Electronic Supplementary Information

Unraveling the Mechanism of Pd-Catalyzed Hydrocyanation of Methylenecyclopropane or Cyclopropene with $Me_2C(OH)CN$: A DFT Study

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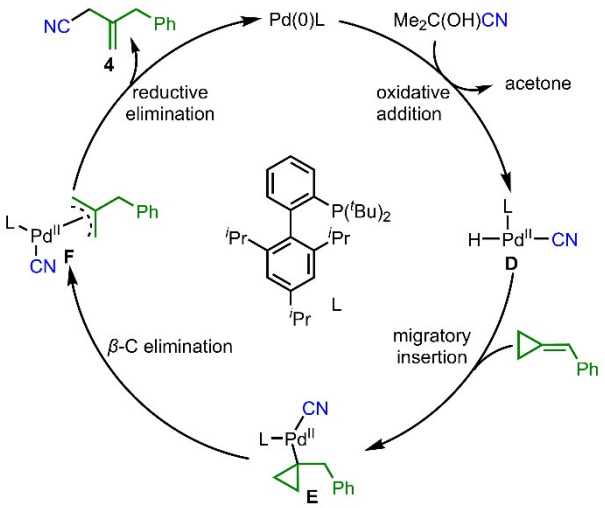
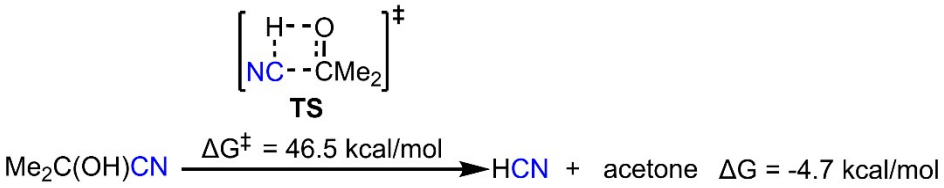


Scheme S1 Proposed mechanisms for the Pd-catalyzed hydrocyanation of methylenecyclopropane.



Scheme S2 The activation energy for the decomposition of $Me_2C(OH)CN$ into HCN and acetone.

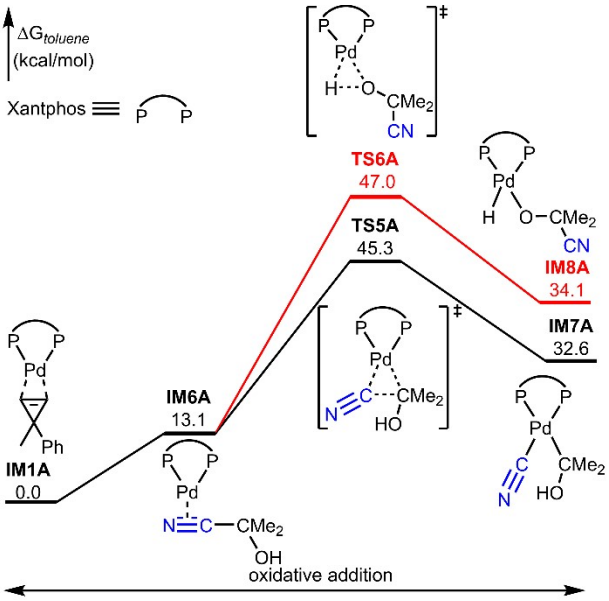


Fig. S1 Calculated free energy profiles for the O–H bond cleavage or C–C bond cleavage of $Me_2C(OH)CN$ in the cyclopropene system.

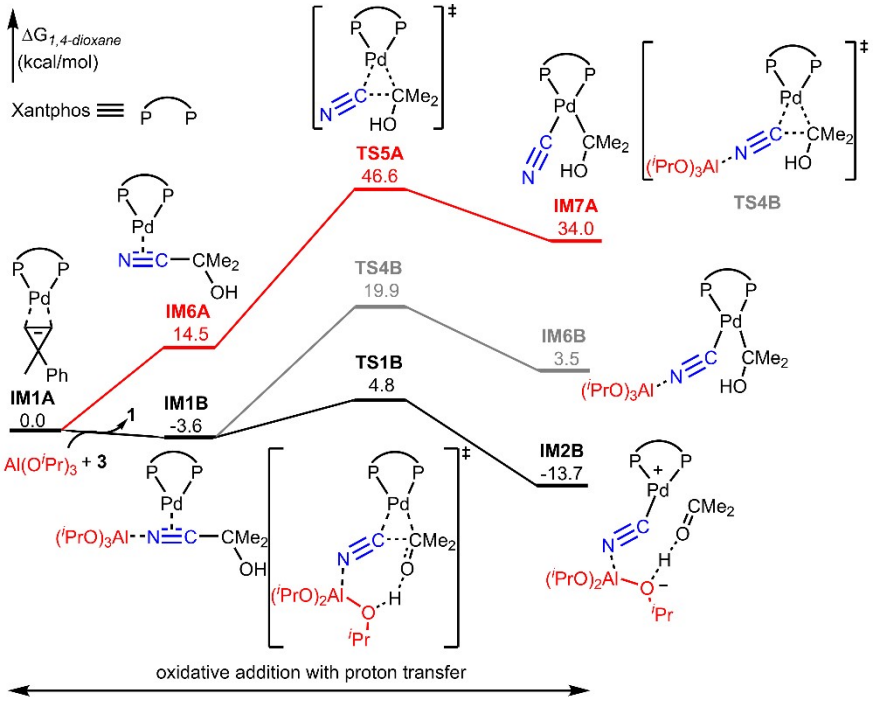


Fig. S2 Calculated free energy profiles for C–C bond activation of $Me_2C(OH)CN$ with or without $Al(O^iPr)_3$ in the cyclopropene system.

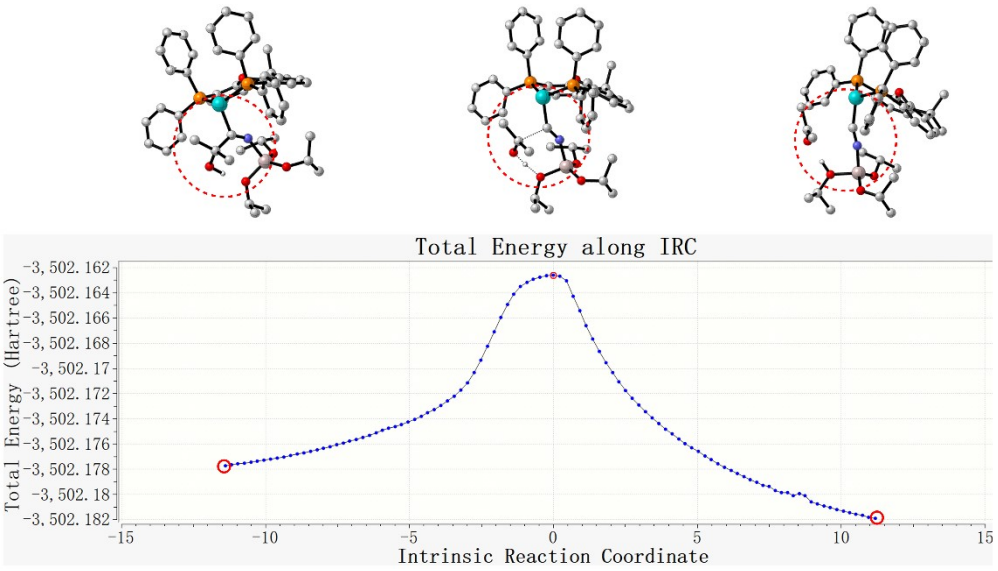


Fig. S3 The IRC for **TS1B** links the reactants and products.

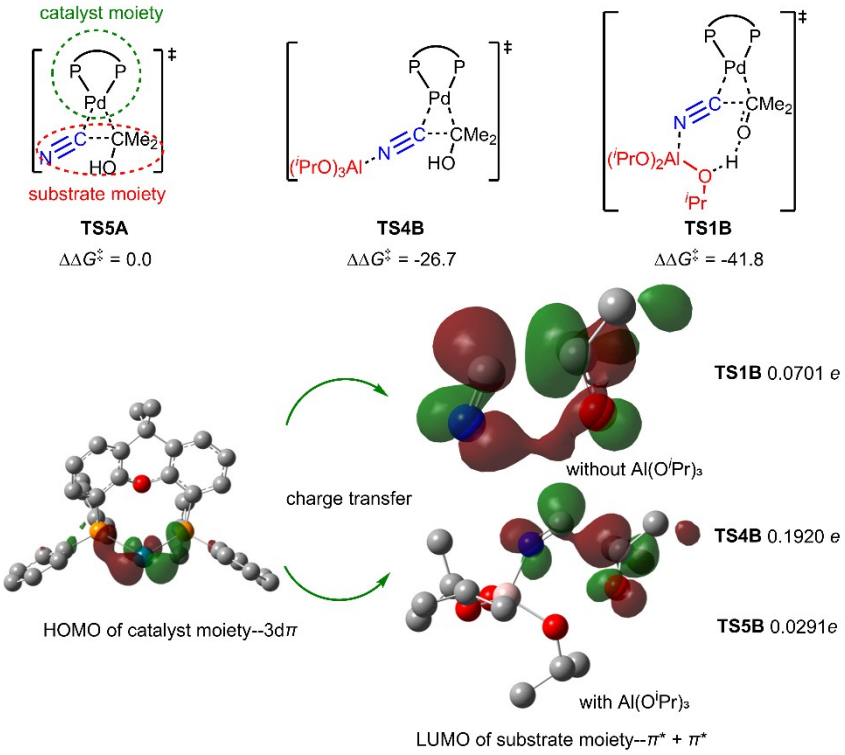


Fig. S4 Fragment molecular orbital analysis and charge transfer of the **TS1B**, **TS4B**, and **TS5A** corresponding to the C−C bond cleavage.

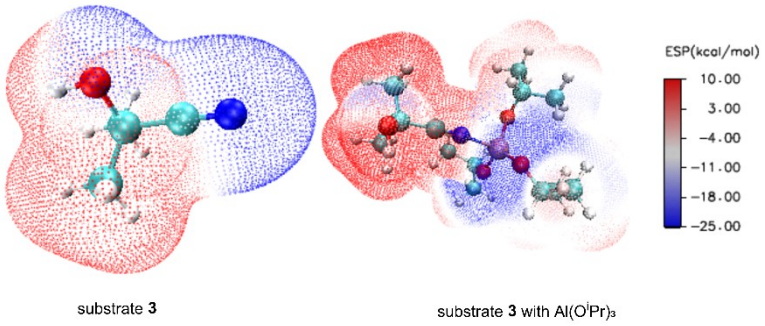


Fig. S5 ESP of the $Me_2C(OH)CN$ with or without $Al(O^iPr)_3$.

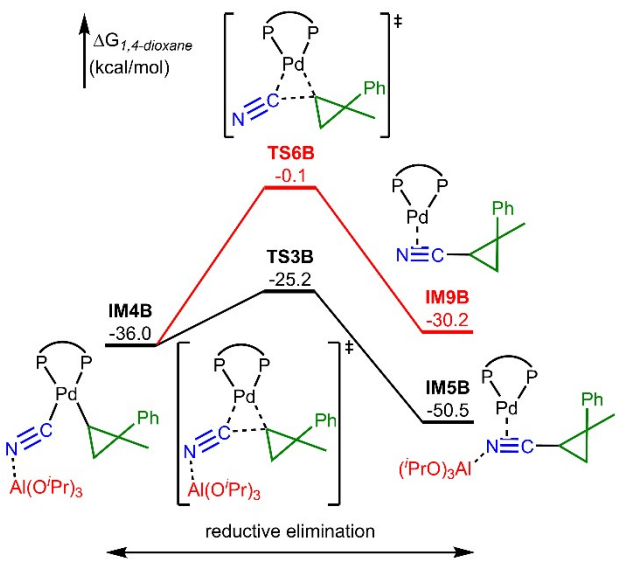


Fig. S6 Calculated free energy profiles for **TS3B** and **TS6B**.

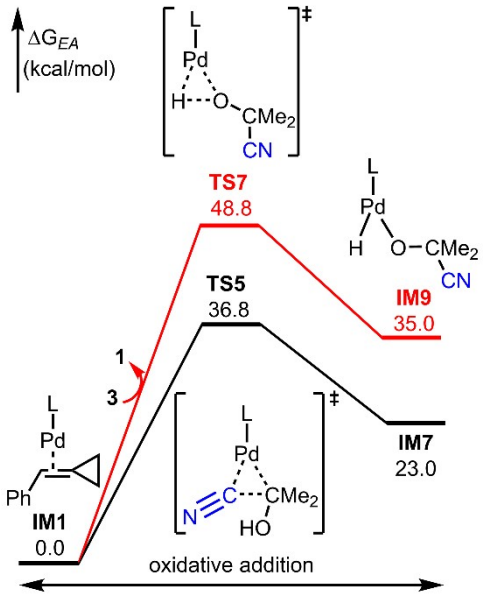


Fig. S7 Calculated free energy profiles for the O–H bond cleavage or C–C bond cleavage of $Me_2C(OH)CN$ in the methylenecyclopropane system.

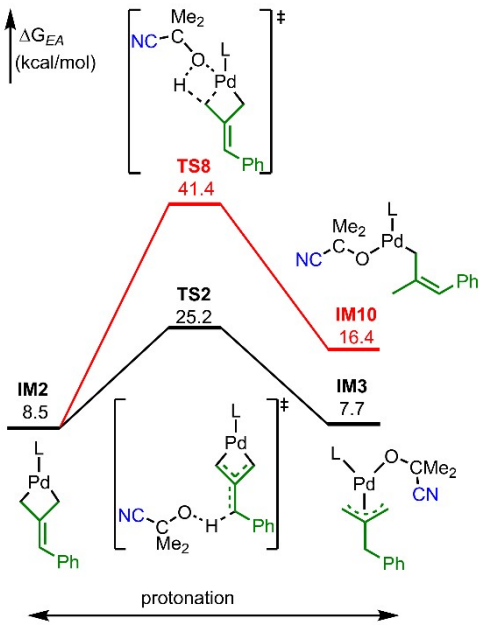


Fig. S8 Calculated free energy profiles for possible protonation transition states **TS2** and **TS8**.

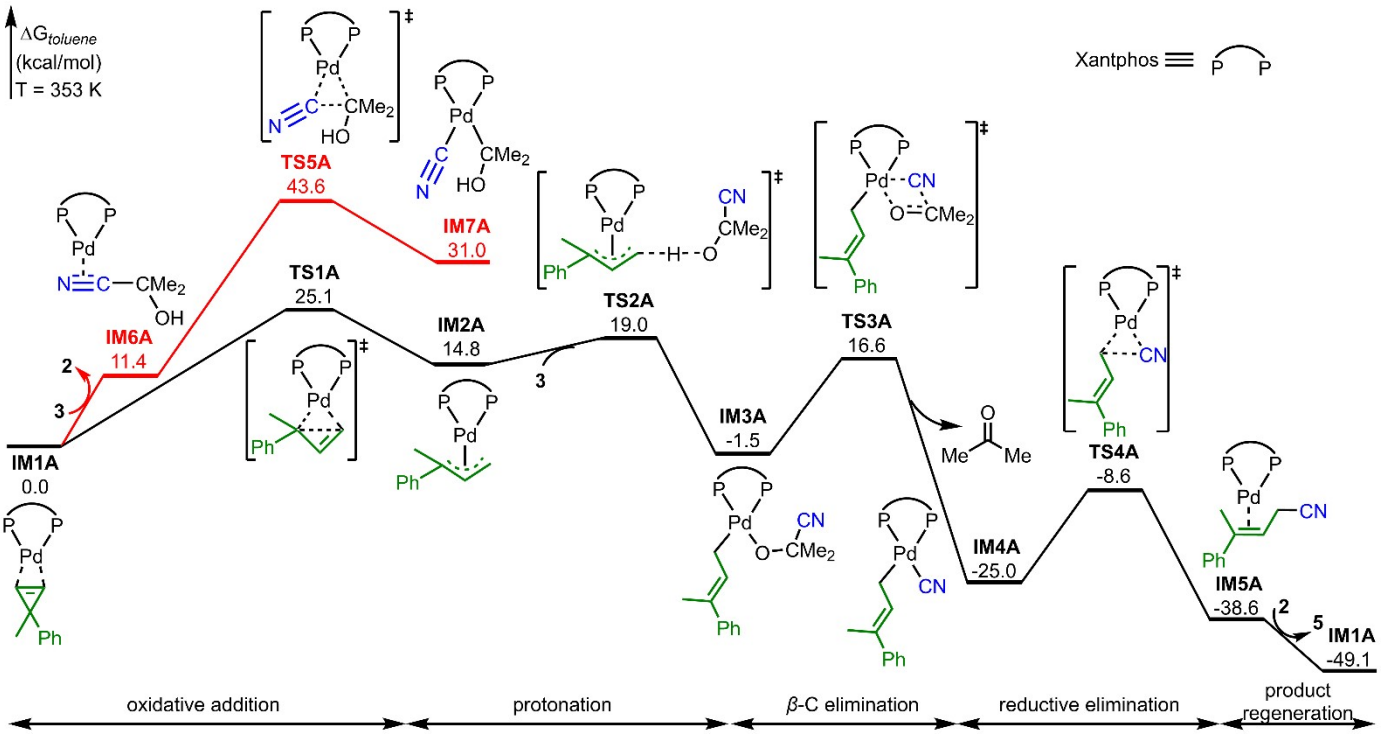


Fig. S9 Calculated free energy profiles for Pd-catalyzed hydrocyanation of **2** with **3** to yield ring-opening product **5** in the absence of $Al(O^iPr)_3$ at 353 K.

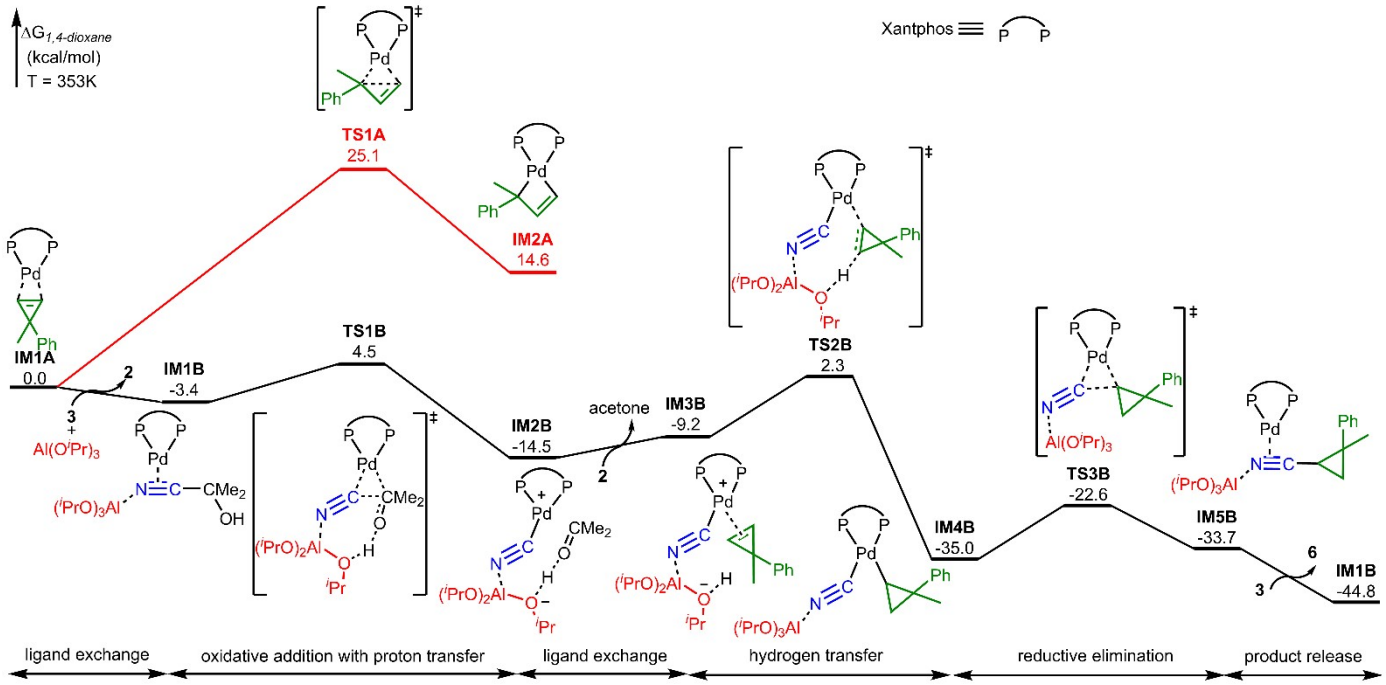


Fig. S10 Calculated free energy profiles for Pd-catalyzed hydrocyanation of **2** with **3** to yield ring-retentive product **6** in the presence of Al(O^{i}Pr)$_3$ at 353 K.

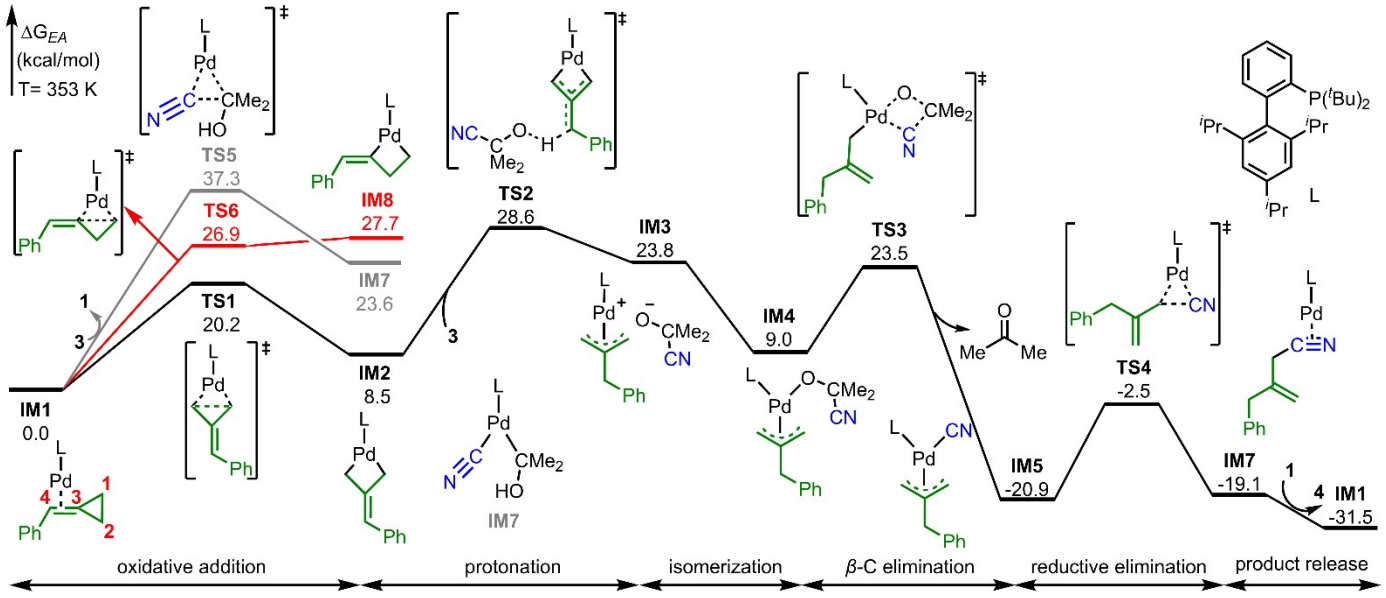


Fig. S11 Calculated free energy profiles for Pd-catalyzed hydrocyanation of **1** with **3** to afford ring-opening product at 353 K.

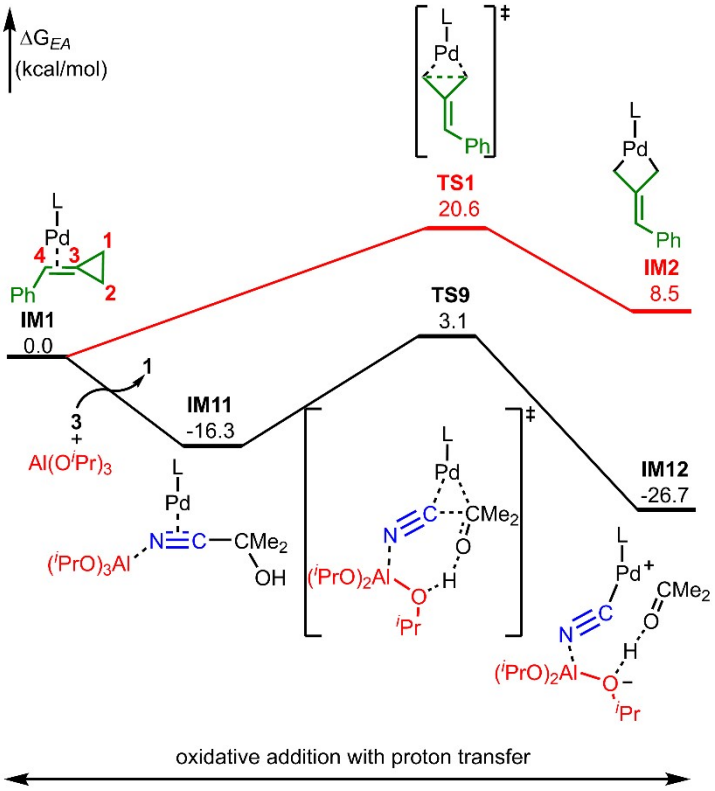


Fig. S12 Calculated free energy profiles for the oxidative addition with proton transfer of $Me_2C(OH)CN$ in the presence of $Al(O^iPr)_3$ in the methylenecyclopropane system.

