6	5.160575	-1.937814	-2.968106	1	-1.707022	-2.547796	-2.032592
1	4.066764	-3.776333	-2.681135	6	-5.447755	-1.600534	-2.424181
1	6.040786	0.028115	-3.043037	1	-5.022903	0.043007	-1.098321
1	5.838753	-2.359136	-3.704014	6	-4.931778	-2.712288	-3.091675
6	0.989632	2.742956	-0.680811	1	-3.181916	-3.916676	-3.470225
8	0.777039	3.916084	-1.324829	1	-6.493882	-1.334962	-2.536189
6	-0.998190	2.395333	-1.681047	1	-5.577468	-3.310926	-3.725942
6	-0.441028	3.781490	-2.112195	6	-0.016463	0.088679	1.855003
7	0.087107	1.835317	-0.833423	8	0.611640	0.613251	2.910586
6	-1.465281	4.854635	-1.704972	6	1.388974	1.574794	0.894406
1	-0.968820	5.676064	-1.178239	6	1.644956	1.535068	2.424936
1	-1.940151	5.284847	-2.594966	7	0.384152	0.498043	0.694309
6	-2.470016	4.107846	-0.857219	6	1.397671	2.947780	2.975918
6	-3.548782	4.625427	-0.141462	1	0.790589	2.905057	3.885221
6	-2.242570	2.728235	-0.888041	1	2.350553	3.416156	3.248284
6	-4.394828	3.745596	0.538717	6	0.733020	3.680403	1.830636
1	-3.731678	5.696242	-0.112656	6	0.153880	4.948216	1.832187
6	-3.100462	1.846317	-0.235979	6	0.781458	2.935194	0.649196
6	-4.175322	2.364993	0.487506	6	-0.374237	5.450502	0.640719

(S)-TS3A

SCF Energy = -2606.390753

Gibbs Free Energy = -2605.738430

1	0.113751	5.539082	2.742478	8	-1.068053	-1.121819	-2.496631
6	0.266175	3.434353	-0.545199	6	-1.733017	-2.253917	-1.961341
6	-0.316655	4.702088	-0.539972	1	-1.098111	-3.127869	-2.122915
1	-0.830595	6.435334	0.629771	1	-2.684837	-2.399157	-2.481936
1	0.315706	2.849650	-1.458749	6	-1.943737	-2.093131	-0.438676
1	-0.730544	5.108290	-1.456803	8	-0.861553	-2.230068	0.300096
1	2.602043	1.102396	2.718018	6	-3.202383	-2.629023	0.175038
1	2.264171	1.365427	0.279611	6	-4.362725	-2.909816	-0.561241
8	-0.471064	0.014693	-2.944774	6	-3.213828	-2.840837	1.562681
1	-0.505373	-0.900025	-3.268088	6	-5.505868	-3.387889	0.076552
1	0.706972	0.241142	-2.847663	1	-4.395772	-2.752499	-1.632566
6	2.487733	-1.671442	0.306573	6	-4.359880	-3.307699	2.200053
6	2.199929	-1.694094	-1.003150	1	-2.309386	-2.639220	2.124672
6	1.426149	-2.714013	-1.809657	6	-5.511328	-3.582230	1.458403
1	1.909254	-3.702323	-1.760354	1	-6.394262	-3.605316	-0.507601
1	0.386031	-2.836068	-1.485528	1	-4.354215	-3.465131	3.274058
8	1.406582	-2.228794	-3.154457	1	-6.404510	-3.950499	1.952874
6	2.556140	-1.384440	-3.303824	6	1.525265	1.987063	1.594094
1	2.408019	-0.746107	-4.176465	6	2.163025	1.002200	2.381850
1	3.465728	-1.984684	-3.439471	6	2.883285	1.378267	3.524639
6	2.620350	-0.593598	-1.983989	6	2.975002	2.716752	3.896493
8	1.600544	0.423717	-2.013592	6	2.363078	3.692922	3.114039
6	3.967629	0.041562	-1.704911	6	1.649855	3.328472	1.970146
6	5.091676	-0.760182	-1.460886	1	3.371141	0.611520	4.113452
6	4.113153	1.432604	-1.704837	1	3.529108	2.993049	4.787082
6	6.335347	-0.181023	-1.219630	1	2.440930	4.740791	3.385234
1	4.990235	-1.841168	-1.444583	1	1.188761	4.100196	1.366848
6	5.359495	2.012404	-1.457036	15	0.646780	1.505295	0.054049
1	3.246655	2.051222	-1.904633	6	1.972254	1.442936	-1.199968
6	6.472755	1.209311	-1.214191	6	3.100255	2.272676	-1.106142
1	7.196742	-0.814461	-1.032104	6	1.835760	0.570456	-2.288572
1	5.458319	3.093695	-1.460862	6	4.079369	2.228714	-2.095571
1	7.441649	1.660126	-1.024106	1	3.216178	2.945035	-0.263038
1	3.140024	-0.862940	0.630397	6	2.818140	0.537858	-3.278341
6	2.031250	-2.539963	1.391287	1	0.978266	-0.089214	-2.359899
6	2.497669	-2.261073	2.691081	6	3.938276	1.362702	-3.183116
6	1.134158	-3.615108	1.233259	1	4.952665	2.868399	-2.017683
6	2.095815	-3.021211	3.785389	1	2.712053	-0.144838	-4.114576
1	3.197416	-1.441922	2.832799	1	4.704530	1.329018	-3.951085
6	0.728825	-4.373089	2.328276	6	-0.344366	2.977813	-0.369397
1	0.750639	-3.872813	0.255518	6	-0.268370	3.552338	-1.645242
6	1.206700	-4.083167	3.607902	6	-1.190939	3.547735	0.594632
1	2.481045	-2.790636	4.773830	6	-1.023508	4.687156	-1.947796
1	0.038552	-5.197788	2.181135	1	0.391004	3.126526	-2.393700
1	0.894378	-4.682977	4.456824	6	-1.921188	4.695907	0.296143
				1	-1.256942	3.109473	1.585545
				6	-1.840591	5.266192	-0.976796
				1	-0.958742	5.125841	-2.938223
				1	-2.558802	5.141116	1.053086
				1	-2.413810	6.157717	-1.209251
28	-0.256941	-0.490945	0.286441	6	2.150742	-0.422844	2.022165
6	-3.003361	0.362997	0.191474	8	3.103372	-1.165601	2.598994
6	-2.036894	-0.125991	-0.618513	6	1.816433	-2.451504	1.098104
6	-1.839908	0.021901	-2.101758	6	2.917495	-2.557288	2.185937
1	-2.783185	0.027015	-2.665482	7	1.347816	-1.042654	1.217309
1	-1.267632	0.911920	-2.373430	6	4.193805	-3.090271	1.518226

(S)-TS3B

SCF Energy = -2456.1104

Gibbs Free Energy = -2455.447734

1	5.061705	-2.493863	1.815695	6	-3.063598	-3.349073	-0.160220
1	4.386195	-4.119736	1.841445	6	-4.267707	-3.573133	0.505583
6	3.889970	-3.028441	0.038280	1	-5.900381	-2.646281	1.570597
6	4.748785	-3.288027	-1.028565	1	-5.019042	-0.372777	1.342680
6	2.548426	-2.712796	-0.199189	1	-1.591501	-1.919246	-0.737901
6	4.245687	-3.235552	-2.330363	1	-2.513666	-4.164344	-0.619958
1	5.791834	-3.534017	-0.852857	1	-4.681098	-4.575321	0.577383
6	2.040398	-2.667473	-1.495006	6	-2.686847	0.415015	0.132555
6	2.899945	-2.932430	-2.561816	6	-3.184167	1.440282	0.867132
1	4.904223	-3.438495	-3.169101	6	-3.072651	2.898479	0.553815
1	1.003386	-2.412126	-1.668374	1	-4.064591	3.349049	0.737527
1	2.520705	-2.903316	-3.578637	1	-2.365545	3.407234	1.219154
1	2.624698	-3.106807	3.082063	8	-2.655942	3.193143	-0.766480
1	0.964621	-3.112151	1.251739	6	-3.247728	2.349269	-1.741027
1	-3.008105	-0.042112	1.206128	1	-3.123319	2.863188	-2.700159
6	-4.183642	1.273465	-0.073894	1	-4.317237	2.208863	-1.549329
6	-4.011739	2.190173	-1.295339	6	-2.495677	1.024178	-1.855005
1	-4.052793	1.630140	-2.232006	8	-1.206430	1.180189	-2.008902
1	-4.825043	2.921283	-1.323015	6	-3.124844	-0.119144	-2.568709
1	-3.070355	2.738487	-1.260235	6	-4.502727	-0.375575	-2.517035
6	-5.397577	0.334104	-0.294982	6	-2.277780	-1.019211	-3.232075
1	-5.548690	-0.342877	0.550063	6	-5.022647	-1.516856	-3.119041
1	-6.300710	0.941139	-0.415865	1	-5.164789	0.285857	-1.968271
1	-5.270758	-0.273501	-1.194265	6	-2.799788	-2.165595	-3.823011
6	-4.450322	2.113262	1.192383	1	-1.210589	-0.832111	-3.243561
1	-3.623476	2.793523	1.401774	6	-4.171522	-2.416280	-3.767664
1	-5.354946	2.713242	1.057127	1	-6.088088	-1.718245	-3.063372
1	-4.599586	1.471441	2.066679	1	-2.122172	-2.873130	-4.288102
				1	-4.579000	-3.317723	-4.216033
				1	-3.828084	1.229332	1.722708
				6	1.608882	-0.320466	1.929215
				6	2.575443	-0.113970	0.924407
				6	3.853879	-0.668157	1.075642
				6	4.175398	-1.421050	2.200738
				6	3.223726	-1.618075	3.197272
				6	1.949784	-1.065921	3.059604
				1	4.579641	-0.533900	0.286324
				1	5.162669	-1.861854	2.285642
				1	3.462262	-2.208367	4.076747
				1	1.205487	-1.239237	3.828289
				15	-0.058816	0.415704	1.773620
				6	0.153750	2.020473	2.630379
				6	0.407985	2.114408	4.006724
				6	0.168570	3.183401	1.848495
				6	0.645185	3.357368	4.590453
				1	0.421243	1.218785	4.619354
				6	0.421826	4.425005	2.431944
				1	0.002828	3.114376	0.780438
				6	0.652881	4.513768	3.804680
				1	0.833696	3.423920	5.657760
				1	0.446451	5.310733	1.804582
				1	0.847297	5.478570	4.263472
				6	-1.120824	-0.626951	2.816988
				6	-1.144796	-2.003919	2.542483
				6	-2.012578	-0.088173	3.751780
				6	-2.038264	-2.830100	3.218489
28	-0.655635	0.711848	-0.307037	6			
8	1.357347	-1.173947	-2.701674	6			
16	0.959714	-2.224869	-1.724259	6			
8	0.123859	-3.313601	-2.277743	1			
8	0.390322	-1.656078	-0.450282	1			
6	2.503510	-2.953397	-1.151352	1			
6	3.709470	-2.623618	-1.761805	1			
6	2.484836	-3.812652	-0.050208	15			
6	4.902837	-3.150647	-1.263043	6			
1	3.699787	-1.947448	-2.608573	6			
6	3.677840	-4.331649	0.438313	6			
1	1.539998	-4.051355	0.425647	6			
6	4.906597	-4.007248	-0.157916	1			
1	5.845373	-2.887347	-1.736836	6			
1	3.663055	-4.990642	1.303075	1			
6	6.193862	-4.581195	0.381199	6			
1	7.065542	-4.069338	-0.035947	1			
1	6.287789	-5.646091	0.136541	1			
1	6.242285	-4.499009	1.472730	1			
6	-4.952301	-2.490112	1.063285	6			
6	-4.440238	-1.201386	0.947618	6			
6	-3.209340	-0.963157	0.306753	6			
6	-2.541635	-2.062682	-0.250917	6			

(S)-TS4D

SCF Energy = -3424.932772

Gibbs Free Energy = -3424.182807

1	-0.492579	-2.406387	1.774025	6	-1.850897	-3.576760	-0.368390
6	-2.910319	-0.921566	4.419284	6	-3.956293	-2.692832	-1.216269
1	-2.012777	0.977404	3.953191	6	-2.225630	-4.852444	-0.783984
6	-2.922433	-2.291259	4.154430	1	-0.893198	-3.417029	0.122115
1	-2.068436	-3.888791	2.985056	6	-4.318554	-3.975625	-1.630910
1	-3.601095	-0.499013	5.142820	1	-4.623835	-1.855116	-1.386564
1	-3.629255	-2.936762	4.666760	6	-3.457113	-5.051830	-1.416086
6	2.306916	0.644976	-0.307745	1	-1.557268	-5.691123	-0.616727
8	3.392604	0.866481	-1.067415	1	-5.272783	-4.131550	-2.123468
6	1.474477	1.815579	-2.039379	1	-3.742631	-6.046733	-1.742289
6	2.959810	1.485801	-2.313658	6	-0.620562	1.112328	1.755270
7	1.191509	1.117380	-0.759256	8	-0.436972	2.293318	2.353940
6	3.706629	2.811844	-2.527272	6	0.668900	2.217187	0.249197
1	4.641522	2.826947	-1.958246	6	0.255909	3.170042	1.405436
1	3.971453	2.930222	-3.584971	7	-0.037473	0.955148	0.610852
6	2.714540	3.869343	-2.094883	6	-0.714155	4.219330	0.816489
6	2.920913	5.239413	-1.938812	1	-1.705631	4.101339	1.266839
6	1.445813	3.319308	-1.882002	1	-0.380932	5.237278	1.041608
6	1.843639	6.049995	-1.571928	6	-0.713974	3.938754	-0.670514
1	3.904204	5.673165	-2.099595	6	-1.380352	4.633029	-1.678715
6	0.360951	4.125138	-1.541114	6	0.099184	2.849382	-0.994052
6	0.572164	5.497360	-1.381019	6	-1.220729	4.219029	-3.003995
1	1.993450	7.118172	-1.443547	1	-2.009680	5.485981	-1.443085
1	-0.621834	3.691881	-1.394588	6	0.279867	2.440664	-2.314933
1	-0.261998	6.139846	-1.113200	6	-0.395201	3.134059	-3.322334
1	3.104468	0.741639	-3.095224	1	-1.730749	4.755984	-3.797946
1	0.796311	1.425876	-2.793952	1	0.937213	1.608965	-2.545003
				1	-0.268990	2.837707	-4.358689
				1	1.092193	3.605151	1.949751
				1	1.734248	1.991192	0.189513
				8	-0.137272	-1.389379	-2.337799
				1	-0.322907	-2.334696	-2.245125
28	-0.156410	-0.393750	-0.700224	1	0.981470	-1.096667	-2.180303
6	-2.156996	-0.871872	1.767038	6	3.520172	0.313853	1.220504
6	-1.435027	0.120053	2.468513	6	2.748633	-0.681646	0.779571
6	-1.486198	0.169095	3.866279	6	1.858940	-1.647932	1.545787
6	-2.222208	-0.781923	4.572027	1	2.448721	-2.257600	2.246531
6	-2.920501	-1.773408	3.884604	1	1.043717	-1.182478	2.099481
6	-2.893939	-1.813319	2.487630	8	1.271239	-2.502402	0.550162
1	-0.938492	0.943743	4.390293	6	2.239587	-2.582310	-0.499213
1	-2.247250	-0.747283	5.655842	1	1.766709	-3.011939	-1.383810
1	-3.492690	-2.515545	4.431611	1	3.079084	-3.223809	-0.201547
1	-3.446538	-2.580893	1.957193	6	2.709912	-1.123823	-0.692009
15	-2.167992	-0.850173	-0.061951	8	1.712092	-0.378861	-1.404043
6	-3.406468	0.388289	-0.528841	6	4.038953	-1.030828	-1.422207
6	-4.595583	0.543085	0.200632	6	5.191955	-1.596422	-0.857873
6	-3.147731	1.207073	-1.638024	6	4.132591	-0.410134	-2.670084
6	-5.523517	1.506681	-0.188051	6	6.409374	-1.547314	-1.531673
1	-4.789900	-0.078935	1.068666	1	5.141473	-2.060390	0.122625
6	-4.081035	2.170402	-2.017836	6	5.354426	-0.358307	-3.344918
1	-2.220464	1.103398	-2.190981	1	3.247727	0.036131	-3.106635
6	-5.266302	2.318866	-1.296189	6	6.494522	-0.927319	-2.780752
1	-6.443846	1.627169	0.374220	1	7.292712	-1.988747	-1.080617
1	-3.872036	2.808295	-2.869091	1	5.411907	0.129455	-4.313220
1	-5.990164	3.071424	-1.592515	1	7.443670	-0.886538	-3.305681
6	-2.724362	-2.493615	-0.582286	1	4.143303	0.792674	0.464956

(S)-TS5B

SCF Energy = -2532.587956

Gibbs Free Energy = -2531.903436

6	3.774735	0.822294	2.627794	1	3.048968	-2.957353	-3.231804
6	5.028781	0.088743	3.157202	6	2.887189	-1.544367	-1.574147
1	5.310177	0.471238	4.144221	8	2.338955	-0.233139	-1.374753
1	4.842453	-0.986056	3.246914	6	4.411181	-1.442696	-1.597719
1	5.879499	0.228418	2.483371	6	5.188684	-2.597140	-1.770025
6	2.604641	0.600901	3.600205	6	5.052048	-0.208180	-1.472931
1	2.841784	1.048093	4.570619	6	6.578834	-2.518676	-1.804074
1	1.687304	1.072125	3.236107	1	4.702168	-3.566190	-1.831702
1	2.405581	-0.458716	3.776206	6	6.445918	-0.129576	-1.503499
6	4.076789	2.332195	2.548904	1	4.448948	0.679269	-1.329439
1	3.216204	2.889722	2.163063	6	7.214197	-1.281534	-1.669150
1	4.319365	2.731041	3.538495	1	7.166844	-3.423588	-1.926071
1	4.925187	2.531445	1.886874	1	6.930918	0.836291	-1.393560
				1	8.298146	-1.219293	-1.690284
				1	0.951093	-4.067177	-0.175726