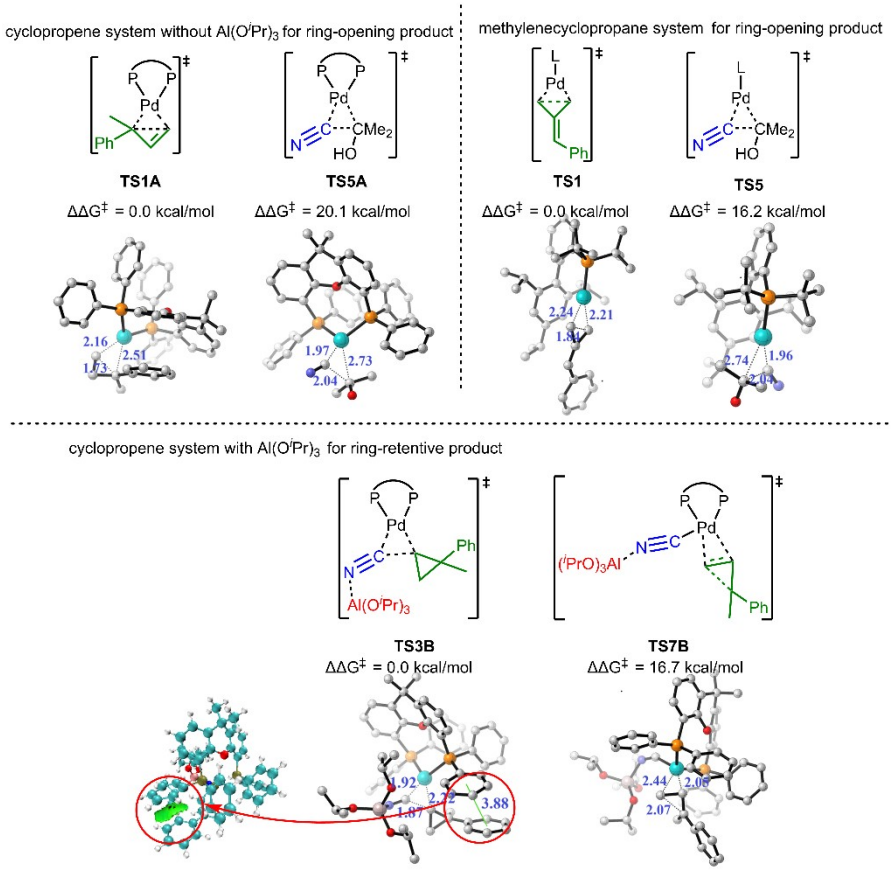
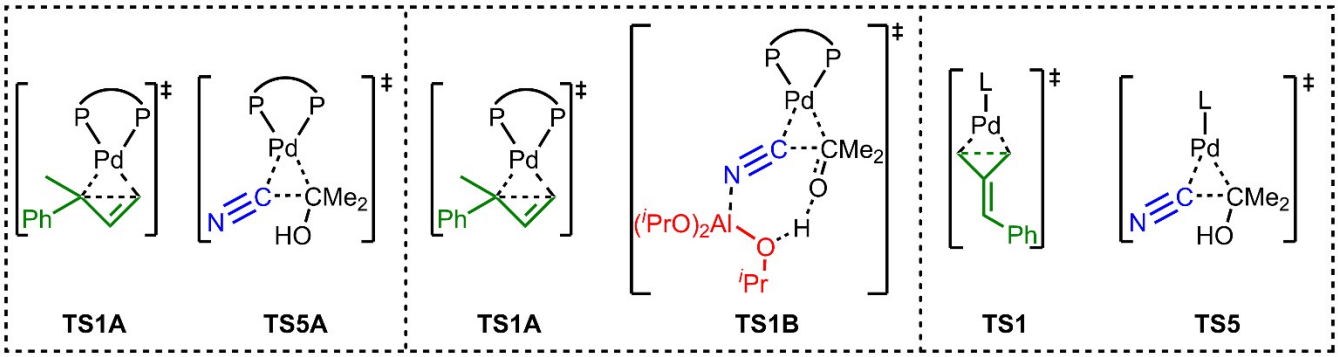
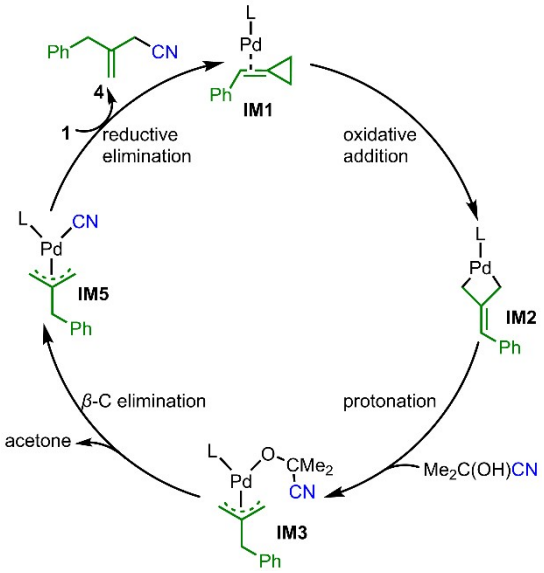


Fig. S13 The chemoselectivity-determining step in the three system.

Table S1 Comparison of activation barrier difference ($\Delta\Delta G^{\ddagger}$) of key transition states obtained with different DFT functionals in single-point energy calculations.



	M06	M06-L	M06-2X	MN15	B3LYP-GD3(BJ)
$\Delta\Delta G^{\ddagger}$(**TS5A-TS1A**)	20.1	16.9	20.6	22.4	20.7
$\Delta\Delta G^{\ddagger}$(**TS1B-TS1A**)	-20.3	-24.7	-18.4	-18.6	-22.9
$\Delta\Delta G^{\ddagger}$(**TS5-TS1**)	17.2	11.6	16.3	17.5	16.2



Scheme S3 Revised mechanisms for the Pd-catalyzed hydrocyanation of methylenecyclopropane system.

Cartesian Coordinates (Å) of Optimized Structures.

1

SCF Energy: -387.051169316

Sum of electronic and zero-point Energies= -386.883472

Sum of electronic and thermal Energies= -386.874934

Sum of electronic and thermal Enthalpies= -386.873990

Sum of electronic and thermal Free Energies= -386.917518

Electronic energy in solution by single point calculation = -386.818836883

6	3.591442	-0.296384	0.000239
6	2.802174	1.023769	0.000012
1	4.118284	-0.574365	-0.912062
1	4.117129	-0.574050	0.913330
1	2.801823	1.618991	-0.912915
1	2.801777	1.619631	0.912504
6	2.125564	-0.278760	-0.000037
6	0.993583	-0.977184	-0.000239
1	1.063384	-2.065051	-0.000319
6	-0.368635	-0.429849	-0.000209
6	-1.461445	-1.312827	-0.000020
6	-0.631883	0.952485	-0.000164
6	-2.771643	-0.837583	0.000136
1	-1.274426	-2.384051	0.000006
6	-1.939682	1.427025	-0.000004
1	0.197617	1.651167	-0.000332
6	-3.017159	0.535860	0.000157
1	-3.600490	-1.540201	0.000286
1	-2.122112	2.498360	-0.000028
1	-4.036879	0.910248	0.000303

2

SCF Energy: -387.016796892

Sum of electronic and zero-point Energies= -386.8513609

Sum of electronic and thermal Energies= -386.8432589

Sum of electronic and thermal Enthalpies= -386.8423149

Sum of electronic and thermal Free Energies= -386.8839259

Electronic energy in solution by single point calculation = -386.788746868

6	-2.280897	-0.986043	0.647246
6	-2.281091	-0.986137	-0.646864
6	-1.502482	0.142266	-0.000046
1	-2.549925	-1.445691	1.587257
1	-2.549942	-1.446523	-1.586578
6	0.005854	0.064721	-0.000092
6	0.803629	1.218416	0.000031

6	0.658416	-1.179343	-0.000176
6	2.196843	1.133412	0.000129
1	0.340014	2.198552	0.000092
6	2.048018	-1.267196	-0.000092
1	0.066522	-2.089111	-0.000282
6	2.827822	-0.109129	0.000054
1	2.788225	2.045296	0.000254
1	2.523951	-2.244389	-0.000139
1	3.912134	-0.175908	0.000123
6	-2.100935	1.543567	-0.000192
1	-1.794802	2.114886	0.885239
1	-1.794723	2.114697	-0.885724
1	-3.192511	1.480992	-0.000235

3

SCF Energy: -286.601018723

Sum of electronic and zero-point Energies= -286.494154

Sum of electronic and thermal Energies= -286.487146

Sum of electronic and thermal Enthalpies= -286.486202

Sum of electronic and thermal Free Energies= -286.524197

Electronic energy in solution by single point calculation = -286.496080559

6	-0.294572	-0.001609	0.034865
6	-0.871079	-1.299251	-0.538689
1	-0.595943	-1.413541	-1.590610
1	-0.497527	-2.157483	0.025085
1	-1.961066	-1.266583	-0.451567
6	-0.816934	1.234227	-0.713650
1	-1.907113	1.262708	-0.626605
1	-0.403311	2.152769	-0.282923
1	-0.541015	1.201921	-1.772101
8	-0.682498	0.026486	1.405542
1	-0.334278	0.841701	1.802370
6	1.190585	-0.032816	-0.055725
7	2.350320	-0.033812	-0.101255

4

SCF Energy: -480.544617993

Sum of electronic and zero-point Energies= -480.354889

Sum of electronic and thermal Energies= -480.343850

Sum of electronic and thermal Enthalpies= -480.342906

Sum of electronic and thermal Free Energies= -480.393602

Electronic energy in solution by single point calculation = -480.273828142

6	-2.788235	-0.002990	0.788783

6	-1.230393	0.004710	-1.180579
1	-2.890087	0.870382	1.449028
1	-2.889921	-0.881246	1.442535
1	-0.233927	0.006426	-1.607665
1	-2.069502	0.007319	-1.868977
6	-1.411231	-0.000434	0.139896
6	-0.286522	-0.004273	1.160959
6	1.104322	-0.002134	0.575609
6	1.753471	1.203136	0.284497
6	1.753788	-1.205225	0.276350
6	3.025345	1.207923	-0.288380
1	1.255401	2.143627	0.507335
6	3.025671	-1.205785	-0.296539
1	1.255988	-2.147346	0.492809
6	3.665377	0.002125	-0.580211
1	3.516758	2.152320	-0.504942
1	3.517339	-2.148565	-0.519479
1	4.656714	0.003758	-1.024245
1	-0.412692	0.868187	1.819348
1	-0.412747	-0.881585	1.812847
6	-3.907943	0.000396	-0.152983
7	-4.787890	0.003147	-0.909000

5

SCF Energy: -480.548787544

Sum of electronic and zero-point Energies= -480.359047

Sum of electronic and thermal Energies= -480.347719

Sum of electronic and thermal Enthalpies= -480.346775

Sum of electronic and thermal Free Energies= -480.398050

Electronic energy in solution by single point calculation = -480.273614107

6	2.858470	-0.144657	0.997925
6	1.369001	-0.372662	0.813148
6	0.528452	0.467189	0.185283
1	3.236228	-0.778852	1.807440
1	0.983805	-1.295221	1.236542
6	0.981398	1.784133	-0.402292
1	2.064957	1.832208	-0.527226
1	0.526127	1.941273	-1.385501
1	0.678847	2.628555	0.230998
6	-0.912599	0.130140	0.057598
6	-1.338454	-1.200545	-0.095181
6	-1.890188	1.138852	0.076492
6	-2.691748	-1.513241	-0.196928

1	-0.597816	-1.990933	-0.166379
6	-3.245164	0.826551	-0.022523
1	-1.592072	2.176805	0.185607
6	-3.652783	-0.501024	-0.156980
1	-2.995689	-2.548656	-0.322740
1	-3.983255	1.623295	0.004953
1	-4.708020	-0.744144	-0.241320
6	3.628466	-0.447043	-0.217347
7	4.214711	-0.677223	-1.192315
1	3.074811	0.890076	1.288663

6

SCF Energy: -480.539599571

Sum of electronic and zero-point Energies= -480.348730

Sum of electronic and thermal Energies= -480.338359

Sum of electronic and thermal Enthalpies= -480.337415

Sum of electronic and thermal Free Energies= -480.384859

Electronic energy in solution by single point calculation = -480.265475031

1	2.293075	-0.403233	1.946817
6	3.004757	-0.397358	-0.700223
7	4.041695	-0.080573	-1.119599
6	1.724458	-0.786515	-0.173720
6	1.476574	-0.748468	1.320217
6	0.789676	0.273898	0.450462
1	1.235204	-1.572333	-0.741593
1	0.889701	-1.555476	1.746512
6	-0.677487	0.103631	0.161338
6	-1.488836	1.215225	-0.104924
6	-1.280879	-1.165231	0.144590
6	-2.849981	1.066453	-0.376872
1	-1.062997	2.211727	-0.101357
6	-2.637883	-1.316379	-0.128945
1	-0.692518	-2.055777	0.346496
6	-3.432557	-0.198968	-0.391265
1	-3.452671	1.947494	-0.578734
1	-3.074970	-2.310915	-0.134984
1	-4.491178	-0.315541	-0.603589
6	1.319899	1.694097	0.521415
1	1.175755	2.223470	-0.426168
1	0.811364	2.254515	1.313209
1	2.390921	1.697761	0.738147

acetone

SCF Energy: -193.161998777

Sum of electronic and zero-point Energies= -193.077811

Sum of electronic and thermal Energies= -193.072434

Sum of electronic and thermal Enthalpies= -193.071490

Sum of electronic and thermal Free Energies= -193.106114

Electronic energy in solution by single point calculation = -193.087806145

6	0.000042	0.186677	0.000002
6	-1.290688	-0.615457	0.000025
1	-1.335447	-1.268900	0.880342
1	-2.147981	0.060318	0.001010
1	-1.336137	-1.267155	-0.881580
6	1.290677	-0.615400	-0.000004
1	1.335402	-1.268578	-0.880550
1	2.148121	0.060198	-0.000711
1	1.336113	-1.267482	0.881322
8	-0.000032	1.402085	0.000003

$Al(O^iPr)_3$

SCF Energy: -823.918543265

Sum of electronic and zero-point Energies= -823.6201493

Sum of electronic and thermal Energies= -823.6017563

Sum of electronic and thermal Enthalpies= -823.6008113

Sum of electronic and thermal Free Energies= -823.6699803

Electronic energy in solution by single point calculation = -823.637529896

13	-0.282970	-0.408079	0.165138
8	-0.539685	1.235331	-0.212286
8	-1.637298	-1.433251	0.218213
8	1.218268	-1.118715	0.519831
6	0.201251	2.432084	-0.041506
6	-3.013468	-1.126842	0.019816
6	2.545409	-0.915862	0.066277
6	-3.247229	-0.611870	-1.400523
1	-2.870242	-1.335340	-2.131510
1	-4.314682	-0.452747	-1.592892
1	-2.724421	0.340806	-1.547094
6	-3.504663	-0.140062	1.079231
1	-3.309492	-0.533701	2.082635
1	-2.984084	0.818670	0.969967
1	-4.581832	0.039485	0.983348
6	0.828844	2.489237	1.351402
1	1.561897	1.682246	1.476510
1	1.342052	3.442949	1.518904
1	0.056285	2.375501	2.119845

6	1.237492	2.585183	-1.153723
1	2.008257	1.809785	-1.075282
1	0.756142	2.495012	-2.132691
1	1.731844	3.561907	-1.098683
6	2.630639	-1.175434	-1.437776
1	2.323304	-2.204267	-1.656408
1	1.970292	-0.493735	-1.988517
1	3.650644	-1.029210	-1.811274
6	3.468426	-1.834416	0.861376
1	3.199381	-2.881410	0.683597
1	4.514706	-1.685884	0.571020
1	3.370590	-1.633705	1.932736
1	-3.555748	-2.074300	0.144151
1	-0.520562	3.256625	-0.129460
1	2.843787	0.127307	0.260808

HCN

SCF Energy: -93.397465

Sum of electronic and zero-point Energies= -93.383042

Sum of electronic and thermal Energies= -93.380054

Sum of electronic and thermal Enthalpies= -93.379109

Sum of electronic and thermal Free Energies= -93.397488

Electronic energy in solution by single point calculation =-93.3691551096

1	0.000920	1.449272	0.000000
6	-0.000071	-0.748452	-0.000000
7	-0.000071	0.434492	0.000000

IM10B

SCF Energy: -3696.133351

Sum of electronic and zero-point Energies= -3695.042054

Sum of electronic and thermal Energies= -3694.973198

Sum of electronic and thermal Enthalpies= -3694.972254

Sum of electronic and thermal Free Energies= -3695.151032

Electronic energy in solution by single point calculation = -3694.48634545

6	-3.524613	-3.364614	1.480652
6	-2.988160	-2.322348	0.708886
6	-2.735581	-2.596366	-0.638296
6	-2.911445	-3.851215	-1.229965
6	-3.414061	-4.869983	-0.417471
6	-3.735335	-4.622364	0.918733
6	-2.597929	-3.991583	-2.724850
6	-1.409536	-3.077907	-3.037967
6	-1.344816	-1.860761	-2.364891

6	-0.365006	-0.892520	-2.583595
6	0.605612	-1.156499	-3.555283
6	0.580770	-2.370813	-4.244243
6	-0.410535	-3.321786	-3.987391
1	-3.755464	-3.200078	2.525422
1	-3.565627	-5.863288	-0.824907
1	-4.142026	-5.421191	1.531291
1	1.386130	-0.430025	-3.750845
1	1.346448	-2.581288	-4.984214
1	-0.401457	-4.257026	-4.536212
8	-2.282923	-1.546515	-1.401489
15	-0.407202	0.545414	-1.456419
15	-2.490577	-0.690002	1.425820
6	0.924251	1.632572	-2.099104
6	0.639755	2.808597	-2.810837
6	2.264642	1.279758	-1.876986
6	1.678656	3.613734	-3.278927
1	-0.386321	3.102998	-2.993036
6	3.300980	2.085868	-2.347175
1	2.528316	0.379329	-1.341483
6	3.008937	3.260253	-3.043363
1	1.443181	4.522381	-3.826706
1	4.318064	1.769677	-2.143654
1	3.813559	3.895259	-3.403695
6	-1.918763	1.461182	-1.930530
6	-2.287993	2.551489	-1.130828
6	-2.654218	1.173244	-3.085890
6	-3.359391	3.360553	-1.499311
1	-1.725046	2.780728	-0.233257
6	-3.743057	1.971265	-3.438746
1	-2.369261	0.337125	-3.716084
6	-4.091514	3.069966	-2.651841
1	-3.621145	4.209239	-0.876956
1	-4.310783	1.740602	-4.336088
1	-4.933780	3.695634	-2.933835
6	-2.756732	-1.060713	3.209536
6	-1.773506	-1.829373	3.855528
6	-3.907644	-0.695945	3.917965
6	-1.936850	-2.218179	5.182859
1	-0.880436	-2.120271	3.308848
6	-4.063665	-1.076498	5.253199
1	-4.688265	-0.123745	3.429815
6	-3.081318	-1.836078	5.887939

1	-1.167613	-2.811579	5.668275
1	-4.959595	-0.782798	5.792829
1	-3.205434	-2.130665	6.925977
6	-3.869769	0.445246	1.011423
6	-3.966538	1.661570	1.706910
6	-4.790629	0.169379	-0.004905
6	-4.984774	2.565223	1.416410
1	-3.255828	1.891756	2.494434
6	-5.797761	1.085908	-0.308553
1	-4.724411	-0.759232	-0.559779
6	-5.904515	2.278551	0.405586
1	-5.053245	3.496369	1.971761
1	-6.499820	0.864381	-1.106839
1	-6.693278	2.986845	0.169266
46	-0.256237	0.000043	0.902535
6	-3.823584	-3.472347	-3.524533
1	-3.623925	-3.527564	-4.600257
1	-4.708147	-4.078012	-3.298726
1	-4.044827	-2.431192	-3.270113
6	-2.319658	-5.447726	-3.118455
1	-3.192327	-6.077047	-2.921303
1	-2.113582	-5.522843	-4.190011
1	-1.464251	-5.855380	-2.570573
1	1.259609	0.396857	3.126718
6	1.664181	-0.567642	0.813520
7	2.804927	-0.810789	0.800915
13	4.719406	-0.672148	0.578876
8	4.967749	-0.282894	-1.108242
8	5.010645	0.684028	1.635976
8	5.354975	-2.240559	0.998005
6	5.162434	-1.161235	-2.195986
6	6.092488	1.586328	1.630887
6	5.078546	-2.958626	2.178603
6	5.932072	2.620222	0.510444
1	4.959506	3.117752	0.588486
1	6.719206	3.383909	0.554581
1	5.981648	2.117564	-0.461199
6	7.435614	0.856302	1.515924
1	7.533325	0.107265	2.307817
1	7.502487	0.340799	0.549156
1	8.278513	1.555302	1.587723
6	6.578377	-1.743384	-2.165098
1	6.703530	-2.354182	-1.264544

1	6.777020	-2.365544	-3.047295
1	7.315079	-0.932744	-2.139122
6	4.102963	-2.269754	-2.228288
1	4.198265	-2.902400	-1.338873
1	3.094240	-1.843603	-2.241814
1	4.219032	-2.901716	-3.118126
6	5.860120	-2.381075	3.363603
1	6.936760	-2.447529	3.164886
1	5.605710	-1.325751	3.505194
1	5.642752	-2.925462	4.291682
6	5.415734	-4.431248	1.942021
1	6.481018	-4.534020	1.703228
1	5.195007	-5.041864	2.826410
1	4.839288	-4.818822	1.095114
1	6.076280	2.120422	2.595249
1	5.052723	-0.560953	-3.115568
1	4.000233	-2.891290	2.416858
6	-0.131281	1.943609	2.475414
6	0.215573	0.612296	2.923268
6	0.676539	2.825941	1.795537
1	-1.179825	2.209661	2.572763
1	-0.455946	0.168172	3.649351
6	0.081469	4.029916	1.181490
6	0.665686	4.591112	0.030711
6	-1.106609	4.615504	1.666318
6	0.059493	5.653178	-0.636904
1	1.576874	4.166711	-0.372303
6	-1.704039	5.683761	1.005145
1	-1.554256	4.243193	2.582167
6	-1.130419	6.202251	-0.160029
1	0.519251	6.043017	-1.540243
1	-2.614907	6.121170	1.405443
1	-1.600743	7.031623	-0.680273
6	2.150708	2.596532	1.599586
1	2.382865	2.299556	0.570656
1	2.707026	3.520347	1.795645
1	2.555748	1.814890	2.240335

IM10

SCF Energy: -2275.44282991

Sum of electronic and zero-point Energies= -2274.485648

Sum of electronic and thermal Energies= -2274.431331

Sum of electronic and thermal Enthalpies= -2274.430387

Sum of electronic and thermal Free Energies= -2274.573628

Electronic energy in solution by single point calculation = -2274.26028085

46	-0.276255	-0.902893	0.460293
15	1.633993	-1.728755	-0.472146
6	3.227423	-0.772970	-0.423427
6	3.336860	0.593560	-0.059618
6	4.411587	-1.465443	-0.747710
6	4.625133	1.152452	0.048777
6	2.230261	1.592182	0.138639
6	5.671294	-0.882083	-0.666403
1	4.352762	-2.492504	-1.071996
6	5.782139	0.438042	-0.238067
1	4.697701	2.192802	0.348300
6	1.946502	2.485797	-0.921125
6	1.637452	1.799176	1.400178
1	6.552903	-1.459685	-0.928427
1	6.754118	0.913762	-0.145541
6	1.088271	3.562387	-0.688438
6	0.750059	2.869271	1.570919
6	0.472162	3.778541	0.547846
1	0.901208	4.261576	-1.497569
1	0.291992	3.003012	2.542283
6	1.923185	-3.222951	0.721608
6	1.472169	-2.359531	-2.275354
6	2.379011	-3.533865	-2.680876
1	2.181567	-3.772187	-3.733862
1	3.442156	-3.296835	-2.603242
1	2.175417	-4.437492	-2.102232
6	0.010119	-2.796852	-2.505245
1	-0.241691	-3.694763	-1.937367
1	-0.704674	-2.023919	-2.224374
1	-0.126032	-3.027246	-3.569662
6	1.865289	-2.659134	2.155888
1	0.923954	-2.145495	2.375981
1	1.961427	-3.491338	2.864988
1	2.689925	-1.966323	2.344358
6	0.751624	-4.206506	0.537370
1	-0.215152	-3.696146	0.568007
1	0.821080	-4.761857	-0.401740
1	0.772233	-4.938369	1.354332
6	2.573184	2.338134	-2.303823
1	3.015149	1.340455	-2.369611
6	2.046540	0.963820	2.603420

1	2.410428	0.008079	2.221258
6	-0.408953	5.010769	0.745705
1	0.247696	5.882281	0.598048
6	3.705175	3.359781	-2.515339
1	4.143473	3.249227	-3.514388
1	3.324426	4.383629	-2.423799
1	4.502799	3.230111	-1.778289
6	1.535298	2.462113	-3.433620
1	1.984661	2.180070	-4.392660
1	0.666205	1.821305	-3.257554
1	1.169876	3.489978	-3.533660
6	-1.008699	5.124347	2.151902
1	-0.234770	5.156174	2.926015
1	-1.600333	6.042305	2.233223
1	-1.673681	4.280163	2.369746
6	-1.525833	5.108200	-0.311415
1	-1.133850	5.056784	-1.331630
1	-2.249377	4.296918	-0.190715
1	-2.062030	6.058177	-0.206514
6	0.905584	0.671828	3.587868
1	1.251000	-0.044721	4.343028
1	0.598893	1.576832	4.125774
1	0.024924	0.249875	3.095829
6	3.222228	1.641408	3.334786
1	2.922920	2.627519	3.708951
1	3.540410	1.035427	4.191556
1	4.084747	1.777274	2.675127
6	3.244131	-4.002037	0.603148
1	3.424591	-4.407014	-0.394110
1	4.102405	-3.394538	0.897379
1	3.195689	-4.852772	1.294829
6	1.795676	-1.162530	-3.187061
1	2.854706	-0.895383	-3.137506
1	1.558792	-1.424503	-4.225691
1	1.214791	-0.277115	-2.926247
6	-2.664179	1.549562	0.282465
6	-0.820725	0.412754	-1.039250
1	-3.546021	2.140524	0.017092
1	-1.837993	2.223789	0.517101
1	-0.577641	-0.000869	-2.015598
1	-0.199306	1.273046	-0.804504
6	-2.258279	0.627387	-0.839754
6	-3.127638	0.009749	-1.689540

6	-4.586837	0.010054	-1.701509
6	-5.383104	0.233180	-0.559175
6	-5.242695	-0.280870	-2.916330
6	-6.772892	0.191170	-0.643393
1	-4.926606	0.394947	0.407252
6	-6.630330	-0.310989	-2.999632
1	-4.643409	-0.474061	-3.803136
6	-7.404227	-0.070339	-1.860703
1	-7.360293	0.352030	0.255989
1	-7.110330	-0.527662	-3.950158
1	-8.488587	-0.100449	-1.920452
1	-2.678843	-0.563678	-2.501536
6	-2.689607	-1.758211	2.252463
6	-3.128134	-2.556728	1.007044
1	-4.041807	-3.131326	1.196757
1	-3.303445	-1.883412	0.166358
1	-2.325016	-3.249805	0.736176
6	-2.406403	-2.717624	3.428142
1	-1.583052	-3.378709	3.136724
1	-2.099539	-2.144945	4.307430
1	-3.281927	-3.325737	3.682579
8	-1.578458	-0.953339	2.041213
1	-2.883740	0.999200	1.200204
6	-3.842689	-0.881460	2.644521
7	-4.720740	-0.171224	2.919259

IM11

SCF Energy: -2712.35901364

Sum of electronic and zero-point Energies= -2711.269923

Sum of electronic and thermal Energies= -2711.207165

Sum of electronic and thermal Enthalpies= -2711.206221

Sum of electronic and thermal Free Energies= -2711.365279

Electronic energy in solution by single point calculation = -2711.14436871

46	0.655657	-0.656478	-0.089749
6	-1.320211	-3.492754	-0.093631
6	-0.298758	-4.454544	0.495578
1	0.639485	-4.428322	-0.057664
1	-0.112461	-4.203004	1.543200
1	-0.711332	-5.466886	0.454754
6	-1.602383	-3.790202	-1.580290
1	-1.947121	-4.825304	-1.668716
1	-2.387673	-3.123873	-1.949823
1	-0.707072	-3.657446	-2.197428

8	-2.482859	-3.624532	0.683630
1	-3.148921	-2.938736	0.392802
6	-0.848516	-2.032723	-0.049453
7	-1.433121	-0.959094	-0.073054
13	-3.176773	-0.147708	0.121938
8	-3.525817	0.879400	-1.234098
8	-4.135160	-1.640687	0.064434
8	-3.112081	0.668018	1.656497
6	-4.288671	0.530866	-2.370423
6	-5.398892	-1.895865	0.668220
6	-2.371835	0.259611	2.789827
6	-6.093884	-2.998207	-0.128056
1	-5.454946	-3.886340	-0.180907
1	-7.046196	-3.282122	0.335026
1	-6.290764	-2.655949	-1.150982
6	-6.243416	-0.624177	0.757147
1	-5.724780	0.139253	1.347355
1	-6.436837	-0.221505	-0.244218
1	-7.208009	-0.830318	1.236095
6	-5.236761	1.682698	-2.703755
1	-4.662670	2.591701	-2.921245
1	-5.861051	1.449264	-3.574836
1	-5.890498	1.891974	-1.850473
6	-3.357503	0.203679	-3.539789
1	-2.759073	1.084776	-3.801131
1	-2.669898	-0.603277	-3.263005
1	-3.921018	-0.106354	-4.428387
6	-2.794259	-1.132059	3.273852
1	-3.861358	-1.128302	3.527471
1	-2.628152	-1.896800	2.509391
1	-2.230425	-1.421711	4.169952
6	-2.555330	1.298060	3.896398
1	-3.613809	1.361692	4.174833
1	-1.974786	1.033289	4.788044
1	-2.236512	2.287085	3.555631
1	-5.223597	-2.262391	1.692375
1	-4.892819	-0.365678	-2.158831
1	-1.300832	0.220647	2.527008
15	2.913949	-1.177663	0.000317
6	3.806452	0.434983	-0.147754
6	3.067148	1.637273	-0.225396
6	5.208089	0.497428	-0.253203
6	3.763191	2.843240	-0.425877

6	1.568557	1.780895	-0.123264
6	5.879309	1.701353	-0.441657
1	5.789589	-0.411530	-0.187131
6	5.149043	2.885472	-0.534681
1	3.187469	3.760374	-0.500540
6	0.778925	1.787951	-1.312604
6	1.006396	2.310030	1.075340
1	6.962503	1.711524	-0.520062
1	5.653168	3.834650	-0.691478
6	-0.516306	2.319049	-1.267927
6	-0.283026	2.846217	1.050550
6	-1.048983	2.903077	-0.117889
1	-1.113623	2.325941	-2.173331
1	-0.685331	3.269730	1.963045
6	3.451014	-1.894918	1.687254
6	3.599922	-2.265800	-1.424949
6	4.994488	-2.878669	-1.211709
1	5.239326	-3.495078	-2.086118
1	5.778982	-2.123733	-1.125918
1	5.040337	-3.528625	-0.335786
6	2.594532	-3.408653	-1.657049
1	2.574879	-4.115557	-0.825510
1	1.583687	-3.018137	-1.799668
1	2.883518	-3.964641	-2.557971
6	2.646217	-1.117014	2.741545
1	1.569891	-1.193970	2.561391
1	2.863083	-1.523138	3.737791
1	2.916913	-0.060011	2.747134
6	3.036557	-3.372138	1.769222
1	1.981535	-3.500941	1.523270
1	3.628574	-4.016360	1.114350
1	3.186039	-3.725594	2.797096
6	1.377310	1.430792	-2.667148
1	2.345160	0.960229	-2.487907
6	1.824021	2.430024	2.355174
1	2.742767	1.851617	2.221081
6	-2.361800	3.662630	-0.224897
1	-3.025146	3.037268	-0.830359
6	1.642923	2.709585	-3.482683
1	2.114642	2.462613	-4.441125
1	0.708759	3.243324	-3.690104
1	2.307477	3.390760	-2.940996
6	0.508219	0.445215	-3.460834

1	1.007041	0.164411	-4.396186
1	0.315570	-0.462268	-2.878158
1	-0.461274	0.879870	-3.719326
6	-2.114500	4.985872	-0.977935
1	-1.660927	4.813788	-1.960362
1	-3.058698	5.522618	-1.127609
1	-1.440654	5.637948	-0.407586
6	-3.063574	3.923341	1.109610
1	-3.270938	2.980540	1.619733
1	-2.468608	4.570735	1.767736
1	-4.015018	4.436668	0.928995
6	1.083209	1.875236	3.581928
1	1.749834	1.860166	4.452095
1	0.218542	2.494108	3.839902
1	0.719684	0.860146	3.406017
6	2.242477	3.891105	2.606015
1	1.361692	4.532770	2.720228
1	2.838483	3.966465	3.523183
1	2.841035	4.283702	1.778778
6	4.942739	-1.748667	2.027424
1	5.597319	-2.257177	1.316630
1	5.241552	-0.699059	2.084459
1	5.120481	-2.196031	3.013625
6	3.627357	-1.409859	-2.702723
1	4.301287	-0.553364	-2.618626
1	3.973463	-2.032620	-3.537131
1	2.629896	-1.046870	-2.954726

IM12

SCF Energy: -2712.35363911

Sum of electronic and zero-point Energies= -2711.269251

Sum of electronic and thermal Energies= -2711.204119

Sum of electronic and thermal Enthalpies= -2711.203175

Sum of electronic and thermal Free Energies= -2711.371747

Electronic energy in solution by single point calculation = -2711.149095

46	0.876975	-0.812802	0.186531
6	-1.891306	-3.541275	-0.205485
6	-0.689758	-4.138512	0.451079
1	-0.001004	-3.283854	0.617697
1	-0.949602	-4.594364	1.408103
1	-0.170634	-4.847308	-0.201081
6	-1.735503	-3.080018	-1.628282
1	-1.441042	-3.918115	-2.270520

1	-2.651905	-2.621771	-2.005374
1	-0.919687	-2.343021	-1.651495
8	-2.931307	-3.359163	0.435786
1	-3.938100	-2.245383	-0.046305
6	-1.038328	-0.439629	0.290934
7	-2.188529	-0.178173	0.269174
13	-3.988471	0.237755	0.161547
8	-4.447179	1.216699	-1.178432
8	-4.603861	-1.510480	-0.262945
8	-4.653525	0.685491	1.684464
6	-4.431354	0.871637	-2.549911
6	-5.958724	-2.017428	-0.013209
6	-4.104871	0.393601	2.959152
6	-6.178889	-3.213579	-0.927528
1	-5.419960	-3.983605	-0.755255
1	-7.162856	-3.654865	-0.737347
1	-6.133458	-2.902504	-1.976862
6	-6.949018	-0.887682	-0.237075
1	-6.772446	-0.068892	0.465787
1	-6.876854	-0.503364	-1.259100
1	-7.964522	-1.265491	-0.077845
6	-5.432032	1.762433	-3.283145
1	-5.143135	2.813625	-3.171302
1	-5.472792	1.521124	-4.351993
1	-6.433360	1.640657	-2.856712
6	-3.019525	1.008615	-3.125801
1	-2.690049	2.051685	-3.058166
1	-2.307956	0.394756	-2.564772
1	-2.989386	0.704065	-4.179204
6	-4.301036	-1.085534	3.304344
1	-5.370498	-1.331138	3.299916
1	-3.791675	-1.729538	2.578441
1	-3.899546	-1.317975	4.297882
6	-4.760861	1.313658	3.985146
1	-5.841101	1.128987	4.018047
1	-4.346748	1.150573	4.987094
1	-4.602872	2.359955	3.705585
1	-5.982633	-2.329080	1.036483
1	-4.749738	-0.179077	-2.673592
1	-3.021506	0.598311	2.951560
15	3.143896	-1.333264	0.113227
6	4.188848	0.179089	-0.164801
6	3.621487	1.474373	-0.291034

6	5.582334	0.047293	-0.316492
6	4.478442	2.556068	-0.567556
6	2.166464	1.847705	-0.174979
6	6.411719	1.131672	-0.585011
1	6.033818	-0.930771	-0.226848
6	5.852760	2.401278	-0.713959
1	4.033703	3.540652	-0.673403
6	1.357334	1.899500	-1.335222
6	1.662338	2.358973	1.040639
1	7.481921	0.981802	-0.696135
1	6.477975	3.263206	-0.929250
6	0.066154	2.419815	-1.241982
6	0.355958	2.860310	1.084443
6	-0.464774	2.894368	-0.041000
1	-0.556963	2.444209	-2.130679
1	-0.024362	3.233044	2.028314
6	3.734122	-2.045009	1.790020
6	3.640074	-2.542733	-1.299271
6	4.951988	-3.326848	-1.135743
1	5.081729	-3.978822	-2.009707
1	5.829740	-2.678034	-1.090935
1	4.950568	-3.968394	-0.251875
6	2.482860	-3.552601	-1.441509
1	2.372697	-4.184962	-0.557475
1	1.534839	-3.030517	-1.598406
1	2.677377	-4.206896	-2.302197
6	3.128382	-1.119934	2.858824
1	2.043343	-1.039692	2.741354
1	3.348854	-1.520194	3.857369
1	3.553146	-0.115582	2.800982
6	3.110780	-3.440974	1.968417
1	2.031257	-3.412723	1.791843
1	3.553512	-4.189418	1.305801
1	3.277084	-3.777042	3.000047
6	1.878124	1.458133	-2.694026
1	2.811922	0.915059	-2.532940
6	2.520910	2.440452	2.294510
1	3.380929	1.779381	2.153716
6	-1.882708	3.442341	-0.016855
1	-2.499879	2.772149	-0.627265
6	2.208506	2.678184	-3.571396
1	2.603178	2.362298	-4.544875
1	1.313008	3.285464	-3.747608

1	2.957415	3.316124	-3.089994
6	0.903281	0.510185	-3.410246
1	1.359609	0.106991	-4.322621
1	0.628134	-0.320839	-2.750712
1	-0.018701	1.023722	-3.702718
6	-1.932909	4.833494	-0.675850
1	-1.538208	4.804433	-1.697414
1	-2.963559	5.205087	-0.717501
1	-1.331458	5.552418	-0.105786
6	-2.506864	3.486371	1.382258
1	-2.418054	2.520700	1.888192
1	-2.029596	4.246631	2.013122
1	-3.571683	3.729479	1.312116
6	1.772953	1.982874	3.557400
1	2.471649	1.876592	4.395481
1	1.012009	2.711437	3.858596
1	1.273230	1.024112	3.395657
6	3.071106	3.866047	2.485573
1	2.249967	4.585251	2.587004
1	3.689802	3.925333	3.389387
1	3.684307	4.173122	1.632754
6	5.249754	-2.113583	2.032333
1	5.775580	-2.739182	1.308297
1	5.701595	-1.118433	2.023347
1	5.426999	-2.544610	3.026461
6	3.709062	-1.732635	-2.604194
1	4.521728	-1.001504	-2.596355
1	3.877093	-2.419067	-3.444269
1	2.771647	-1.205514	-2.787750

IM1A

SCF Energy: -2778.63612588

Sum of electronic and zero-point Energies= -2777.868037

Sum of electronic and thermal Energies= -2777.821345

Sum of electronic and thermal Enthalpies= -2777.820401

Sum of electronic and thermal Free Energies= -2777.947905

Electronic energy in solution by single point calculation = -2777.35576074

6	3.339728	-1.265796	1.438950
6	2.191472	-0.517536	1.143920
6	1.118309	-0.629054	2.031802
6	1.114782	-1.451444	3.161142
6	2.273366	-2.188956	3.414278
6	3.377421	-2.090131	2.563726

6	-0.140470	-1.439346	4.040639
6	-1.351544	-1.313939	3.110852
6	-1.212227	-0.497973	1.988614
6	-2.230037	-0.251883	1.065514
6	-3.474585	-0.843060	1.311663
6	-3.653958	-1.662974	2.426982
6	-2.602443	-1.902901	3.314778
1	4.196603	-1.218736	0.777775
1	2.321716	-2.847144	4.274853
1	4.272973	-2.666536	2.776537
1	-4.294565	-0.674875	0.622871
1	-4.622011	-2.122000	2.605547
1	-2.765102	-2.551124	4.169009
8	-0.002848	0.116316	1.738666
15	-1.791095	0.748504	-0.418673
15	1.951472	0.438208	-0.422348
6	-3.422415	0.837379	-1.269622
6	-4.276513	1.943326	-1.171963
6	-3.827509	-0.270944	-2.030167
6	-5.509565	1.942352	-1.827575
1	-3.980770	2.804954	-0.583415
6	-5.065634	-0.276460	-2.669873
1	-3.161553	-1.122012	-2.116336
6	-5.908634	0.833749	-2.574529
1	-6.159907	2.809403	-1.749239
1	-5.368316	-1.143388	-3.251044
1	-6.869363	0.834657	-3.081958
6	-1.625005	2.439065	0.277025
6	-1.022821	3.413204	-0.530688
6	-2.093157	2.797479	1.547132
6	-0.912093	4.728368	-0.085157
1	-0.630948	3.129318	-1.503187
6	-1.963351	4.110981	2.000171
1	-2.563071	2.050732	2.179249
6	-1.378768	5.079206	1.182862
1	-0.437510	5.472285	-0.716758
1	-2.324810	4.378170	2.989653
1	-1.278679	6.101963	1.535687
6	3.595357	0.164480	-1.215337
6	3.716715	-0.851571	-2.171560
6	4.740140	0.882950	-0.836916
6	4.957030	-1.146375	-2.740025
1	2.828797	-1.396817	-2.469335

6	5.977346	0.593429	-1.411346
1	4.662661	1.667377	-0.091263
6	6.089074	-0.422725	-2.363726
1	5.035777	-1.936845	-3.481428
1	6.855560	1.159608	-1.113024
1	7.053948	-0.646544	-2.810357
6	2.110478	2.198302	0.090607
6	2.363090	3.143110	-0.917609
6	1.958905	2.639020	1.409141
6	2.493231	4.493962	-0.606652
1	2.475569	2.811896	-1.946697
6	2.068027	3.996537	1.715779
1	1.760942	1.926534	2.201060
6	2.344713	4.925363	0.713857
1	2.704671	5.210983	-1.395442
1	1.939304	4.325378	2.743098
1	2.436710	5.980119	0.957367
46	0.013882	-0.129249	-1.630101
6	-0.090521	-0.172647	4.937404
1	-0.988794	-0.116198	5.562270
1	0.790426	-0.203023	5.588214
1	-0.039091	0.735055	4.328929
6	-0.227171	-2.681374	4.935321
1	0.631806	-2.732110	5.610902
1	-1.121832	-2.642203	5.563518
1	-0.258343	-3.601708	4.343671
6	0.519728	-1.350812	-3.308236
6	-0.860489	-1.145951	-3.266438
6	-0.355083	-2.549052	-2.999829
1	1.273797	-1.203216	-4.073858
1	-1.600646	-0.770692	-3.964609
6	-0.552021	-3.614523	-4.072434
1	-0.524708	-3.169371	-5.073437
1	0.232674	-4.380035	-4.014610
1	-1.515467	-4.126726	-3.951976
6	-0.408966	-3.088034	-1.589863
6	-1.639182	-3.402981	-0.997700
6	0.756547	-3.268988	-0.834568
6	-1.708277	-3.856050	0.318890
1	-2.552423	-3.266252	-1.571761
6	0.696134	-3.724795	0.482110
1	1.714559	-3.015605	-1.277628
6	-0.538705	-4.014046	1.064386

1	-2.673503	-4.063879	0.770836
1	1.609912	-3.830843	1.058510
1	-0.591141	-4.355933	2.094039

IM1B

SCF Energy: -3502.18515982

Sum of electronic and zero-point Energies= -3501.175522

Sum of electronic and thermal Energies= -3501.111376

Sum of electronic and thermal Enthalpies= -3501.110431

Sum of electronic and thermal Free Energies= -3501.277099

Electronic energy in solution by single point calculation = -3500.71409348

6	-2.680286	1.995142	2.641901
6	-2.350973	1.118848	1.595673
6	-2.558797	-0.247927	1.822697
6	-3.000257	-0.772168	3.044370
6	-3.287840	0.135201	4.065778
6	-3.147493	1.508401	3.859604
6	-3.190339	-2.290139	3.150500
6	-2.095391	-2.952505	2.311495
6	-1.737574	-2.324401	1.121417
6	-0.805815	-2.838200	0.216987
6	-0.191499	-4.053794	0.532596
6	-0.511711	-4.703182	1.726275
6	-1.453772	-4.161542	2.604798
1	-2.542428	3.061405	2.513675
1	-3.628188	-0.224956	5.030054
1	-3.385413	2.201947	4.660204
1	0.548164	-4.471519	-0.141869
1	-0.023015	-5.639985	1.975998
1	-1.683924	-4.688032	3.524389
8	-2.297362	-1.106210	0.781631
15	-0.390048	-1.765543	-1.202810
15	-1.533419	1.716341	0.043651
6	0.735432	-2.796053	-2.216710
6	0.261820	-3.728476	-3.152288
6	2.116782	-2.630388	-2.039770
6	1.160833	-4.487365	-3.900591
1	-0.806125	-3.854958	-3.298886
6	3.010514	-3.399868	-2.787487
1	2.503152	-1.935768	-1.299189
6	2.536810	-4.323937	-3.719783
1	0.787290	-5.205188	-4.625823
1	4.078380	-3.270145	-2.635387

1	3.235290	-4.915182	-4.305763
6	-1.946190	-1.744695	-2.176860
6	-2.116925	-0.711817	-3.108474
6	-2.961605	-2.695872	-2.017037
6	-3.278443	-0.636131	-3.874251
1	-1.344994	0.045927	-3.211693
6	-4.129751	-2.612569	-2.776084
1	-2.841492	-3.497060	-1.294118
6	-4.289510	-1.583589	-3.705708
1	-3.404822	0.178688	-4.579048
1	-4.914591	-3.351836	-2.640270
1	-5.201599	-1.516099	-4.292132
6	-1.054290	3.403696	0.608442
6	0.126436	3.512550	1.365755
6	-1.823839	4.550762	0.369130
6	0.511774	4.745087	1.891573
1	0.750658	2.638923	1.535628
6	-1.417512	5.788181	0.875586
1	-2.736017	4.475976	-0.213598
6	-0.256123	5.886360	1.643321
1	1.420738	4.811258	2.482412
1	-2.013995	6.673248	0.673439
1	0.054062	6.848426	2.040493
6	-2.898486	2.006343	-1.136565
6	-2.591715	2.656073	-2.344827
6	-4.198993	1.543690	-0.911743
6	-3.588292	2.865949	-3.294818
1	-1.575360	2.994102	-2.532585
6	-5.186839	1.733374	-1.879802
1	-4.439594	1.034664	0.015765
6	-4.887316	2.401565	-3.066515
1	-3.348117	3.382095	-4.220349
1	-6.191918	1.361863	-1.701604
1	-5.659703	2.555018	-3.814943
46	0.288032	0.480517	-0.682800
6	-4.562657	-2.649796	2.519485
1	-4.719392	-3.733707	2.549069
1	-5.373411	-2.161462	3.071534
1	-4.610784	-2.324376	1.475952
6	-3.163918	-2.771042	4.606671
1	-3.977052	-2.318059	5.181153
1	-3.310416	-3.853861	4.655152
1	-2.214152	-2.526330	5.092958

6	1.919700	3.156602	-1.765143
6	2.489741	2.871832	-3.160904
1	3.471277	2.398061	-3.083499
1	1.817327	2.212810	-3.717458
1	2.580786	3.820132	-3.699436
6	2.858732	4.050386	-0.941306
1	3.025287	4.984555	-1.487206
1	2.414355	4.286167	0.028289
1	3.815298	3.553425	-0.763959
8	0.663537	3.776364	-1.973835
1	0.271521	3.965393	-1.104280
6	1.793254	1.804719	-1.072603
7	2.554708	0.921723	-0.725967
13	3.460875	0.211784	0.862819
8	3.635733	-1.480064	0.469710
8	4.901041	1.194128	0.925174
8	2.386728	0.630439	2.175747
6	4.535564	-2.459645	0.942040
6	5.766832	1.460899	-0.152330
6	1.183855	0.034310	2.604344
6	6.490997	0.194704	-0.623594
1	5.767577	-0.558244	-0.952597
1	7.171280	0.411719	-1.456646
1	7.075340	-0.231191	0.200663
6	6.751575	2.550049	0.272809
1	6.208139	3.442827	0.600701
1	7.356344	2.195999	1.115701
1	7.423167	2.827598	-0.548884
6	5.125530	-2.091662	2.307109
1	4.331867	-2.024516	3.059653
1	5.851736	-2.844342	2.638005
1	5.633446	-1.122469	2.257226
6	3.830947	-3.819043	0.984773
1	3.006726	-3.800026	1.706451
1	3.416858	-4.066445	0.002643
1	4.529534	-4.612625	1.277335
6	0.665497	0.779043	3.834876
1	1.385871	0.681950	4.655734
1	0.534712	1.844867	3.625475
1	-0.299590	0.374056	4.159342
6	1.336190	-1.459686	2.893747
1	2.079523	-1.613405	3.685462
1	0.384972	-1.894133	3.219618

1	1.671212	-1.987980	1.999917
1	5.186915	1.845137	-1.013763
1	5.373187	-2.537096	0.227459
1	0.426900	0.134831	1.799986

IM1

SCF Energy: -1988.81566427

Sum of electronic and zero-point Energies= -1987.968249

Sum of electronic and thermal Energies= -1987.922348

Sum of electronic and thermal Enthalpies= -1987.921404

Sum of electronic and thermal Free Energies= -1988.043718

Electronic energy in solution by single point calculation = -1987.77147542

46	-0.106717	0.720264	-0.559410
15	2.158294	0.690013	-0.066720
6	2.509693	-0.887766	0.840853
6	1.460681	-1.820782	1.032625
6	3.766160	-1.165922	1.408039
6	1.720709	-2.982302	1.781339
6	0.047854	-1.699730	0.511073
6	4.004828	-2.322464	2.145098
1	4.576564	-0.461656	1.274680
6	2.971616	-3.238822	2.334389
1	0.910202	-3.688898	1.931316
6	-0.965869	-1.123912	1.324661
6	-0.335776	-2.445378	-0.640548
1	4.988254	-2.502335	2.570063
1	3.135201	-4.144834	2.910910
6	-2.312736	-1.284833	0.956384
6	-1.688394	-2.587637	-0.945834
6	-2.696712	-2.019581	-0.159802
1	-3.079996	-0.836057	1.578615
1	-1.965102	-3.175341	-1.815552
6	3.311254	0.665992	-1.592857
6	2.719847	2.092907	1.118903
6	4.228731	2.368742	1.216441
1	4.389955	3.193428	1.923185
1	4.788363	1.509894	1.595858
1	4.665642	2.671941	0.262759
6	2.002645	3.378129	0.655699
1	2.343068	3.716572	-0.325518
1	0.922162	3.219760	0.599378
1	2.204932	4.183002	1.374748
6	2.657953	-0.309226	-2.585239

1	1.618541	-0.035667	-2.784195
1	3.215014	-0.298657	-3.531389
1	2.673251	-1.331902	-2.202792
6	3.306289	2.065515	-2.232607
1	2.287773	2.436673	-2.373215
1	3.862212	2.799394	-1.644238
1	3.782762	2.008993	-3.219722
6	-0.649923	-0.509588	2.681771
1	0.428292	-0.343631	2.727091
6	0.688900	-3.166836	-1.503840
1	1.675772	-2.773279	-1.246464
6	-4.164620	-2.250113	-0.474098
1	-4.744252	-1.579783	0.173906
6	-1.001264	-1.504484	3.803704
1	-0.741610	-1.085309	4.783021
1	-2.074030	-1.729599	3.804059
1	-0.458123	-2.447528	3.681798
6	-1.347250	0.838853	2.905748
1	-1.034325	1.271825	3.863375
1	-1.107297	1.543600	2.105959
1	-2.437368	0.742334	2.927268
6	-4.568583	-3.695227	-0.128710
1	-4.356381	-3.921387	0.921690
1	-5.638245	-3.856426	-0.307970
1	-4.010992	-4.411120	-0.744335
6	-4.521059	-1.920606	-1.932500
1	-4.243479	-0.893530	-2.190608
1	-4.003553	-2.589304	-2.629687
1	-5.597838	-2.037638	-2.100430
6	0.457961	-2.930203	-3.005510
1	1.306455	-3.310969	-3.585584
1	-0.438819	-3.451163	-3.359182
1	0.336036	-1.866184	-3.224070
6	0.705235	-4.675653	-1.196490
1	-0.276409	-5.121823	-1.394129
1	1.444094	-5.188778	-1.823597
1	0.957825	-4.866270	-0.149235
6	4.756616	0.200911	-1.357958
1	5.300558	0.829040	-0.649845
1	4.789839	-0.831679	-1.000665
1	5.299540	0.236202	-2.311761
6	2.194650	1.755151	2.524042
1	2.647734	0.846905	2.930917

1	2.430528	2.585063	3.202475
1	1.111063	1.632112	2.517845
6	-0.442801	2.287345	-3.361544
6	-0.488001	3.435837	-2.353494
1	-1.193402	2.272868	-4.150823
1	0.534442	1.929641	-3.676604
1	-1.268311	4.187087	-2.468730
1	0.458958	3.833457	-1.995775
6	-0.891831	2.061271	-1.962698
6	-2.004279	1.449577	-1.362037
1	-2.473748	0.609880	-1.874464
6	-2.801222	2.069898	-0.290981
6	-4.030736	1.502941	0.089753
6	-2.374283	3.222670	0.398819
6	-4.785232	2.037693	1.131846
1	-4.390098	0.627002	-0.440487
6	-3.130365	3.760302	1.436342
1	-1.431059	3.681338	0.123394
6	-4.337527	3.168177	1.818804
1	-5.729171	1.572259	1.405220
1	-2.772738	4.646323	1.955214
1	-4.923037	3.586740	2.632425

IM2A

SCF Energy: -2778.62744287

Sum of electronic and zero-point Energies= -2777.858986

Sum of electronic and thermal Energies= -2777.812463

Sum of electronic and thermal Enthalpies= -2777.811519

Sum of electronic and thermal Free Energies= -2777.937857

Electronic energy in solution by single point calculation = -2777.33369837

6	-3.428264	-1.308992	-1.012358
6	-2.191519	-0.657910	-0.941945
6	-1.112403	-1.265269	-1.590948
6	-1.187436	-2.469354	-2.286026
6	-2.441313	-3.083658	-2.344979
6	-3.548154	-2.506345	-1.719081
6	0.091625	-2.973794	-2.961453
6	1.278095	-2.599255	-2.064227
6	1.220624	-1.382055	-1.384051
6	2.246790	-0.880317	-0.575943
6	3.416715	-1.645441	-0.490707
6	3.509575	-2.871045	-1.151952
6	2.448900	-3.348461	-1.923746