(S)-TS5D

SCF Energy = -3501.417372

Gibbs Free Energy = -3500.642817

28	0.437265	0.274999	-0.837816	6	-3.755536	0.468373	3.152230
8	-1.262847	-2.255880	1.633725	6	-4.439968	0.830183	1.992966
16	-1.852041	-2.553548	0.299381	6	-3.734828	1.089446	0.819944
8	-1.661654	-3.947515	-0.163109	1	-1.826832	0.070880	4.027550
8	-1.463166	-1.543355	-0.751416	1	-4.302749	0.248069	4.062770
6	-3.621653	-2.313652	0.520303	1	-5.522865	0.883598	1.990415
6	-4.197234	-2.597042	1.757582	1	-4.272352	1.349393	-0.083554
6	-4.414325	-1.864344	-0.534265	15	-1.413411	1.366290	-0.731715
6	-5.567919	-2.422470	1.936396	6	-0.957966	3.132481	-0.612409
1	-3.561060	-2.921536	2.573089	6	-0.978904	3.828811	0.601272
6	-5.782207	-1.683481	-0.342635	6	-0.446830	3.756208	-1.762547
1	-3.956368	-1.630710	-1.486447	6	-0.504475	5.139278	0.662544
6	-6.381330	-1.961730	0.892915	1	-1.364653	3.352089	1.495824
1	-6.013890	-2.635823	2.904851	6	0.007418	5.070397	-1.698274
1	-6.393236	-1.315942	-1.163542	1	-0.402522	3.206018	-2.697386
6	-7.868197	-1.792256	1.087409	6	-0.018278	5.763141	-0.485345
1	-8.267382	-0.996172	0.451478	1	-0.513718	5.670014	1.609275
1	-8.112171	-1.553372	2.127051	1	0.393795	5.550303	-2.592408
1	-8.407366	-2.712703	0.831381	1	0.349398	6.783358	-0.434345
6	2.133639	-2.762945	3.254102	6	-2.589656	1.284144	-2.118889
6	1.797508	-2.719204	1.902952	6	-2.680026	0.122193	-2.898495
6	2.770155	-2.470388	0.912739	6	-3.414118	2.382119	-2.408331
6	4.085913	-2.216626	1.347167	6	-3.593646	0.063455	-3.950142
6	4.413062	-2.237672	2.704200	1	-2.066423	-0.733995	-2.647574
6	3.446076	-2.525503	3.667706	6	-4.330186	2.312294	-3.457164
1	1.352673	-2.962346	3.982518	1	-3.335053	3.290616	-1.820697
1	0.757349	-2.836158	1.624969	6	-4.419614	1.153503	-4.230053
1	4.870922	-2.015570	0.635459	1	-3.660066	-0.839135	-4.549795
1	5.440031	-2.045515	3.002278	1	-4.968124	3.164065	-3.672349
1	3.709555	-2.555407	4.721315	1	-5.129206	1.101796	-5.050409
6	2.342855	-2.512793	-0.517110	6	-0.185796	0.559015	2.011254
6	1.372340	-3.366729	-0.889196	8	0.360049	0.717445	3.225087
6	0.734176	-3.419721	-2.240241	6	2.009781	0.756604	1.542920
1	0.999988	-4.362633	-2.750920	6	1.818332	0.721683	3.079328
1	-0.348858	-3.395186	-2.111512	7	0.648834	0.469710	1.026033
8	1.089884	-2.317836	-3.075505	6	2.395585	2.024926	3.650303
6	2.477339	-2.054238	-2.980763	1	1.718466	2.456884	4.393860
1	2.716112	-1.283772	-3.719063	1	3.345204	1.819491	4.159186

6	2.605323	2.901744	2.435330	6	-2.137791	-0.988913	2.163106
6	2.967698	4.247264	2.389475	6	-2.694977	-1.384141	3.382882
6	2.430477	2.180195	1.250422	6	-3.147274	-2.692552	3.553837
6	3.151013	4.856558	1.146523	6	-3.068570	-3.597088	2.497238
1	3.106158	4.814994	3.305588	6	-2.540792	-3.198862	1.264644
6	2.618714	2.781813	0.007278	1	-2.766869	-0.666207	4.192026
6	2.980667	4.128501	-0.035588	1	-3.564246	-2.998834	4.507183
1	3.427517	5.905668	1.097087	1	-3.425546	-4.614094	2.623510
1	2.481477	2.210205	-0.903587	1	-2.497724	-3.903093	0.441689
1	3.118152	4.617043	-0.994601	15	-1.345784	-1.330519	-0.503550
1	2.186645	-0.183959	3.554879	6	-2.607152	-0.221591	-1.205556
1	2.704813	0.013271	1.163498	6	-3.929956	-0.206490	-0.743706
8	0.568172	0.401375	-2.740003	6	-2.217937	0.648987	-2.233934
1	0.271854	-0.466329	-3.074753	6	-4.852830	0.676221	-1.306355
1	1.676266	0.115822	-2.339163	1	-4.239308	-0.879990	0.048293

(S)-TS5_iso

SCF Energy = -2529.907656

Gibbs Free Energy = -2529.277998

28	0.470985	-0.325254	0.286448	1	-5.183023	2.217233	-2.774142
6	3.395684	3.966438	0.001671	6	-1.274003	-2.795728	-1.570807
6	2.937313	2.940423	0.823792	6	-0.280757	-3.760766	-1.332393
6	2.611100	1.677888	0.294723	6	-2.198729	-2.986382	-2.607732
6	2.749760	1.489744	-1.093326	6	-0.225077	-4.907346	-2.121332
6	3.227443	2.510313	-1.913103	1	0.443111	-3.600552	-0.542991
6	3.549865	3.754594	-1.370494	6	-2.129887	-4.133776	-3.397218
1	3.631999	4.934566	0.432101	1	-2.966664	-2.244181	-2.795018
1	2.819060	3.129313	1.886358	6	-1.146794	-5.094148	-3.154354
1	2.477890	0.536657	-1.528736	1	0.541205	-5.653003	-1.934366
1	3.336560	2.334781	-2.978831	1	-2.846635	-4.277908	-4.199278
1	3.910997	4.554486	-2.008743	1	-1.097436	-5.986778	-3.769884
6	2.072910	0.592117	1.140122	6	-1.684380	0.400711	2.002262
6	2.143722	0.552247	2.485849	8	-2.321196	1.320396	2.737730
6	1.571952	-0.583868	3.282123	6	-0.697729	2.316516	1.313814
1	2.254476	-0.852401	4.104123	6	-1.870021	2.633289	2.290237
1	0.615723	-0.299233	3.738991	7	-0.751530	0.833461	1.213037
8	1.294912	-1.730898	2.490063	6	-2.974567	3.343003	1.478237
6	2.445168	-2.139200	1.769325	1	-3.833743	2.671916	1.366964
1	2.299569	-3.192632	1.507818	1	-3.332206	4.244996	1.983540
1	3.345308	-2.056540	2.386931	6	-2.320185	3.643473	0.150769
6	2.613209	-1.394418	0.442108	6	-2.820153	4.424928	-0.888859
8	1.664439	-1.558755	-0.433751	6	-1.053246	3.061095	0.048087
6	3.994565	-1.186417	-0.057050	6	-2.035358	4.619970	-2.027352
6	5.026945	-0.730714	0.776860	1	-3.799756	4.886994	-0.811225
6	4.270671	-1.482967	-1.400600	6	-0.265308	3.255458	-1.083926
6	6.312298	-0.569320	0.272878	6	-0.766979	4.038914	-2.124271
1	4.811255	-0.456050	1.803927	1	-2.409750	5.236738	-2.838660
6	5.561548	-1.332330	-1.898666	1	0.723354	2.823543	-1.153069
1	3.464653	-1.835935	-2.033920	1	-0.158724	4.209644	-3.007064
6	6.582497	-0.871197	-1.065287	1	-1.570949	3.182279	3.182731
1	7.103307	-0.200629	0.917604	1	0.288181	2.590126	1.693818
1	5.772050	-1.572387	-2.935863				
1	7.587027	-0.744464	-1.456257				
1	2.635807	1.333812	3.069460				
6	-2.066563	-1.900315	1.084930				

(S)-TS5

SCF Energy = -2529.919805

Gibbs Free Energy = -2529.289366

28	-0.162661	-0.555004	0.109563	1	4.017222	-0.521449	-3.034367
6	-5.078981	1.390427	0.463983	1	5.611260	1.368127	-2.764400
6	-4.183456	0.754013	-0.390324	6	-0.499467	2.684980	-1.146312
6	-2.937463	0.303794	0.076572	6	-1.717827	3.143537	-0.619258
6	-2.646753	0.458488	1.442863	6	-0.136586	3.031146	-2.456357
6	-3.541761	1.095104	2.300984	6	-2.562594	3.928755	-1.400030
6	-4.757945	1.573203	1.811634	1	-2.015331	2.877485	0.387921
1	-6.034148	1.736616	0.081368	6	-0.990571	3.812765	-3.234089
1	-4.451131	0.602131	-1.430861	1	0.807909	2.690331	-2.866218
1	-1.704126	0.084127	1.832894	6	-2.205360	4.257971	-2.709760
1	-3.291180	1.212936	3.350613	1	-3.504631	4.272502	-0.985796
1	-5.458522	2.067212	2.477188	1	-0.703672	4.077646	-4.246745
6	-1.944277	-0.297439	-0.838300	1	-2.868686	4.865506	-3.317156
6	-1.884463	0.011522	-2.153193	6	1.785533	0.043172	2.214342
6	-0.947673	-0.658076	-3.105369	8	2.713272	-0.455930	3.039841
1	-1.490812	-0.927812	-4.026663	6	1.978708	-2.092314	1.483792
1	-0.144865	0.029979	-3.399233	6	2.989870	-1.832927	2.637772
8	-0.318069	-1.801431	-2.555481	7	1.305151	-0.773050	1.330491
6	-1.273035	-2.691126	-1.988495	6	4.413690	-1.955729	2.055312
1	-0.787439	-3.668055	-1.908573	1	4.941615	-1.001959	2.159935
1	-2.144431	-2.786173	-2.643691	1	4.997896	-2.705163	2.599030
6	-1.662735	-2.275078	-0.566913	6	4.196696	-2.353958	0.612870
8	-0.665277	-2.325458	0.293201	6	5.161329	-2.643431	-0.351161
6	-3.011538	-2.670016	-0.065508	6	2.838944	-2.469270	0.302599
6	-4.147671	-2.648700	-0.888107	6	4.747736	-3.059844	-1.618708
6	-3.145291	-3.038184	1.279298	1	6.219004	-2.560998	-0.119160
6	-5.391062	-3.005557	-0.377594	6	2.420612	-2.897017	-0.955090
1	-4.071196	-2.319177	-1.919015	6	3.386810	-3.191658	-1.918070
6	-4.391112	-3.395799	1.788950	1	5.490627	-3.296659	-2.374233
1	-2.261119	-3.044310	1.905191	1	1.365724	-2.981835	-1.176501
6	-5.515829	-3.380517	0.962896	1	3.079592	-3.528503	-2.903240
1	-6.265148	-2.984022	-1.020414	1	2.829030	-2.448543	3.522497
1	-4.485260	-3.686340	2.830454	1	1.209108	-2.832874	1.705673
1	-6.487420	-3.655830	1.360694				
1	-2.527572	0.779569	-2.584249				
6	0.841627	2.250542	1.425837				
6	1.433427	1.455525	2.434845				
6	1.735727	2.022301	3.679901				
6	1.439194	3.359245	3.937873	28	0.146700	-0.861060	-0.571379
6	0.858834	4.144906	2.944654	6	1.874570	-1.705549	0.040779
6	0.570342	3.593875	1.693511	6	2.013457	-2.006164	1.350270
1	2.201540	1.407364	4.440373	6	0.891936	-2.524251	2.191934
1	1.668123	3.783921	4.909361	1	1.262538	-3.327026	2.849686
1	0.634553	5.189411	3.135250	1	0.501221	-1.731487	2.842286
1	0.131116	4.215495	0.922413	8	-0.209629	-2.991376	1.428412
15	0.519622	1.503254	-0.211502	6	0.213157	-3.892952	0.415645
6	2.151725	1.483271	-1.020153	1	-0.660579	-4.494970	0.143687
6	3.054159	2.545055	-0.858573	1	1.000648	-4.559694	0.787957
6	2.500540	0.381167	-1.812786	6	0.671188	-3.171026	-0.853971
6	4.295092	2.501659	-1.490002	8	-0.232438	-2.460784	-1.463148
1	2.790378	3.395609	-0.238051	1	2.965189	-1.873289	1.865934
6	3.745113	0.343803	-2.441004	6	0.488013	2.374008	-0.595959
1	1.816219	-0.453221	-1.920963	6	-0.428058	2.369778	-1.673412
6	4.640524	1.401357	-2.279860	6	-0.471168	3.457782	-2.554862
1	4.993779	3.322471	-1.363338	6	0.396410	4.535626	-2.388784
				6	1.297125	4.543538	-1.326117

(S)-TS5_p

SCF Energy = -2338.15764

Gibbs Free Energy = -2337.575454

6	1.335278	3.471610	-0.430684	1	6.417223	-1.437058	-0.977704
1	-1.186533	3.449888	-3.368273	1	3.670909	0.634086	-3.557252
1	0.361181	5.367401	-3.084084	1	6.005901	0.045030	-2.930894
1	1.967969	5.384665	-1.184441	6	1.686143	-3.883911	-1.712223
1	2.029168	3.492531	0.401103	1	2.529817	-4.258333	-1.130499
15	0.475999	0.971721	0.576693	1	1.174857	-4.735231	-2.179947
6	-0.973621	1.286468	1.634022	1	2.045175	-3.227066	-2.504298
6	-1.310266	2.589311	2.030446				
6	-1.757605	0.201812	2.050548				
6	-2.423373	2.800721	2.840999				
1	-0.710037	3.431950	1.702257				
6	-2.870746	0.421149	2.861538				
1	-1.515858	-0.804554	1.726546	28	-0.164969	0.828549	-0.353814
6	-3.203351	1.717438	3.255492	6	-1.915669	1.455245	0.428680
1	-2.684612	3.808954	3.146186	6	-2.048503	1.480441	1.772536
1	-3.484970	-0.419489	3.162698	6	-0.935860	1.862382	2.694467
1	-4.073685	1.887026	3.881554	1	-1.325935	2.504606	3.500707
6	1.936880	1.155143	1.644705	1	-0.509703	0.971268	3.172472
6	3.220731	1.252984	1.083520	8	0.138414	2.511323	2.032529
6	1.794521	1.062328	3.037067	6	-0.328308	3.584969	1.227056
6	4.343379	1.246541	1.907580	1	0.522384	4.257414	1.077714
1	3.347175	1.318063	0.009545	1	-1.130057	4.135407	1.734927
6	2.923794	1.050909	3.855462	6	-0.786533	3.119440	-0.158218
1	0.806154	0.998323	3.478870	8	0.134150	2.587631	-0.909584
6	4.198229	1.137663	3.292732	1	-2.987065	1.207407	2.256003
1	5.331083	1.316919	1.463995	6	-0.379328	-2.346081	-1.027368
1	2.806497	0.979518	4.932052	6	0.513969	-2.085416	-2.092360
1	5.075612	1.127754	3.931549	6	0.580198	-2.968548	-3.177777
6	-1.381491	1.268410	-1.885949	6	-0.242961	-4.092043	-3.224768
8	-2.458688	1.572534	-2.619451	6	-1.120778	-4.352990	-2.175009
6	-2.510804	-0.694194	-1.915125	6	-1.180825	-3.488329	-1.079077
6	-3.329412	0.400739	-2.658186	1	1.278404	-2.766190	-3.980933
7	-1.302828	0.048113	-1.457850	1	-0.190798	-4.762700	-4.075672
6	-4.621333	0.653041	-1.851944	1	-1.756439	-5.232151	-2.199776
1	-4.635570	1.685930	-1.487991	1	-1.855806	-3.706786	-0.260289
1	-5.509620	0.523009	-2.478314	15	-0.397606	-1.210143	0.405059
6	-4.569570	-0.362458	-0.732972	6	1.085830	-1.668827	1.357428
6	-5.528888	-0.606496	0.248722	6	1.489495	-3.007722	1.467273
6	-3.409337	-1.139548	-0.787670	6	1.827122	-0.658555	1.985702
6	-5.315357	-1.642264	1.161296	6	2.626968	-3.329897	2.204263
1	-6.436106	-0.011623	0.297111	1	0.921865	-3.790978	0.975015
6	-3.197238	-2.181761	0.111281	6	2.964424	-0.988762	2.722140
6	-4.159856	-2.429011	1.090890	1	1.533010	0.380363	1.883234
1	-6.060383	-1.847089	1.924014	6	3.364078	-2.321006	2.830619
1	-2.294918	-2.774152	0.050272	1	2.940143	-4.365713	2.287580
1	-4.012562	-3.238657	1.798780	1	3.544824	-0.201279	3.188633
1	-3.510607	0.187558	-3.711316	1	4.253237	-2.575448	3.398827
1	-2.173826	-1.519072	-2.544525	6	-1.826758	-1.668090	1.432942
6	3.011542	-1.279241	-0.802065	6	-3.117575	-1.705721	0.880528
6	4.335497	-1.635440	-0.488698	6	-1.658231	-1.852230	2.813189
6	2.795411	-0.474323	-1.935583	6	-4.221689	-1.913161	1.703488
6	5.402654	-1.155984	-1.242663	1	-3.264225	-1.558742	-0.182669
1	4.528646	-2.291404	0.354040	6	-2.769290	-2.054133	3.631755
6	3.862868	0.005543	-2.693285	1	-0.663802	-1.836839	3.245678
1	1.778895	-0.211325	-2.215984	6	-4.051186	-2.079577	3.080028
6	5.172404	-0.325143	-2.342761	1	-5.215192	-1.934701	1.267830