1	-4.287348	-0.898641	-0.495001
1	-2.559624	-4.024972	-2.870001
1	-4.511378	-3.005645	-1.767422
1	4.249970	-1.290757	0.103421
1	4.419231	-3.458114	-1.066497
1	2.542421	-4.307619	-2.420752
8	0.093689	-0.599858	-1.499193
15	1.938794	0.700559	0.339964
15	-1.760242	0.801555	0.085677
6	3.519476	0.931310	1.250096
6	4.352933	2.038079	1.039236
6	3.878048	-0.008693	2.232149
6	5.515843	2.202165	1.793923
1	4.098075	2.772114	0.283212
6	5.046233	0.151509	2.974930
1	3.240154	-0.867365	2.409626
6	5.867524	1.260775	2.761176
1	6.150548	3.066341	1.617828
1	5.310217	-0.588036	3.725772
1	6.774683	1.389135	3.344919
6	2.069138	1.956363	-0.991371
6	1.608444	3.250217	-0.712732
6	2.642509	1.687800	-2.240597
6	1.745915	4.265822	-1.656502
1	1.136835	3.454595	0.244180
6	2.759608	2.700683	-3.192382
1	3.002564	0.689090	-2.465251
6	2.319388	3.992095	-2.899288
1	1.382002	5.263067	-1.431152
1	3.202467	2.482092	-4.160397
1	2.412918	4.780980	-3.640420
6	-3.332408	1.371962	0.842937
6	-3.313094	1.751576	2.189622
6	-4.499077	1.581787	0.089924
6	-4.450746	2.297621	2.787824
1	-2.398241	1.616869	2.758240
6	-5.638553	2.112098	0.690415
1	-4.506207	1.351079	-0.970896
6	-5.616976	2.467469	2.042709
1	-4.423116	2.586683	3.834619
1	-6.539332	2.262655	0.101910
1	-6.504803	2.886723	2.507860
6	-1.567091	2.176096	-1.140180

6	-1.776348	3.488171	-0.684989
6	-1.228634	1.976470	-2.483490
6	-1.670717	4.569413	-1.556476
1	-2.047827	3.662985	0.351684
6	-1.114004	3.061883	-3.352564
1	-1.061179	0.976795	-2.862135
6	-1.340796	4.359426	-2.896332
1	-1.849353	5.576060	-1.188015
1	-0.847234	2.888016	-4.391122
1	-1.256205	5.201256	-3.577790
46	-0.016648	0.281810	1.644718
6	0.256575	-2.215027	-4.306310
1	1.176054	-2.533574	-4.809927
1	-0.594975	-2.419733	-4.964662
1	0.313640	-1.134523	-4.142460
6	0.033152	-4.480659	-3.238245
1	-0.803489	-4.717865	-3.902105
1	0.942261	-4.817263	-3.745109
1	-0.084039	-5.046116	-2.310005
6	0.930760	-0.111940	3.407077
6	0.127855	-1.035856	3.926478
6	-0.970568	-1.245916	2.907357
1	1.811210	0.350403	3.849786
1	0.183218	-1.570124	4.885754
6	-2.357671	-1.026670	3.487580
1	-2.364179	-0.147662	4.137053
1	-3.136627	-0.885235	2.733286
1	-2.648317	-1.893889	4.105461
6	-0.821012	-2.464187	2.056479
6	0.450671	-3.016554	1.781482
6	-1.934214	-3.127220	1.501399
6	0.598064	-4.166723	1.015077
1	1.328497	-2.519934	2.176069
6	-1.787044	-4.282273	0.735423
1	-2.931466	-2.740363	1.674342
6	-0.522513	-4.816748	0.490315
1	1.594539	-4.554416	0.822793
1	-2.670707	-4.765877	0.328247
1	-0.411290	-5.727917	-0.091442

IM2B

SCF Energy: -3502.18687082

Sum of electronic and zero-point Energies= -3501.180520

Sum of electronic and thermal Energies= -3501.114580

Sum of electronic and thermal Enthalpies= -3501.113635

Sum of electronic and thermal Free Energies= -3501.287592

Electronic energy in solution by single point calculation = -3500.72153043

6	-1.235963	2.881127	2.598623
6	-1.589502	1.875012	1.687058
6	-2.038622	0.662108	2.224407
6	-2.112746	0.398942	3.596641
6	-1.725640	1.419040	4.468751
6	-1.301947	2.653493	3.972280
6	-2.656760	-0.968356	4.024761
6	-2.127349	-1.999793	3.024709
6	-2.056790	-1.611970	1.686082
6	-1.623548	-2.449855	0.652920
6	-1.253709	-3.755698	1.000669
6	-1.307691	-4.175226	2.330699
6	-1.738588	-3.306211	3.334925
1	-0.880357	3.835625	2.229615
1	-1.755963	1.257589	5.540531
1	-1.011756	3.440456	4.662177
1	-0.911413	-4.436937	0.229802
1	-1.010792	-5.187940	2.587321
1	-1.764983	-3.651271	4.362531
8	-2.410729	-0.323221	1.334364
15	-1.480377	-1.728605	-1.036686
15	-1.317040	2.013186	-0.137512
6	-0.920546	-3.203579	-1.988482
6	-1.795037	-4.159818	-2.522130
6	0.463048	-3.379417	-2.143773
6	-1.293280	-5.274432	-3.196042
1	-2.867157	-4.032121	-2.409915
6	0.962896	-4.502753	-2.801977
1	1.140364	-2.626178	-1.752756
6	0.085236	-5.451037	-3.332387
1	-1.979912	-6.007222	-3.611761
1	2.036554	-4.630480	-2.907233
1	0.473282	-6.321491	-3.854519
6	-3.244792	-1.555972	-1.523364
6	-3.541735	-0.662392	-2.561823
6	-4.291956	-2.243876	-0.896035
6	-4.857496	-0.475482	-2.979762
1	-2.735806	-0.096834	-3.021000
6	-5.611502	-2.044820	-1.305088

1	-4.074512	-2.931722	-0.084504
6	-5.895852	-1.163751	-2.349578
1	-5.074070	0.229757	-3.775503
1	-6.416849	-2.579310	-0.807934
1	-6.923767	-1.006021	-2.664657
6	-0.542405	3.685714	-0.232097
6	0.856008	3.741541	-0.290530
6	-1.271369	4.883951	-0.207052
6	1.519437	4.968942	-0.309961
1	1.418393	2.814154	-0.338559
6	-0.609734	6.112103	-0.240617
1	-2.355618	4.853575	-0.161123
6	0.786375	6.157129	-0.288182
1	2.603866	4.983278	-0.363055
1	-1.183947	7.034759	-0.226266
1	1.298330	7.115441	-0.313392
6	-2.999001	2.339260	-0.808089
6	-3.094510	2.821198	-2.124391
6	-4.175883	2.049938	-0.108518
6	-4.337671	3.034565	-2.714337
1	-2.186737	3.037536	-2.682122
6	-5.421064	2.244789	-0.708378
1	-4.124260	1.672943	0.906537
6	-5.507588	2.744120	-2.007203
1	-4.394334	3.420803	-3.728723
1	-6.325285	2.006852	-0.155038
1	-6.478331	2.899753	-2.469592
46	-0.170513	0.222574	-1.098487
6	-4.204651	-0.931512	3.910212
1	-4.626248	-1.906034	4.180635
1	-4.616460	-0.170549	4.582552
1	-4.515774	-0.695160	2.888545
6	-2.269960	-1.315252	5.467326
1	-2.679351	-0.578655	6.164980
1	-2.685058	-2.286154	5.753271
1	-1.183282	-1.350799	5.595428
6	3.698369	2.466964	-2.545928
6	2.494609	3.008054	-3.261863
1	1.664750	2.323932	-3.023837
1	2.227314	3.996938	-2.886483
1	2.628840	3.016362	-4.347472
6	4.538271	1.448652	-3.271461
1	5.067914	1.953114	-4.091087

1	5.261479	0.976063	-2.605833
1	3.898062	0.680036	-3.713741
8	3.965647	2.840472	-1.401133
1	4.624572	1.766353	-0.390940
6	1.756026	0.048938	-1.452726
7	2.892478	-0.205770	-1.201668
13	4.062758	-0.615664	0.173054
8	5.384960	-1.662915	-0.212460
8	4.911473	1.068851	0.275239
8	3.194128	-0.961730	1.620682
6	5.364489	-3.081101	-0.163246
6	6.211666	1.390764	0.867645
6	1.946362	-0.439561	2.052156
6	7.303483	1.134220	-0.161667
1	7.155098	1.755992	-1.051597
1	8.285539	1.374846	0.260197
1	7.284637	0.080122	-0.453863
6	6.364358	0.565706	2.134828
1	5.513045	0.718821	2.803394
1	6.428292	-0.497359	1.885420
1	7.282669	0.859509	2.653795
6	5.534529	-3.565311	1.278605
1	4.695876	-3.215079	1.890491
1	5.575838	-4.660347	1.328233
1	6.462080	-3.166757	1.704553
6	4.086906	-3.641481	-0.797899
1	3.206816	-3.357478	-0.206319
1	3.961402	-3.247594	-1.812389
1	4.115343	-4.736545	-0.848993
6	2.093460	1.017275	2.493672
1	2.826833	1.092501	3.306732
1	2.438258	1.642328	1.662490
1	1.138409	1.420470	2.844734
6	1.417062	-1.322081	3.178371
1	2.136202	-1.345144	4.006341
1	0.461632	-0.940736	3.551316
1	1.263150	-2.345653	2.823164
1	6.154305	2.455632	1.117628
1	6.223504	-3.431298	-0.755184
1	1.221002	-0.468262	1.220260

IM2

SCF Energy: -1988.80693068

Sum of electronic and zero-point Energies= -1987.959621

Sum of electronic and thermal Energies= -1987.914124

Sum of electronic and thermal Enthalpies= -1987.913180

Sum of electronic and thermal Free Energies= -1988.035630

Electronic energy in solution by single point calculation = -1987.75733699

46	-0.267164	-0.419301	1.146788
15	-2.325375	-0.951515	0.110568
6	-2.587737	0.355840	-1.175911
6	-1.599838	1.350013	-1.376784
6	-3.763441	0.414406	-1.946172
6	-1.828522	2.339925	-2.350131
6	-0.301159	1.512612	-0.621156
6	-3.974899	1.406114	-2.899074
1	-4.529713	-0.335045	-1.803264
6	-2.995088	2.375516	-3.106999
1	-1.067339	3.100202	-2.496565
6	-0.269132	2.328335	0.548684
6	0.931069	1.193337	-1.262768
1	-4.896284	1.418221	-3.474062
1	-3.139066	3.157595	-3.846850
6	0.963542	2.796510	1.022256
6	2.125250	1.710381	-0.759474
6	2.166277	2.525937	0.374088
1	0.977674	3.422027	1.910539
1	3.049302	1.454022	-1.263915
6	-2.235339	-2.598995	-0.867396
6	-3.898716	-0.958293	1.203306
6	-5.159249	-1.613002	0.613698
1	-5.957645	-1.572539	1.366047
1	-5.528428	-1.086756	-0.270129
1	-5.013272	-2.662539	0.354010
6	-3.517449	-1.677240	2.515031
1	-3.302555	-2.737404	2.366591
1	-2.635598	-1.217398	2.969678
1	-4.354705	-1.602278	3.220961
6	-0.813090	-2.670685	-1.448552
1	-0.048738	-2.633593	-0.668159
1	-0.697319	-3.611203	-2.002902
1	-0.627563	-1.852309	-2.146012
6	-2.414758	-3.794020	0.086018
1	-1.743490	-3.733746	0.944438
1	-3.437708	-3.894991	0.454481
1	-2.172181	-4.714380	-0.459937

6	-1.543035	2.853587	1.193394
1	-2.379560	2.284687	0.786346
6	0.987886	0.339396	-2.519275
1	-0.013511	-0.066644	-2.688811
6	3.451959	3.145050	0.900791
1	3.418568	3.061972	1.996343
6	-1.767702	4.326499	0.805864
1	-2.703371	4.699047	1.239083
1	-0.948931	4.957960	1.169420
1	-1.826004	4.441247	-0.281544
6	-1.546512	2.673473	2.718687
1	-2.513880	2.975948	3.136229
1	-1.356549	1.627524	2.984319
1	-0.776124	3.285451	3.200469
6	3.494331	4.645099	0.549278
1	2.615420	5.171960	0.935617
1	4.390188	5.117948	0.968336
1	3.514639	4.780128	-0.538815
6	4.725715	2.443551	0.417646
1	4.688199	1.365991	0.598285
1	4.883752	2.596664	-0.656659
1	5.599636	2.851708	0.936881
6	1.965504	-0.836955	-2.351766
1	1.878814	-1.528012	-3.198248
1	3.005992	-0.498605	-2.310408
1	1.771909	-1.389364	-1.430241
6	1.348096	1.183756	-3.754560
1	2.332659	1.650233	-3.635971
1	1.379593	0.554001	-4.651265
1	0.614736	1.979403	-3.922589
6	-3.231344	-2.723335	-2.031624
1	-4.274178	-2.667757	-1.710709
1	-3.061515	-1.955748	-2.790641
1	-3.088245	-3.699993	-2.511635
6	-4.234245	0.499912	1.556822
1	-4.486717	1.094846	0.674434
1	-5.099330	0.512446	2.231938
1	-3.404084	0.978763	2.076948
6	1.691949	-0.407987	1.960600
6	0.225178	-2.118768	2.299825
1	2.404230	0.114006	1.326620
1	1.620381	0.018666	2.965233
1	-0.245946	-3.051167	1.990541

1	-0.015700	-1.851072	3.332510
6	1.627880	-1.885291	1.889975
6	2.390706	-2.770553	1.189158
6	3.631990	-2.506399	0.470706
6	4.530261	-1.468295	0.801745
6	3.980009	-3.326131	-0.624618
6	5.682788	-1.242659	0.052739
1	4.329627	-0.852210	1.671357
6	5.130038	-3.098095	-1.374898
1	3.315471	-4.144348	-0.893616
6	5.988934	-2.045426	-1.049401
1	6.356116	-0.438477	0.339996
1	5.356661	-3.744207	-2.219694
1	6.887024	-1.863482	-1.632910
1	1.976174	-3.769537	1.048604

IM3A

SCF Energy: -3065.30911556

Sum of electronic and zero-point Energies= -3064.429450

Sum of electronic and thermal Energies= -3064.374931

Sum of electronic and thermal Enthalpies= -3064.373987

Sum of electronic and thermal Free Energies= -3064.518764

Electronic energy in solution by single point calculation = -3063.87981046

6	-0.398152	-3.640877	0.307697
6	-0.169211	-2.296608	0.627018
6	-1.231133	-1.594024	1.200577
6	-2.478451	-2.146120	1.492705
6	-2.679419	-3.479916	1.129088
6	-1.649759	-4.216119	0.539092
6	-3.467540	-1.270227	2.268969
6	-3.330396	0.157437	1.734794
6	-2.049677	0.585554	1.383856
6	-1.757432	1.855309	0.878127
6	-2.810927	2.778418	0.821332
6	-4.101578	2.391921	1.184299
6	-4.364470	1.087729	1.611834
1	0.397986	-4.231736	-0.129110
1	-3.639407	-3.950838	1.307238
1	-1.819008	-5.254471	0.269615
1	-2.627952	3.787253	0.471908
1	-4.913013	3.111058	1.123566
1	-5.381094	0.800954	1.855612
8	-0.984078	-0.272351	1.513048

15	-0.070410	2.089100	0.184801
15	1.408881	-1.371568	0.358994
6	-0.157800	3.773643	-0.564715
6	0.787628	4.760939	-0.251085
6	-1.133945	4.070162	-1.533254
6	0.761595	6.001718	-0.889633
1	1.548254	4.566512	0.494960
6	-1.163512	5.312694	-2.163310
1	-1.887493	3.335604	-1.789610
6	-0.211456	6.283410	-1.847551
1	1.504828	6.750209	-0.629799
1	-1.930614	5.518438	-2.904472
1	-0.230419	7.249906	-2.342742
6	1.020003	2.349776	1.625576
6	2.402861	2.396221	1.394675
6	0.525934	2.560068	2.917448
6	3.274791	2.698610	2.438008
1	2.797954	2.177570	0.406919
6	1.406781	2.827298	3.965777
1	-0.542834	2.518781	3.101891
6	2.778802	2.912157	3.724997
1	4.343190	2.731888	2.246891
1	1.019112	2.976975	4.969519
1	3.461165	3.127087	4.542437
6	2.482115	-2.685718	-0.348711
6	2.172749	-3.175406	-1.629041
6	3.584858	-3.216135	0.332310
6	2.946058	-4.182590	-2.203901
1	1.342796	-2.755001	-2.179193
6	4.368054	-4.210865	-0.255515
1	3.838298	-2.855484	1.321796
6	4.050707	-4.698743	-1.522761
1	2.692732	-4.551236	-3.194111
1	5.223735	-4.606715	0.284395
1	4.659263	-5.475378	-1.977876
6	2.045476	-1.191736	2.075600
6	3.288069	-0.563701	2.248978
6	1.359032	-1.666784	3.201464
6	3.834643	-0.429647	3.524588
1	3.829137	-0.189014	1.385710
6	1.900415	-1.510208	4.476972
1	0.406675	-2.171496	3.087844
6	3.141454	-0.894045	4.642418

1	4.799750	0.054669	3.642554
1	1.354391	-1.880314	5.340593
1	3.565330	-0.777654	5.636124
46	0.767091	0.443799	-1.220180
6	-3.022845	-1.267336	3.758219
1	-3.682630	-0.620936	4.347588
1	-3.070406	-2.283141	4.165854
1	-1.997301	-0.901319	3.864957
6	-4.905577	-1.789605	2.177919
1	-4.972140	-2.801226	2.590022
1	-5.577127	-1.162956	2.773164
1	-5.261981	-1.806422	1.145732
6	-0.375782	1.136055	-2.833746
6	-1.685652	0.621348	-2.438902
6	-2.150418	-0.655461	-2.544531
1	-0.329385	2.217228	-2.948542
1	-2.329749	1.333374	-1.928680
6	-1.286350	-1.762165	-3.097279
1	-0.329754	-1.388378	-3.464320
1	-1.061987	-2.497538	-2.313269
1	-1.793066	-2.301446	-3.907995
6	-3.508452	-1.018726	-2.086895
6	-4.495236	-0.054379	-1.789985
6	-3.883043	-2.371557	-1.960905
6	-5.777597	-0.420856	-1.398166
1	-4.266969	1.001091	-1.884541
6	-5.169610	-2.740911	-1.573367
1	-3.155143	-3.149354	-2.155813
6	-6.131136	-1.769540	-1.294997
1	-6.510474	0.352562	-1.183875
1	-5.419540	-3.795427	-1.489784
1	-7.137836	-2.055295	-1.003023
6	3.090323	0.057704	-2.987700
6	3.909296	-0.889519	-3.888901
1	4.886054	-0.464424	-4.145720
1	4.053046	-1.849309	-3.388193
1	3.337736	-1.054969	-4.807832
6	2.941466	1.439885	-3.667510
1	2.388953	1.304560	-4.602962
1	2.373591	2.116908	-3.022805
1	3.915483	1.890290	-3.889983
8	1.876077	-0.541855	-2.698454
6	3.876714	0.286928	-1.725012

7	4.442343	0.486690	-0.728675
1	0.112596	0.624890	-3.659103

IM3B

SCF Energy: -3696.04048818

Sum of electronic and zero-point Energies= -3694.952745

Sum of electronic and thermal Energies= -3694.882818

Sum of electronic and thermal Enthalpies= -3694.881874

Sum of electronic and thermal Free Energies= -3695.064566

Electronic energy in solution by single point calculation = -3694.41580614

6	-0.262214	-3.948192	1.624047
6	-0.955017	-2.823698	1.153589
6	-1.978047	-3.046783	0.222459
6	-2.304668	-4.307240	-0.286078
6	-1.575484	-5.399337	0.192125
6	-0.571883	-5.221439	1.147296
6	-3.460729	-4.384784	-1.289905
6	-3.382262	-3.137215	-2.176355
6	-3.010715	-1.940920	-1.562410
6	-2.938751	-0.711044	-2.227459
6	-3.286236	-0.692347	-3.582983
6	-3.659581	-1.871564	-4.230656
6	-3.701847	-3.083480	-3.537388
1	0.536577	-3.819747	2.345822
1	-1.787942	-6.396892	-0.176463
1	-0.021400	-6.082292	1.515504
1	-3.247358	0.243706	-4.130252
1	-3.919367	-1.847353	-5.285045
1	-3.990485	-3.986989	-4.063317
8	-2.674774	-1.943050	-0.221783
15	-2.281840	0.721837	-1.276877
15	-0.453518	-1.087338	1.521501
6	-2.396487	2.104413	-2.491344
6	-3.527453	2.918678	-2.634636
6	-1.255084	2.381202	-3.258677
6	-3.512959	3.995757	-3.523102
1	-4.413353	2.719488	-2.040425
6	-1.245565	3.448968	-4.155744
1	-0.371857	1.761648	-3.120889
6	-2.373026	4.264461	-4.283639
1	-4.392911	4.626433	-3.619957
1	-0.353984	3.654201	-4.742263
1	-2.361973	5.107030	-4.969685

6	-3.688656	1.076335	-0.147232
6	-3.429545	1.850353	0.989709
6	-4.992011	0.612655	-0.376843
6	-4.459301	2.173028	1.871324
1	-2.420411	2.193169	1.185355
6	-6.018046	0.921236	0.516514
1	-5.203071	0.009210	-1.254316
6	-5.753410	1.705818	1.640921
1	-4.240723	2.774372	2.746661
1	-7.023678	0.551989	0.332384
1	-6.552232	1.946344	2.337514
6	1.041484	-1.349773	2.576364
6	2.283968	-1.406549	1.926500
6	1.003477	-1.481991	3.972755
6	3.464739	-1.585743	2.647769
1	2.322241	-1.303520	0.848450
6	2.184395	-1.652554	4.697252
1	0.051700	-1.446692	4.492333
6	3.415764	-1.702557	4.038403
1	4.403448	-1.625408	2.105369
1	2.141401	-1.749788	5.778998
1	4.331844	-1.834425	4.608333
6	-1.674170	-0.515351	2.770515
6	-1.411436	0.699777	3.425217
6	-2.865592	-1.191040	3.055116
6	-2.299824	1.205293	4.369118
1	-0.505868	1.252213	3.191850
6	-3.768488	-0.670232	3.984024
1	-3.087953	-2.127627	2.555211
6	-3.484729	0.520378	4.651907
1	-2.076387	2.143314	4.870421
1	-4.693677	-1.201867	4.188685
1	-4.186695	0.919685	5.378661
46	-0.168390	0.106352	-0.475265
6	-4.795043	-4.328784	-0.497779
1	-5.645459	-4.350718	-1.188418
1	-4.869402	-5.186424	0.180246
1	-4.859172	-3.412382	0.096031
6	-3.421826	-5.678232	-2.112388
1	-3.507005	-6.553111	-1.460983
1	-4.266067	-5.717959	-2.807024
1	-2.494052	-5.761545	-2.687616
1	3.672086	1.579552	0.783058

6	1.656452	0.165767	-1.210773
7	2.833513	0.181079	-1.381569
13	4.603167	0.007096	-0.915268
8	5.740311	0.868811	-1.892020
8	4.523466	1.109139	0.634534
8	5.022532	-1.540094	-0.277609
6	6.459571	0.418532	-3.024446
6	5.622671	1.831327	1.298074
6	5.004225	-2.852917	-0.805905
6	5.903843	3.120280	0.540748
1	5.018165	3.764009	0.513998
1	6.713160	3.672387	1.031189
1	6.196209	2.880573	-0.485229
6	6.809916	0.887229	1.366882
1	6.529015	-0.059839	1.834281
1	7.190557	0.684962	0.362156
1	7.607051	1.353161	1.955222
6	7.701602	-0.363130	-2.588991
1	7.407433	-1.257759	-2.027852
1	8.301239	-0.674570	-3.452655
1	8.329796	0.254957	-1.938313
6	5.568450	-0.405153	-3.957940
1	5.253628	-1.337387	-3.468451
1	4.670282	0.160582	-4.225946
1	6.097413	-0.678200	-4.878613
6	3.586061	-3.282929	-1.190561
1	2.934315	-3.279811	-0.310075
1	3.151660	-2.601387	-1.928968
1	3.588516	-4.293954	-1.615124
6	5.618003	-3.796277	0.227585
1	5.002109	-3.813857	1.134028
1	5.687868	-4.817956	-0.163346
1	6.622864	-3.456822	0.500412
1	5.246750	2.037036	2.305783
1	6.788630	1.314680	-3.571501
1	5.633541	-2.888601	-1.712231
6	1.763247	2.197069	1.466007
6	2.333947	3.329778	1.758015
6	1.331550	3.378024	0.620702
1	1.562071	1.156180	1.672664
1	2.972832	3.907356	2.413091
6	-0.031355	3.959980	0.903359
6	-0.880146	4.366990	-0.137499

6	-0.489092	4.114915	2.222347
6	-2.133491	4.917838	0.130476
1	-0.576682	4.243466	-1.169288
6	-1.737956	4.672259	2.492276
1	0.143424	3.802868	3.048087
6	-2.566498	5.080877	1.445722
1	-2.773527	5.202399	-0.698767
1	-2.063998	4.785089	3.523029
1	-3.544885	5.504000	1.653054
6	1.825784	3.512819	-0.811339
1	1.186186	2.958602	-1.503782
1	1.848454	4.564707	-1.122223
1	2.834184	3.102923	-0.909807

IM3

SCF Energy: -2275.46272946

Sum of electronic and zero-point Energies= -2274.503813

Sum of electronic and thermal Energies= -2274.450677

Sum of electronic and thermal Enthalpies= -2274.449733

Sum of electronic and thermal Free Energies= -2274.585718

Electronic energy in solution by single point calculation = -2274.28195338

46	-0.637196	-0.731824	0.143575
15	-0.918771	1.660368	0.375932
6	0.645269	2.674131	0.451431
6	1.920261	2.241356	0.003019
6	0.521678	4.006493	0.890306
6	2.964909	3.182997	-0.044174
6	2.328362	0.830566	-0.318226
6	1.575547	4.913808	0.857476
1	-0.428176	4.350812	1.268478
6	2.809278	4.503055	0.361782
1	3.936694	2.842309	-0.383088
6	2.693994	-0.013056	0.763209
6	2.586850	0.416248	-1.643511
1	1.425798	5.929823	1.210952
1	3.647955	5.191461	0.312243
6	3.197157	-1.286117	0.487344
6	3.101408	-0.868938	-1.865684
6	3.413045	-1.738344	-0.819011
1	3.467423	-1.937673	1.311822
1	3.314483	-1.170133	-2.885272
6	-1.798313	2.516802	-1.101098
6	-1.890816	1.995044	2.002249