(S)-TS5_q

SCF Energy = -2377.479034

Gibbs Free Energy = -2376.870045

1	-2.631741	-2.196503	4.698860	1	-3.462605	-0.822838	3.318152
1	-4.914363	-2.235855	3.719162	15	-1.518050	-0.394692	1.120270
6	1.421352	-0.926206	-2.086182	6	-2.367250	0.434289	-0.269627
8	2.496881	-1.031922	-2.875787	6	-3.706507	0.843988	-0.162741
6	2.474506	1.046089	-1.727380	6	-1.648505	0.703687	-1.437657
6	3.325101	0.154179	-2.677144	6	-4.323945	1.491084	-1.230586
7	1.303917	0.177858	-1.418735	1	-4.259538	0.665326	0.754326
6	4.631549	-0.208741	-1.938908	6	-2.265513	1.369031	-2.496794
1	4.680366	-1.291735	-1.782897	1	-0.613895	0.398158	-1.509969
1	5.510130	0.068491	-2.530073	6	-3.601335	1.755737	-2.398204
6	4.557963	0.567035	-0.643222	1	-5.361370	1.801093	-1.147599
6	5.519424	0.649480	0.362869	1	-1.691074	1.587365	-3.388678
6	3.370698	1.297015	-0.539699	1	-4.079191	2.274937	-3.223975
6	5.280255	1.478451	1.461458	6	-2.288750	-2.025996	1.336291
1	6.447297	0.090009	0.290024	6	-1.671831	-2.933097	2.214289
6	3.133110	2.135722	0.546255	6	-3.442276	-2.405242	0.633922
6	4.097549	2.221499	1.551210	6	-2.221588	-4.202425	2.390905
1	6.026242	1.557128	2.246371	1	-0.744098	-2.646034	2.700135
1	2.210986	2.696917	0.604726	6	-3.979456	-3.678531	0.815183
1	3.930408	2.871561	2.404318	1	-3.905458	-1.718116	-0.063987
1	3.490697	0.582410	-3.665315	6	-3.372072	-4.576950	1.694890
1	2.095281	1.964090	-2.178692	1	-1.738158	-4.905542	3.062111
6	-3.047542	1.155997	-0.474007	1	-4.869126	-3.970095	0.265069
6	-4.379383	1.391130	-0.088322	1	-3.789919	-5.570193	1.829415
6	-2.817579	0.595737	-1.743907	6	-0.528208	2.474206	1.788242
6	-5.438420	1.024978	-0.913995	8	-0.371874	3.807827	1.814158
1	-4.584834	1.863241	0.867015	6	1.190515	2.783725	0.343096
6	-3.876828	0.229839	-2.573257	6	0.756167	4.150140	0.955854
1	-1.795920	0.433976	-2.077050	7	0.282541	1.814870	1.023791
6	-5.192815	0.433541	-2.156271	6	0.292668	5.067530	-0.189663
1	-6.458968	1.208579	-0.592520	1	-0.732555	5.405340	-0.005337
1	-3.673581	-0.210635	-3.544362	1	0.920127	5.963825	-0.249487
1	-6.020074	0.151709	-2.799599	6	0.428974	4.217135	-1.430199
6	-1.845504	3.954260	-0.846069	6	0.148330	4.584838	-2.745580
1	-2.684925	4.128474	-0.167034	6	0.966330	2.957802	-1.146128
1	-2.219468	3.398582	-1.708143	6	0.434338	3.686117	-3.774737
6	-1.237055	5.291547	-1.309817	1	-0.272321	5.561448	-2.968621
1	-1.989931	5.873179	-1.847674	6	1.282708	2.068048	-2.172580
1	-0.889597	5.897008	-0.466888	6	1.007342	2.441926	-3.489018
1	-0.392437	5.118307	-1.981506	1	0.224724	3.962018	-4.804190
				1	1.696011	1.093572	-1.940881
				1	1.240335	1.755511	-4.297301
				1	1.507503	4.607777	1.601399
				1	2.217817	2.487834	0.572375
				14	3.388851	-0.255109	1.596897
28	0.645693	-0.076715	1.260345	8	4.047514	0.987028	0.709944
8	1.080653	-1.691185	1.968986	8	3.779862	-1.605913	0.771785
6	-2.101081	0.632037	2.526532	6	4.528275	0.828063	-0.640385
6	-1.576608	1.938869	2.676265	1	3.939373	0.066647	-1.157545
6	-2.050850	2.761776	3.705995	1	4.360718	1.790206	-1.137951
6	-3.012288	2.294127	4.600294	6	6.003419	0.463613	-0.652080
6	-3.513050	1.001078	4.466017	1	6.149516	-0.516149	-0.189927
6	-3.063600	0.179416	3.429044	1	6.372570	0.414094	-1.682348
1	-1.651026	3.763692	3.804919	1	6.593617	1.205679	-0.104874
1	-3.362548	2.938272	5.400106	6	3.880865	-2.960603	1.218961
1	-4.258247	0.628837	5.162306	1	4.402876	-2.991688	2.185604

(S)-TS6D

SCF Energy = -3332.475813

Gibbs Free Energy = -3331.795010

1	2.877477	-3.364325	1.353251	8	1.630966	-0.997898	-1.037772
6	4.632747	-3.744132	0.159157	6	3.650825	-2.268092	-0.536031
1	4.110691	-3.654059	-0.795919	6	4.669719	-2.645028	0.348484
1	5.651447	-3.360697	0.039740	6	3.781229	-2.577234	-1.892906
1	4.689520	-4.801238	0.440593	6	5.802594	-3.307975	-0.116249
6	3.982538	-0.288936	3.365757	1	4.585134	-2.398021	1.402522
1	3.345610	-0.960476	3.948847	6	4.919021	-3.239449	-2.358609
1	5.017135	-0.640946	3.425707	1	3.013344	-2.281812	-2.598564
1	3.928443	0.710976	3.807229	6	5.931674	-3.606955	-1.474051
1	2.040545	0.441123	1.835273	1	6.587141	-3.585305	0.580676
1	1.075048	-2.304634	1.205350	1	5.011237	-3.464675	-3.416546
8	2.641224	-2.164654	-2.362041	1	6.816193	-4.119494	-1.838325
16	1.482580	-1.981222	-1.469274	1	1.966501	0.176546	2.961294
8	1.453939	-0.595710	-0.848627	6	-1.586320	2.142130	-1.428294
8	1.239135	-3.050565	-0.460018	6	-2.558644	1.474589	-2.206188
6	0.016579	-1.985018	-2.508040	6	-3.263849	2.159330	-3.203901
6	0.038585	-1.308253	-3.727601	6	-2.996991	3.503485	-3.451632
6	-1.161329	-2.566256	-2.042905	6	-2.039307	4.168402	-2.688678
6	-1.138203	-1.181747	-4.461207	6	-1.342708	3.493835	-1.682600
1	0.973841	-0.894994	-4.090094	1	-4.014373	1.629845	-3.778720
6	-2.331559	-2.433669	-2.788022	1	-3.536647	4.026643	-4.233564
1	-1.148011	-3.110408	-1.106342	1	-1.829122	5.217210	-2.871269
6	-2.344288	-1.723187	-3.993437	1	-0.604064	4.026873	-1.097283
1	-1.126379	-0.648760	-5.408722	15	-0.656486	1.259436	-0.098674
1	-3.251530	-2.878650	-2.418377	6	-1.767572	1.276696	1.351272
6	-3.632660	-1.500920	-4.743530	6	-3.160741	1.316409	1.200379
1	-4.321938	-2.341166	-4.617700	6	-1.222338	1.176289	2.640639
1	-3.457677	-1.359773	-5.814086	6	-3.990447	1.243478	2.316826
1	-4.139304	-0.601972	-4.369755	1	-3.607842	1.418269	0.219602
				6	-2.056495	1.112378	3.755440
				1	-0.147168	1.171690	2.771449
				6	-3.442238	1.137749	3.594745
				1	-5.066621	1.263188	2.185007
				1	-1.622346	1.046072	4.748060
				1	-4.091657	1.080906	4.462112
28	-0.313839	-0.749550	-0.973805	6	0.715471	2.396204	0.234612
6	5.287765	2.050623	1.860303	6	1.773882	2.405297	-0.684849
6	4.239965	1.148009	2.014398	6	0.657161	3.372145	1.242306
6	3.747825	0.407864	0.925200	6	2.755071	3.390293	-0.603293
6	4.362416	0.600520	-0.324636	6	1.829457	1.641634	-1.452988
6	5.429633	1.482321	-0.474334	1	1.665436	4.329009	1.339312
6	5.895553	2.217920	0.614486	6	-0.174365	3.397830	1.935815
1	5.647254	2.605760	2.721153	1	2.711683	4.341693	0.414743
1	3.823179	1.001633	3.004920	6	3.571703	3.392397	-1.314190
1	4.000710	0.063735	-1.189933	1	1.624334	5.073275	2.128129
1	5.892834	1.597391	-1.449653	1	3.491635	5.092450	0.487140
1	6.728470	2.904313	0.498993	6	-2.899220	0.075754	-1.941144
6	2.640991	-0.564958	1.101198	6	-4.110875	-0.330325	-2.323919
6	1.831668	-0.562708	2.176831	8	-2.997432	-2.015120	-1.099700
6	0.749558	-1.571142	2.431687	6	-4.254907	-1.747874	-1.975064
1	1.069918	-2.270448	3.224347	6	-2.172462	-0.798744	-1.321232
1	-0.169571	-1.091898	2.775351	7	-5.492571	-1.939747	-1.089258
8	0.399166	-2.308949	1.266048	6	-6.213092	-1.133166	-1.254466
6	1.574774	-2.784287	0.633716	1	-5.997116	-2.877785	-1.348091
1	1.272679	-3.481757	-0.149455	1	-4.934172	-1.989435	0.314991
1	2.200900	-3.331916	1.349437	6	-5.631025	-1.999552	1.522554
6	2.384258	-1.622908	0.023186	6			

(S)-TS6_iso

SCF Energy = -2606.379719

Gibbs Free Energy = -2605.722730

6	-3.540011	-2.092959	0.310098
6	-4.913565	-2.119247	2.714496
1	-6.714365	-1.925288	1.538149
6	-2.819160	-2.229591	1.494082
6	-3.519433	-2.239631	2.700382
1	-5.444571	-2.128786	3.661271
1	-1.741424	-2.336929	1.469730
1	-2.979054	-2.340447	3.636048
1	-4.284833	-2.296603	-2.917184
1	-2.426435	-2.892030	-1.408296
8	0.062985	-2.242398	-2.173405
1	-0.128320	-3.121069	-1.819012
1	1.150307	-1.817779	-1.745696

(S)-TS6

SCF Energy = -2606.395347

Gibbs Free Energy = -2605.742477

28	-0.098777	-0.447816	-0.566295
6	0.232142	-1.942845	3.199156
6	0.674700	-2.367378	1.949533
6	1.881399	-1.898838	1.392349
6	2.624463	-0.968638	2.139858
6	2.180367	-0.541423	3.391350
6	0.985664	-1.022437	3.928018
1	-0.706695	-2.316964	3.595483
1	0.078965	-3.073966	1.381602
1	3.564573	-0.596011	1.759713
1	2.786435	0.157797	3.960106
1	0.647072	-0.686528	4.902816
6	2.286824	-2.416109	0.055397
6	2.091848	-3.714790	-0.237320
6	2.231935	-4.283039	-1.619262
1	3.163715	-4.868520	-1.714109
1	1.402881	-4.966565	-1.832373
8	2.189921	-3.265695	-2.607158
6	3.159620	-2.279299	-2.302356
1	3.217546	-1.594987	-3.151001
1	4.143198	-2.746503	-2.153419
6	2.768968	-1.460264	-1.046014
8	1.702932	-0.587282	-1.430303
6	4.010020	-0.655428	-0.674683
6	5.087049	-1.276589	-0.027016
6	4.135161	0.679094	-1.070214
6	6.248147	-0.562502	0.261266
1	5.002277	-2.317092	0.274252
6	5.298173	1.396360	-0.778643
1	3.320141	1.149126	-1.606462
6	6.354297	0.781388	-0.107545
1	7.069594	-1.053451	0.773725
1	5.378813	2.434672	-1.086328
1	7.257935	1.338550	0.118355
1	1.786110	-4.406095	0.544557
6	-2.559447	-0.152153	1.593263
6	-1.672557	0.591155	2.399957
6	-1.978401	0.805501	3.749619

6	-3.133180	0.259318	4.305292
6	-3.999195	-0.495583	3.514370
6	-3.716270	-0.692627	2.161411
1	-1.295990	1.386176	4.357704
1	-3.353670	0.421407	5.354995
1	-4.898007	-0.925089	3.944418
1	-4.397517	-1.267311	1.543768
15	-2.215257	-0.355599	-0.180437
6	-2.868042	1.114121	-1.019608
6	-3.628206	2.080405	-0.348957
6	-2.527210	1.293216	-2.371069
6	-4.045803	3.223786	-1.030458
1	-3.889990	1.944570	0.694833
6	-2.958123	2.433012	-3.043842
1	-1.923721	0.547664	-2.880098
6	-3.711660	3.400081	-2.373799
1	-4.632741	3.974747	-0.511616
1	-2.696101	2.572781	-4.087486
1	-4.036831	4.292353	-2.899076
6	-3.164627	-1.800456	-0.724330
6	-2.700343	-3.076527	-0.364981
6	-4.328354	-1.669173	-1.491238
6	-3.400750	-4.210439	-0.766841
1	-1.798770	-3.175545	0.232615
6	-5.023701	-2.810775	-1.893495
1	-4.683506	-0.684815	-1.775996
6	-4.562238	-4.077259	-1.533810
1	-3.042827	-5.195943	-0.486548
1	-5.924558	-2.708615	-2.489692
1	-5.104700	-4.961797	-1.851474
6	-0.426179	1.159893	1.867142
8	0.096465	2.168099	2.569757
6	1.339719	1.775265	0.601797
6	1.332517	2.602298	1.912841
7	0.220283	0.815330	0.798224
6	1.235999	4.086756	1.531341
1	0.486414	4.595012	2.145304
1	2.194424	4.585227	1.717197
6	0.906060	4.067898	0.054998
6	0.561541	5.139554	-0.766783
6	1.024572	2.781624	-0.481328
6	0.339391	4.905481	-2.125999
1	0.468283	6.142300	-0.360376
6	0.822401	2.544919	-1.840656
6	0.474613	3.620003	-2.660299
1	0.067434	5.731909	-2.775120
1	0.942293	1.547342	-2.249033
1	0.310268	3.456841	-3.720591
1	2.143553	2.365975	2.601332
1	2.256718	1.215376	0.432626
8	-0.306159	-1.412695	-2.197404
1	-0.446922	-2.366347	-2.111068
1	0.831449	-1.200910	-2.147882

TS1B

SCF Energy = -3351.100152

Gibbs Free Energy = -3350.328213

				6	-2.979136	-0.564684	-2.801961
				6	-4.060938	-0.183606	-0.672444
28	-0.897250	0.456448	0.993503	6	-4.042887	-1.380422	-3.191932
8	2.010888	2.562037	2.065329	1	-2.151482	-0.397275	-3.482006
16	1.949379	2.235741	0.625003	6	-5.132620	-0.975955	-1.074449
8	1.485885	3.325589	-0.269168	1	-4.052856	0.255379	0.319309
8	1.230961	0.931720	0.339760	6	-5.121928	-1.582888	-2.331647
6	3.620878	1.835975	0.110613	1	-4.030300	-1.847964	-4.172046
6	3.903253	1.722750	-1.251753	1	-5.959440	-1.144698	-0.394215
6	4.587484	1.527136	1.064653	1	-5.949995	-2.215716	-2.636212
6	5.159576	1.278065	-1.652735	6	-2.213129	2.808790	-1.386474
1	3.141232	1.979874	-1.978279	6	-1.410764	3.913604	-1.057514
6	5.839597	1.073186	0.648217	6	-3.460596	3.011892	-1.995651
1	4.345052	1.644601	2.115182	6	-1.858525	5.202517	-1.344806
6	6.139833	0.928405	-0.711283	1	-0.435136	3.764277	-0.603749
1	5.385453	1.193211	-2.713240	6	-3.902894	4.306435	-2.267458
1	6.593931	0.824309	1.389968	1	-4.085512	2.165900	-2.256262
6	7.469327	0.373552	-1.157173	6	-3.103791	5.403362	-1.943059
1	7.402070	-0.709628	-1.320225	1	-1.228915	6.050289	-1.092557
1	8.246834	0.543004	-0.407194	1	-4.871149	4.454914	-2.736238
1	7.797983	0.825190	-2.098112	1	-3.450249	6.410289	-2.156758
6	-0.931532	1.228901	2.813006	6	-0.099287	-1.539626	-1.138622
6	-0.414880	0.078899	2.872379	8	-0.047528	-2.819110	-1.565697
6	0.235942	-0.992201	3.682483	6	-0.918859	-2.645917	0.628763
1	-0.065634	-0.858153	4.726493	6	-0.644194	-3.647623	-0.529043
1	-0.105459	-1.982924	3.365688	7	-0.539332	-1.337481	0.055937
8	1.655103	-0.942403	3.708005	6	-2.007791	-4.219829	-0.978137
6	2.281524	-1.098315	2.454747	1	-2.246725	-3.852856	-1.982692
1	3.331056	-0.812070	2.587831	1	-1.993081	-5.313523	-1.025195
1	1.862424	-0.411023	1.707563	6	-2.989460	-3.699145	0.048984
6	2.225311	-2.516217	1.913714	6	-4.336110	-4.026104	0.196306
8	1.646698	-3.411098	2.521090	6	-2.388713	-2.794086	0.927781
6	2.868912	-2.789152	0.591143	6	-5.069732	-3.432669	1.226305
6	3.403329	-1.774052	-0.214823	1	-4.810619	-4.733990	-0.477403
6	2.933330	-4.123061	0.157247	6	-3.117058	-2.189891	1.950240
6	4.008648	-2.098058	-1.429617	6	-4.467422	-2.515058	2.093681
1	3.333851	-0.735646	0.078879	1	-6.118129	-3.686063	1.354491
6	3.526141	-4.440907	-1.059219	1	-2.640811	-1.477503	2.615783
1	2.517092	-4.889475	0.802641	1	-5.050571	-2.060499	2.888971
6	4.071459	-3.425938	-1.852972	1	0.089354	-4.413298	-0.279759
1	4.416629	-1.301929	-2.041823	1	-0.304261	-2.837973	1.506037
1	3.574509	-5.474773	-1.387969	6	-1.332282	2.531585	3.423151
1	4.543127	-3.672710	-2.800019	6	-0.340994	2.792991	4.576937
1	-2.084596	1.108484	1.445267	1	-0.593655	3.734880	5.075811
6	-0.268192	0.755191	-2.150853	1	-0.381649	1.989963	5.319845
6	0.330583	-0.523252	-2.112908	1	0.674540	2.856636	4.180935
6	1.331796	-0.856622	-3.027897	6	-1.254095	3.676233	2.401634
6	1.783090	0.089151	-3.948168	1	-1.957825	3.516712	1.580837
6	1.214907	1.360656	-3.969607	1	-1.509701	4.622388	2.890575
6	0.185286	1.687127	-3.081670	1	-0.247465	3.754845	1.988148
1	1.766599	-1.847255	-2.992696	6	-2.772845	2.399867	3.955925
1	2.575780	-0.169957	-4.642892	1	-3.469915	2.174327	3.141196
1	1.563490	2.103942	-4.680014	1	-2.846712	1.603088	4.702469
1	-0.257632	2.675006	-3.109725	1	-3.087614	3.340335	4.420063
15	-1.621629	1.131062	-0.969589				
6	-2.979099	0.036543	-1.536884	TS1_iso1			

SCF Energy = -4151.474674				28	0.845483	-0.195173	-0.234149
Gibbs Free Energy = -4150.682896				8	-1.068582	-0.850145	-1.446484
				8	1.610392	1.350801	-1.042794
6	0.299918	0.325192	2.934496	16	-2.041075	-1.778185	-2.132502
6	0.669692	-1.027062	3.099173	16	1.242142	1.776040	-2.586794
6	1.095850	-1.483557	4.356193	8	-2.656770	-1.191819	-3.343664
6	1.166526	-0.614728	5.441120	8	-1.476879	-3.142275	-2.298682
6	0.800828	0.721055	5.283206	8	1.372176	0.585445	-3.427218
6	0.371223	1.181940	4.038571	8	2.021979	2.977699	-2.877984
1	1.373924	-2.524159	4.468026	6	-0.457022	2.276837	-2.464350
1	1.507430	-0.981206	6.403795	6	-1.434455	1.544423	-3.126966
1	0.852068	1.406590	6.123203	6	-0.758958	3.458168	-1.779217
1	0.093765	2.222677	3.915667	6	-2.753261	1.999173	-3.086109
15	-0.302297	0.956433	1.317703	1	-1.192266	0.621180	-3.632279
6	0.072003	2.743211	1.405036	6	-2.078570	3.889405	-1.746674
6	-0.944517	3.700269	1.516293	1	0.024289	4.023090	-1.288372
6	1.411516	3.156152	1.322631	6	-3.093052	3.169047	-2.400078
6	-0.625765	5.058650	1.531466	1	-3.516486	1.401745	-3.572963
1	-1.980442	3.388110	1.570277	1	-2.327165	4.797779	-1.205366
6	1.720883	4.514274	1.336437	6	-3.381270	-1.965153	-0.944971
1	2.198921	2.417351	1.240137	6	-4.700642	-1.925326	-1.383142
6	0.704356	5.468270	1.433035	6	-3.099326	-2.179272	0.406601
1	-1.419456	5.795168	1.612832	6	-5.739182	-2.092287	-0.464291
1	2.757893	4.826505	1.259956	1	-4.897214	-1.751078	-2.435046
1	0.949106	6.526114	1.432537	6	-4.138226	-2.348210	1.312024
6	-2.115863	0.876340	1.448338	1	-2.072310	-2.171413	0.750279
6	-2.845220	1.012516	0.259759	6	-5.476279	-2.302232	0.892180
6	-2.787455	0.782291	2.675468	1	-6.770006	-2.052729	-0.807285
6	-4.236019	1.069212	0.302641	1	-3.914358	-2.491482	2.365932
1	-2.327255	1.033632	-0.688498	14	3.317264	0.211828	-0.737353
6	-4.180147	0.829609	2.708314	1	2.024477	-0.843124	-1.009277
1	-2.230201	0.674242	3.599518	8	3.289759	0.565083	0.905189
6	-4.904232	0.975699	1.522844	8	4.204550	1.353682	-1.532780
1	-4.792191	1.145633	-0.624246	6	3.927966	-0.258924	1.880336
1	-4.699479	0.748667	3.658553	1	4.917342	-0.572070	1.526081
1	-5.989239	0.998936	1.550141	1	3.331920	-1.167825	2.038366
6	0.619457	-2.013694	2.005014	6	4.054575	0.520477	3.176943
8	0.566399	-3.299405	2.400378	1	3.073026	0.843154	3.528785
6	0.492963	-3.135094	0.036925	1	4.514183	-0.101194	3.952085
6	0.708229	-4.123692	1.205358	1	4.677182	1.407846	3.029545
7	0.624946	-1.811304	0.728250	6	4.332904	2.737930	-1.193940
6	2.138229	-4.690986	1.059130	1	4.510075	3.275551	-2.127570
1	2.809008	-4.176948	1.759881	1	3.395758	3.119685	-0.782292
1	2.185318	-5.758251	1.294690	6	5.480141	2.936118	-0.212802
6	2.485507	-4.385569	-0.382395	1	5.621431	4.002648	-0.002780
6	3.526855	-4.902133	-1.151142	1	5.271631	2.421715	0.729890
6	1.572912	-3.488031	-0.947693	1	6.413918	2.540519	-0.623531
6	3.632280	-4.509949	-2.488605	6	4.402551	-1.277920	-1.107686
1	4.236162	-5.607076	-0.726565	1	5.443418	-1.038861	-0.868737
6	1.662510	-3.103842	-2.284233	1	4.084939	-2.168368	-0.562120
6	2.707753	-3.622680	-3.050436	1	4.344151	-1.508900	-2.173308
1	4.435201	-4.908727	-3.101533	6	-4.522001	3.644891	-2.329457
1	0.920561	-2.441418	-2.711112	1	-4.892659	3.610500	-1.298289
1	2.795781	-3.339825	-4.094522	1	-4.614224	4.681045	-2.672537
1	-0.054584	-4.898584	1.268819	1	-5.178848	3.024508	-2.944334
1	-0.485027	-3.177721	-0.441961	6	-6.592416	-2.438636	1.896723

1	-6.593269	-1.593467	2.596209	1	3.512939	5.305269	1.804840
1	-7.570060	-2.469667	1.408416	1	0.398365	2.470156	0.950905
1	-6.485289	-3.349848	2.495350	1	1.574021	3.954639	2.543842
TS1_iso				1	1.731323	2.478722	-3.989652
SCF Energy = -3256.452952				1	0.095051	2.477563	-2.133081
Gibbs Free Energy = -3255.786054				28	-0.093466	-0.051807	-0.467205
6	2.536058	-1.834552	-0.832537	8	-1.603388	-0.831124	0.345175
6	2.753552	-1.084508	-2.013082	16	-1.991612	-0.228463	1.818306
6	3.514366	-1.618313	-3.059917	8	-0.772397	0.455108	2.279626
6	4.032151	-2.908452	-2.960945	8	-2.574223	-1.315421	2.591179
6	3.805878	-3.658621	-1.808702	6	-3.226764	0.999867	1.474567
6	3.069941	-3.121310	-0.748391	6	-2.851290	2.210423	0.889261
1	3.687002	-1.020713	-3.947474	6	-4.558958	0.717703	1.771622
1	4.608948	-3.322823	-3.780694	6	-3.840660	3.136632	0.569098
1	4.206152	-4.663887	-1.726196	1	-1.808682	2.429556	0.693694
1	2.912082	-3.708039	0.149005	6	-5.530110	1.663446	1.459227
15	1.565976	-1.117252	0.553763	1	-4.816621	-0.230636	2.227678
6	2.696510	0.011070	1.431042	6	-5.191164	2.879604	0.847152
6	3.865821	0.505355	0.838956	1	-3.559822	4.080905	0.111931
6	2.336840	0.429355	2.722864	1	-6.570622	1.454262	1.689285
6	4.669473	1.408683	1.532938	14	-2.445643	-0.462162	-1.470134
1	4.165387	0.180276	-0.150833	1	-1.227368	0.716561	-1.207255
6	3.156508	1.316758	3.415114	8	-3.839946	-0.939718	-0.721466
1	1.419867	0.069771	3.174248	8	-1.607943	-1.692126	-2.184208
6	4.319799	1.810588	2.821687	6	-5.170408	-0.787591	-1.227237
1	5.572253	1.790684	1.067795	1	-5.299359	0.206752	-1.669466
1	2.879990	1.628983	4.417139	1	-5.830794	-0.841119	-0.357359
1	4.951378	2.508533	3.361905	6	-5.511978	-1.880900	-2.227394
6	1.239269	-2.487602	1.695544	1	-5.364736	-2.866316	-1.776366
6	2.211713	-2.872940	2.634427	1	-6.556650	-1.798292	-2.543379
6	0.030251	-3.192575	1.613423	1	-4.881024	-1.814021	-3.119639
6	1.971706	-3.956026	3.476198	6	-1.622431	-3.065756	-1.757365
1	3.144243	-2.324511	2.710076	1	-0.606803	-3.320421	-1.434253
6	-0.203884	-4.270690	2.465634	1	-2.293351	-3.182810	-0.899791
1	-0.732706	-2.882746	0.913902	6	-2.058307	-3.951239	-2.910014
6	0.763900	-4.654115	3.393654	1	-2.020455	-5.004251	-2.612948
1	2.723698	-4.250547	4.201125	1	-3.082200	-3.714947	-3.212474
1	-1.150030	-4.798755	2.411924	1	-1.401947	-3.809747	-3.773148
1	0.576459	-5.490760	4.059137	6	-2.949293	0.749232	-2.822620
6	2.219923	0.274037	-2.154191	1	-3.737010	0.341365	-3.463385
8	2.879394	1.112157	-2.958042	1	-3.304826	1.689513	-2.388413
6	1.116744	2.215456	-1.848776	1	-2.076557	0.965517	-3.445503
6	2.155027	2.391982	-2.988023	6	-6.251871	3.901440	0.531192
7	1.179332	0.766212	-1.558046	1	-5.938976	4.568601	-0.275912
6	3.081905	3.549293	-2.593875	1	-7.191651	3.424191	0.240548
1	4.127068	3.293599	-2.792483	1	-6.460800	4.522974	1.409888
1	2.848794	4.433957	-3.197868	TS1			
6	2.781277	3.777976	-1.128470	SCF Energy = -3256.469528			
6	3.451844	4.602442	-0.226594	Gibbs Free Energy = -3255.800943			
6	1.667393	3.044067	-0.710646	6	-0.049169	-2.840961	-0.461780
6	2.997929	4.669178	1.091918	6	0.638432	-2.623914	-1.678229
1	4.315513	5.181077	-0.540427	6	0.618414	-3.601870	-2.678791
6	1.222475	3.088956	0.609181	6	-0.101029	-4.781883	-2.492231
6	1.896758	3.913726	1.509346	6	-0.786353	-4.995814	-1.297628

6	-0.755640	-4.032073	-0.286041	6	-2.979997	-1.559998	-2.121317
1	1.160531	-3.424596	-3.600338	1	-1.179359	-0.706589	-2.957733
1	-0.122925	-5.529442	-3.277831	6	-4.507146	0.015372	-1.121422
1	-1.345885	-5.913149	-1.146555	1	-3.868358	2.086135	-1.131501
1	-1.292083	-4.207443	0.639125	6	-4.189948	-1.309554	-1.458472
15	-0.047303	-1.562862	0.850371	1	-2.727730	-2.574463	-2.415452
6	1.504852	-1.712970	1.779532	1	-5.455809	0.228244	-0.636954
6	2.641715	-2.303775	1.213241	14	-0.993191	2.406062	1.139394
6	1.589154	-1.095965	3.038120	1	-1.184519	0.762449	0.858931
6	3.851468	-2.280830	1.904073	8	-2.344261	3.111001	0.535109
1	2.587517	-2.785343	0.243516	8	0.427945	3.223213	1.255780
6	2.799129	-1.088907	3.727168	6	-3.235701	3.954383	1.281692
1	0.711556	-0.635530	3.480513	1	-3.475660	3.491966	2.246993
6	3.931214	-1.676326	3.158742	1	-4.159039	4.004712	0.697472
1	4.731753	-2.732395	1.459590	6	-2.642953	5.341218	1.469638
1	2.859068	-0.620017	4.703969	1	-2.394509	5.777525	0.498563
1	4.875521	-1.660646	3.692876	1	-3.358429	5.997382	1.974906
6	-1.414367	-1.979739	1.964293	1	-1.731433	5.300725	2.075524
6	-1.242299	-2.871616	3.033560	6	1.011165	4.132338	0.299082
6	-2.680616	-1.435908	1.701381	1	1.594584	3.551093	-0.419995
6	-2.332751	-3.210671	3.834283	1	0.216636	4.642776	-0.253029
1	-0.263403	-3.289394	3.243618	6	1.893201	5.109805	1.050460
6	-3.766032	-1.784546	2.502495	1	2.360010	5.807395	0.348341
1	-2.820274	-0.749140	0.874479	1	1.310237	5.685604	1.774690
6	-3.592586	-2.669187	3.569811	1	2.684826	4.578474	1.586975
1	-2.197494	-3.895194	4.665271	6	-1.269937	1.949801	2.945598
1	-4.743252	-1.359817	2.296511	1	-1.423215	2.846066	3.554836
1	-4.437361	-2.933615	4.197653	1	-2.127999	1.282555	3.071810
6	1.386525	-1.382734	-1.919474	1	-0.379196	1.441307	3.326806
8	2.386080	-1.430577	-2.799052	6	-5.112093	-2.442890	-1.091559
6	2.250292	0.693925	-1.766036	1	-5.077152	-3.243594	-1.835068
6	2.952552	-0.071729	-2.917639	1	-4.819121	-2.876319	-0.127238
7	1.176563	-0.240924	-1.352922	1	-6.147337	-2.104918	-1.000248
6	4.454427	-0.100328	-2.606348				
1	4.873456	-1.092707	-2.798065				
1	4.982370	0.601806	-3.261969				
6	4.538468	0.331178	-1.157701				
6	5.649478	0.327921	-0.315348				
6	3.311210	0.817050	-0.696231	28	1.085415	1.023196	-0.027556
6	5.511244	0.813554	0.986791	8	-2.400787	1.426708	-2.385646
1	6.609337	-0.040903	-0.664785	16	-1.609567	0.244506	-1.953671
6	3.165378	1.300991	0.603005	8	-0.584940	-0.198754	-2.928141
6	4.279768	1.296668	1.442708	8	-1.072325	0.424254	-0.550396
1	6.369549	0.817801	1.651445	6	-2.750549	-1.132776	-1.777805
1	2.212638	1.677464	0.961002	6	-3.393436	-1.362737	-0.562893
1	4.187253	1.666188	2.458588	6	-2.991737	-1.962997	-2.871486
1	2.697315	0.276499	-3.918244	6	-4.289392	-2.423263	-0.449274
1	1.793080	1.632721	-2.074402	1	-3.182658	-0.726440	0.286576
28	-0.157905	0.337512	-0.142824	6	-3.886893	-3.022842	-2.745051
8	-0.412635	2.077026	-0.887798	1	-2.457853	-1.785386	-3.798343
16	-1.218762	2.079008	-2.292961	6	-4.552530	-3.266563	-1.535629
8	-0.271984	1.608652	-3.310692	1	-4.791416	-2.596354	0.498973
8	-1.882440	3.365624	-2.437738	1	-4.069216	-3.675548	-3.595233
6	-2.422212	0.780088	-2.031508	6	-5.545201	-4.396678	-1.415418
6	-2.098942	-0.523431	-2.417713	1	-6.543543	-4.081545	-1.743502
6	-3.632900	1.064807	-1.400150	1	-5.257166	-5.251383	-2.035220

TS2B

SCF Energy = -3351.096942

Gibbs Free Energy = -3350.325164

1	-5.636986	-4.740578	-0.380959	1	4.488955	-4.235504	1.805765
6	0.886435	2.829650	-0.800703	1	5.327182	-0.319398	3.372189
6	0.543957	2.835505	0.420232	1	6.021250	-2.674193	2.985176
6	-0.199642	3.427932	1.570478	6	-0.169264	-0.846174	2.637715
1	0.443080	4.119947	2.125354	6	-1.348768	-0.087277	2.593703
1	-0.526753	2.647128	2.264021	6	0.127683	-1.612546	3.772847
8	-1.300773	4.202923	1.115658	6	-2.220917	-0.093464	3.680337
6	-2.346889	3.429905	0.560132	1	-1.572640	0.489330	1.703464
1	-2.955645	4.108401	-0.046489	6	-0.752043	-1.617880	4.855425
1	-1.967098	2.652935	-0.116101	1	1.041439	-2.196372	3.809934
6	-3.231918	2.782645	1.621285	6	-1.922733	-0.858425	4.809994
8	-2.967692	2.884063	2.812351	1	-3.112119	0.521226	3.646176
6	-4.418016	2.004231	1.154524	1	-0.519152	-2.209904	5.735556
6	-4.646105	1.728101	-0.201596	1	-2.599748	-0.856209	5.659099
6	-5.315815	1.520208	2.120116	6	1.959759	-1.368407	-1.649127
6	-5.750502	0.964205	-0.578294	8	2.900158	-1.941471	-2.435244
1	-3.946599	2.042702	-0.967606	6	3.439717	0.295244	-1.882077
6	-6.416953	0.761808	1.738982	6	4.001113	-0.999760	-2.537104
1	-5.131062	1.762185	3.161393	7	2.148177	-0.139581	-1.316429
6	-6.634317	0.480704	0.385681	6	5.211878	-1.453530	-1.686921
1	-5.899671	0.729070	-1.626945	1	4.950693	-2.366502	-1.139822
1	-7.107826	0.390634	2.490333	1	6.083216	-1.684638	-2.308097
1	-7.489253	-0.119004	0.086845	6	5.461432	-0.297645	-0.743597
1	1.631405	1.580810	1.166197	6	6.520415	-0.123664	0.145331
6	0.930142	3.604515	-2.084651	6	4.462351	0.674441	-0.840938
6	-0.434145	4.322849	-2.213483	6	6.559573	1.027032	0.936190
1	-0.416133	4.982294	-3.088665	1	7.304233	-0.871372	0.225605
1	-0.642869	4.921658	-1.323254	6	4.491437	1.821301	-0.050763
1	-1.232633	3.588596	-2.345869	6	5.549991	1.991003	0.844166
6	1.144781	2.723836	-3.326069	1	7.382816	1.174859	1.629109
1	2.178837	2.373548	-3.386134	1	3.702392	2.561465	-0.129261
1	0.955747	3.317006	-4.226882	1	5.594705	2.881072	1.464535
1	0.482339	1.856715	-3.331160	1	4.236610	-0.897273	-3.596449
6	2.063701	4.646382	-1.979260	1	3.248306	1.102117	-2.589589
1	3.035628	4.159304	-1.845797				
1	1.898298	5.322106	-1.134997				
1	2.108063	5.243002	-2.897080				
6	0.313477	-2.114781	0.078393				
6	0.868641	-2.249655	-1.210842				
6	0.418815	-3.258045	-2.066295	28	0.278183	-0.193765	-0.723349
6	-0.599583	-4.117791	-1.661117	6	0.344982	-2.867425	-1.776427
6	-1.151334	-3.989078	-0.388965	6	-1.680015	-2.419425	-2.846404
6	-0.692039	-2.996018	0.477373	6	-2.201126	-1.426839	-1.790992
1	0.854077	-3.341651	-3.054993	6	-1.187475	-2.068140	0.027966
1	-0.968009	-4.877513	-2.341959	8	-0.794530	-3.431197	-2.398816
1	-1.956960	-4.643570	-0.074786	1	-1.173940	-1.797552	-3.604616
1	-1.131132	-2.894865	1.462796	1	-2.508902	-2.944633	-3.324687
15	0.930564	-0.792771	1.189800	8	-1.602603	-0.276824	-1.729608
6	2.542890	-1.439631	1.765744	6	-3.642904	-1.496984	-1.434185
6	2.937924	-2.766437	1.548389	6	-4.362273	-2.705481	-1.477611
6	3.417126	-0.562519	2.423986	6	-4.313574	-0.336494	-1.020878
6	4.189788	-3.206658	1.982810	6	-5.699235	-2.750914	-1.095931
1	2.270635	-3.453230	1.039681	1	-3.853041	-3.621199	-1.760938
6	4.656333	-1.009647	2.872723	6	-5.649746	-0.384325	-0.631649
1	3.132790	0.475024	2.563992	1	-3.766895	0.596673	-1.006732
6	5.047704	-2.331176	2.648148	6	-6.349998	-1.591109	-0.662043