6	-2.668817	3.315794	2.146758
1	-3.086752	3.340791	3.161207
1	-2.068134	4.219366	2.031208
1	-3.511559	3.369514	1.452809
6	-2.935972	0.864970	2.126287
1	-3.650522	0.873650	1.298600
1	-2.441593	-0.103734	2.165975
1	-3.499734	1.013101	3.057508
6	-0.855776	2.368164	-2.307040
1	-0.448765	1.365568	-2.396819
1	-1.404194	2.600960	-3.228610
1	-0.018315	3.066103	-2.229645
6	-3.118616	1.776402	-1.353791
1	-2.983383	0.697265	-1.420428
1	-3.846955	1.971667	-0.562029
1	-3.559583	2.123606	-2.296247
6	2.760958	0.527639	2.189990
1	2.030176	1.334996	2.285528
6	2.500481	1.375128	-2.830186
1	1.933791	2.254608	-2.516180
6	4.050698	-3.105793	-1.039737
1	4.802486	-3.221754	-0.246339
6	4.160617	1.127292	2.436894
1	4.219353	1.548763	3.447479
1	4.926996	0.348236	2.348105
1	4.400873	1.920937	1.724564
6	2.437844	-0.503439	3.272623
1	2.434673	-0.014295	4.254419
1	1.453248	-0.924081	3.082672
1	3.174583	-1.312734	3.312902
6	4.779281	-3.232527	-2.383487
1	5.495530	-2.417464	-2.535872
1	5.326040	-4.180743	-2.425981
1	4.074512	-3.226671	-3.223911
6	3.038776	-4.253561	-0.865471
1	2.548360	-4.214632	0.111528
1	2.267463	-4.208145	-1.644203
1	3.546800	-5.221417	-0.953871
6	1.817876	0.794315	-4.080009
1	1.765738	1.559925	-4.862527
1	2.380712	-0.051556	-4.489827
1	0.800515	0.452134	-3.880931
6	3.916860	1.848958	-3.217666

1	4.526357	1.002268	-3.553605
1	3.869026	2.578963	-4.034534
1	4.434818	2.315254	-2.375494
6	-2.092087	4.022976	-0.976814
1	-2.815729	4.262459	-0.199554
1	-1.185242	4.607466	-0.808085
1	-2.518426	4.357109	-1.931747
6	-0.870674	1.865095	3.150106
1	-0.152472	2.690313	3.153889
1	-1.412547	1.885683	4.105105
1	-0.340190	0.912596	3.086843
6	-0.714520	-0.980857	-1.986155
6	-0.091954	-2.764473	-0.531064
1	-1.465937	-0.477211	-2.585124
1	0.317910	-0.794729	-2.264239
1	-0.310270	-3.647817	0.056596
1	0.958871	-2.510884	-0.621378
6	-1.032961	-2.252074	-1.429708
6	-2.381675	-2.928253	-1.613184
6	-3.584250	-2.013766	-1.658333
6	-4.100141	-1.562057	-2.877802
6	-4.207523	-1.605834	-0.471937
6	-5.215847	-0.723244	-2.915200
1	-3.629908	-1.878702	-3.805893
6	-5.327743	-0.776881	-0.505617
1	-3.807901	-1.936445	0.480520
6	-5.835882	-0.332267	-1.728081
1	-5.604427	-0.383978	-3.871356
1	-5.801523	-0.475353	0.424414
1	-6.708870	0.313578	-1.754810
1	-2.321663	-3.491131	-2.554749
6	-0.745177	-2.281188	2.850840
6	-0.782268	-2.049574	4.380369
1	-0.918393	-2.987103	4.930891
1	0.139935	-1.571921	4.716829
1	-1.620054	-1.379855	4.598869
6	-2.049836	-2.995428	2.432791
1	-2.895399	-2.353913	2.701530
1	-2.069235	-3.158830	1.354540
1	-2.165730	-3.961137	2.937521
8	-0.548146	-1.063279	2.224838
1	-2.509293	-3.672729	-0.820233
6	0.399931	-3.213696	2.562205

7	1.305161	-3.895016	2.302674

IM4A

SCF Energy: -2872.13490390

Sum of electronic and zero-point Energies= -2871.343844

Sum of electronic and thermal Energies= -2871.294426

Sum of electronic and thermal Enthalpies= -2871.293482

Sum of electronic and thermal Free Energies= -2871.427257

Electronic energy in solution by single point calculation = -2870.8002728

6	-3.266926	1.379121	0.717040
6	-2.064520	0.658890	0.796942
6	-1.010217	1.269331	1.479055
6	-1.092826	2.516096	2.104014
6	-2.300886	3.205457	1.990123
6	-3.374801	2.641309	1.298988
6	0.124283	2.979253	2.911806
6	1.367790	2.570533	2.120539
6	1.321959	1.343314	1.460436
6	2.372131	0.817769	0.704735
6	3.565248	1.551026	0.669205
6	3.651291	2.780651	1.325260
6	2.560493	3.292468	2.032591
1	-4.112165	0.956008	0.189016
1	-2.409308	4.186802	2.437432
1	-4.308060	3.190169	1.215982
1	4.419188	1.168762	0.122992
1	4.578058	3.345259	1.285075
1	2.646786	4.256433	2.521664
8	0.181463	0.572543	1.522304
15	1.991458	-0.726878	-0.220196
15	-1.791315	-0.963992	-0.044512
6	3.577968	-1.088291	-1.082849
6	4.221612	-2.324460	-0.926496
6	4.123274	-0.159555	-1.987391
6	5.376229	-2.621757	-1.651178
1	3.822153	-3.058964	-0.237144
6	5.281790	-0.455571	-2.703794
1	3.651550	0.806134	-2.129095
6	5.911461	-1.690440	-2.540707
1	5.858610	-3.585530	-1.514931
1	5.687327	0.279037	-3.393646
1	6.810532	-1.923968	-3.103476
6	1.956835	-2.000033	1.094143

6	1.372425	-3.238548	0.796833
6	2.538847	-1.794958	2.351048
6	1.394685	-4.266500	1.737627
1	0.899627	-3.387879	-0.170070
6	2.537349	-2.818071	3.298399
1	2.994504	-0.838629	2.586948
6	1.971427	-4.056336	2.990628
1	0.936880	-5.220758	1.500278
1	2.984003	-2.649585	4.274480
1	1.972457	-4.853652	3.728443
6	-3.475252	-1.244092	-0.730554
6	-3.764222	-0.864327	-2.046254
6	-4.513350	-1.722290	0.085705
6	-5.065035	-0.966297	-2.540965
1	-2.971280	-0.517358	-2.692594
6	-5.810762	-1.827198	-0.412074
1	-4.307873	-2.008822	1.111387
6	-6.089618	-1.449088	-1.727755
1	-5.268337	-0.682968	-3.569406
1	-6.603704	-2.203707	0.228196
1	-7.100467	-1.535731	-2.116465
6	-1.740600	-2.218267	1.292707
6	-1.969378	-3.551921	0.913215
6	-1.467993	-1.924499	2.631931
6	-1.957416	-4.565661	1.867044
1	-2.174379	-3.787904	-0.127585
6	-1.434336	-2.947802	3.580996
1	-1.290325	-0.901581	2.941163
6	-1.687647	-4.266153	3.204918
1	-2.152768	-5.590741	1.564518
1	-1.216066	-2.709081	4.618023
1	-1.670219	-5.058071	3.948376
46	0.032177	-0.888802	-1.634934
6	0.134478	2.200177	4.256031
1	1.007059	2.489102	4.852308
1	-0.772354	2.424179	4.828230
1	0.178411	1.120161	4.087444
6	0.088768	4.481644	3.209995
1	-0.793721	4.731708	3.806656
1	0.962397	4.777118	3.798969
1	0.066735	5.068921	2.289049
6	1.049354	-0.006905	-3.288385
6	0.905517	1.304032	-2.667306

6	-0.195811	2.116799	-2.658836
1	2.065668	-0.381848	-3.373979
1	1.732466	1.605706	-2.031223
6	-1.422633	1.788729	-3.474250
1	-1.278698	0.895761	-4.082500
1	-2.291874	1.606352	-2.831868
1	-1.685029	2.622356	-4.138161
6	-0.240986	3.337578	-1.827674
6	0.907263	3.895281	-1.224627
6	-1.463671	4.004674	-1.610101
6	0.836209	5.057317	-0.466481
1	1.876718	3.429018	-1.357863
6	-1.536768	5.163634	-0.840878
1	-2.376171	3.608010	-2.037789
6	-0.386504	5.706491	-0.271048
1	1.744531	5.459206	-0.026911
1	-2.499442	5.645115	-0.692249
1	-0.437714	6.622285	0.311424
6	-0.974170	-1.916955	-3.019459
7	-1.519699	-2.568631	-3.824598
1	0.474016	-0.202368	-4.187126

IM4B

SCF Energy: -3696.10683104

Sum of electronic and zero-point Energies= -3695.015515

Sum of electronic and thermal Energies= -3694.947252

Sum of electronic and thermal Enthalpies= -3694.946307

Sum of electronic and thermal Free Energies= -3695.123994

Electronic energy in solution by single point calculation = -3694.4627839

6	-1.981748	3.869855	0.319097
6	-0.907540	3.010873	0.048253
6	-0.432293	2.965524	-1.274952
6	-0.960749	3.769055	-2.291810
6	-2.035080	4.604406	-1.979724
6	-2.547099	4.650635	-0.684420
6	-0.279014	3.710741	-3.658732
6	0.070869	2.246594	-3.923690
6	0.542093	1.489312	-2.843412
6	0.955464	0.152032	-2.984331
6	0.879261	-0.416671	-4.263972
6	0.400829	0.312282	-5.347728
6	-0.003610	1.635057	-5.176039
1	-2.400884	3.898635	1.316837

1	-2.478775	5.224911	-2.749622
1	-3.390731	5.294371	-0.456122
1	1.170755	-1.450924	-4.402387
1	0.337731	-0.152424	-6.326815
1	-0.376950	2.191763	-6.027666
8	0.603608	2.093925	-1.593894
15	1.512748	-0.871610	-1.552323
15	-0.216143	1.911652	1.357103
6	1.219520	-2.596716	-2.062823
6	2.083486	-3.298676	-2.918434
6	0.054149	-3.220339	-1.590022
6	1.774347	-4.601795	-3.306398
1	2.996441	-2.829130	-3.271891
6	-0.257918	-4.517894	-1.994821
1	-0.603361	-2.707072	-0.897192
6	0.600170	-5.208605	-2.851792
1	2.448436	-5.142219	-3.965021
1	-1.169606	-4.978453	-1.628335
1	0.360098	-6.222069	-3.160778
6	3.318012	-0.623050	-1.507794
6	4.161193	-1.621111	-1.003568
6	3.852655	0.636545	-1.816814
6	5.519523	-1.369261	-0.821758
1	3.757266	-2.589180	-0.730702
6	5.211170	0.885572	-1.631203
1	3.207238	1.422819	-2.194382
6	6.046777	-0.116320	-1.132573
1	6.152434	-2.142229	-0.400039
1	5.616367	1.863885	-1.874879
1	7.103267	0.082090	-0.977189
6	-1.445252	1.869650	2.695344
6	-2.169612	0.681337	2.863777
6	-1.716255	2.975801	3.520986
6	-3.178478	0.612756	3.826844
1	-1.967851	-0.190679	2.247819
6	-2.714593	2.894635	4.488309
1	-1.144018	3.892014	3.407802
6	-3.451536	1.713949	4.636292
1	-3.759632	-0.298498	3.912867
1	-2.922029	3.751045	5.123707
1	-4.238271	1.658506	5.383490
6	1.235990	2.817024	1.999564
6	1.554301	2.802138	3.363477

6	2.144588	3.380292	1.090332
6	2.755920	3.352622	3.811767
1	0.870001	2.352307	4.074165
6	3.343335	3.927488	1.541345
1	1.927550	3.364440	0.027925
6	3.653563	3.914695	2.903712
1	2.990832	3.335236	4.872246
1	4.039613	4.358400	0.827397
1	4.590216	4.338902	3.253813
46	0.364048	-0.040752	0.266047
6	1.043318	4.521838	-3.578578
1	1.574546	4.472063	-4.535308
1	0.829166	5.571158	-3.348481
1	1.702174	4.127679	-2.799621
6	-1.152984	4.308251	-4.768150
1	-1.369188	5.360259	-4.561561
1	-0.629923	4.278466	-5.728167
1	-2.101203	3.770941	-4.870715
1	0.812253	-0.644093	3.294586
6	-1.438789	-0.184500	-0.684127
7	-2.527579	-0.528015	-0.955725
13	-3.473470	-1.766969	0.240051
8	-4.008530	-3.138069	-0.685161
8	-2.136782	-2.235851	1.288535
8	-4.623901	-0.776082	1.088380
6	-5.115629	-3.313654	-1.535409
6	-2.124420	-3.329200	2.187399
6	-5.524166	0.220237	0.669839
6	-1.725226	-4.614454	1.457210
1	-0.747557	-4.494429	0.980295
1	-1.670728	-5.465174	2.148082
1	-2.465455	-4.833593	0.679778
6	-3.468234	-3.495619	2.903923
1	-3.769100	-2.558458	3.382295
1	-4.248649	-3.775501	2.185658
1	-3.413164	-4.278941	3.669819
6	-6.416425	-3.384156	-0.728547
1	-6.593741	-2.434480	-0.211439
1	-7.278246	-3.597454	-1.373373
1	-6.344480	-4.171702	0.029155
6	-5.176446	-2.225250	-2.612527
1	-5.355410	-1.242295	-2.158347
1	-4.226754	-2.175888	-3.155145

1	-5.983345	-2.418987	-3.330177
6	-4.824037	1.577959	0.532060
1	-4.413921	1.887535	1.499345
1	-3.999515	1.516445	-0.183081
1	-5.524959	2.349275	0.187670
6	-6.673025	0.287830	1.677886
1	-6.280209	0.554927	2.666299
1	-7.421259	1.034992	1.386078
1	-7.163680	-0.687819	1.759624
1	-1.357417	-3.110241	2.948003
1	-4.981818	-4.281368	-2.046201
1	-5.955115	-0.038537	-0.314499
6	2.020577	-0.185463	1.472173
6	1.820873	-0.451570	2.931604
6	2.428829	-1.538113	2.043784
1	2.837085	0.481580	1.204610
1	2.468476	0.031523	3.659005
6	3.890648	-1.815139	2.220146
6	4.406667	-3.113444	2.084772
6	4.801457	-0.784281	2.516030
6	5.771493	-3.372239	2.229225
1	3.738108	-3.937445	1.861361
6	6.161968	-1.039188	2.659257
1	4.447104	0.236245	2.624619
6	6.659961	-2.336850	2.515847
1	6.136477	-4.390375	2.119867
1	6.838476	-0.218375	2.883218
1	7.721841	-2.535967	2.630265
6	1.532735	-2.726929	1.748241
1	1.814465	-3.226210	0.813717
1	1.568029	-3.470421	2.554189
1	0.494720	-2.401483	1.634102

IM4

SCF Energy: -2275.45171423

Sum of electronic and zero-point Energies= -2274.502176

Sum of electronic and thermal Energies= -2274.448591

Sum of electronic and thermal Enthalpies= -2274.447647

Sum of electronic and thermal Free Energies= -2274.587402

Electronic energy in solution by single point calculation = -2274.26586607

46	0.460718	-0.787344	0.134526
15	-1.696439	-1.403663	-0.800276
6	-3.118868	-0.200464	-0.697020

6	-3.074598	1.066452	-0.061915
6	-4.346240	-0.605402	-1.258267
6	-4.270980	1.795671	0.069693
6	-1.845226	1.786033	0.412303
6	-5.510320	0.148550	-1.151462
1	-4.398281	-1.538995	-1.795929
6	-5.480040	1.352479	-0.452785
1	-4.226925	2.750866	0.582124
6	-1.350979	1.605723	1.721595
6	-1.292073	2.788648	-0.419455
1	-6.430384	-0.210724	-1.603237
1	-6.378953	1.950174	-0.332699
6	-0.235944	2.347208	2.129682
6	-0.207872	3.534190	0.052139
6	0.359619	3.304922	1.308451
1	0.166992	2.190727	3.125870
1	0.217168	4.303135	-0.585512
6	-1.469679	-1.713931	-2.688633
6	-2.394242	-2.987183	0.035824
6	-3.737095	-3.564727	-0.452347
1	-3.894633	-4.510788	0.081242
1	-4.576802	-2.914354	-0.198979
1	-3.771654	-3.788126	-1.518240
6	-1.309694	-4.071028	-0.116047
1	-1.257482	-4.450669	-1.141548
1	-0.330879	-3.697192	0.186436
1	-1.564378	-4.918719	0.532855
6	-1.587020	-0.343957	-3.380745
1	-0.998586	0.422225	-2.875911
1	-1.224462	-0.424876	-4.413411
1	-2.624341	0.000721	-3.411017
6	-0.053983	-2.287106	-2.902203
1	0.717604	-1.629076	-2.507906
1	0.069785	-3.259870	-2.419743
1	0.119825	-2.420742	-3.977917
6	-2.106766	0.749591	2.727171
1	-2.675284	0.005733	2.165554
6	-1.875270	3.119809	-1.791458
1	-2.505094	2.281903	-2.103145
6	1.559175	4.106193	1.785680
1	1.881774	3.670095	2.740755
6	-3.120470	1.631940	3.483158
1	-3.695804	1.027110	4.193936

1	-2.601298	2.416890	4.045866
1	-3.825560	2.116098	2.800797
6	-1.211468	-0.004268	3.715461
1	-1.830533	-0.651335	4.348559
1	-0.492807	-0.631073	3.184030
1	-0.674834	0.680448	4.383449
6	1.169669	5.571731	2.048272
1	0.350174	5.637857	2.771888
1	2.023008	6.137661	2.439806
1	0.839160	6.058438	1.122966
6	2.743702	4.019883	0.807987
1	3.041916	2.982332	0.627106
1	2.491583	4.467542	-0.160317
1	3.609914	4.560165	1.206658
6	-0.811070	3.328284	-2.882296
1	-1.297694	3.445900	-3.857046
1	-0.218378	4.232377	-2.704128
1	-0.118936	2.485717	-2.948450
6	-2.769469	4.371846	-1.706556
1	-2.185597	5.238048	-1.373793
1	-3.197533	4.607159	-2.688201
1	-3.593183	4.231675	-1.001959
6	-2.448401	-2.681293	-3.376174
1	-2.350474	-3.702652	-3.002144
1	-3.492517	-2.373022	-3.294178
1	-2.206843	-2.704496	-4.446759
6	-2.592992	-2.636634	1.522713
1	-3.389867	-1.894971	1.641744
1	-2.909693	-3.544975	2.053165
1	-1.669077	-2.282802	1.977828
6	1.169409	0.672898	-1.307750
6	2.409966	0.072015	0.643421
1	0.990966	0.566774	-2.372725
1	0.798660	1.588482	-0.864217
1	3.175813	-0.522619	1.127431
1	2.026762	0.920397	1.204518
6	2.312232	0.041755	-0.758486
6	3.238341	-0.834047	-1.584640
6	4.665327	-0.333905	-1.482518
6	5.603944	-1.028363	-0.711315
6	5.051272	0.853251	-2.117314
6	6.906599	-0.542975	-0.579235
1	5.305421	-1.949777	-0.218862

6	6.351327	1.339259	-1.985484
1	4.325998	1.399026	-2.717153
6	7.283629	0.641220	-1.213940
1	7.627602	-1.093366	0.019222
1	6.638005	2.260817	-2.485076
1	8.297524	1.017994	-1.110981
1	3.188760	-1.864358	-1.222376
6	1.385752	-2.729517	2.388883
6	2.038971	-1.863652	3.491435
1	2.921718	-2.348926	3.923331
1	2.326485	-0.888163	3.096155
1	1.301745	-1.705752	4.284257
6	0.872863	-4.044993	3.023425
1	0.076114	-3.786973	3.727940
1	0.458166	-4.700311	2.254108
1	1.666366	-4.578572	3.558490
8	0.323585	-2.099126	1.762427
1	2.904641	-0.824551	-2.628099
6	2.442244	-3.108581	1.395953
7	3.236330	-3.397291	0.596986

IM5A

SCF Energy: -2872.15116130

Sum of electronic and zero-point Energies= -2871.359685

Sum of electronic and thermal Energies= -2871.310465

Sum of electronic and thermal Enthalpies= -2871.309520

Sum of electronic and thermal Free Energies= -2871.443257

Electronic energy in solution by single point calculation = -2870.82218717

6	-3.503006	1.138477	0.824093
6	-2.200895	0.639495	0.955310
6	-1.231414	1.520235	1.451701
6	-1.489143	2.837798	1.826468
6	-2.802953	3.293028	1.689587
6	-3.797788	2.450025	1.193978
6	-0.321323	3.657686	2.385459
6	0.941917	3.256128	1.615552
6	1.073421	1.917741	1.241923
6	2.177811	1.404533	0.547296
6	3.226984	2.290685	0.272218
6	3.132694	3.634277	0.639033
6	1.997148	4.115403	1.293533
1	-4.279839	0.511652	0.403613
1	-3.054856	4.313402	1.955221

1	-4.810385	2.824845	1.078297
1	4.107824	1.933751	-0.249027
1	3.949840	4.312302	0.410936
1	1.940829	5.165978	1.556268
8	0.060975	1.032153	1.537417
15	2.066701	-0.330217	-0.079997
15	-1.607058	-0.979219	0.309394
6	3.665802	-0.539587	-0.970636
6	4.655204	-1.438967	-0.552909
6	3.865708	0.174062	-2.165435
6	5.812044	-1.623428	-1.313866
1	4.522229	-1.999099	0.365861
6	5.026749	0.000972	-2.915512
1	3.108885	0.875980	-2.498493
6	6.003428	-0.905568	-2.493781
1	6.566707	-2.329089	-0.977549
1	5.167483	0.569442	-3.830902
1	6.905030	-1.049816	-3.082189
6	2.331611	-1.333568	1.429092
6	1.938543	-2.678108	1.392420
6	2.935503	-0.824318	2.585386
6	2.170696	-3.507816	2.487350
1	1.440331	-3.063594	0.507325
6	3.147131	-1.651337	3.688598
1	3.241633	0.216781	2.619708
6	2.771323	-2.994677	3.638128
1	1.855733	-4.545440	2.452437
1	3.610178	-1.247796	4.585128
1	2.935913	-3.638315	4.497799
6	-3.105307	-1.850942	-0.297431
6	-3.023957	-2.491990	-1.539280
6	-4.265056	-2.008426	0.479303
6	-4.098524	-3.246163	-2.017843
1	-2.107088	-2.419886	-2.114343
6	-5.341819	-2.747200	-0.005202
1	-4.315247	-1.566878	1.470063
6	-5.261738	-3.363394	-1.258431
1	-4.018290	-3.743893	-2.979959
1	-6.238426	-2.856075	0.598899
1	-6.099984	-3.945743	-1.630993
6	-1.303212	-1.993339	1.826828
6	-1.395301	-3.389980	1.708295
6	-0.958208	-1.445158	3.067958

6	-1.167843	-4.213757	2.808217
1	-1.663082	-3.834432	0.754437
6	-0.721034	-2.273016	4.165664
1	-0.874341	-0.372889	3.186820
6	-0.830543	-3.657505	4.043404
1	-1.255422	-5.291489	2.698964
1	-0.450681	-1.829811	5.120047
1	-0.649810	-4.298619	4.901720
46	0.059224	-0.462197	-1.263748
6	-0.120058	3.264908	3.873715
1	0.724141	3.817520	4.301148
1	-1.021829	3.495681	4.451508
1	0.086929	2.195033	3.971259
6	-0.592277	5.164713	2.297227
1	-1.476602	5.430837	2.883456
1	0.243858	5.734882	2.712288
1	-0.754271	5.480475	1.262133
6	0.995887	-0.924703	-4.134410
6	0.487154	0.221016	-3.264012
6	-0.884730	0.507206	-3.042596
1	2.089445	-0.950189	-4.065615
1	1.183874	1.053529	-3.259617
6	-1.972172	-0.234803	-3.793677
1	-1.646451	-1.224510	-4.115164
1	-2.872671	-0.376677	-3.191604
1	-2.262079	0.329712	-4.693395
6	-1.248027	1.858148	-2.516892
6	-0.293034	2.719950	-1.932324
6	-2.571794	2.330994	-2.582861
6	-0.640160	3.981498	-1.463433
1	0.732012	2.391792	-1.810881
6	-2.921900	3.592497	-2.101157
1	-3.346233	1.708214	-3.014689
6	-1.960303	4.431574	-1.543170
1	0.128311	4.606736	-1.018438
1	-3.957372	3.916853	-2.165605
1	-2.233395	5.414508	-1.169398
6	0.513866	-2.252849	-3.730734
7	0.130146	-3.308821	-3.434354
1	0.746742	-0.783244	-5.197751

IM5B

SCF Energy: -3696.12343013

Sum of electronic and zero-point Energies= -3695.030725

Sum of electronic and thermal Energies= -3694.962578

Sum of electronic and thermal Enthalpies= -3694.961634

Sum of electronic and thermal Free Energies= -3695.139390

Electronic energy in solution by single point calculation = -3694.48717614

6	-0.156260	-1.556807	-3.904795
6	-0.456292	-1.619623	-2.535762
6	-1.780942	-1.903804	-2.182058
6	-2.809425	-2.080085	-3.114861
6	-2.473537	-1.978257	-4.466498
6	-1.156324	-1.731948	-4.858416
6	-4.204222	-2.426784	-2.581746
6	-4.402834	-1.642887	-1.282470
6	-3.297702	-1.503466	-0.445448
6	-3.328566	-0.836054	0.781872
6	-4.551027	-0.298057	1.197548
6	-5.679716	-0.420329	0.385403
6	-5.606279	-1.080132	-0.843508
1	0.857325	-1.339789	-4.219941
1	-3.239395	-2.096945	-5.224705
1	-0.911066	-1.665705	-5.913974
1	-4.607558	0.234510	2.140824
1	-6.623875	0.007730	0.708655
1	-6.495008	-1.152398	-1.460592
8	-2.067123	-2.001311	-0.837915
15	-1.720424	-0.569206	1.616222
15	0.786892	-1.202106	-1.240189
6	-2.189714	0.316034	3.151198
6	-2.675626	-0.347624	4.287877
6	-2.051607	1.711819	3.169223
6	-3.021039	0.376984	5.428120
1	-2.775831	-1.428637	4.281837
6	-2.403340	2.431264	4.312949
1	-1.681813	2.250719	2.301422
6	-2.885154	1.767808	5.442283
1	-3.393289	-0.143815	6.306251
1	-2.288988	3.511337	4.314678
1	-3.150333	2.329882	6.333705
6	-1.281009	-2.253078	2.202002
6	0.057194	-2.499106	2.539309
6	-2.214100	-3.291884	2.309508
6	0.452830	-3.756168	2.990073
1	0.788766	-1.704509	2.418956