TS2C

SCF Energy = -2529.40065

Gibbs Free Energy = -2528.785810

1	-6.234399	-3.696025	-1.124219	1	0.880810	-2.223613	-2.495008
1	-6.145258	0.525219	-0.303215	1	1.012910	-3.701109	-1.533762
1	-7.391329	-1.630323	-0.356159	6	-0.003723	-2.094373	-0.525904
6	3.201500	1.104074	0.001900	6	-1.852037	-1.566984	1.220357
6	2.715884	2.320669	-0.532654	6	-3.075619	-2.146443	1.610951
6	3.580278	3.431736	-0.596418	6	-1.311508	-0.565811	2.054405
6	4.890109	3.352623	-0.141172	6	-3.732889	-1.735906	2.767136
6	5.372249	2.152195	0.381068	1	-3.509739	-2.917544	0.987416
6	4.530949	1.045731	0.442586	6	-1.959911	-0.165732	3.219131
1	3.205735	4.359106	-1.009026	1	-0.379760	-0.094453	1.771217
1	5.533393	4.224844	-0.199734	6	-3.178566	-0.744667	3.580182
1	6.396324	2.075896	0.733222	1	-4.681349	-2.192821	3.033823
1	4.909305	0.108657	0.837292	1	-1.512888	0.607094	3.837736
15	2.180239	-0.430645	0.132474	1	-3.689326	-0.428092	4.485183
6	2.113929	-0.741375	1.936468				
6	1.621808	-1.977471	2.388908				
6	2.372692	0.273047	2.867891				
6	1.415858	-2.196231	3.747731				
1	1.355481	-2.741405	1.666502				
6	2.147350	0.053649	4.228073	28	0.071880	-0.280402	-1.100650
1	2.739639	1.237429	2.535314	6	-4.562770	1.518082	-1.276880
6	1.673048	-1.180344	4.671140	6	-3.259192	1.105369	-1.536638
1	1.026549	-3.152480	4.082744	6	-2.992909	-0.242660	-1.824743
1	2.343119	0.850737	4.939149	6	-4.050708	-1.167849	-1.870106
1	1.492941	-1.347344	5.728712	6	-5.350709	-0.745957	-1.615778
6	3.358239	-1.663290	-0.544116	6	-5.608926	0.593806	-1.313459
6	3.544843	-1.671073	-1.935292	1	-4.761866	2.560017	-1.048056
6	4.062099	-2.581444	0.244298	1	-2.443609	1.817408	-1.522521
6	4.415539	-2.582059	-2.526516	1	-3.836360	-2.211352	-2.069389
1	2.996290	-0.964848	-2.552673	1	-6.162463	-1.465398	-1.639103
6	4.927660	-3.500352	-0.352326	1	-6.624680	0.916478	-1.108132
1	3.931094	-2.584385	1.320477	6	-1.651031	-0.699436	-2.071658
6	5.106136	-3.504097	-1.735528	6	-0.739691	-1.406564	-2.555958
1	4.548521	-2.579903	-3.604153	6	-0.189907	-2.399471	-3.510064
1	5.463702	-4.212613	0.267982	1	-1.037824	-2.845482	-4.039141
1	5.777494	-4.221944	-2.196700	1	0.448886	-1.888249	-4.245707
6	1.347731	2.524164	-1.047698	8	0.501849	-3.479471	-2.913347
8	1.116858	3.759759	-1.557061	6	1.825898	-3.202828	-2.532553
6	-0.829235	2.458423	-1.577340	1	2.287376	-2.474815	-3.212023
6	-0.219423	3.763189	-2.140282	1	2.396768	-4.135888	-2.631677
7	0.347775	1.706024	-1.077888	6	1.978039	-2.757471	-1.078154
6	-1.034955	4.940358	-1.588263	8	1.070314	-2.903757	-0.271587
1	-0.379684	5.768048	-1.299231	6	3.304896	-2.224563	-0.654644
1	-1.712028	5.319971	-2.363697	6	4.167841	-1.547429	-1.530835
6	-1.802140	4.334717	-0.434005	6	3.676797	-2.383739	0.688565
6	-2.552891	4.979566	0.547409	6	5.370990	-1.019703	-1.063060
6	-1.710546	2.939090	-0.444589	1	3.900838	-1.407281	-2.572237
6	-3.202864	4.210128	1.516937	6	4.888459	-1.876930	1.147479
1	-2.629964	6.063388	0.563621	1	2.999684	-2.905634	1.354696
6	-2.355873	2.168874	0.517626	6	5.734119	-1.186514	0.275224
6	-3.104161	2.814726	1.503423	1	6.029705	-0.490570	-1.744557
1	-3.787570	4.702189	2.288839	1	5.175810	-2.018601	2.184346
1	-2.268879	1.091946	0.502918	1	6.677789	-0.788371	0.634771
1	-3.601676	2.220618	2.263344	1	0.909181	-0.427066	-2.292553
1	-0.091382	3.783425	-3.225554	6	0.230190	-0.794227	2.114979
1	-1.361417	1.833038	-2.293813	6	1.543845	-0.281417	2.079996

TS2D

SCF Energy = -2529.874044

Gibbs Free Energy = -2529.247947

6	2.428365	-0.548272	3.133506	28	-0.308597	0.376454	1.057485
6	2.036436	-1.363548	4.192173	8	-0.399382	-2.254101	-1.707688
6	0.752715	-1.906451	4.207889	16	0.582002	-2.379773	-0.606281
6	-0.148540	-1.608950	3.182741	8	0.330458	-3.478865	0.359998
1	3.426974	-0.131504	3.099077	8	0.845154	-1.063717	0.102260
1	2.731591	-1.575319	4.997584	6	2.201892	-2.635481	-1.326296
1	0.443083	-2.552025	5.023494	6	2.500826	-2.021297	-2.541541
1	-1.152501	-2.015820	3.214354	6	3.200123	-3.252472	-0.574490
15	-0.996920	-0.231551	0.865636	6	3.817584	-2.008206	-2.992663
6	-1.453011	1.395398	1.557647	1	1.709472	-1.549620	-3.110820
6	-1.956911	1.508541	2.863657	6	4.513590	-3.234389	-1.040171
6	-1.216740	2.553953	0.806970	1	2.942168	-3.732250	0.362178
6	-2.254686	2.762336	3.391466	6	4.845185	-2.598756	-2.244463
1	-2.110257	0.620298	3.467769	1	4.053726	-1.520379	-3.934725
6	-1.507224	3.808995	1.343098	1	5.295451	-3.714570	-0.457437
1	-0.794100	2.481611	-0.186991	6	6.278335	-2.521310	-2.708705
6	-2.033400	3.913731	2.630284	1	6.348894	-2.557824	-3.799872
1	-2.651712	2.842702	4.398369	1	6.877144	-3.340437	-2.300655
1	-1.315613	4.696848	0.750614	1	6.742744	-1.581663	-2.384000
1	-2.263079	4.889587	3.046469	6	4.091565	0.198554	3.803472
6	-2.398964	-1.369451	1.063948	6	2.757164	0.502540	3.554035
6	-2.188603	-2.704866	0.675476	6	1.903098	-0.473249	3.014452
6	-3.662000	-0.957310	1.502018	6	2.407776	-1.749828	2.707436
6	-3.238171	-3.617464	0.751358	6	3.744441	-2.041347	2.964107
1	-1.214509	-3.020396	0.313059	6	4.588403	-1.073325	3.512210
6	-4.706816	-1.879202	1.570574	1	4.748488	0.960491	4.210352
1	-3.839724	0.078499	1.764628	1	2.368484	1.493512	3.762996
6	-4.496673	-3.207336	1.200720	1	1.745729	-2.485508	2.265500
1	-3.073687	-4.649111	0.456491	1	4.130336	-3.029187	2.729946
1	-5.686378	-1.554462	1.906326	1	5.631909	-1.305303	3.703204
1	-5.312042	-3.921768	1.256290	6	0.523034	-0.180977	2.740378
6	2.033879	0.519112	0.952699	6	-0.736319	-0.204269	2.895694
8	3.094405	1.300237	1.196987	6	-1.904797	-0.670860	3.706148
6	2.390630	1.495038	-1.052901	1	-1.780778	-0.335476	4.740537
6	3.400175	2.055110	-0.013372	1	-2.840531	-0.256918	3.320210
7	1.582392	0.536941	-0.261619	8	-1.974262	-2.089353	3.780294
6	3.088578	3.554780	0.178832	6	-2.182647	-2.732760	2.541373
1	2.849867	3.756256	1.228009	1	-2.058680	-3.806532	2.721390
1	3.956753	4.171577	-0.076222	1	-1.411844	-2.459540	1.809919
6	1.923905	3.822547	-0.749567	6	-3.578048	-2.492277	1.965185
6	1.225707	5.015730	-0.935547	8	-4.410637	-1.849581	2.591074
6	1.575717	2.688099	-1.486729	6	-3.884539	-3.022929	0.602109
6	0.179215	5.052618	-1.860745	6	-2.909688	-3.616266	-0.211662
1	1.489249	5.905508	-0.371533	6	-5.190365	-2.849743	0.111412
6	0.544409	2.721942	-2.425061	6	-3.239027	-4.020852	-1.506729
6	-0.159153	3.915116	-2.604201	1	-1.887165	-3.739062	0.126070
1	-0.370084	5.976394	-2.013443	6	-5.517906	-3.270214	-1.172230
1	0.285244	1.834057	-2.993134	1	-5.921480	-2.376310	0.757892
1	-0.966178	3.963495	-3.328309	6	-4.538271	-3.855484	-1.985513
1	4.443448	1.846410	-0.247093	1	-2.464457	-4.439051	-2.139838
1	2.851850	0.947648	-1.877859	1	-6.529895	-3.141936	-1.545331
				1	-4.789979	-4.171728	-2.993770
				1	-1.194439	1.093126	1.925392
				6	1.101314	1.363178	-1.801887
				6	-0.055185	0.819611	-2.408174
				6	-0.037333	0.515528	-3.779982

TS2_iso

SCF Energy = -3424.889474

Gibbs Free Energy = -3424.149528

6	1.094568	0.745652	-4.554253	8	-2.058993	2.693855	-0.928384
6	2.234923	1.282732	-3.960822	16	-1.474712	1.365158	-1.255975
6	2.230609	1.581495	-2.599960	8	-0.431240	1.431613	-2.306713
1	-0.921618	0.079018	-4.224305	8	-1.058118	0.623234	-0.007667
1	1.085485	0.497109	-5.610627	6	-2.780226	0.327934	-1.924940
1	3.129836	1.462557	-4.548983	6	-3.512840	-0.509558	-1.086283
1	3.130847	1.973743	-2.142181	6	-3.048852	0.366896	-3.292263
15	1.147638	1.819832	-0.008648	6	-4.525019	-1.302248	-1.620253
6	0.680227	3.592243	-0.098262	1	-3.285637	-0.544630	-0.029396
6	1.381954	4.536364	-0.863870	6	-4.063490	-0.431680	-3.815725
6	-0.487293	3.986011	0.567606	1	-2.445709	1.000518	-3.933012
6	0.929250	5.851073	-0.945256	6	-4.819355	-1.273739	-2.988872
1	2.278536	4.240942	-1.398972	1	-5.097598	-1.948725	-0.960814
6	-0.949739	5.299275	0.472785	1	-4.269461	-0.407024	-4.882979
1	-1.040448	3.251095	1.140483	6	-5.941157	-2.109716	-3.553948
6	-0.239172	6.233842	-0.279156	1	-5.762736	-2.365553	-4.602625
1	1.480660	6.576475	-1.536154	1	-6.069456	-3.040104	-2.992394
1	-1.867924	5.582996	0.978011	1	-6.895562	-1.570294	-3.508937
1	-0.595197	7.257027	-0.354353	6	1.160059	2.464045	1.344271
6	2.937909	1.768027	0.354242	6	0.534217	1.850213	2.232841
6	3.601458	0.540773	0.169180	6	-0.373454	1.716346	3.406079
6	3.640099	2.853640	0.891767	1	0.210005	1.814286	4.328045
6	4.951729	0.423357	0.478374	1	-0.846406	0.732330	3.414591
1	3.053127	-0.314440	-0.204283	8	-1.339410	2.753666	3.441154
6	4.994030	2.724205	1.211069	6	-2.329279	2.659102	2.433603
1	3.136817	3.800720	1.054532	1	-2.844781	3.625255	2.416625
6	5.653794	1.514894	0.996830	1	-1.894092	2.510427	1.436525
1	5.445140	-0.531779	0.330284	6	-3.352089	1.557183	2.703778
1	5.531273	3.573803	1.622673	8	-3.223485	0.806157	3.663729
1	6.707173	1.418869	1.243199	6	-4.498691	1.406589	1.759317
6	-1.315153	0.531393	-1.697251	6	-4.634210	2.194121	0.607051
8	-2.364260	0.258237	-2.494552	6	-5.458629	0.419398	2.036439
6	-2.997616	0.234880	-0.242739	6	-5.707029	1.983895	-0.258083
6	-3.468767	-0.190567	-1.653549	1	-3.877739	2.918795	0.337563
7	-1.559180	0.512772	-0.427972	6	-6.528259	0.214922	1.172684
6	-4.736971	0.604452	-1.979643	1	-5.345406	-0.170028	2.939554
1	-4.719603	0.969528	-3.010971	6	-6.652351	0.998219	0.020284
1	-5.611941	-0.048391	-1.877200	1	-5.785443	2.576942	-1.163359
6	-4.758181	1.705079	-0.941862	1	-7.265629	-0.551685	1.392385
6	-5.594731	2.818181	-0.876537	1	-7.480753	0.831715	-0.662149
6	-3.813972	1.472812	0.064603	1	1.363566	-0.021260	2.251823
6	-5.481964	3.690662	0.208183	6	0.027001	-1.975039	-0.951068
1	-6.326506	3.005823	-1.657344	6	0.603832	-1.327433	-2.061800
6	-3.717583	2.327379	1.160887	6	0.101424	-1.567389	-3.344026
6	-4.553975	3.443395	1.225306	6	-0.981101	-2.423972	-3.528794
1	-6.126490	4.562589	0.267493	6	-1.556465	-3.061316	-2.432855
1	-3.002710	2.129485	1.952508	6	-1.048593	-2.841753	-1.151443
1	-4.488445	4.118699	2.073180	1	0.542723	-1.045199	-4.183623
1	-3.557970	-1.266080	-1.795463	1	-1.385210	-2.575732	-4.523831
1	-3.117373	-0.541999	0.507610	1	-2.414447	-3.711521	-2.566352
				1	-1.505604	-3.331246	-0.299456
				15	0.706869	-1.676529	0.724465
				6	2.209681	-2.716030	0.741218
				6	2.296401	-3.886691	-0.027471
				6	3.312175	-2.309872	1.503576
28	1.069650	0.444161	0.932543	6	3.467590	-4.642905	-0.021816

TS2

SCF Energy = -3424.896778

Gibbs Free Energy = -3424.156720

1	1.453759	-4.196931	-0.636575	16	1.407562	1.544692	1.106832
6	4.483370	-3.065551	1.502925	8	0.343468	1.502784	2.142028
1	3.259016	-1.388337	2.070706	8	1.152892	0.630689	-0.068869
6	4.562204	-4.232289	0.741947	6	2.860888	0.819026	1.873824
1	3.527844	-5.547302	-0.619779	6	3.762174	0.081090	1.108481
1	5.337997	-2.727666	2.078461	6	3.076819	0.999483	3.238803
1	5.477668	-4.816369	0.735872	6	4.887138	-0.471046	1.714800
6	-0.490797	-2.453890	1.852207	1	3.576703	-0.066259	0.052785
6	-1.611149	-1.694283	2.223396	6	4.205675	0.441111	3.835105
6	-0.325752	-3.749278	2.357761	1	2.347176	1.549730	3.822333
6	-2.554858	-2.226027	3.098924	6	5.128898	-0.298101	3.083443
1	-1.732215	-0.694775	1.821535	1	5.589469	-1.041251	1.112820
6	-1.279196	-4.279593	3.228536	1	4.370962	0.574398	4.901423
1	0.543042	-4.336042	2.078900	6	6.367484	-0.871855	3.726625
6	-2.389526	-3.519658	3.600041	1	7.204538	-0.164695	3.670598
1	-3.391156	-1.608279	3.404823	1	6.203443	-1.095990	4.784923
1	-1.148076	-5.283040	3.622612	1	6.687988	-1.791841	3.228344
1	-3.121453	-3.931730	4.288464	6	-1.397979	1.912231	-1.464735
6	1.717723	-0.378156	-1.911508	6	-0.686922	1.372678	-2.340406
8	2.530941	-0.266544	-2.983363	6	0.218109	1.329083	-3.522025
6	3.237186	1.099514	-1.188252	1	-0.383810	1.254639	-4.434637
6	3.596335	0.658323	-2.635162	1	0.862638	0.448998	-3.477224
7	2.010061	0.338480	-0.882556	8	0.980399	2.517792	-3.654507
6	4.962129	-0.061440	-2.579887	6	1.983513	2.676847	-2.668379
1	4.858720	-1.084965	-2.955239	1	2.321254	3.716375	-2.737632
1	5.699373	0.441419	-3.215678	1	1.593002	2.534114	-1.652135
6	5.359926	-0.013493	-1.120215	6	3.181194	1.752399	-2.877882
6	6.512988	-0.522785	-0.524026	8	3.176536	0.911886	-3.770075
6	4.410769	0.661266	-0.347913	6	4.348114	1.883827	-1.954952
6	6.705170	-0.340904	0.847620	6	4.356322	2.774557	-0.871993
1	7.255951	-1.049938	-1.116056	6	5.464265	1.061145	-2.178903
6	4.594844	0.840790	1.021371	6	5.459400	2.826258	-0.020970
6	5.753259	0.337745	1.616519	1	3.486889	3.374773	-0.640292
1	7.603087	-0.727774	1.320689	6	6.563110	1.117455	-1.329438
1	3.840353	1.347547	1.612298	1	5.446988	0.390437	-3.030664
1	5.915443	0.471717	2.681981	6	6.560433	2.001456	-0.245300
1	3.562987	1.466346	-3.366421	1	5.442686	3.496168	0.832470
1	3.021894	2.163390	-1.098503	1	7.421568	0.476400	-1.507782
6	1.763412	3.490850	0.541087	1	7.412963	2.038453	0.426665
6	3.019338	4.017848	0.896637	1	-1.098777	-0.618931	-2.205733
6	1.129668	3.940991	-0.632762	6	0.499423	-1.987547	1.186080
6	3.644868	4.953329	0.076908	6	-0.255595	-1.394224	2.217721
1	3.499070	3.680125	1.808791	6	0.220157	-1.415762	3.531470
6	1.764428	4.881247	-1.440218	6	1.453398	-1.993585	3.822935
1	0.156713	3.550667	-0.903353	6	2.207203	-2.572376	2.804995
6	3.023567	5.381648	-1.098597	6	1.727498	-2.574731	1.494566
1	4.617456	5.347352	0.356070	1	-0.368175	-0.945144	4.309705
1	1.270186	5.218942	-2.345940	1	1.831062	-1.975503	4.839650
1	3.514708	6.107729	-1.739615	1	3.179697	-3.001298	3.021113
				1	2.320356	-3.019624	0.704146
TS2_c				15	-0.156972	-1.984075	-0.525510
SCF Energy = -3539.427817				6	-1.441612	-3.284670	-0.474247
Gibbs Free Energy = -3538.659219				6	-1.414093	-4.308722	0.483717
				6	-2.496087	-3.232555	-1.396004
28	-0.920041	-0.003903	-0.927130	6	-2.425213	-5.269338	0.512262
8	1.749252	2.921308	0.668959	1	-0.608719	-4.348110	1.209434

6	-3.499916	-4.198234	-1.369176				
1	-2.542247	-2.419362	-2.111194	28	0.613285	0.503864	-1.199726
6	-3.467652	-5.215800	-0.414441	8	-1.552013	-3.044006	-0.144051
1	-2.398543	-6.057134	1.259213	16	-1.269475	-1.807254	0.637531
1	-4.318633	-4.138222	-2.077295	8	-0.101857	-1.950274	1.539473
1	-4.257196	-5.960925	-0.387423	8	-1.234518	-0.590034	-0.254002
6	1.199427	-2.631528	-1.550094	6	-2.677340	-1.486047	1.705858
6	2.127533	-1.708608	-2.055080	6	-3.680361	-0.607323	1.302827
6	1.332650	-3.993335	-1.850305	6	-2.752704	-2.122088	2.944111
6	3.175635	-2.145082	-2.862285	6	-4.769253	-0.376879	2.138649
1	2.021648	-0.659242	-1.807633	1	-3.602038	-0.105631	0.348195
6	2.390561	-4.425723	-2.651067	6	-3.846820	-1.883097	3.772950
1	0.611377	-4.707895	-1.467552	1	-1.945568	-2.776098	3.255238
6	3.308128	-3.503672	-3.158521	6	-4.873442	-1.013109	3.381324
1	3.857790	-1.410907	-3.274890	1	-5.552680	0.303374	1.816110
1	2.491076	-5.481284	-2.885843	1	-3.904338	-2.374274	4.741162
1	4.121316	-3.843369	-3.793258	6	-6.076561	-0.787743	4.263362
6	-1.550334	-0.753967	1.941417	1	-5.839912	-0.958593	5.317670
8	-2.457526	-0.811666	2.942358	1	-6.463481	0.230788	4.160796
6	-3.328767	0.244861	1.011609	1	-6.892515	-1.471547	3.997571
6	-3.710776	-0.297138	2.418149	6	1.071607	-1.163122	-2.373307
7	-1.922096	-0.179365	0.851206	6	0.176145	-0.472387	-2.893765
6	-4.739937	-1.433658	2.210654	6	-0.932830	-0.181547	-3.843948
1	-4.293034	-2.389232	2.506878	1	-0.515834	0.228345	-4.770230
1	-5.632638	-1.289264	2.828288	1	-1.609809	0.565459	-3.425556
6	-5.054267	-1.393456	0.731093	8	-1.627653	-1.360919	-4.212465
6	-5.993744	-2.146572	0.029163	6	-2.422079	-1.912898	-3.178605
6	-4.267835	-0.452642	0.060964	1	-2.692227	-2.923217	-3.503952
6	-6.132004	-1.946556	-1.346610	1	-1.865684	-2.016930	-2.237767
1	-6.611651	-2.878670	0.541472	6	-3.700918	-1.118467	-2.920472
6	-4.398100	-0.250791	-1.311275	8	-3.916284	-0.070462	-3.518280
6	-5.337905	-1.007732	-2.014189	6	-4.670414	-1.641353	-1.912712
1	-6.864711	-2.524269	-1.902746	6	-4.419009	-2.791283	-1.150623
1	-3.775487	0.477292	-1.818465	6	-5.866559	-0.931836	-1.716298
1	-5.457545	-0.862435	-3.083702	6	-5.347107	-3.213302	-0.199695
1	-4.053345	0.470771	3.111912	1	-3.479484	-3.320493	-1.237821
1	-3.374820	1.330914	0.930587	6	-6.790695	-1.358068	-0.769770
6	-2.221277	2.859480	-0.768479	1	-6.048488	-0.051539	-2.322868
6	-1.913164	3.276023	0.544824	6	-6.529707	-2.501411	-0.007053
6	-3.382168	3.357379	-1.380359	1	-5.129000	-4.085765	0.407447
6	-2.749120	4.159379	1.207912	1	-7.712671	-0.803339	-0.621772
1	-1.035072	2.883611	1.044683	1	-7.244943	-2.828619	0.742023
6	-4.229726	4.239177	-0.711735	1	0.547105	1.454480	-2.266115
1	-3.623818	3.044814	-2.391164	6	-0.677269	1.754557	1.498003
1	-2.520831	4.489818	2.215528	6	0.167455	0.922930	2.258677
1	-5.119813	4.600916	-1.211155	6	-0.209963	0.549637	3.552209
6	-3.913504	4.644273	0.590841	6	-1.422192	0.979025	4.086935
8	-4.669624	5.496496	1.337849	6	-2.257965	1.802132	3.337256
6	-5.847668	6.027382	0.753991	6	-1.882112	2.192366	2.050890
1	-6.290042	6.681095	1.506757	1	0.438917	-0.111086	4.112718
1	-5.622998	6.612472	-0.146767	1	-1.719970	0.653686	5.077908
1	-6.563146	5.235689	0.496487	1	-3.212923	2.124260	3.738889
				1	-2.541366	2.821796	1.464807
TS2_g				15	-0.178918	2.243422	-0.195461
SCF Energy = -3652.789602				6	1.022993	3.586132	0.099328
Gibbs Free Energy = -3652.013346				6	0.929586	4.412943	1.229237

6	2.083228	3.762687	-0.797895	1	7.293163	-4.349833	2.086087
6	1.880443	5.408290	1.447903				
1	0.122623	4.267730	1.939915				
6	3.037171	4.753517	-0.571774				
1	2.172761	3.103454	-1.652881				
6	2.936039	5.577677	0.549101				
1	1.803371	6.043844	2.324931	6	0.140412	-2.959430	-0.536507
1	3.869902	4.861802	-1.258167	6	-1.216595	-3.278809	-0.299793
1	3.683901	6.344132	0.729151	6	-1.791224	-4.390522	-0.929789
6	-1.671863	3.010608	-0.899930	6	-1.051871	-5.185312	-1.798700
6	-2.649822	2.150543	-1.423745	6	0.284168	-4.877523	-2.037000
6	-1.865214	4.396438	-0.942492	6	0.869306	-3.780398	-1.407795
6	-3.808976	2.674932	-1.990315	1	-2.831733	-4.613194	-0.731022
1	-2.492133	1.078510	-1.382083	1	-1.518428	-6.036340	-2.284478
6	-3.032151	4.916121	-1.506012	1	0.879300	-5.488504	-2.708751
1	-1.108946	5.064148	-0.543724	1	1.910685	-3.562535	-1.602578
6	-4.000490	4.058536	-2.030000	15	1.005660	-1.526139	0.246423
1	-4.533187	1.995407	-2.424560	6	2.767180	-1.953080	-0.085411
1	-3.178846	5.991593	-1.541568	6	3.498804	-2.868171	0.682898
1	-4.900784	4.468211	-2.478416	6	3.388304	-1.321066	-1.173000
6	1.433315	0.394275	1.723203	6	4.827213	-3.147721	0.363464
8	2.365242	0.099773	2.649113	1	3.037527	-3.350166	1.537381
6	3.130776	-0.329200	0.464232	6	4.714298	-1.605383	-1.493803
6	3.513264	-0.475503	1.957777	1	2.838884	-0.587545	-1.752779
7	1.744939	0.183806	0.489728	6	5.435565	-2.520851	-0.726422
6	4.788534	0.353106	2.196529	1	5.389619	-3.851797	0.969344
1	4.663201	1.021968	3.054070	1	5.186448	-1.094478	-2.326642
1	5.625797	-0.318248	2.413993	1	6.472314	-2.734948	-0.967281
6	5.013774	1.087433	0.891675	6	0.835872	-1.824228	2.047617
6	5.990015	2.034987	0.585777	6	0.892229	-0.731049	2.920906
6	4.110769	0.672488	-0.091363	6	0.658757	-3.111530	2.571473
6	6.057213	2.548505	-0.712092	6	0.776481	-0.921956	4.296945
1	6.694865	2.367604	1.342873	1	1.012104	0.269010	2.520908
6	4.174197	1.179149	-1.386955	6	0.539500	-3.300059	3.948200
6	5.158696	2.120098	-1.695264	1	0.593472	-3.964069	1.903232
1	6.816954	3.283908	-0.960760	6	0.598471	-2.206434	4.813737
1	3.456039	0.858118	-2.134543	1	0.819749	-0.065908	4.963518
1	5.224409	2.525688	-2.700856	1	0.397301	-4.301441	4.343541
1	3.603456	-1.508528	2.287551	1	0.503451	-2.354357	5.885187
1	3.157094	-1.276215	-0.060833	6	-2.067548	-2.492931	0.602276
6	2.040276	-2.144354	-1.988972	8	-3.203462	-3.125389	1.025224
6	3.359799	-2.055596	-2.471270	6	-2.986761	-0.927664	1.870254
6	1.715621	-3.119880	-1.026113	6	-3.892852	-2.205084	1.905852
6	4.361095	-2.853279	-1.928649	7	-1.840797	-1.311659	1.025712
1	3.602133	-1.320200	-3.229750	6	-5.270254	-1.827807	1.328479
6	2.719836	-3.917075	-0.487058	1	-5.538424	-2.516484	0.520828
1	0.695436	-3.212775	-0.673323	1	-6.050972	-1.909786	2.094185
6	4.033246	-3.747383	-0.914443	6	-5.107494	-0.399991	0.862995
1	5.391099	-2.761011	-2.254477	6	-6.033477	0.390081	0.183122
1	2.494259	-4.638535	0.290358	6	-3.860752	0.123389	1.219528
8	5.049551	-4.500783	-0.312615	6	-5.703010	1.713660	-0.117724
6	5.704902	-3.911167	0.731598	1	-7.000412	-0.014108	-0.104184
8	5.456054	-2.801500	1.142750	6	-3.530762	1.444567	0.931703
6	6.756460	-4.841293	1.275818	6	-4.465049	2.240739	0.265119
1	6.284724	-5.758311	1.640627	1	-6.415769	2.340251	-0.645826
1	7.450415	-5.126499	0.480342	1	-2.564766	1.845757	1.204041

TS3C
SCF Energy = -3168.535744
Gibbs Free Energy = -3167.735978

1	-4.218529	3.273308	0.045530	1	2.383462	4.530693	0.232805
1	-3.954575	-2.685874	2.884478	1	2.034831	3.898826	1.836571
1	-2.613553	-0.617546	2.852013	1	2.256291	0.934428	0.699837
28	0.871807	0.604318	-0.343264				
6	-1.342756	-2.234794	-3.732354				
6	-0.679256	-1.252540	-3.001402				
6	-1.384387	-0.376898	-2.159039				
6	-2.780335	-0.523587	-2.067057				
6	-3.442328	-1.517791	-2.784579	28	-0.137407	-0.067299	-1.256912
6	-2.727380	-2.377657	-3.620653	6	5.134166	0.108447	-2.776362
1	-0.777320	-2.901546	-4.376128	6	3.794915	-0.236479	-2.884932
1	0.399347	-1.149352	-3.077284	6	2.840251	0.299191	-1.984288
1	-3.335175	0.138634	-1.414892	6	3.271346	1.238039	-1.023672
1	-4.520085	-1.617568	-2.688696	6	4.610183	1.589343	-0.923323
1	-3.242465	-3.154480	-4.178160	6	5.544402	1.014518	-1.788830
6	-0.689301	0.691464	-1.430223	1	5.861634	-0.310420	-3.464044
6	-1.055049	1.980662	-1.543067	1	3.466379	-0.914350	-3.664466
6	-2.008223	2.688368	-2.464320	1	2.535258	1.687624	-0.375074
1	-3.015025	2.808185	-2.046510	1	4.927471	2.304979	-0.172388
1	-2.098660	2.174897	-3.430556	1	6.593068	1.283404	-1.708607
8	-1.448921	4.011999	-2.640273	6	1.461692	-0.070787	-2.067737
6	-0.134330	4.043944	-2.072805	6	0.754360	-1.038416	-2.770121
1	0.622870	3.713569	-2.796966	6	1.135562	-2.512892	-2.879959
1	0.073183	5.074828	-1.771959	1	0.334207	-3.038417	-3.403804
6	-0.161417	3.028257	-0.912102	1	2.057549	-2.649694	-3.464478
8	1.077995	2.414591	-0.652413	8	1.269522	-3.189665	-1.633919
6	-0.786174	3.600016	0.365397	6	2.475067	-2.980708	-0.939622
6	-1.744502	4.622099	0.327523	1	3.271356	-2.654093	-1.617898
6	-0.449730	3.053832	1.610610	1	2.792202	-3.943737	-0.515098
6	-2.338284	5.086187	1.503442	6	2.347674	-2.006615	0.237102
1	-2.038598	5.039457	-0.629781	8	1.245742	-1.624551	0.611446
6	-1.039730	3.516402	2.785540	6	3.586566	-1.578418	0.939283
1	0.278144	2.253361	1.647877	6	4.867730	-1.737938	0.390106
6	-1.990753	4.537205	2.737781	6	3.449784	-0.955457	2.191836
1	-3.078714	5.879538	1.451226	6	5.986241	-1.258883	1.069110
1	-0.758650	3.075793	3.738226	1	5.003710	-2.206682	-0.576922
1	-2.455035	4.899097	3.650149	6	4.567698	-0.485816	2.871278
14	3.150214	2.180313	0.440635	1	2.457294	-0.858915	2.617021
8	3.852406	2.018462	-1.050892	6	5.839152	-0.630597	2.306280
8	4.315750	1.731439	1.549930	1	6.972493	-1.375452	0.631916
6	3.537521	2.726519	-2.247609	1	4.454528	-0.019629	3.845100
1	4.475204	3.157185	-2.620484	1	6.713110	-0.262845	2.834726
1	2.846650	3.547296	-2.035253	1	-0.017059	-0.706548	-3.469211
6	2.929930	1.799766	-3.289541	6	-1.796165	2.517730	-0.893582
1	1.973102	1.411221	-2.932054	6	-2.852851	1.849476	-1.564178
1	2.757135	2.341753	-4.226210	6	-3.724384	2.568597	-2.389381
1	3.605130	0.963821	-3.501449	6	-3.525069	3.931045	-2.609873
6	5.027433	0.500343	1.573782	6	-2.447533	4.576524	-2.009066
1	5.243921	0.272092	2.624724	6	-1.594239	3.875004	-1.152039
1	4.405442	-0.313757	1.186904	1	-4.543236	2.047136	-2.871355
6	6.321887	0.599604	0.777206	1	-4.200210	4.477498	-3.259518
1	6.882143	-0.339505	0.838291	1	-2.269278	5.630610	-2.195610
1	6.100563	0.809629	-0.271816	1	-0.765443	4.394743	-0.688151
1	6.946427	1.408326	1.168879	15	-0.716141	1.512964	0.192027
6	2.777358	3.907502	1.036449	6	-1.859044	0.819690	1.448454
1	3.704518	4.337907	1.425994	6	-3.101483	1.399520	1.731783