6	-1.814290	-4.554848	2.749224
1	-3.251642	-3.114452	2.043247
6	-0.481687	-4.788205	3.091620
1	1.495045	-3.937438	3.230903
1	-2.544826	-5.355986	2.823255
1	-0.169991	-5.773182	3.427835
6	2.157582	-0.528378	-2.265873
6	2.050984	0.822363	-2.647577
6	3.302851	-1.254598	-2.611908
6	3.084134	1.430534	-3.356402
1	1.181395	1.406885	-2.350989
6	4.343202	-0.633071	-3.309464
1	3.395690	-2.295169	-2.320533
6	4.237490	0.707969	-3.680067
1	2.994410	2.476344	-3.635052
1	5.235099	-1.200825	-3.560794
1	5.050034	1.190026	-4.216650
6	1.401941	-2.815088	-0.633148
6	2.560787	-2.826939	0.160688
6	0.715854	-4.013448	-0.858220
6	3.045063	-4.022799	0.684172
1	3.093194	-1.904086	0.363754
6	1.187096	-5.206137	-0.307074
1	-0.185732	-4.017715	-1.460910
6	2.355497	-5.216315	0.454221
1	3.954064	-4.011953	1.276967
1	0.640401	-6.128871	-0.479693
1	2.724192	-6.148406	0.873435
46	0.120964	0.320171	0.356406
6	-4.228114	-3.941717	-2.242504
1	-5.202866	-4.220164	-1.826994
1	-4.047508	-4.535262	-3.145611
1	-3.458138	-4.190467	-1.506195
6	-5.303591	-2.125542	-3.607471
1	-5.160035	-2.718768	-4.515257
1	-6.285516	-2.394449	-3.207459
1	-5.318110	-1.065836	-3.881791
1	3.941133	3.066140	1.293932
6	1.761093	1.513629	0.542876
7	1.040628	2.398060	0.986122
13	-0.067973	3.669996	0.011185
8	-1.442009	4.045440	0.997442
8	1.042293	4.977234	-0.318174

8	-0.430076	2.699180	-1.422275
6	-2.244572	5.192018	1.161395
6	2.177820	4.827836	-1.142323
6	-1.649481	2.698055	-2.139903
6	3.282314	5.754076	-0.633488
1	3.517243	5.521070	0.410884
1	4.197395	5.655625	-1.230898
1	2.945381	6.796267	-0.677798
6	1.817371	5.110190	-2.603723
1	1.041947	4.411622	-2.932746
1	1.428653	6.130564	-2.702718
1	2.691400	5.008033	-3.261007
6	-2.170124	6.123066	-0.052490
1	-2.560451	5.610273	-0.941373
1	-2.767183	7.029462	0.106600
1	-1.134138	6.416027	-0.250524
6	-3.685097	4.751438	1.434569
1	-4.084272	4.218424	0.563219
1	-3.724737	4.072831	2.292375
1	-4.331343	5.613438	1.640434
6	-2.693857	1.855547	-1.408636
1	-2.326307	0.829335	-1.318979
1	-2.856396	2.248029	-0.401497
1	-3.652816	1.835373	-1.941877
6	-1.395606	2.167095	-3.550894
1	-1.051574	1.127863	-3.508434
1	-2.310261	2.199083	-4.155367
1	-0.626340	2.763817	-4.053286
1	2.560195	3.790835	-1.088955
1	-1.882544	5.751922	2.040737
1	-2.033310	3.729161	-2.228423
6	3.174851	1.181897	0.412475
6	4.259837	2.117393	0.873209
6	3.986418	0.877281	1.694185
1	3.391506	0.526678	-0.417151
1	5.164470	2.164303	0.274786
6	4.910980	-0.301550	1.567445
6	5.077634	-1.202345	2.628986
6	5.604793	-0.563850	0.372033
6	5.904314	-2.321341	2.504001
1	4.559925	-1.036147	3.566357
6	6.421239	-1.683646	0.242958
1	5.496976	0.096876	-0.482189

6	6.578340	-2.571146	1.309911
1	6.016284	-2.998230	3.346685
1	6.935405	-1.863161	-0.697066
1	7.217053	-3.443819	1.209728
6	3.295314	1.073761	3.030244
1	2.675321	0.208459	3.291478
1	4.032775	1.224571	3.826158
1	2.641597	1.947744	3.003199

IM5

SCF Energy: -2082.28769650

Sum of electronic and zero-point Energies= -2081.428325

Sum of electronic and thermal Energies= -2081.380059

Sum of electronic and thermal Enthalpies= -2081.379115

Sum of electronic and thermal Free Energies= -2081.507381

Electronic energy in solution by single point calculation = -2081.20190946

46	1.024314	0.083762	0.105274
15	-0.125733	-2.000349	-0.218825
6	-1.979958	-1.990011	-0.049770
6	-2.758628	-0.855157	0.288839
6	-2.653400	-3.211352	-0.252639
6	-4.140254	-1.030463	0.496243
6	-2.298834	0.575114	0.347068
6	-4.025013	-3.354538	-0.074536
1	-2.092670	-4.078860	-0.562754
6	-4.776310	-2.254504	0.330485
1	-4.722881	-0.159166	0.775298
6	-1.789159	1.142997	1.537581
6	-2.577020	1.405085	-0.766879
1	-4.495044	-4.318640	-0.245311
1	-5.846157	-2.340468	0.496685
6	-1.478702	2.508101	1.552123
6	-2.275149	2.767359	-0.688650
6	-1.702011	3.335214	0.451612
1	-1.061476	2.943657	2.454201
1	-2.489931	3.402106	-1.542900
6	0.185999	-2.595174	-2.024619
6	0.436112	-3.350860	1.031484
6	-0.176979	-4.761736	0.914100
1	0.350680	-5.405126	1.628992
1	-1.231073	-4.772760	1.197777
1	-0.070059	-5.218745	-0.068657
6	1.966457	-3.478557	0.899610

1	2.247867	-3.975061	-0.035180
1	2.468774	-2.512602	0.962913
1	2.341149	-4.095663	1.725191
6	-0.809188	-1.822826	-2.907610
1	-0.815710	-0.758985	-2.668284
1	-0.524110	-1.932954	-3.961599
1	-1.828121	-2.201418	-2.789710
6	1.623275	-2.194799	-2.408559
1	1.784245	-1.124631	-2.290508
1	2.369255	-2.715018	-1.802240
1	1.802326	-2.459348	-3.458749
6	-1.702252	0.332268	2.823978
1	-1.446459	-0.692725	2.549408
6	-3.257177	0.878354	-2.029508
1	-3.182462	-0.212268	-2.027228
6	-1.369136	4.816367	0.508337
1	-0.864811	4.999847	1.466351
6	-3.078109	0.302272	3.521965
1	-3.014659	-0.273325	4.452756
1	-3.398848	1.320069	3.774345
1	-3.849635	-0.152700	2.896610
6	-0.646067	0.829347	3.818989
1	-0.550725	0.108141	4.637836
1	0.337093	0.933150	3.359240
1	-0.936766	1.787837	4.266009
6	-2.648778	5.670523	0.481447
1	-3.322035	5.396329	1.300560
1	-2.407634	6.735826	0.574645
1	-3.192713	5.530277	-0.460224
6	-0.405342	5.234328	-0.615103
1	0.518331	4.647231	-0.585458
1	-0.860961	5.090321	-1.601674
1	-0.142082	6.294205	-0.521795
6	-2.616355	1.382643	-3.333916
1	-3.079729	0.882015	-4.191544
1	-2.763553	2.459916	-3.468469
1	-1.542403	1.187571	-3.368370
6	-4.753834	1.245884	-2.026591
1	-4.881369	2.334571	-2.009444
1	-5.246543	0.860284	-2.927014
1	-5.269587	0.834461	-1.155361
6	0.042793	-4.095827	-2.326317
1	0.802725	-4.692735	-1.816842

1	-0.943679	-4.494761	-2.082718
1	0.187568	-4.241030	-3.404737
6	0.058546	-2.849443	2.438319
1	-1.029573	-2.797727	2.550814
1	0.433689	-3.570680	3.175325
1	0.498272	-1.883807	2.675470
6	0.703552	1.266165	-1.775933
6	1.910731	2.061135	0.146470
1	0.701144	0.826383	-2.768817
1	-0.204782	1.779641	-1.483719
1	2.838804	2.195710	0.689650
1	1.041591	2.586737	0.533399
6	1.936423	1.644364	-1.205052
6	3.246541	1.373874	-1.932838
6	4.414260	1.020434	-1.041092
6	4.491945	-0.244596	-0.445996
6	5.407115	1.961980	-0.753037
6	5.531244	-0.558206	0.426071
1	3.713087	-0.974247	-0.641650
6	6.455244	1.649793	0.115073
1	5.356687	2.948184	-1.209297
6	6.517414	0.388835	0.708657
1	5.558447	-1.534230	0.900845
1	7.218262	2.392874	0.329944
1	7.324934	0.147063	1.393645
1	3.078927	0.588799	-2.679118
1	3.482000	2.285176	-2.499359
6	1.928607	-0.276339	1.857629
7	2.569760	-0.423543	2.825140

IM6A

SCF Energy: -2678.18521594

Sum of electronic and zero-point Energies= -2677.477200

Sum of electronic and thermal Energies= -2677.431662

Sum of electronic and thermal Enthalpies= -2677.430718

Sum of electronic and thermal Free Energies= -2677.558057

Electronic energy in solution by single point calculation = -2677.03148373

6	-4.176100	0.090414	-1.185413
6	-2.899535	0.269460	-0.633423
6	-2.429718	1.581765	-0.529218
6	-3.138535	2.702935	-0.967345
6	-4.401250	2.482364	-1.523408
6	-4.916706	1.188041	-1.623118

6	-2.481066	4.070739	-0.765432
6	-0.983290	3.891006	-1.030974
6	-0.390081	2.709394	-0.578706
6	0.974182	2.427092	-0.695208
6	1.781274	3.408481	-1.286681
6	1.220968	4.595618	-1.759436
6	-0.149248	4.834073	-1.637542
1	-4.578669	-0.910298	-1.289836
1	-4.989977	3.319362	-1.882490
1	-5.901700	1.033898	-2.053853
1	2.846835	3.238533	-1.386327
1	1.857947	5.342520	-2.223997
1	-0.563506	5.763954	-2.011432
8	-1.173774	1.746593	0.022429
15	1.584402	0.793854	-0.081010
15	-1.743778	-1.100359	-0.202471
6	3.384490	0.986593	-0.418442
6	4.318598	1.351558	0.558085
6	3.830206	0.722216	-1.722902
6	5.675823	1.436448	0.237884
1	3.988084	1.560157	1.569961
6	5.181303	0.827095	-2.046352
1	3.109264	0.420176	-2.478656
6	6.109970	1.177389	-1.062163
1	6.393303	1.707190	1.007612
1	5.512229	0.620106	-3.060279
1	7.165932	1.243125	-1.308303
6	1.469203	1.021852	1.739578
6	1.425111	-0.123802	2.545546
6	1.424213	2.285883	2.343405
6	1.347943	-0.007775	3.932270
1	1.427485	-1.102523	2.076343
6	1.336663	2.399844	3.731077
1	1.455032	3.179882	1.728448
6	1.300063	1.253596	4.527365
1	1.298856	-0.903197	4.542977
1	1.296562	3.384248	4.189659
1	1.226758	1.343678	5.607690
6	-2.730168	-2.575082	-0.675686
6	-2.385828	-3.254386	-1.850703
6	-3.819478	-3.026494	0.085320
6	-3.130852	-4.357894	-2.269425
1	-1.516244	-2.932515	-2.413857

6	-4.558888	-4.132282	-0.331331
1	-4.084326	-2.511159	1.003734
6	-4.216987	-4.797491	-1.512030
1	-2.852317	-4.882113	-3.179230
1	-5.399996	-4.476220	0.264530
1	-4.791609	-5.661666	-1.834113
6	-1.814674	-1.180619	1.633968
6	-1.273171	-2.326021	2.242520
6	-2.310899	-0.151022	2.439156
6	-1.251389	-2.443179	3.629684
1	-0.873388	-3.123504	1.621626
6	-2.270533	-0.263738	3.830557
1	-2.733885	0.738442	1.985511
6	-1.748164	-1.409351	4.428912
1	-0.840402	-3.338861	4.087799
1	-2.652762	0.546358	4.445462
1	-1.723311	-1.496468	5.511634
46	0.605051	-1.201787	-0.710803
6	-2.660999	4.485038	0.720293
1	-2.173046	5.448436	0.905464
1	-3.725987	4.577876	0.960293
1	-2.219188	3.742485	1.391018
6	-3.102558	5.147183	-1.662953
1	-4.166074	5.269260	-1.437462
1	-2.628618	6.117251	-1.486344
1	-2.998650	4.897161	-2.723755
6	3.381266	-3.223620	-0.829289
6	4.076568	-2.505920	0.324133
1	4.100519	-1.429835	0.153665
1	3.552977	-2.706611	1.263340
1	5.101759	-2.880129	0.408773
6	4.050247	-2.916496	-2.177537
1	5.099919	-3.223615	-2.130341
1	3.556139	-3.471413	-2.982547
1	4.000749	-1.849846	-2.406833
8	3.475035	-4.620754	-0.537429
1	2.832166	-5.075179	-1.105611
6	1.921954	-2.840388	-0.917709
7	0.845682	-3.358427	-1.115010

IM6B

SCF Energy: -3502.16870208

Sum of electronic and zero-point Energies= -3501.160766

Sum of electronic and thermal Energies= -3501.095854

Sum of electronic and thermal Enthalpies= -3501.094910

Sum of electronic and thermal Free Energies= -3501.263891

Electronic energy in solution by single point calculation = -3500.69949759

6	-3.126009	0.590179	3.117899
6	-2.584985	0.082154	1.925796
6	-2.093251	-1.225829	1.960325
6	-2.046555	-2.012100	3.117893
6	-2.555854	-1.450559	4.289880
6	-3.107312	-0.168552	4.285127
6	-1.500444	-3.439757	3.003666
6	-0.385548	-3.430038	1.956201
6	-0.538222	-2.583698	0.862020
6	0.360228	-2.507538	-0.202604
6	1.472308	-3.354910	-0.176136
6	1.664585	-4.211794	0.908603
6	0.750987	-4.246708	1.964338
1	-3.542675	1.588416	3.141603
1	-2.533308	-2.015228	5.214921
1	-3.516764	0.246255	5.200943
1	2.194228	-3.325181	-0.982688
1	2.540268	-4.852218	0.934113
1	0.930609	-4.916930	2.797314
8	-1.627366	-1.737277	0.775208
15	-0.001773	-1.208190	-1.435777
15	-2.446177	1.106369	0.388788
6	1.320887	-1.398709	-2.687302
6	1.036137	-1.686047	-4.030180
6	2.652349	-1.181092	-2.298122
6	2.069431	-1.749597	-4.966693
1	0.013633	-1.861271	-4.346306
6	3.679422	-1.252523	-3.236499
1	2.923463	-0.956474	-1.274232
6	3.391407	-1.532390	-4.573953
1	1.837665	-1.972490	-6.004663
1	4.695599	-1.070558	-2.901534
1	4.191539	-1.579664	-5.307530
6	-1.501617	-1.827732	-2.286316
6	-2.251674	-0.922244	-3.048735
6	-1.911170	-3.165039	-2.213398
6	-3.383865	-1.349526	-3.739902
1	-1.951008	0.121062	-3.092567
6	-3.056533	-3.586387	-2.888256

1	-1.334477	-3.874782	-1.628972
6	-3.792653	-2.680797	-3.654459
1	-3.959264	-0.637250	-4.321124
1	-3.370410	-4.624349	-2.819965
1	-4.684263	-3.010394	-4.180201
6	-2.836890	2.745721	1.133532
6	-1.840911	3.324292	1.939906
6	-4.060973	3.407710	0.977465
6	-2.066434	4.544699	2.572986
1	-0.893114	2.809580	2.071109
6	-4.278019	4.638844	1.602822
1	-4.841503	2.965543	0.368233
6	-3.284676	5.208040	2.400173
1	-1.288941	4.979706	3.193902
1	-5.228016	5.147932	1.468511
1	-3.457047	6.164129	2.885433
6	-3.939269	0.666171	-0.579641
6	-4.269273	1.447536	-1.700621
6	-4.720691	-0.451716	-0.266788
6	-5.389792	1.131630	-2.465899
1	-3.644460	2.295108	-1.965100
6	-5.823798	-0.779881	-1.056006
1	-4.471554	-1.065995	0.591207
6	-6.168016	0.015755	-2.148114
1	-5.647298	1.751235	-3.320579
1	-6.417298	-1.655677	-0.810149
1	-7.033876	-0.235717	-2.754021
46	-0.335899	1.174703	-0.766269
6	-2.643246	-4.349934	2.477900
1	-2.281511	-5.376520	2.354145
1	-3.480933	-4.354224	3.184108
1	-3.010167	-3.996956	1.509068
6	-1.008183	-3.974047	4.355015
1	-1.825924	-4.011487	5.080433
1	-0.635621	-4.996829	4.250292
1	-0.205636	-3.351768	4.763445
6	-0.482673	3.215282	-1.415491
6	0.006873	3.053565	-2.851160
1	1.076506	2.842909	-2.887112
1	-0.522135	2.247635	-3.372974
1	-0.194859	3.987241	-3.396691
6	0.308149	4.240929	-0.620582
1	0.191246	5.228909	-1.092251

1	-0.049517	4.315553	0.409442
1	1.368560	3.986797	-0.590252
8	-1.839663	3.585402	-1.513075
1	-2.137213	3.886070	-0.638056
6	1.633662	1.438734	-0.688440
7	2.746723	1.456093	-0.337555
13	4.228089	0.936657	0.806627
8	4.794650	-0.429440	-0.138380
8	5.281617	2.307585	0.959975
8	3.447011	0.536512	2.312620
6	5.771925	-1.391180	0.187472
6	5.801610	3.048880	-0.120104
6	2.361038	-0.347933	2.441910
6	6.902316	2.266146	-0.846052
1	6.508102	1.313616	-1.214200
1	7.304567	2.833714	-1.694935
1	7.723926	2.050624	-0.151933
6	6.317631	4.386323	0.411111
1	5.512244	4.923327	0.923071
1	7.122502	4.212553	1.135079
1	6.704549	5.017763	-0.398443
6	6.499595	-1.065791	1.496402
1	5.791644	-1.058024	2.333642
1	7.282928	-1.803578	1.709668
1	6.963752	-0.075466	1.438078
6	5.122366	-2.777333	0.238217
1	4.357232	-2.800473	1.022646
1	4.636395	-3.001471	-0.717795
1	5.861779	-3.561406	0.444026
6	1.098845	0.435778	2.819311
1	1.282851	1.007751	3.736565
1	0.839859	1.138302	2.019896
1	0.244014	-0.229318	2.985083
6	2.688656	-1.410649	3.493591
1	2.908158	-0.927340	4.452761
1	1.854029	-2.109132	3.627762
1	3.571982	-1.983174	3.191864
1	4.999455	3.261931	-0.852105
1	6.523245	-1.398920	-0.621221
1	2.159421	-0.871900	1.489758

IM6

SCF Energy: -2082.29524946

Sum of electronic and zero-point Energies= -2081.425766

Sum of electronic and thermal Energies= -2081.377204

Sum of electronic and thermal Enthalpies= -2081.376260

Sum of electronic and thermal Free Energies= -2081.506181

Electronic energy in solution by single point calculation = -2081.2063888

46	-0.260673	-0.371960	-1.039265
15	-2.174465	-1.152275	-0.051868
6	-2.801908	0.204105	1.049966
6	-2.043396	1.392269	1.210186
6	-4.004403	0.076828	1.768402
6	-2.542701	2.398679	2.055849
6	-0.705538	1.695287	0.577782
6	-4.476561	1.081851	2.608033
1	-4.586426	-0.829449	1.673749
6	-3.741754	2.257553	2.747630
1	-1.958822	3.306634	2.170583
6	0.483502	1.508088	1.334475
6	-0.637403	2.427251	-0.640346
1	-5.409840	0.944842	3.146832
1	-4.093509	3.056423	3.394225
6	1.691486	2.010309	0.844510
6	0.600879	2.911413	-1.080590
6	1.775353	2.712662	-0.358209
1	2.599159	1.849363	1.417442
1	0.640805	3.462472	-2.014250
6	-3.555869	-1.451131	-1.349022
6	-2.054117	-2.694813	1.086472
6	-3.365835	-3.408939	1.446985
1	-3.136599	-4.241673	2.125003
1	-4.069652	-2.756523	1.969581
1	-3.866354	-3.833639	0.573715
6	-1.115903	-3.704037	0.396395
1	-1.531115	-4.096101	-0.534472
1	-0.154315	-3.242124	0.168188
1	-0.941744	-4.553970	1.069392
6	-3.477566	-0.276349	-2.337502
1	-2.473770	-0.179058	-2.758588
1	-4.188050	-0.443770	-3.157705
1	-3.743006	0.668439	-1.856754
6	-3.207671	-2.736349	-2.122288
1	-2.167070	-2.721635	-2.463185
1	-3.369233	-3.639708	-1.528329
1	-3.853151	-2.807202	-3.007047

6	0.468120	0.847209	2.705217
1	-0.494663	0.345299	2.824947
6	-1.893473	2.821751	-1.403779
1	-2.700272	2.162655	-1.075632
6	3.103146	3.263709	-0.844013
1	3.869493	2.927591	-0.133385
6	0.571748	1.906482	3.818092
1	0.548947	1.430628	4.805889
1	1.509374	2.467739	3.732839
1	-0.255466	2.621386	3.765798
6	1.574270	-0.207290	2.863595
1	1.442733	-0.756670	3.803212
1	1.559963	-0.922902	2.038706
1	2.573022	0.240042	2.880458
6	3.102746	4.802490	-0.830641
1	2.872881	5.189628	0.168167
1	4.080051	5.194598	-1.136387
1	2.351434	5.198336	-1.524199
6	3.477746	2.723231	-2.233776
1	3.446913	1.631111	-2.255795
1	2.773617	3.079049	-2.994835
1	4.480420	3.063323	-2.519989
6	-1.741867	2.669940	-2.925131
1	-2.716792	2.773138	-3.415138
1	-1.084052	3.441072	-3.341481
1	-1.319178	1.695621	-3.184864
6	-2.307701	4.261163	-1.044990
1	-1.513891	4.968807	-1.311142
1	-3.216428	4.547809	-1.587921
1	-2.505633	4.362454	0.026533
6	-5.004687	-1.525317	-0.839895
1	-5.167848	-2.312151	-0.101752
1	-5.324684	-0.573162	-0.409258
1	-5.664322	-1.735382	-1.692121
6	-1.369195	-2.237900	2.383338
1	-1.992989	-1.547491	2.957703
1	-1.162311	-3.113538	3.011976
1	-0.418219	-1.748494	2.169633
6	1.590655	-2.791050	-2.357773
6	3.987929	-3.386974	-2.058510
1	0.773116	-3.452772	-2.053221
1	1.805801	-2.979371	-3.415482
1	4.880741	-3.518561	-1.453348

1	4.088342	-3.552730	-3.127600
6	2.829024	-3.020789	-1.509688
6	2.666836	-2.775773	-0.015779
6	3.748731	-1.925656	0.614684
6	4.046513	-0.661222	0.086256
6	4.416980	-2.348956	1.766724
6	4.991135	0.156121	0.702483
1	3.524572	-0.318503	-0.801597
6	5.359810	-1.527706	2.390445
1	4.191746	-3.327334	2.185057
6	5.649255	-0.271102	1.859747
1	5.214891	1.130378	0.277204
1	5.867699	-1.872698	3.287057
1	6.384530	0.369249	2.339219
1	1.705568	-2.273312	0.150389
1	2.602108	-3.738859	0.507818
6	1.161705	-1.367706	-2.186986
7	1.485610	-0.214426	-2.324527

IM7A

SCF Energy: -2678.16186408

Sum of electronic and zero-point Energies= -2677.454743

Sum of electronic and thermal Energies= -2677.408907

Sum of electronic and thermal Enthalpies= -2677.407963

Sum of electronic and thermal Free Energies= -2677.534841

Electronic energy in solution by single point calculation = -2677.00019916

6	-2.942095	2.264250	-1.187648
6	-1.816946	1.681123	-0.581854
6	-0.646050	2.446613	-0.568837
6	-0.537308	3.725561	-1.128817
6	-1.675002	4.254279	-1.740369
6	-2.867786	3.530974	-1.762318
6	0.795484	4.469449	-0.971627
6	1.913446	3.432930	-1.093029
6	1.674964	2.178205	-0.540272
6	2.591893	1.127362	-0.554205
6	3.845805	1.364937	-1.127342
6	4.127137	2.615740	-1.680625
6	3.171017	3.635558	-1.672607
1	-3.876231	1.720613	-1.226136
1	-1.638707	5.236532	-2.197934
1	-3.748249	3.956269	-2.234269
1	4.581848	0.568819	-1.159733

1	5.098087	2.797026	-2.131696
1	3.412391	4.591982	-2.123274
8	0.456045	1.892995	0.045080
15	1.940239	-0.479414	0.020171
15	-1.854242	-0.048585	0.105089
6	3.396764	-1.585785	-0.144011
6	4.293052	-1.797180	0.914767
6	3.628417	-2.216177	-1.376582
6	5.401691	-2.625921	0.742590
1	4.124805	-1.315430	1.871984
6	4.743791	-3.037078	-1.545065
1	2.932473	-2.080231	-2.196941
6	5.630232	-3.246244	-0.487247
1	6.087192	-2.785714	1.570409
1	4.909851	-3.520585	-2.503414
1	6.493276	-3.893171	-0.618401
6	1.797049	-0.267515	1.836113
6	1.067584	-1.231696	2.546467
6	2.385629	0.793864	2.533821
6	0.946137	-1.147912	3.930946
1	0.584873	-2.041751	2.005583
6	2.251193	0.884902	3.919974
1	2.952171	1.545798	1.993423
6	1.536163	-0.087012	4.620478
1	0.368864	-1.893753	4.467763
1	2.708995	1.714419	4.452150
1	1.428588	-0.013160	5.698838
6	-3.574421	-0.492467	-0.369006
6	-3.761257	-1.027720	-1.652238
6	-4.690029	-0.240051	0.440047
6	-5.044356	-1.314635	-2.113806
1	-2.897733	-1.245820	-2.271083
6	-5.973092	-0.535987	-0.022901
1	-4.559849	0.190034	1.427025
6	-6.152561	-1.073026	-1.299068
1	-5.174046	-1.740659	-3.104148
1	-6.832154	-0.342078	0.613409
1	-7.152172	-1.304719	-1.655891
6	-1.958228	0.197817	1.925563
6	-2.486966	-0.835518	2.717190
6	-1.459614	1.343604	2.557220
6	-2.537887	-0.712099	4.104000
1	-2.881216	-1.729423	2.246630