TS3D

SCF Energy = -2529.880704

Gibbs Free Energy = -2529.252596

6	-1.430144	-0.305714	2.166000	1	-3.900584	2.747114	-1.677381
6	-3.914977	0.848654	2.723336	6	-6.094448	1.625076	0.699526
1	-3.438110	2.273423	1.184162	1	-5.528167	1.124426	2.718271
6	-2.240544	-0.838320	3.165768	1	-6.326354	2.239933	-1.350175
1	-0.480573	-0.772720	1.928768	6	-7.546552	1.264116	0.890061
6	-3.484542	-0.268222	3.441169	1	-7.891909	1.510595	1.898782
1	-4.878847	1.299064	2.939756	1	-7.703469	0.187759	0.745882
1	-1.912354	-1.717756	3.707405	1	-8.186484	1.786434	0.173603
1	-4.118450	-0.694955	4.211999	6	1.325408	1.368124	-2.292822
6	0.331353	2.583204	1.237753	6	0.443072	0.547960	-2.729988
6	1.514316	2.000875	1.716853	6	-0.261041	0.043187	-3.942260
6	-0.064208	3.834506	1.733036	1	0.122200	0.570364	-4.822731
6	2.323529	2.683494	2.623441	1	-0.044855	-1.026323	-4.058786
1	1.785403	1.001383	1.396963	8	-1.666554	0.260878	-3.977547
6	0.751502	4.518231	2.633914	6	-2.383577	-0.158501	-2.839006
1	-1.012563	4.269026	1.439348	1	-3.412935	0.195398	-2.969790
6	1.950762	3.951334	3.071233	1	-1.993736	0.309055	-1.925862
1	3.239184	2.219604	2.976487	6	-2.402222	-1.660742	-2.630490
1	0.443387	5.490772	3.004350	8	-1.825286	-2.420483	-3.402633
1	2.580636	4.489556	3.772325	6	-3.112032	-2.194424	-1.427002
6	-3.035364	0.388250	-1.473355	6	-3.635562	-1.362296	-0.427111
8	-4.284394	-0.067867	-1.644812	6	-3.248383	-3.586601	-1.308869
6	-2.733160	-1.841553	-1.354496	6	-4.291357	-1.920590	0.669788
6	-4.253007	-1.513904	-1.447735	1	-3.512521	-0.289793	-0.477206
7	-2.105889	-0.497427	-1.304675	6	-3.895658	-4.140743	-0.209875
6	-4.892840	-1.912357	-0.100196	1	-2.840980	-4.208015	-2.099502
1	-5.147437	-1.008277	0.464582	6	-4.422506	-3.305466	0.780804
1	-5.817450	-2.479766	-0.241357	1	-4.684584	-1.263458	1.437452
6	-3.814341	-2.710666	0.595519	1	-3.999641	-5.218479	-0.125245
6	-3.916348	-3.447814	1.772894	1	-4.933787	-3.736290	1.637187
6	-2.598740	-2.654037	-0.091765	1	2.102955	0.545970	-1.205131
6	-2.785676	-4.114296	2.251725	6	0.060546	0.027814	2.313974
1	-4.858308	-3.507477	2.309927	6	-0.674412	-1.142506	2.023001
6	-1.466365	-3.314683	0.376616	6	-1.731185	-1.526880	2.853448
6	-1.569622	-4.043380	1.563330	6	-2.090682	-0.733902	3.942522
1	-2.853886	-4.697702	3.165041	6	-1.383426	0.436224	4.214264
1	-0.530066	-3.259275	-0.166175	6	-0.308208	0.811734	3.404863
1	-0.702098	-4.570912	1.947778	1	-2.276078	-2.433662	2.623207
1	-4.753831	-1.955714	-2.308676	1	-2.922735	-1.030292	4.573561
1	-2.331526	-2.361253	-2.230531	1	-1.665126	1.062598	5.055043
				1	0.232549	1.727795	3.607653
				15	1.470790	0.471228	1.235289
TS3				6	2.724365	-0.797947	1.669332
SCF Energy = -3424.890985				6	2.582857	-1.661679	2.762766
Gibbs Free Energy = -3424.152378				6	3.861840	-0.906705	0.856213
				6	3.562071	-2.620308	3.034126
28	0.751008	0.232119	-0.823005	6	3.562071	-2.620308	3.034126
8	-1.445796	3.157440	-1.194407	1	1.710062	-1.589539	3.401715
16	-1.614647	2.355212	0.035835	6	4.843982	-1.850638	1.138232
8	-1.016222	2.910908	1.269586	1	3.967300	-0.260060	-0.008727
8	-1.240120	0.893818	-0.165191	6	4.693526	-2.714537	2.225343
6	-3.377791	2.192989	0.323753	1	3.439935	-3.287081	3.882690
6	-3.823292	1.744006	1.567853	1	5.712476	-1.931242	0.493845
6	-4.273148	2.382096	-0.726476	1	5.453311	-3.461197	2.435476
6	-5.175794	1.469103	1.748801	6	2.191554	2.030223	1.832213
1	-3.110828	1.612144	2.373837	6	1.968591	3.198427	1.090876
6	-5.625077	2.096470	-0.532331	6	3.006114	2.071187	2.974184

1	-2.584026	-1.794931	0.657707	1	1.572812	-3.130799	2.429580
6	-4.232035	-0.408793	3.883182	6	2.749760	-5.458112	-0.433042
1	-2.749692	1.149691	3.795154	1	1.031336	-4.696549	-1.517092
6	-4.745162	-1.552626	3.265515	6	3.489791	-5.415547	0.754741
1	-4.553075	-2.927725	1.612451	1	3.595740	-4.549770	2.726216
1	-4.692256	-0.023512	4.788163	1	3.071199	-6.114066	-1.237831
1	-5.607920	-2.056225	3.691821	6	4.752941	-6.225214	0.910371
6	1.657787	1.692287	0.676883	1	4.889634	-6.560405	1.942970
8	2.542141	2.713970	0.720496	1	5.634418	-5.629700	0.641222
6	1.307101	2.691148	-1.300908	1	4.745609	-7.107121	0.263812
6	2.327471	3.522032	-0.469493	6	-1.640487	0.135623	-2.067071
7	0.955176	1.575216	-0.396499	6	-0.488542	0.025403	-2.619001
6	1.650018	4.866717	-0.116210	6	0.224406	-0.185699	-3.911638
1	1.464265	4.911203	0.962747	1	-0.513719	-0.276526	-4.715949
1	2.285693	5.720631	-0.372911	1	0.851177	0.691904	-4.115677
6	0.357505	4.855258	-0.901997	8	1.003554	-1.371370	-4.004306
6	-0.578584	5.879027	-1.035243	6	1.913544	-1.595086	-2.951493
6	0.159674	3.635955	-1.554746	1	2.330022	-2.597425	-3.105986
6	-1.713014	5.663285	-1.820904	1	1.405624	-1.601558	-1.979044
1	-0.431055	6.832064	-0.535249	6	3.050756	-0.593791	-2.885413
6	-0.970554	3.413519	-2.338063	8	3.143047	0.323191	-3.695960
6	-1.911625	4.437359	-2.464720	6	4.040647	-0.727112	-1.771972
1	-2.446882	6.455933	-1.934586	6	3.874351	-1.635899	-0.717123
1	-1.112892	2.461403	-2.837961	6	5.172971	0.102419	-1.797059
1	-2.796062	4.285111	-3.076146	6	4.833805	-1.714493	0.292128
1	3.298590	3.635821	-0.949032	1	2.993166	-2.258093	-0.654803
1	1.720076	2.280821	-2.223143	6	6.123943	0.027584	-0.785177
6	-3.103792	-1.151870	-1.938394	1	5.281558	0.792841	-2.627005
6	-3.120783	-2.546938	-2.074625	6	5.956271	-0.886032	0.260844
6	-4.292636	-0.487826	-1.587353	1	4.686224	-2.418485	1.103621
6	-4.300302	-3.264385	-1.877405	1	6.998865	0.670516	-0.811388
1	-2.188441	-3.066110	-2.261225	1	6.701242	-0.949595	1.049132
6	-5.469415	-1.192547	-1.400041	1	-1.455587	1.266141	-1.013332
1	-4.281596	0.589279	-1.446239	6	0.641583	0.195904	2.341959
6	-5.479588	-2.589489	-1.540483	6	1.968438	0.426210	1.916274
1	-4.279398	-4.343107	-1.968480	6	3.037452	-0.072660	2.666570
1	-6.391600	-0.692836	-1.124600	6	2.796988	-0.832829	3.810428
8	-6.678698	-3.195693	-1.311888	6	1.486994	-1.083946	4.215829
6	-6.737303	-4.609639	-1.413568	6	0.413864	-0.567118	3.485168
1	-6.068965	-5.093906	-0.690352	1	4.048599	0.124141	2.333285
1	-7.769166	-4.885550	-1.192473	1	3.632120	-1.229013	4.379562
1	-6.478564	-4.952666	-2.423154	1	1.293742	-1.683445	5.100065
				1	-0.604374	-0.771593	3.792733
				15	-0.732605	0.916846	1.372601
				6	-0.582329	2.710373	1.739469
				6	0.259032	3.214696	2.739012
				6	-1.341649	3.605048	0.971455
				6	0.341452	4.591373	2.961938
				1	0.851121	2.536856	3.343344
				6	-1.270970	4.974296	1.206231
				1	-1.977210	3.225439	0.177968
				6	-0.423858	5.471854	2.199036
				1	0.999894	4.970947	3.737818
				1	-1.854961	5.654936	0.596530
				1	-0.357873	6.541857	2.371272
				6	-2.308867	0.442113	2.142597
28	-0.269209	0.497918	-0.731999				
8	-0.890419	-3.142623	-1.011628				
16	-0.132020	-2.662717	0.164441				
8	-0.884370	-2.546442	1.432313				
8	0.666335	-1.402493	-0.134675				
6	1.203808	-3.829688	0.433214				
6	1.911607	-3.784501	1.634802				
6	1.610024	-4.670982	-0.600212				
6	3.044163	-4.578945	1.789364				

TS3_g

SCF Energy = -3652.781311

Gibbs Free Energy = -3652.006938

6	-3.110417	-0.511179	1.499981	6	-1.236500	-1.426394	2.158265
6	-2.762600	1.058772	3.319144	6	-2.402806	-0.684450	2.468745
6	-4.359990	-0.841459	2.023131	6	-2.862121	-0.650153	3.793208
1	-2.753452	-1.004266	0.607264	6	-2.189825	-1.331823	4.802446
6	-4.005314	0.715365	3.847299	6	-1.050223	-2.070649	4.495934
1	-2.152129	1.811423	3.808441	6	-0.581142	-2.112612	3.184081
6	-4.804082	-0.228909	3.195856	1	-3.746854	-0.070370	4.021793
1	-4.983938	-1.563654	1.508124	1	-2.553833	-1.278984	5.823334
1	-4.354422	1.191728	4.758797	1	-0.517100	-2.607223	5.274578
1	-5.778315	-0.485472	3.602070	1	0.318831	-2.671169	2.958125
6	2.264170	1.230523	0.716093	15	-0.516122	-1.368125	0.479406
8	3.389016	1.977490	0.780302	6	-1.525680	-2.530411	-0.514268
6	2.205622	2.324254	-1.242212	6	-2.420716	-3.436674	0.065715
6	3.403594	2.838196	-0.391973	6	-1.380306	-2.513585	-1.909339
7	1.561943	1.327621	-0.359729	6	-3.157017	-4.310225	-0.735533
6	3.103222	4.306820	-0.011249	1	-2.543620	-3.455463	1.143432
1	2.920817	4.376033	1.066991	6	-2.095157	-3.405351	-2.706417
1	3.946242	4.966376	-0.242236	1	-0.718286	-1.786740	-2.368483
6	1.864424	4.655892	-0.806076	6	-2.989892	-4.303138	-2.120310
6	1.238036	5.895031	-0.925390	1	-3.858588	-4.999569	-0.275667
6	1.354687	3.545415	-1.483588	1	-1.969082	-3.386289	-3.785099
6	0.095645	6.004162	-1.721516	1	-3.559759	-4.987867	-2.740952
1	1.629861	6.765243	-0.406532	6	1.106929	-2.214094	0.617618
6	0.214397	3.646818	-2.277147	6	2.150648	-1.519832	1.256717
6	-0.417102	4.887177	-2.389487	6	1.359694	-3.474015	0.056940
1	-0.397975	6.966198	-1.824369	6	3.416756	-2.095077	1.345883
1	-0.171628	2.776124	-2.796413	1	1.954642	-0.548119	1.700703
1	-1.303320	4.987960	-3.008985	6	2.638902	-4.031647	0.129597
1	4.373351	2.700932	-0.867957	1	0.562703	-4.018028	-0.437871
1	2.501837	1.834682	-2.170595	6	3.668292	-3.346919	0.776878
6	-3.053314	-0.203516	-1.990464	1	4.213531	-1.553440	1.845322
6	-3.430976	-1.555116	-2.069557	1	2.825152	-5.006311	-0.312328
6	-4.027945	0.774766	-1.745444	1	4.663137	-3.777764	0.829074
6	-4.767256	-1.914978	-1.916772	6	-3.184543	0.046592	1.459020
1	-2.660131	-2.309430	-2.177014	8	-4.390785	0.497132	1.894953
6	-5.364125	0.417839	-1.600162	6	-4.078429	0.905406	-0.381532
1	-3.732371	1.815842	-1.655027	6	-4.977326	1.283510	0.824885
6	-5.719309	-0.925247	-1.686826	7	-2.887393	0.279886	0.225793
1	-5.065044	-2.956255	-1.954516	6	-6.399748	0.794737	0.519043
1	-6.131050	1.160767	-1.411309	1	-6.857756	0.344953	1.405228
8	-7.078056	-1.239400	-1.594467	1	-7.031655	1.641297	0.222622
6	-7.508786	-2.021457	-0.557976	6	-6.210391	-0.177613	-0.624150
8	-6.794391	-2.441799	0.319095	6	-7.132403	-1.072305	-1.164151
6	-8.990045	-2.265983	-0.684699	6	-4.916862	-0.095326	-1.151195
1	-9.525420	-1.312697	-0.709665	6	-6.743010	-1.885174	-2.231680
1	-9.200773	-2.782820	-1.625423	1	-8.137403	-1.144238	-0.757386
1	-9.331130	-2.867409	0.156744	6	-4.523456	-0.907290	-2.210866
				6	-5.446374	-1.805123	-2.749408
				1	-7.450896	-2.590536	-2.657069
				1	-3.509342	-0.866713	-2.589113
				1	-5.149203	-2.454495	-3.566735
				1	-4.921531	2.332515	1.125228
28	-0.590106	0.763432	-0.272645	1	-3.783251	1.763647	-0.985979
6	0.444603	0.770796	-1.662049	6	1.575861	-0.086718	-2.117509
6	0.122890	2.111506	-1.668249	1	1.417937	-1.126431	-1.804591
1	0.898810	2.799196	-1.323370	1	1.614251	-0.069553	-3.222550

TS4B

SCF Energy = -3351.083698

Gibbs Free Energy = -3350.310154

8	2.796263	0.389220	-1.565084	6	-3.473174	3.856903	2.553982
6	3.827481	-0.551299	-1.714856	6	-2.146329	4.035818	2.937782
1	3.475220	-1.563557	-1.467241	6	-1.118929	3.415651	2.223299
1	4.203681	-0.581389	-2.753242	1	-4.798015	2.887545	1.155586
6	4.981731	-0.216324	-0.780950	1	-4.274887	4.345872	3.097980
8	4.983424	0.798480	-0.105819	1	-1.903530	4.665269	3.788577
6	6.108421	-1.196608	-0.707795	1	-0.088974	3.579349	2.517350
6	7.143927	-0.933972	0.200417	15	-0.061436	1.721720	0.192176
6	6.152243	-2.366558	-1.480329	6	1.492150	2.278575	0.976675
6	8.201686	-1.826673	0.339379	6	1.979610	3.588711	0.855006
1	7.088082	-0.024786	0.788986	6	2.215529	1.333220	1.714919
6	7.214531	-3.258116	-1.343823	6	3.166164	3.955366	1.486861
1	5.358558	-2.594379	-2.183172	1	1.430890	4.313872	0.261428
6	8.238436	-2.991073	-0.432726	6	3.397740	1.708417	2.355750
1	8.997092	-1.619004	1.048408	1	1.863107	0.309020	1.751494
1	7.242316	-4.161757	-1.944800	6	3.872111	3.016000	2.244821
1	9.063080	-3.689174	-0.324424	1	3.541822	4.969640	1.388660
8	-0.865935	1.724728	1.395114	1	3.953409	0.974327	2.928777
16	0.257916	2.133814	2.368833	1	4.796191	3.302653	2.738275
8	1.079910	0.965590	2.754424	6	-0.059482	2.635424	-1.411612
8	-0.315078	2.949737	3.447220	6	0.841611	2.204951	-2.399614
6	1.297180	3.196568	1.370746	6	-0.937688	3.685606	-1.709266
6	2.455606	2.696817	0.783006	6	0.860495	2.812030	-3.653694
6	0.862557	4.495382	1.098874	1	1.546679	1.408528	-2.189255
6	3.177436	3.501109	-0.098407	6	-0.923669	4.284853	-2.971224
1	2.783059	1.685151	0.980302	1	-1.634836	4.042733	-0.959815
6	1.591350	5.287934	0.216343	6	-0.027563	3.849999	-3.947107
1	-0.037750	4.867469	1.575486	1	1.571452	2.469922	-4.400076
6	2.756037	4.801455	-0.398467	1	-1.612208	5.097169	-3.186002
1	4.065695	3.086879	-0.562715	1	-0.017185	4.318375	-4.926855
1	1.254023	6.298232	-0.001938	6	-3.139281	1.479196	-0.329419
6	3.548785	5.672020	-1.342021	8	-4.305112	1.774526	-0.953433
1	4.271842	6.290164	-0.795372	6	-3.343344	-0.222941	-1.769676
1	2.899201	6.352086	-1.901923	6	-4.490936	0.800729	-2.019958
1	4.112404	5.068552	-2.059198	7	-2.510627	0.428587	-0.733317
6	-0.977164	2.807426	-2.476726	6	-5.828141	0.064065	-1.846558
6	-1.901861	1.788560	-3.155457	1	-6.509660	0.649041	-1.220962
1	-2.722457	2.293399	-3.676090	1	-6.318439	-0.068723	-2.818767
1	-1.350197	1.192290	-3.891166	6	-5.442499	-1.267540	-1.243833
1	-2.326226	1.095314	-2.428302	6	-6.284208	-2.266953	-0.757513
6	-0.274292	3.656392	-3.557522	6	-4.056283	-1.453622	-1.251775
1	-1.010310	4.205441	-4.156519	6	-5.721553	-3.454181	-0.283538
1	0.402568	4.384120	-3.098489	1	-7.361623	-2.126609	-0.747234
1	0.313332	3.025276	-4.232497	6	-3.491679	-2.646189	-0.801835
6	-1.770510	3.744793	-1.547827	6	-4.335849	-3.644481	-0.311391
1	-1.101854	4.479732	-1.090555	1	-6.365945	-4.238373	0.102921
1	-2.546735	4.282427	-2.105378	1	-2.419334	-2.787246	-0.826642
1	-2.233342	3.188982	-0.728871	1	-3.910560	-4.575647	0.050617
				1	-4.411693	1.349201	-2.960970
				1	-2.719087	-0.429455	-2.641949
TS4C				28	-0.823456	-0.300991	0.156952
SCF Energy = -3168.563399				6	-0.449373	-0.743329	5.093475
Gibbs Free Energy = -3167.771728				6	0.128644	-0.983838	3.847968
6	-1.394407	2.585862	1.133646	6	-0.659954	-1.328786	2.735216
6	-2.749542	2.381329	0.768671	6	-2.053359	-1.422181	2.918408
6	-3.770585	3.038954	1.465684	6	-2.628884	-1.189262	4.165224