6	-1.498319	1.457583	3.946813
1	-1.035493	2.148356	1.970916
6	-2.042298	0.436196	4.724274
1	-2.965323	-1.514424	4.699187
1	-1.099235	2.349794	4.420342
1	-2.075729	0.530892	5.805893
46	-0.176005	-1.423342	-0.899651
6	0.846274	5.071053	0.458868
1	1.798655	5.588957	0.617217
1	0.028419	5.786437	0.598721
1	0.753036	4.288082	1.217515
6	0.949420	5.600222	-1.996064
1	0.162103	6.348986	-1.869285
1	1.902512	6.118046	-1.854340
1	0.909016	5.221425	-3.022258
6	-1.216030	-3.319896	-1.017277
6	-2.205958	-3.482791	0.121431
1	-1.726133	-3.258753	1.078694
1	-3.088876	-2.859067	-0.001146
1	-2.539939	-4.530828	0.150594
6	-0.018331	-4.259947	-0.798248
1	-0.401370	-5.267306	-0.571035
1	0.624414	-4.316541	-1.676151
1	0.597204	-3.938545	0.049986
8	-1.884215	-3.559319	-2.215388
1	-1.233636	-3.429401	-2.930980
6	0.570023	-2.028688	-2.677529
7	0.849599	-2.376864	-3.761781

IM7

SCF Energy: -1888.33083532

Sum of electronic and zero-point Energies= -1887.544546

Sum of electronic and thermal Energies= -1887.499759

Sum of electronic and thermal Enthalpies= -1887.498814

Sum of electronic and thermal Free Energies= -1887.618076

Electronic energy in solution by single point calculation = -1887.4080774

46	0.126756	-1.161907	0.384419
6	0.221540	-3.245971	-0.094955
6	-0.577059	-3.552950	-1.344251
1	-1.644105	-3.421506	-1.192000
1	-0.249071	-2.941283	-2.185372
1	-0.395531	-4.604450	-1.611032
6	-0.214667	-4.083279	1.100436

1	-0.083499	-5.146023	0.843886
1	0.375670	-3.862970	1.990204
1	-1.269879	-3.915593	1.326834
8	1.553690	-3.431379	-0.452626
1	2.107074	-3.238596	0.328325
6	1.652672	-1.615154	1.630799
7	2.511729	-1.992128	2.333965
15	-2.067465	-0.194557	-0.003193
6	-1.763952	1.626494	-0.252606
6	-0.458930	2.162889	-0.377705
6	-2.850807	2.521894	-0.288923
6	-0.317910	3.543000	-0.615984
6	0.846405	1.425904	-0.237150
6	-2.688030	3.887849	-0.495698
1	-3.853017	2.149556	-0.147545
6	-1.407541	4.403292	-0.681336
1	0.686413	3.936321	-0.735024
6	1.603023	1.592691	0.952467
6	1.463140	0.837715	-1.376254
1	-3.557364	4.538655	-0.514409
1	-1.255277	5.463726	-0.859972
6	2.932621	1.154536	0.978021
6	2.783800	0.401013	-1.286300
6	3.540333	0.556197	-0.120187
1	3.504525	1.263010	1.893812
1	3.240640	-0.064994	-2.152782
6	-3.332586	-0.684509	-1.367466
6	-2.931056	-0.271763	1.715257
6	-4.394462	0.191921	1.774874
1	-4.739658	0.112071	2.813612
1	-4.515831	1.236419	1.479888
1	-5.060505	-0.424162	1.166897
6	-2.838231	-1.717772	2.236611
1	-3.376492	-2.431581	1.608512
1	-1.794847	-2.032404	2.304302
1	-3.277583	-1.763390	3.241301
6	-2.521406	-0.824260	-2.668695
1	-1.652027	-1.469370	-2.554547
1	-3.162612	-1.246515	-3.452953
1	-2.176711	0.153612	-3.016884
6	-3.956740	-2.041249	-0.984185
1	-3.225085	-2.762659	-0.620613
1	-4.721579	-1.928964	-0.211912

1	-4.442122	-2.474644	-1.867250
6	1.040104	2.288087	2.185101
1	-0.040146	2.385146	2.052777
6	0.740519	0.776576	-2.711808
1	-0.330506	0.816301	-2.505361
6	4.974381	0.065576	-0.049686
1	5.368969	0.356708	0.932354
6	1.615844	3.709916	2.323966
1	1.209649	4.200976	3.216179
1	2.706854	3.677735	2.422765
1	1.373801	4.329754	1.455548
6	1.290030	1.490071	3.476897
1	0.721294	1.930837	4.303962
1	1.005794	0.440901	3.368780
1	2.348183	1.506483	3.758929
6	5.853979	0.726316	-1.124403
1	5.817946	1.819110	-1.051820
1	6.897166	0.408304	-1.014905
1	5.527136	0.446102	-2.132745
6	5.036654	-1.469490	-0.139101
1	4.468981	-1.921956	0.677950
1	4.615446	-1.823975	-1.087771
1	6.075962	-1.814383	-0.080918
6	1.021591	-0.516173	-3.490093
1	0.317628	-0.617476	-4.323837
1	2.031393	-0.520257	-3.915418
1	0.933131	-1.393114	-2.843746
6	1.087313	2.008231	-3.569144
1	2.163917	2.043240	-3.772184
1	0.559725	1.969847	-4.529848
1	0.806659	2.937281	-3.063941
6	-4.488805	0.284703	-1.674461
1	-5.116050	0.498658	-0.806910
1	-4.130919	1.227142	-2.093328
1	-5.130640	-0.185607	-2.430866
6	-2.097567	0.609822	2.659833
1	-2.168990	1.669586	2.402513
1	-2.463871	0.482755	3.686154
1	-1.045691	0.314915	2.645045

IM8A

SCF Energy: -2678.16625319

Sum of electronic and zero-point Energies= -2677.461418

Sum of electronic and thermal Energies= -2677.416275

Sum of electronic and thermal Enthalpies= -2677.415330

Sum of electronic and thermal Free Energies= -2677.540951

Electronic energy in solution by single point calculation = -2676.9961198

6	-3.242978	-2.211478	-0.729273
6	-2.225455	-1.248601	-0.726213
6	-1.173678	-1.421309	-1.634075
6	-1.055514	-2.521296	-2.486489
6	-2.083230	-3.467887	-2.450330
6	-3.173302	-3.304774	-1.592822
6	0.181118	-2.583708	-3.391559
6	1.360083	-2.036175	-2.579009
6	1.110397	-0.939307	-1.756513
6	2.083318	-0.303095	-0.982549
6	3.385157	-0.811813	-1.029615
6	3.670497	-1.918185	-1.831769
6	2.672281	-2.522506	-2.600609
1	-4.069274	-2.123965	-0.033688
1	-2.036426	-4.342400	-3.089710
1	-3.964684	-4.048126	-1.582201
1	4.156237	-0.373729	-0.406524
1	4.676921	-2.324032	-1.842429
1	2.920681	-3.385315	-3.208753
8	-0.185313	-0.458394	-1.637200
15	1.513387	0.978948	0.195852
15	-2.050497	0.042806	0.578568
6	3.069051	1.646894	0.909217
6	3.843085	2.566556	0.182385
6	3.500946	1.228274	2.176379
6	5.032334	3.059268	0.715703
1	3.515529	2.900190	-0.796666
6	4.693550	1.727802	2.702549
1	2.922942	0.482730	2.710791
6	5.458999	2.641676	1.978538
1	5.624697	3.769461	0.145221
1	5.026921	1.390289	3.679682
1	6.387474	3.025328	2.392753
6	0.993227	2.368773	-0.883721
6	0.445243	3.498129	-0.259867
6	1.182966	2.380592	-2.270494
6	0.116186	4.626438	-1.005759
1	0.282051	3.492142	0.814331
6	0.841728	3.508464	-3.018857

1	1.613408	1.516290	-2.764937
6	0.315339	4.635139	-2.387964
1	-0.308889	5.494012	-0.510635
1	0.997715	3.507866	-4.094304
1	0.054346	5.514613	-2.969959
6	-3.560894	-0.165070	1.601784
6	-3.476714	-0.609785	2.925619
6	-4.821754	0.136894	1.058542
6	-4.634217	-0.761713	3.692840
1	-2.503000	-0.833185	3.348111
6	-5.974764	-0.023839	1.822422
1	-4.896479	0.500623	0.038283
6	-5.882424	-0.473450	3.143094
1	-4.555569	-1.103092	4.720962
1	-6.944593	0.206776	1.390804
1	-6.781997	-0.592350	3.740427
6	-2.434766	1.641721	-0.235813
6	-2.795557	2.719726	0.587781
6	-2.409212	1.818274	-1.622924
6	-3.154274	3.943558	0.029591
1	-2.817960	2.591332	1.666416
6	-2.759440	3.049405	-2.178140
1	-2.122111	0.999930	-2.271466
6	-3.141274	4.109246	-1.356985
1	-3.444397	4.766936	0.676230
1	-2.729673	3.178142	-3.255873
1	-3.418107	5.064284	-1.794234
46	-0.034912	-0.360718	1.525301
6	-0.051937	-1.643441	-4.604405
1	0.830710	-1.639282	-5.253235
1	-0.915429	-1.982558	-5.187375
1	-0.240049	-0.617348	-4.274911
6	0.446746	-4.004387	-3.902586
1	-0.395046	-4.364158	-4.501743
1	1.326995	-4.019087	-4.551854
1	0.612264	-4.704622	-3.077585
6	2.000478	-2.471063	2.318222
6	1.564836	-3.062904	3.672046
1	1.831722	-4.121830	3.766470
1	2.028145	-2.502248	4.488554
1	0.477326	-2.958434	3.749717
6	1.396796	-3.292170	1.157077
1	0.305622	-3.240362	1.223136

1	1.710748	-2.878391	0.197091
1	1.711164	-4.341284	1.208412
8	1.727492	-1.106961	2.251704
1	-0.861135	-1.455291	2.295700
6	3.489491	-2.573480	2.193125
7	4.643080	-2.610381	2.061050

IM8

SCF Energy: -1988.77778664

Sum of electronic and zero-point Energies= -1987.930430

Sum of electronic and thermal Energies= -1987.884546

Sum of electronic and thermal Enthalpies= -1987.883602

Sum of electronic and thermal Free Energies= -1988.007855

Electronic energy in solution by single point calculation = -1987.72486796

46	-0.279532	-0.929611	-0.310928
15	-1.168399	1.346371	-0.035412
6	0.254224	2.500700	0.282060
6	1.590706	2.040708	0.325570
6	0.019354	3.870248	0.512310
6	2.618472	2.969933	0.580765
6	2.090691	0.624774	0.184507
6	1.045857	4.772975	0.767721
1	-0.993724	4.243395	0.487736
6	2.362939	4.318773	0.797663
1	3.639295	2.602509	0.620515
6	2.259541	-0.157319	1.358126
6	2.756006	0.233453	-1.005646
1	0.815756	5.820258	0.941131
1	3.182443	5.003714	0.995495
6	3.082329	-1.284257	1.315587
6	3.569417	-0.902602	-0.994539
6	3.760029	-1.668423	0.157305
1	3.222096	-1.870071	2.220043
1	4.084251	-1.184564	-1.908051
6	-1.879678	1.978277	-1.701267
6	-2.424255	1.697740	1.373448
6	-3.273181	2.975214	1.261750
1	-3.972867	2.995867	2.107305
1	-2.680288	3.891021	1.319745
1	-3.871354	3.005585	0.349381
6	-3.365571	0.481212	1.425880
1	-3.976006	0.375919	0.528167
1	-2.802458	-0.444019	1.554336

1	-4.047407	0.592352	2.279078
6	-0.933799	1.422127	-2.778695
1	-0.844362	0.332529	-2.705550
1	-1.324533	1.669379	-3.774394
1	0.063821	1.857891	-2.697289
6	-3.261752	1.349136	-1.920455
1	-3.234701	0.272094	-1.764394
1	-4.029061	1.764297	-1.263091
1	-3.579511	1.535647	-2.954763
6	1.672896	0.276515	2.691984
1	0.984110	1.099300	2.498124
6	2.682178	1.062812	-2.278589
1	1.931563	1.842117	-2.123179
6	4.703267	-2.859078	0.167198
1	4.638881	-3.315419	1.163871
6	2.778262	0.820990	3.614410
1	2.349603	1.172986	4.560086
1	3.517533	0.045250	3.844983
1	3.303481	1.659440	3.144830
6	0.875621	-0.843130	3.376919
1	0.427256	-0.473634	4.306695
1	0.076388	-1.205842	2.723553
1	1.513973	-1.694956	3.637186
6	6.157831	-2.403066	-0.045771
1	6.453188	-1.662685	0.705466
1	6.845087	-3.254520	0.019874
1	6.283523	-1.945626	-1.034182
6	4.306134	-3.930059	-0.862226
1	3.285830	-4.285864	-0.689456
1	4.353547	-3.534374	-1.883441
1	4.987105	-4.787089	-0.805103
6	2.248997	0.213674	-3.485199
1	2.062089	0.852212	-4.356249
1	3.026276	-0.506522	-3.764011
1	1.337813	-0.349550	-3.264321
6	4.017972	1.772862	-2.561287
1	4.828109	1.046761	-2.694198
1	3.947964	2.372881	-3.476171
1	4.293866	2.438994	-1.737811
6	-1.968124	3.500263	-1.888168
1	-2.612054	3.983772	-1.150302
1	-0.983977	3.973865	-1.853152
1	-2.397052	3.703288	-2.878218

6	-1.644201	1.737560	2.697628
1	-0.937059	2.570609	2.744690
1	-2.356821	1.850935	3.524442
1	-1.100874	0.805082	2.858824
6	0.005720	-3.402575	0.656169
6	0.624055	-2.768798	-0.597588
1	-0.150905	-4.494213	0.656076
1	0.599375	-3.134562	1.538021
1	0.295150	-3.242127	-1.525157
1	1.695266	-2.577817	-0.587469
6	-1.222419	-2.563541	0.493988
6	-2.475231	-3.011067	0.674143
1	-2.564020	-3.934701	1.260283
6	-3.754258	-2.500220	0.168221
6	-4.914690	-2.572130	0.958841
6	-3.873777	-2.005682	-1.139520
6	-6.141398	-2.121819	0.477271
1	-4.840486	-2.971262	1.967624
6	-5.104471	-1.567916	-1.628834
1	-2.984835	-1.982921	-1.762894
6	-6.241895	-1.612845	-0.820702
1	-7.022298	-2.171097	1.112125
1	-5.176507	-1.191663	-2.646181
1	-7.199824	-1.270806	-1.202649

IM9B

SCF Energy: -2872.12962783

Sum of electronic and zero-point Energies= -2871.337357

Sum of electronic and thermal Energies= -2871.288577

Sum of electronic and thermal Enthalpies= -2871.287633

Sum of electronic and thermal Free Energies= -2871.421471

Electronic energy in solution by single point calculation = -2870.78994931

6	0.067368	-3.978384	-0.832928
6	-0.380899	-2.717465	-0.410703
6	-1.748765	-2.589005	-0.145011
6	-2.677806	-3.621181	-0.316046
6	-2.192148	-4.853056	-0.759526
6	-0.829233	-5.031641	-1.004554
6	-4.137601	-3.326296	0.045086
6	-4.426465	-1.884036	-0.379537
6	-3.410348	-0.948876	-0.184446
6	-3.535245	0.414914	-0.464583
6	-4.765875	0.855918	-0.967011

6	-5.802930	-0.053178	-1.184461
6	-5.636641	-1.409780	-0.896111
1	1.118379	-4.130421	-1.046309
1	-2.874087	-5.682355	-0.912047
1	-0.464424	-5.998300	-1.339154
1	-4.904164	1.906430	-1.197508
1	-6.750725	0.298399	-1.581519
1	-6.457518	-2.096118	-1.073206
8	-2.185647	-1.361773	0.304218
15	-2.025700	1.444406	-0.264185
15	0.709901	-1.221945	-0.329410
6	-2.663190	3.133813	-0.608774
6	-3.569463	3.784738	0.242657
6	-2.219782	3.782885	-1.768435
6	-4.038648	5.058625	-0.071918
1	-3.901374	3.294201	1.153023
6	-2.693687	5.059072	-2.081668
1	-1.482061	3.297981	-2.399727
6	-3.603413	5.696089	-1.237716
1	-4.739750	5.556610	0.592544
1	-2.341097	5.557564	-2.980292
1	-3.967191	6.691082	-1.479863
6	-1.813271	1.476138	1.565052
6	-0.588311	1.946456	2.061104
6	-2.795825	1.053101	2.467876
6	-0.357897	2.007121	3.432897
1	0.188088	2.243635	1.361464
6	-2.559015	1.103202	3.843001
1	-3.745249	0.678574	2.097683
6	-1.342158	1.582625	4.327785
1	0.600660	2.357663	3.802208
1	-3.327439	0.767108	4.534351
1	-1.156165	1.615736	5.397763
6	2.265456	-1.943720	-1.011877
6	2.467475	-1.846358	-2.396947
6	3.222819	-2.605380	-0.232427
6	3.601592	-2.399081	-2.991326
1	1.734436	-1.316827	-3.000987
6	4.361501	-3.152583	-0.825771
1	3.082484	-2.687354	0.839870
6	4.554278	-3.052047	-2.204402
1	3.745341	-2.313064	-4.064818
1	5.100051	-3.654311	-0.207036

1	5.442347	-3.477119	-2.663911
6	1.100866	-1.053006	1.457401
6	2.216349	-0.275742	1.809542
6	0.302634	-1.596343	2.469163
6	2.543431	-0.074284	3.147410
1	2.843620	0.152755	1.035590
6	0.619348	-1.372662	3.810159
1	-0.567155	-2.191540	2.216326
6	1.742142	-0.620550	4.153531
1	3.426392	0.506670	3.396483
1	-0.015504	-1.789971	4.586581
1	1.989376	-0.455942	5.198701
46	0.069410	0.810026	-1.217188
6	-4.282634	-3.412074	1.588786
1	-5.310759	-3.175848	1.884881
1	-4.038862	-4.422050	1.936718
1	-3.612027	-2.704605	2.085274
6	-5.105028	-4.323193	-0.603818
1	-4.898137	-5.341611	-0.261936
1	-6.136912	-4.097688	-0.318974
1	-5.033395	-4.301300	-1.696039
1	3.941126	3.393237	-2.627803
6	1.768382	1.758295	-2.007681
7	0.937424	2.587536	-2.294206
6	3.186155	1.446391	-1.859498
6	4.260760	2.437147	-2.224016
6	3.979991	2.178330	-0.756812
1	3.416015	0.395383	-1.964060
1	5.181967	2.044643	-2.645602
6	4.957064	1.343052	0.023410
6	5.261726	1.656001	1.357668
6	5.587685	0.221098	-0.540305
6	6.150252	0.876696	2.100422
1	4.798944	2.514227	1.830454
6	6.474147	-0.557225	0.199184
1	5.377713	-0.072225	-1.563652
6	6.760877	-0.236980	1.526815
1	6.362952	1.145956	3.131614
1	6.933233	-1.424529	-0.266082
1	7.449317	-0.846924	2.104501
6	3.262629	3.275133	0.008299
1	2.719295	2.865584	0.867929
1	3.973300	4.025061	0.373176

1	2.534364	3.778686	-0.629988

IM9

SCF Energy: -1888.31552556

Sum of electronic and zero-point Energies= -1887.533068

Sum of electronic and thermal Energies= -1887.488418

Sum of electronic and thermal Enthalpies= -1887.487474

Sum of electronic and thermal Free Energies= -1887.607881

Electronic energy in solution by single point calculation = -1887.38389299

46	0.199863	-0.832115	0.184965
6	0.598720	-3.741685	-0.429458
6	-0.126737	-5.102845	-0.410636
1	0.547132	-5.926460	-0.669255
1	-0.548775	-5.283402	0.581436
1	-0.943559	-5.068035	-1.138652
6	1.196974	-3.475307	-1.825185
1	0.376269	-3.441311	-2.549976
1	1.709236	-2.508655	-1.827325
1	1.905245	-4.256673	-2.123193
8	-0.332248	-2.773639	-0.051544
1	1.677325	-1.305333	0.170604
15	-2.098825	-0.113248	-0.033127
6	-1.905946	1.715867	-0.065393
6	-0.591914	2.234471	-0.002571
6	-2.990739	2.608242	-0.098134
6	-0.419261	3.628117	0.030500
6	0.682775	1.418394	0.069607
6	-2.800265	3.987110	-0.070752
1	-4.000436	2.217668	-0.142844
6	-1.504380	4.499604	-0.004565
1	0.589578	4.023949	0.095884
6	1.189348	1.017746	1.351891
6	1.610798	1.500091	-1.033102
1	-3.656279	4.655092	-0.096560
1	-1.338164	5.572532	0.026018
6	2.572025	0.719401	1.482839
6	2.949344	1.211708	-0.824283
6	3.457849	0.824197	0.429220
1	2.943077	0.415185	2.456537
1	3.630267	1.276228	-1.667292
6	-2.775385	-0.597708	-1.745506
6	-3.372593	-0.550317	1.320607
6	-4.852520	-0.391469	0.936349

1	-5.469395	-0.675905	1.798606
1	-5.111415	0.640191	0.680570
1	-5.141525	-1.036960	0.105085
6	-3.098712	-2.019384	1.709096
1	-3.329317	-2.714132	0.899842
1	-2.050354	-2.175116	1.975433
1	-3.726605	-2.281605	2.570702
6	-1.605833	-0.403614	-2.724654
1	-0.738987	-1.000027	-2.431228
1	-1.919747	-0.716499	-3.728883
1	-1.303530	0.644310	-2.782982
6	-3.129111	-2.096448	-1.723390
1	-2.304324	-2.681959	-1.305048
1	-4.038102	-2.302657	-1.152276
1	-3.310218	-2.430230	-2.753541
6	0.390018	1.226859	2.630650
1	-0.648357	1.396767	2.346136
6	1.160719	1.943345	-2.417647
1	0.072116	2.041969	-2.400227
6	4.906924	0.410801	0.596063
1	5.100568	0.333102	1.674155
6	0.873378	2.502362	3.345248
1	0.268617	2.688854	4.240205
1	1.920099	2.408848	3.655326
1	0.790100	3.375924	2.690199
6	0.438409	0.011512	3.567709
1	-0.198601	0.182836	4.443219
1	0.099158	-0.893978	3.054095
1	1.453141	-0.179273	3.932544
6	5.893610	1.433919	0.014593
1	5.739339	2.428212	0.448364
1	6.925259	1.126462	0.219000
1	5.788681	1.521137	-1.073124
6	5.118062	-0.987416	-0.017233
1	4.439184	-1.722747	0.426437
1	4.932074	-0.965454	-1.098200
1	6.148690	-1.326050	0.141457
6	1.528494	0.901983	-3.489350
1	1.078927	1.170492	-4.452285
1	2.613389	0.849293	-3.633406
1	1.180567	-0.094948	-3.207953
6	1.738249	3.320861	-2.790118
1	2.833765	3.297994	-2.795812

1	1.401563	3.617801	-3.790189
1	1.421169	4.093070	-2.082941
6	-3.956764	0.244391	-2.250965
1	-4.841186	0.171204	-1.616304
1	-3.683992	1.299807	-2.343670
1	-4.239498	-0.111464	-3.250258
6	-3.099299	0.323369	2.556997
1	-3.207463	1.391937	2.349974
1	-3.818975	0.056537	3.340966
1	-2.101881	0.143253	2.957883
6	1.727274	-3.804814	0.551351
7	2.601673	-3.836673	1.316424

TS1A

SCF Energy: -2778.59378553

Sum of electronic and zero-point Energies= -2777.828492

Sum of electronic and thermal Energies= -2777.781583

Sum of electronic and thermal Enthalpies= -2777.780639

Sum of electronic and thermal Free Energies= -2777.908400

Electronic energy in solution by single point calculation = -2777.31278758

6	3.123147	-2.041089	0.950162
6	2.071957	-1.113786	0.930904
6	0.929725	-1.439185	1.673437
6	0.794378	-2.602871	2.434342
6	1.869295	-3.495097	2.433918
6	3.019802	-3.218052	1.692172
6	-0.503262	-2.782266	3.230314
6	-1.649893	-2.230762	2.377205
6	-1.387505	-1.100060	1.604078
6	-2.335718	-0.470434	0.791430
6	-3.631515	-1.000555	0.793796
6	-3.933934	-2.123339	1.565641
6	-2.952309	-2.737995	2.345107
1	4.018193	-1.850545	0.369969
1	1.812384	-4.416028	3.003621
1	3.844325	-3.925082	1.694372
1	-4.397908	-0.540978	0.179799
1	-4.942735	-2.526050	1.556387
1	-3.208179	-3.616220	2.927744
8	-0.121786	-0.549217	1.615151
15	-1.763529	0.912021	-0.284358
15	2.000659	0.374286	-0.164260
6	-3.357799	1.437425	-1.052211

6	-4.291837	2.257076	-0.401556
6	-3.648051	0.965461	-2.340133
6	-5.494914	2.588621	-1.024826
1	-4.076378	2.636098	0.592203
6	-4.855593	1.291275	-2.959305
1	-2.915149	0.355657	-2.856358
6	-5.781713	2.103390	-2.302971
1	-6.209696	3.226462	-0.511626
1	-5.067800	0.917925	-3.957649
1	-6.719513	2.363328	-2.786400
6	-1.495184	2.254007	0.945451
6	-0.766433	3.376370	0.529862
6	-2.001769	2.216985	2.250839
6	-0.573320	4.453330	1.391526
1	-0.335733	3.388076	-0.467621
6	-1.793594	3.289335	3.119694
1	-2.562328	1.350256	2.586947
6	-1.085677	4.411744	2.689433
1	0.002756	5.311532	1.060575
1	-2.187914	3.247672	4.131722
1	-0.920678	5.245262	3.366556
6	3.687649	0.412546	-0.913205
6	3.788853	0.445687	-2.307416
6	4.860615	0.479122	-0.143425
6	5.038287	0.513959	-2.929596
1	2.874927	0.433953	-2.892731
6	6.107378	0.541711	-0.761462
1	4.791370	0.492089	0.940409
6	6.198344	0.554971	-2.157460
1	5.101966	0.540043	-4.014035
1	7.009251	0.589203	-0.157145
1	7.171717	0.608001	-2.637391
6	2.204489	1.787937	1.009983
6	2.690975	2.996347	0.484649
6	1.879260	1.728966	2.369540
6	2.869791	4.108380	1.303231
1	2.948478	3.058873	-0.569089
6	2.047170	2.848298	3.186107
1	1.497627	0.812142	2.800025
6	2.548781	4.037826	2.660546
1	3.259653	5.030807	0.880781
1	1.783434	2.785840	4.238172
1	2.682387	4.905536	3.300555