6	-1.831462	-0.844139	5.259244	6	-1.953839	4.924655	1.650277
1	0.181862	-0.473320	5.935715	6	-1.300169	4.081724	0.761491
1	1.202249	-0.886852	3.722178	6	-1.603351	2.701516	0.732228
1	-2.678074	-1.681620	2.069392	6	-2.638669	2.210738	1.553265
1	-3.705657	-1.274855	4.282836	6	-3.301629	3.064802	2.428071
1	-2.282510	-0.654786	6.228887	6	-2.950565	4.414629	2.491786
6	-0.038719	-1.520843	1.398415	1	-1.701602	5.980216	1.683541
6	1.074165	-2.293604	1.269504	1	-0.549367	4.474231	0.084360
6	1.650959	-3.291196	2.242700	1	-2.952588	1.181739	1.420319
1	0.926840	-3.670134	2.966997	1	-4.106790	2.679752	3.046237
1	2.530483	-2.913814	2.796415	1	-3.467985	5.078741	3.178090
8	2.069320	-4.377627	1.397283	6	-0.939432	1.818297	-0.180109
6	2.666557	-3.761100	0.270456	6	-0.058772	1.975479	-1.249323
1	3.704189	-3.474023	0.494282	6	1.255054	2.699856	-1.138536
1	2.665902	-4.472605	-0.558025	1	1.280210	3.579709	-1.804673
6	1.860324	-2.457091	-0.020560	1	1.420779	3.029016	-0.110154
8	2.763923	-1.340050	-0.139969	8	2.301231	1.799953	-1.532409
6	0.941286	-2.560492	-1.225032	6	3.601896	2.293943	-1.374123
6	0.245100	-3.749353	-1.476891	1	3.720992	3.295836	-1.823496
6	0.691361	-1.451238	-2.038504	1	4.261562	1.610336	-1.918571
6	-0.645919	-3.836896	-2.545750	6	4.073657	2.355137	0.083934
1	0.387586	-4.599518	-0.816507	8	3.299182	2.145762	1.005899
6	-0.199863	-1.536369	-3.112043	6	5.511805	2.662281	0.341451
1	1.216301	-0.528156	-1.843988	6	6.427069	2.934880	-0.686210
6	-0.869774	-2.730927	-3.372039	6	5.954081	2.661284	1.673114
1	-1.173898	-4.767773	-2.730688	6	7.761367	3.201451	-0.384551
1	-0.362602	-0.661220	-3.735075	1	6.108487	2.942138	-1.722891
1	-1.563605	-2.803526	-4.204355	6	7.286196	2.923807	1.972496
14	3.926532	-0.935590	-1.241608	1	5.229224	2.449103	2.451377
8	5.372245	-0.733014	-0.451678	6	8.192390	3.194690	0.943044
8	3.592491	0.553864	-1.878724	1	8.464469	3.412183	-1.184226
6	5.927273	-1.652984	0.481579	1	7.621945	2.918824	3.004918
1	7.017350	-1.567696	0.406602	1	9.233019	3.399891	1.175569
1	5.671918	-2.687824	0.211253	1	-0.440511	1.793384	-2.254861
6	5.466128	-1.349882	1.900158	6	-1.863319	-2.840737	-0.110937
1	4.377347	-1.418258	1.963291	6	-1.257987	-3.209610	-1.335976
1	5.910078	-2.054851	2.611265	6	-1.878154	-4.144868	-2.175955
1	5.765209	-0.335782	2.179984	6	-3.120146	-4.676263	-1.847784
6	4.165336	1.781292	-1.401209	6	-3.752689	-4.263412	-0.678372
1	3.412387	2.558377	-1.559874	6	-3.127235	-3.360020	0.179586
1	4.354938	1.719280	-0.326591	1	-1.389843	-4.417373	-3.103527
6	5.444983	2.108969	-2.152777	1	-3.602856	-5.380548	-2.517286
1	5.836706	3.080088	-1.829741	1	-4.744909	-4.628876	-0.434316
1	6.203523	1.346155	-1.958712	1	-3.653007	-3.018458	1.059485
1	5.257025	2.152947	-3.230150	15	-1.090480	-1.566387	0.966556
6	4.063486	-2.179289	-2.623726	6	0.512056	-2.320568	1.508247
1	4.880820	-1.898797	-3.294757	6	0.988369	-3.569734	1.099078
1	4.270807	-3.183334	-2.239343	6	1.274926	-1.567132	2.413292
1	3.138123	-2.228284	-3.202550	6	2.209182	-4.050733	1.576332
1	-1.095928	-1.777063	0.471358	1	0.410739	-4.175085	0.409739
				6	2.478491	-2.059426	2.908665
				1	0.921215	-0.591019	2.733088
				6	2.953688	-3.302051	2.485472
				1	2.573959	-5.015877	1.237508
				1	3.055267	-1.463657	3.609954
				1	3.903141	-3.678075	2.853626
28	-0.583227	0.130218	-0.528754				

TS4

SCF Energy = -3424.882968

Gibbs Free Energy = -3424.140233

6	-1.934118	-1.674443	2.597037	6	-3.030280	2.767593	-2.218146
6	-2.074196	-0.510224	3.358645	6	-2.968764	4.154443	-2.090668
6	-2.268507	-2.907509	3.178700	6	-1.983954	4.737339	-1.295822
6	-2.587716	-0.564428	4.655248	6	-1.056663	3.933713	-0.627498
1	-1.768269	0.440976	2.944424	1	-3.796672	2.304377	-2.827678
6	-2.789748	-2.961378	4.469081	1	-3.689884	4.775014	-2.611643
1	-2.111301	-3.827532	2.626568	1	-1.932879	5.816194	-1.192032
6	-2.959455	-1.788220	5.208676	1	-0.292205	4.392269	-0.010340
1	-2.693815	0.351842	5.228645	15	0.107961	1.501437	0.137171
1	-3.053750	-3.921554	4.902435	6	-0.652690	1.042285	1.722499
1	-3.365291	-1.832901	6.214935	6	-1.913006	1.514853	2.106451
6	-0.025607	-2.582868	-1.825216	6	0.048426	0.155026	2.556688
8	0.673431	-3.282261	-2.749257	6	-2.466291	1.106370	3.320477
6	1.728637	-1.252284	-2.218344	1	-2.460467	2.196377	1.464564
6	1.740628	-2.420676	-3.240411	6	-0.501366	-0.229484	3.776131
7	0.454140	-1.430837	-1.499142	1	1.005177	-0.253435	2.247934
6	3.102333	-3.125276	-3.137025	6	-1.760322	0.242257	4.157100
1	2.970643	-4.211289	-3.095573	1	-3.446432	1.468538	3.612909
1	3.709205	-2.909155	-4.024781	1	0.045841	-0.909084	4.421651
6	3.723867	-2.547347	-1.884403	1	-2.191928	-0.068550	5.103051
6	4.921048	-2.907081	-1.266511	6	1.516260	2.588334	0.507607
6	2.951163	-1.504891	-1.364129	6	1.758010	3.078339	1.797005
6	5.331710	-2.208092	-0.128876	6	2.390683	2.916153	-0.541177
1	5.529023	-3.715281	-1.664225	6	2.874197	3.882408	2.035074
6	3.339428	-0.825867	-0.213907	1	1.086039	2.826308	2.609855
6	4.544791	-1.177051	0.394825	6	3.495811	3.727427	-0.299225
1	6.265800	-2.473999	0.357628	1	2.206820	2.534676	-1.541974
1	2.717454	-0.040291	0.191941	6	3.741512	4.205853	0.991440
1	4.863908	-0.650313	1.288459	1	3.063422	4.255704	3.036272
1	1.471489	-2.135653	-4.260331	1	4.167732	3.982464	-1.112426
1	1.746933	-0.255953	-2.661835	1	4.608563	4.830293	1.181095
8	-3.754566	-0.435688	0.119909	6	-2.223691	0.495820	-1.695759
16	-3.749305	-0.199827	-1.357264	8	-3.396126	0.038822	-2.145721
8	-4.809405	-0.901020	-2.101586	6	-1.998397	-1.730580	-1.498038
8	-2.377241	-0.390101	-1.971934	6	-3.289046	-1.424758	-2.291952
6	-4.028177	1.574160	-1.499430	7	-1.339801	-0.406007	-1.404330
6	-4.904788	2.202600	-0.614655	6	-4.452113	-2.106294	-1.565706
6	-3.320172	2.327292	-2.432650	1	-5.348279	-1.479207	-1.579637
6	-5.029249	3.587813	-0.634039	1	-4.705349	-3.042519	-2.077658
1	-5.443457	1.605254	0.112348	6	-3.901951	-2.360003	-0.179599
6	-3.446433	3.716085	-2.440100	6	-4.586768	-2.735251	0.974309
1	-2.653733	1.819626	-3.119973	6	-2.516170	-2.172541	-0.145263
6	-4.283206	4.368442	-1.527844	6	-3.868059	-2.908274	2.159807
1	-5.690083	4.077215	0.076743	1	-5.662329	-2.884143	0.957517
1	-2.872748	4.303830	-3.152661	6	-1.797695	-2.329732	1.036132
6	-4.348998	5.873562	-1.467548	6	-2.485007	-2.701832	2.192318
1	-3.969326	6.330339	-2.385927	1	-4.390130	-3.198079	3.066321
1	-3.743625	6.250453	-0.633361	1	-0.731791	-2.142149	1.063769
1	-5.373230	6.226265	-1.309767	1	-1.943526	-2.821627	3.124533
				1	-3.241121	-1.624235	-3.363939
				1	-1.305062	-2.425246	-1.972359
TS7_iso				1	0.528483	-0.279463	-1.048874
SCF Energy = -2437.450569				28	0.850480	-1.880902	-1.881025
Gibbs Free Energy = -2436.890072				8	2.793706	-1.209103	-0.247334
				14	2.011476	0.006352	-0.952703
6	-1.101050	2.543429	-0.750919	1	3.594407	-1.865566	-1.524250
6	-2.100021	1.953849	-1.559853	8			

8	2.060609	-2.208322	0.817200	6	5.118895	-3.300927	0.618294
6	5.017107	-1.788526	-1.749606	1	4.709023	-3.854189	-1.425772
1	5.385313	-0.792574	-1.476364	1	5.304116	-2.537196	2.626439
1	5.155151	-1.908818	-2.827110	1	5.910808	-4.032860	0.740454
6	5.762999	-2.868034	-0.984399	6	0.408286	2.166349	-1.502039
1	5.408852	-3.861322	-1.271117	8	-0.219640	3.322883	-1.720496
1	6.834116	-2.807937	-1.201186	6	-1.760980	1.607292	-1.247501
1	5.628147	-2.753516	0.095842	6	-1.665070	3.059406	-1.780315
6	1.495597	-3.523801	0.602967	7	-0.351131	1.129062	-1.324672
1	0.918830	-3.741217	1.505668	6	-2.397428	3.970590	-0.790080
1	0.822405	-3.475307	-0.254619	1	-1.839055	4.897022	-0.626138
6	2.581356	-4.563236	0.389877	1	-3.374685	4.252855	-1.199094
1	2.131619	-5.559570	0.332486	6	-2.546612	3.112796	0.446274
1	3.116995	-4.375635	-0.543385	6	-2.986791	3.493346	1.712942
1	3.297513	-4.557047	1.216844	6	-2.226893	1.776403	0.184045
6	3.866449	-0.086041	0.787099	6	-3.107642	2.519197	2.706066
1	4.662608	-0.659354	1.271752	1	-3.239294	4.528253	1.924097
1	4.317928	0.710951	0.189982	6	-2.347854	0.798883	1.169850
1	3.273007	0.392241	1.570908	6	-2.794374	1.183174	2.434739
1	1.594715	-1.853166	-2.498632	1	-3.452981	2.801528	3.695795

TS7

SCF Energy = -2437.458557

Gibbs Free Energy = -2436.896551

28	0.085536	-0.710738	-1.190932	8	-3.412691	-1.188256	-1.670494
8	0.329851	-2.496784	-1.242911	8	-2.131311	-2.350189	0.247214
6	2.629848	1.243867	-0.765834	6	-4.643336	-1.211270	-0.930940
6	1.875083	2.224844	-1.449391	1	-4.434048	-0.979508	0.118887
6	2.524354	3.311896	-2.048014	1	-5.254348	-0.400682	-1.339268
6	3.912898	3.418412	-1.992671	6	-5.374474	-2.539513	-1.051775
6	4.658989	2.448882	-1.325175	1	-4.799551	-3.349281	-0.590767
6	4.019216	1.369387	-0.710817	1	-6.341312	-2.485463	-0.541392
1	1.934063	4.064674	-2.556584	1	-5.554269	-2.790083	-2.101269
1	4.407740	4.257554	-2.469526	6	-1.503037	-3.340863	1.057820
1	5.740022	2.528846	-1.277888	1	-1.692586	-4.338328	0.643295
1	4.605474	0.620995	-0.190045	1	-0.418958	-3.182839	1.049286
15	1.793532	-0.169821	0.034125	6	-2.051136	-3.225964	2.468902
6	1.214658	0.398484	1.661850	1	-1.843617	-2.232194	2.877354
6	1.133953	1.758929	1.982145	1	-3.133289	-3.380680	2.476235
6	0.745452	-0.561696	2.573119	1	-1.589183	-3.974611	3.120004
6	0.594957	2.153929	3.205987	6	-2.075477	-3.687523	-2.439585
1	1.492857	2.509184	1.286476	1	-1.434578	-4.461714	-2.015738
6	0.226543	-0.160750	3.800986	1	-3.097738	-4.064886	-2.534782
1	0.796838	-1.617979	2.329214	1	-1.702695	-3.453721	-3.440864
6	0.146595	1.197751	4.116390	1	-1.194475	-1.064878	-2.094946
1	0.526994	3.209495	3.446548	1	0.919386	-2.843519	-0.562294
1	-0.120930	-0.907440	4.507708				
1	-0.268443	1.509310	5.069251				
6	3.075022	-1.422421	0.309529				
6	3.422813	-2.266676	-0.759859				
6	3.758833	-1.521224	1.531432				
6	4.444151	-3.201617	-0.600352	6	0.297340	2.590938	0.965232
1	2.891200	-2.195561	-1.703114	6	-0.982030	3.038776	0.540678
6	4.777111	-2.461517	1.680876	6	-1.590673	4.127323	1.187705
1	3.496470	-0.869613	2.357417	6	-0.971093	4.766962	2.256070

TS8

SCF Energy = -3257.194467

Gibbs Free Energy = -3256.519582

6	0.282138	4.330808	2.679711	1	-4.481752	-3.293118	-1.583645
6	0.903240	3.261468	2.035638	1	-3.574621	2.934367	-2.950050
1	-2.562734	4.458859	0.844339	1	-2.155654	0.916421	-3.032001
1	-1.463920	5.598490	2.749095	28	-0.783824	-0.336127	-0.433500
1	0.782765	4.821532	3.508866	8	-0.290967	-2.058661	0.197319
1	1.880162	2.936176	2.372345	16	0.095791	-3.285713	-0.754478
15	1.126282	1.147866	0.160253	8	-0.943769	-3.481282	-1.771687
6	2.570609	0.859681	1.250930	8	0.496241	-4.418210	0.076678
6	3.894248	1.143635	0.889180	6	1.547942	-2.602520	-1.542933
6	2.320214	0.200225	2.468484	6	1.652136	-2.623123	-2.930561
6	4.947582	0.779024	1.730770	6	2.577789	-2.091829	-0.750388
1	4.101108	1.644129	-0.050376	6	2.806876	-2.118920	-3.530621
6	3.373190	-0.145065	3.312918	1	0.833034	-3.018919	-3.519860
1	1.301225	-0.046435	2.753997	6	3.717706	-1.585674	-1.364887
6	4.690930	0.137753	2.943264	1	2.480277	-2.073228	0.328094
1	5.969965	1.001567	1.438694	6	3.848895	-1.587206	-2.761408
1	3.161980	-0.650485	4.249680	1	2.894396	-2.130393	-4.613654
1	5.512136	-0.144692	3.594965	1	4.508315	-1.167405	-0.749857
6	1.842187	1.943117	-1.332435	14	-1.283032	-1.720647	1.941726
6	1.929691	1.170592	-2.498062	1	-1.377242	-0.345892	1.085281
6	2.319334	3.262539	-1.345661	8	-1.046082	-0.692600	3.277024
6	2.501254	1.703220	-3.654352	8	-0.475241	-3.027965	2.567928
1	1.540105	0.160374	-2.495185	6	-1.607481	0.602285	3.402798
6	2.886272	3.794363	-2.503229	1	-2.681921	0.521948	3.625759
1	2.247350	3.871339	-0.449716	1	-1.515306	1.156320	2.458714
6	2.980959	3.013900	-3.658697	6	-0.899215	1.352870	4.520414
1	2.565701	1.091932	-4.549534	1	0.165358	1.461186	4.294582
1	3.253856	4.816349	-2.504879	1	-1.324926	2.354573	4.638693
1	3.421872	3.430075	-4.559804	1	-0.997162	0.812869	5.466618
6	-1.754560	2.422022	-0.551159	6	0.901727	-3.135125	2.887726
8	-2.684450	3.223400	-1.126340	1	1.224270	-4.137958	2.592387
6	-2.698745	1.068003	-2.095356	1	1.495429	-2.426668	2.295287
6	-3.493858	2.395880	-2.006167	6	1.142405	-2.896554	4.373112
7	-1.697347	1.216886	-1.010640	1	2.204052	-3.024184	4.615842
6	-4.868853	2.060744	-1.380832	1	0.824272	-1.889070	4.653904
1	-4.919168	2.473045	-0.366275	1	0.564988	-3.610224	4.968443
1	-5.690594	2.509949	-1.948217	6	-3.014662	-2.353960	1.670295
6	-4.920348	0.547879	-1.384368	1	-3.325147	-2.955643	2.529262
6	-5.985051	-0.280164	-1.031817	1	-3.726877	-1.538402	1.518285
6	-3.710503	-0.010714	-1.807197	1	-3.038371	-2.985401	0.778973
6	-5.816540	-1.665495	-1.108640	6	5.060635	-0.972897	-3.413069
1	-6.931703	0.141002	-0.704712	1	4.946256	0.116428	-3.474103
6	-3.533579	-1.390802	-1.888652	1	5.969947	-1.175997	-2.839703
6	-4.603211	-2.215833	-1.534939	1	5.204931	-1.349010	-4.429619
1	-6.637642	-2.321204	-0.834407	1	-0.416016	-0.532825	-1.827196
1	-2.584185	-1.822166	-2.187486				