46	0.128928	0.320124	-1.558280
6	-0.403784	-1.922270	4.518829
1	-1.327027	-2.008065	5.102690
1	0.436907	-2.257816	5.136340
1	-0.252009	-0.867097	4.272878
6	-0.734830	-4.246738	3.621963
1	0.080601	-4.612536	4.252892
1	-1.655029	-4.349944	4.204125
1	-0.807802	-4.890616	2.739476
6	-0.471187	0.343921	-3.636100
6	-0.779098	-0.641403	-4.450926
6	0.169032	-1.266857	-3.504155
1	-0.365396	1.427581	-3.735273
1	-1.130857	-0.827981	-5.458606
6	1.541686	-1.589829	-4.078022
1	1.866847	-0.791221	-4.750621
1	2.316197	-1.730912	-3.322808
1	1.474923	-2.518922	-4.663572
6	-0.346203	-2.199579	-2.440924
6	-1.727749	-2.409879	-2.283537
6	0.526888	-2.931534	-1.615989
6	-2.217496	-3.294411	-1.327399
1	-2.414431	-1.859981	-2.918714
6	0.037351	-3.825793	-0.666707
1	1.598025	-2.789330	-1.696934
6	-1.337152	-4.009198	-0.513111
1	-3.289467	-3.421479	-1.212067
1	0.737370	-4.366272	-0.038032
1	-1.720678	-4.696085	0.235068

TS1B

SCF Energy: -3502.16259746

Sum of electronic and zero-point Energies= -3501.158258

Sum of electronic and thermal Energies= -3501.093779

Sum of electronic and thermal Enthalpies= -3501.092835

Sum of electronic and thermal Free Energies= -3501.263206

Electronic energy in solution by single point calculation = -3500.69206

6	-1.375933	3.196806	2.083906
6	-1.566378	1.974056	1.425347
6	-1.413281	0.801172	2.180683
6	-1.041182	0.805127	3.529801
6	-0.841537	2.044482	4.142242
6	-1.018184	3.231319	3.429671

6	-0.955975	-0.542508	4.249270
6	-0.430826	-1.574048	3.248243
6	-0.862284	-1.470395	1.923392
6	-0.542932	-2.411205	0.933774
6	0.247323	-3.502789	1.312930
6	0.711344	-3.622224	2.622178
6	0.379315	-2.664140	3.579579
1	-1.485062	4.122356	1.530484
1	-0.550210	2.090243	5.185298
1	-0.865083	4.185965	3.923750
1	0.519538	-4.247663	0.574267
1	1.340368	-4.463537	2.895618
1	0.749506	-2.775189	4.592340
8	-1.651682	-0.399924	1.548507
15	-1.141311	-2.127590	-0.785192
15	-1.891130	1.872999	-0.384936
6	-0.318866	-3.482946	-1.709108
6	-0.995764	-4.585235	-2.242992
6	1.064935	-3.354265	-1.931294
6	-0.301276	-5.546290	-2.983304
1	-2.063134	-4.695073	-2.081812
6	1.755861	-4.323172	-2.654249
1	1.596826	-2.497730	-1.528506
6	1.072631	-5.421567	-3.186440
1	-0.838120	-6.395821	-3.396721
1	2.826704	-4.217830	-2.804894
1	1.610090	-6.173350	-3.757517
6	-2.903482	-2.624117	-0.649647
6	-3.865470	-1.835406	-1.292170
6	-3.317542	-3.721065	0.120784
6	-5.222039	-2.140313	-1.176476
1	-3.546764	-0.964221	-1.856366
6	-4.672870	-4.027758	0.233387
1	-2.578355	-4.324968	0.639181
6	-5.626259	-3.237151	-0.414894
1	-5.956605	-1.506330	-1.662477
1	-4.986739	-4.877937	0.832932
1	-6.682583	-3.472317	-0.316786
6	-1.533140	3.588786	-0.929388
6	-0.200950	3.877593	-1.266365
6	-2.497831	4.601345	-1.015032
6	0.160971	5.160329	-1.673683
1	0.550759	3.095633	-1.214123

6	-2.134242	5.882410	-1.434736
1	-3.529761	4.387861	-0.754414
6	-0.806318	6.164475	-1.762184
1	1.195397	5.366929	-1.932253
1	-2.888901	6.661333	-1.502405
1	-0.527487	7.162395	-2.088900
6	-3.717294	1.737603	-0.501526
6	-4.300585	1.782254	-1.779177
6	-4.531039	1.476226	0.606706
6	-5.670281	1.589142	-1.940198
1	-3.673597	1.967836	-2.648115
6	-5.901293	1.263931	0.441670
1	-4.094468	1.435857	1.599025
6	-6.475525	1.324209	-0.827698
1	-6.109235	1.637003	-2.933037
1	-6.520080	1.054770	1.309808
1	-7.542622	1.163557	-0.952867
46	-0.723852	0.086185	-1.338048
6	-2.396592	-0.961599	4.651907
1	-2.381710	-1.941756	5.141148
1	-2.823930	-0.228043	5.344756
1	-3.046051	-1.026641	3.773815
6	-0.086951	-0.469468	5.511278
1	-0.499846	0.250286	6.223983
1	-0.068412	-1.437093	6.020815
1	0.940536	-0.177430	5.276470
6	1.883020	1.090559	-3.100504
6	0.652378	1.440613	-3.893494
1	-0.014589	0.580094	-3.987624
1	0.121933	2.278685	-3.441219
1	0.980278	1.740472	-4.901146
6	2.652488	-0.134944	-3.541725
1	3.103146	0.101484	-4.517676
1	3.452415	-0.383111	-2.844273
1	1.990355	-0.994315	-3.662155
8	2.536109	2.106842	-2.624296
1	3.388504	1.815652	-1.986709
6	1.264504	0.183068	-1.237416
7	2.121480	-0.032822	-0.443589
13	3.881526	0.235228	0.164494
8	4.907347	-1.136123	-0.124747
8	4.330048	1.467894	-1.087095
8	3.785341	0.795342	1.805376

6	5.117403	-2.253442	0.715390
6	5.657602	1.903448	-1.413512
6	2.663355	1.434976	2.381146
6	6.256420	0.979596	-2.472926
1	5.636234	0.975536	-3.376480
1	7.264825	1.306179	-2.753439
1	6.305661	-0.040076	-2.077930
6	6.515756	1.968854	-0.152906
1	6.031550	2.583595	0.611661
1	6.662969	0.962425	0.254469
1	7.499997	2.394643	-0.379603
6	5.994800	-1.870283	1.910831
1	5.484469	-1.115293	2.518797
1	6.217236	-2.742199	2.539014
1	6.942852	-1.446648	1.561136
6	3.788198	-2.864991	1.167758
1	3.228618	-2.154434	1.787485
1	3.167158	-3.121029	0.303060
1	3.947729	-3.775767	1.758645
6	2.415669	2.804204	1.740259
1	3.299183	3.441806	1.866492
1	2.224027	2.700170	0.666978
1	1.550285	3.301210	2.191615
6	2.900338	1.553993	3.885544
1	3.790884	2.163761	4.078360
1	2.042210	2.015786	4.386727
1	3.071755	0.561434	4.316959
1	5.557889	2.916964	-1.827548
1	5.655145	-3.007397	0.118608
1	1.761531	0.819656	2.222368

TS1

SCF Energy: -1988.77201778

Sum of electronic and zero-point Energies= -1987.927683

Sum of electronic and thermal Energies= -1987.881603

Sum of electronic and thermal Enthalpies= -1987.880659

Sum of electronic and thermal Free Energies= -1988.006505

Electronic energy in solution by single point calculation = -1987.7321332

46	0.419728	-1.409678	0.357859
15	2.646319	-0.969935	0.006275
6	3.038609	0.816289	-0.349992
6	2.038358	1.822563	-0.405179
6	4.366837	1.193275	-0.627386

6	2.426261	3.138961	-0.719551
6	0.555864	1.662498	-0.184117
6	4.728888	2.500188	-0.938624
1	5.143405	0.442546	-0.604917
6	3.746705	3.486696	-0.982680
1	1.652249	3.899118	-0.762207
6	-0.301926	1.497139	-1.295683
6	-0.003115	1.914388	1.086316
1	5.767760	2.740298	-1.146697
1	4.001836	4.514680	-1.224100
6	-1.683461	1.550945	-1.103644
6	-1.395477	1.944122	1.232721
6	-2.258770	1.764322	0.152948
1	-2.341675	1.422533	-1.959586
1	-1.809974	2.130508	2.216740
6	3.674062	-1.402475	1.569263
6	3.369507	-1.928803	-1.501049
6	4.888283	-2.161884	-1.538857
1	5.133472	-2.722659	-2.450510
1	5.459895	-1.231419	-1.575753
1	5.242204	-2.754092	-0.692059
6	2.665794	-3.301726	-1.538487
1	2.923369	-3.925688	-0.679707
1	1.578358	-3.181893	-1.543574
1	2.970571	-3.837325	-2.447841
6	2.939389	-0.749063	2.751287
1	1.895069	-1.069456	2.790235
1	3.432129	-1.034435	3.690245
1	2.961317	0.341102	2.681411
6	3.611273	-2.928845	1.761901
1	2.579744	-3.290530	1.694248
1	4.216818	-3.468542	1.029089
1	3.999669	-3.180448	2.757350
6	0.240291	1.303448	-2.703682
1	1.308731	1.092392	-2.623197
6	0.870716	2.238507	2.288608
1	1.887631	1.913703	2.054869
6	-3.773668	1.838279	0.275073
1	-4.183699	1.000422	-0.302894
6	0.089670	2.593464	-3.528876
1	0.495755	2.458154	-4.538590
1	-0.965323	2.876966	-3.621664
1	0.621031	3.426053	-3.056409

6	-0.415534	0.113355	-3.422631
1	0.079201	-0.072453	-4.383077
1	-0.346714	-0.795083	-2.815103
1	-1.475164	0.300363	-3.630641
6	-4.297033	3.139970	-0.362003
1	-3.979170	3.230962	-1.405918
1	-5.392594	3.170444	-0.334735
1	-3.915983	4.013561	0.180878
6	-4.293540	1.701445	1.709233
1	-3.895189	0.804116	2.191612
1	-4.023402	2.571687	2.320064
1	-5.385686	1.625152	1.703058
6	0.427903	1.513325	3.568164
1	1.170135	1.656710	4.361739
1	-0.527458	1.898422	3.941850
1	0.317024	0.439646	3.394318
6	0.920180	3.759783	2.523058
1	-0.083352	4.152805	2.724133
1	1.558657	3.998950	3.382136
1	1.317783	4.282156	1.647514
6	5.136143	-0.931233	1.619517
1	5.745112	-1.320061	0.801496
1	5.206137	0.159495	1.616879
1	5.585219	-1.284836	2.557030
6	2.957326	-1.162521	-2.768322
1	3.440805	-0.184215	-2.837775
1	3.243643	-1.746978	-3.652256
1	1.876194	-1.018021	-2.801410
6	-1.710036	-1.784251	-0.121387
6	-1.329934	-1.881136	1.674010
1	-1.736688	-0.857862	-0.695714
1	-1.526532	-2.697192	-0.692086
1	-1.098832	-1.011987	2.291378
1	-0.938430	-2.835127	2.029978
6	-2.628260	-1.884374	1.006864
6	-3.925470	-1.789752	1.304789
6	-5.021547	-1.580724	0.354980
6	-4.842346	-1.614419	-1.041966
6	-6.304284	-1.284069	0.848297
6	-5.902880	-1.345725	-1.902569
1	-3.866628	-1.851649	-1.450640
6	-7.364855	-1.013466	-0.013763
1	-6.460175	-1.254563	1.923847

6	-7.168777	-1.039549	-1.395306
1	-5.741406	-1.375708	-2.976850
1	-8.344894	-0.780875	0.393849
1	-7.992805	-0.827244	-2.070383
1	-4.208310	-1.812071	2.357063

TS2A

SCF Energy: -3065.26346594

Sum of electronic and zero-point Energies= -3064.389118

Sum of electronic and thermal Energies= -3064.334896

Sum of electronic and thermal Enthalpies= -3064.333952

Sum of electronic and thermal Free Energies= -3064.477589

Electronic energy in solution by single point calculation = -3063.84287831

6	-2.429800	-3.042670	0.669684
6	-1.768812	-1.821190	0.845148
6	-2.555667	-0.665568	0.849498
6	-3.939549	-0.656547	0.698548
6	-4.566509	-1.895498	0.543600
6	-3.817279	-3.073300	0.529991
6	-4.634485	0.708033	0.719469
6	-3.718579	1.697849	-0.012561
6	-2.342092	1.567029	0.185640
6	-1.381720	2.421355	-0.370716
6	-1.856879	3.493581	-1.137434
6	-3.225019	3.649154	-1.367299
6	-4.147741	2.756000	-0.818712
1	-1.859887	-3.962220	0.612880
1	-5.641222	-1.947790	0.410225
1	-4.319262	-4.025098	0.385609
1	-1.156698	4.200464	-1.565648
1	-3.575105	4.477918	-1.975373
1	-5.205356	2.896330	-1.013385
8	-1.875060	0.533705	0.966539
15	0.404271	2.017036	-0.086245
15	0.042030	-1.545919	0.838644
6	1.274286	3.365707	-0.981652
6	2.173114	4.224059	-0.335811
6	1.100181	3.487315	-2.371539
6	2.881654	5.182148	-1.063586
1	2.322499	4.143866	0.734970
6	1.796521	4.455016	-3.092549
1	0.410719	2.826762	-2.887100
6	2.694728	5.303125	-2.440254

1	3.577703	5.837897	-0.548038
1	1.644756	4.539248	-4.164975
1	3.245295	6.051286	-3.003341
6	0.623541	2.475229	1.672709
6	1.784544	2.042207	2.326178
6	-0.299469	3.277981	2.357365
6	2.025415	2.429403	3.644065
1	2.497966	1.404845	1.814141
6	-0.062184	3.643807	3.681409
1	-1.199129	3.620141	1.856752
6	1.103700	3.224766	4.325028
1	2.926467	2.085677	4.141492
1	-0.785058	4.261662	4.207439
1	1.288824	3.512025	5.356526
6	0.837517	-3.196307	0.842953
6	1.975103	-3.384929	0.048209
6	0.438582	-4.210527	1.729407
6	2.679093	-4.590233	0.110402
1	2.335853	-2.596171	-0.606365
6	1.135535	-5.415364	1.777121
1	-0.401563	-4.047359	2.397580
6	2.255865	-5.609076	0.962393
1	3.558273	-4.721230	-0.514089
1	0.815862	-6.197520	2.460199
1	2.801985	-6.547474	1.006028
6	0.439358	-1.046340	2.569915
6	1.768764	-1.204822	2.991022
6	-0.508259	-0.558495	3.476690
6	2.135781	-0.897603	4.298202
1	2.521055	-1.560033	2.296719
6	-0.133766	-0.241358	4.782716
1	-1.541356	-0.434744	3.178173
6	1.185090	-0.416521	5.199725
1	3.169641	-1.025643	4.605859
1	-0.879329	0.139907	5.474860
1	1.471830	-0.172320	6.218865
46	0.670157	-0.177686	-0.967391
6	-4.755585	1.174180	2.195678
1	-5.228682	2.161303	2.243072
1	-5.363578	0.464396	2.767268
1	-3.771113	1.243532	2.667489
6	-6.035243	0.645255	0.099825
1	-6.672132	-0.042257	0.664222

1	-6.519025	1.625753	0.134384
1	-6.000486	0.308013	-0.940522
6	1.810052	0.240119	-2.797317
6	0.547403	-0.174995	-3.220675
6	0.024101	-1.439973	-2.748356
1	2.049245	1.266457	-3.089285
1	-0.148155	0.489951	-3.745688
6	0.849902	-2.696698	-2.929009
1	1.915959	-2.485373	-2.883960
1	0.615876	-3.457392	-2.180534
1	0.631322	-3.126698	-3.918355
6	-1.453656	-1.601625	-2.767599
6	-2.306025	-0.484804	-2.642575
6	-2.058365	-2.859891	-2.941347
6	-3.686714	-0.614194	-2.737323
1	-1.881819	0.493177	-2.446847
6	-3.443657	-2.991047	-3.023602
1	-1.440607	-3.745775	-3.030487
6	-4.266816	-1.869272	-2.932757
1	-4.308376	0.270970	-2.642274
1	-3.879650	-3.976705	-3.163487
1	-5.346347	-1.972094	-3.000443
6	4.779483	-0.876421	-1.399524
6	5.849095	-1.957230	-1.163647
1	6.733196	-1.553757	-0.657947
1	5.430994	-2.767260	-0.558829
1	6.142471	-2.363016	-2.136602
6	5.348445	0.289278	-2.235581
1	5.627916	-0.102593	-3.218658
1	4.590788	1.065253	-2.372107
1	6.230098	0.735075	-1.761603
8	3.679157	-1.469095	-2.006584
6	4.392916	-0.333045	-0.054285
7	4.086185	0.062417	0.994142
1	2.914138	-0.700723	-2.314721

TS2B

SCF Energy: -3696.02980738

Sum of electronic and zero-point Energies= -3694.942846

Sum of electronic and thermal Energies= -3694.873931

Sum of electronic and thermal Enthalpies= -3694.872987

Sum of electronic and thermal Free Energies= -3695.051300

Electronic energy in solution by single point calculation = -3694.40084378

6	0.667591	4.417015	1.135772
6	1.209468	3.158639	0.838847
6	2.290627	3.123495	-0.052102
6	2.827675	4.255339	-0.670384
6	2.249539	5.488873	-0.357225
6	1.185996	5.568365	0.544246
6	4.033677	4.055757	-1.595120
6	3.838407	2.728990	-2.336209
6	3.260134	1.675555	-1.626444
6	3.085838	0.386538	-2.144786
6	3.537394	0.151883	-3.449003
6	4.109037	1.185204	-4.192387
6	4.254520	2.461958	-3.644600
1	-0.177192	4.488506	1.811380
1	2.627147	6.396617	-0.814684
1	0.752359	6.535797	0.779868
1	3.423286	-0.835331	-3.883546
1	4.447080	0.994937	-5.206803
1	4.702491	3.248140	-4.242302
8	2.827127	1.882621	-0.332554
15	2.165420	-0.830511	-1.117605
15	0.430306	1.568599	1.346997
6	2.128985	-2.326262	-2.193189
6	3.082954	-3.350638	-2.127749
6	1.053614	-2.451875	-3.085612
6	2.954437	-4.486138	-2.929074
1	3.917375	-3.268034	-1.439907
6	0.935443	-3.579041	-3.898577
1	0.300145	-1.668484	-3.112951
6	1.881235	-4.604300	-3.814409
1	3.694560	-5.278996	-2.860944
1	0.095232	-3.665347	-4.582087
1	1.780597	-5.491064	-4.434185
6	3.414121	-1.316993	0.146842
6	3.045889	-2.293514	1.085768
6	4.699448	-0.765296	0.215442
6	3.942738	-2.711673	2.065134
1	2.066487	-2.753437	1.037542
6	5.595850	-1.181221	1.201505
1	5.008574	-0.019458	-0.508940
6	5.221723	-2.155077	2.127465
1	3.633766	-3.472331	2.775199
1	6.590999	-0.745581	1.240034

1	5.921281	-2.477122	2.894047
6	-1.046305	2.110048	2.301175
6	-2.302686	1.950522	1.704853
6	-0.969929	2.648716	3.596235
6	-3.468062	2.315310	2.382336
1	-2.362204	1.537593	0.705610
6	-2.131662	3.015629	4.274152
1	-0.002013	2.769214	4.073531
6	-3.381827	2.846469	3.669387
1	-4.422509	2.174371	1.885775
1	-2.062977	3.431004	5.276128
1	-4.284762	3.128991	4.204423
6	1.502465	0.902850	2.685306
6	0.939183	-0.004360	3.600673
6	2.882200	1.142454	2.741123
6	1.734890	-0.648614	4.546303
1	-0.129823	-0.194382	3.582258
6	3.674409	0.497898	3.689574
1	3.343246	1.824791	2.038084
6	3.107275	-0.400850	4.593121
1	1.280110	-1.343444	5.247546
1	4.742902	0.689133	3.711000
1	3.730716	-0.907482	5.324268
46	0.065079	0.135329	-0.519312
6	5.303533	3.925705	-0.710884
1	6.185144	3.751496	-1.337797
1	5.457860	4.842625	-0.131331
1	5.209338	3.089232	-0.011843
6	4.216797	5.232192	-2.561869
1	4.386129	6.162192	-2.011385
1	5.094657	5.077130	-3.195835
1	3.341207	5.363225	-3.205736
1	-3.169540	-1.253257	0.837117
6	-1.694783	0.148275	-1.411722
7	-2.862582	0.099512	-1.620352
13	-4.558196	0.004025	-0.886139
8	-5.628490	-1.121976	-1.643813
8	-4.101507	-0.892194	0.713341
8	-5.162965	1.533106	-0.355695
6	-6.503097	-0.939503	-2.739280
6	-5.021192	-1.647343	1.580316
6	-5.356945	2.759432	-1.036156
6	-5.180739	-3.057347	1.032336

1	-4.214562	-3.569246	0.988392
1	-5.849613	-3.635506	1.679775
1	-5.603668	-3.009033	0.025170
6	-6.323492	-0.870942	1.673203
1	-6.141737	0.163308	1.975595
1	-6.837002	-0.870641	0.707944
1	-6.973864	-1.350066	2.412544
6	-7.794972	-0.255096	-2.284268
1	-7.577384	0.746859	-1.896288
1	-8.509318	-0.160990	-3.111037
1	-8.268203	-0.833454	-1.483427
6	-5.822093	-0.169171	-3.873595
1	-5.591365	0.858199	-3.558911
1	-4.883731	-0.656883	-4.156356
1	-6.466490	-0.107903	-4.758581
6	-4.022130	3.467892	-1.280355
1	-3.531692	3.686879	-0.325660
1	-3.348288	2.836812	-1.867943
1	-4.172962	4.411165	-1.819104
6	-6.314840	3.619682	-0.213212
1	-5.869153	3.852054	0.761147
1	-6.537855	4.563474	-0.724347
1	-7.254191	3.083529	-0.041464
1	-4.527324	-1.660275	2.557223
1	-6.758044	-1.941887	-3.115147
1	-5.831884	2.570190	-2.014825
6	-0.564190	-1.730303	1.118321
6	-1.711020	-2.189014	1.616313
6	-1.016532	-3.054276	0.558916
1	0.374841	-1.330080	1.472008
1	-2.143376	-2.281356	2.608492
6	-0.101647	-4.172564	0.981672
6	0.530657	-4.987716	0.027876
6	0.248717	-4.341783	2.331318
6	1.490201	-5.923211	0.410647
1	0.303512	-4.869077	-1.025019
6	1.195001	-5.290567	2.716854
1	-0.211520	-3.708933	3.083786
6	1.827029	-6.082013	1.755950
1	1.983469	-6.520742	-0.350792
1	1.444214	-5.405343	3.768598
1	2.576066	-6.810938	2.052120
6	-1.654346	-3.204435	-0.811005

1	-0.911109	-3.183952	-1.611527
1	-2.197536	-4.155877	-0.871692
1	-2.357376	-2.396636	-1.003275

TS2

SCF Energy: -2275.41601990

Sum of electronic and zero-point Energies= -2274.464619

Sum of electronic and thermal Energies= -2274.411198

Sum of electronic and thermal Enthalpies= -2274.410254

Sum of electronic and thermal Free Energies= -2274.549302

Electronic energy in solution by single point calculation = -2274.24376542

46	0.094925	0.102449	-0.631726
15	1.014165	2.143030	0.058489
6	2.685721	1.675372	0.682069
6	3.113066	0.333084	0.554581
6	3.555450	2.612288	1.266835
6	4.418594	0.004121	0.957942
6	2.263696	-0.838867	0.111401
6	4.837666	2.262151	1.679565
1	3.225854	3.634295	1.401709
6	5.278813	0.950738	1.506273
1	4.744299	-1.026538	0.858221
6	1.551544	-1.571580	1.113301
6	2.531895	-1.482293	-1.137154
1	5.486380	3.008540	2.128426
1	6.279288	0.660518	1.813519
6	1.102062	-2.868369	0.828434
6	2.104365	-2.794519	-1.341875
6	1.400768	-3.514812	-0.370258
1	0.547135	-3.407539	1.589479
1	2.348231	-3.272984	-2.283928
6	1.367053	3.368922	-1.369094
6	0.081541	3.034488	1.465907
6	0.459692	4.507169	1.692127
1	-0.129377	4.886376	2.536374
1	1.513883	4.636298	1.953064
1	0.234476	5.140523	0.831910
6	-1.424022	2.925640	1.144779
1	-1.683039	3.362257	0.176738
1	-1.759684	1.885108	1.170930
1	-1.986148	3.471901	1.913339
6	1.933986	2.532482	-2.527648
1	1.256963	1.726330	-2.814473

1	2.090113	3.180737	-3.399204
1	2.899132	2.092894	-2.264121
6	0.045417	4.007194	-1.833569
1	-0.705638	3.254055	-2.076635
1	-0.377917	4.686900	-1.090914
1	0.237571	4.592505	-2.741468
6	1.488813	-1.081952	2.551360
1	1.733698	-0.019342	2.556187
6	3.358043	-0.802335	-2.218063
1	3.516778	0.232920	-1.908238
6	0.975209	-4.964314	-0.559212
1	1.161849	-5.464588	0.401440
6	2.567646	-1.798655	3.387801
1	2.551110	-1.426960	4.418838
1	2.383632	-2.878527	3.412966
1	3.570816	-1.632872	2.982761
6	0.107451	-1.256133	3.186426
1	0.098155	-0.781779	4.175235
1	-0.678624	-0.808355	2.570932
1	-0.147031	-2.310979	3.326511
6	1.780837	-5.707148	-1.631619
1	2.860357	-5.621710	-1.463389
1	1.518352	-6.770263	-1.626666
1	1.561216	-5.323958	-2.635541
6	-0.536448	-5.079337	-0.836361
1	-1.129346	-4.600704	-0.050806
1	-0.786553	-4.615948	-1.798219
1	-0.829252	-6.134627	-0.886704
6	2.631508	-0.785193	-3.572643
1	3.192054	-0.186836	-4.299833
1	2.528578	-1.795777	-3.983403
1	1.629078	-0.359531	-3.475076
6	4.744243	-1.457058	-2.357338
1	4.654152	-2.511344	-2.641967
1	5.332268	-0.947361	-3.129443
1	5.303328	-1.408703	-1.417923
6	2.391363	4.475514	-1.062520
1	2.099731	5.117276	-0.230368
1	3.380140	4.060863	-0.852882
1	2.485336	5.113302	-1.950708
6	0.329822	2.258950	2.768893
1	1.382745	2.265432	3.066390
1	-0.252254	2.728720	3.571336

1	-0.015363	1.229618	2.681634
6	-1.456562	0.752233	-1.937700
6	-0.955681	-1.511884	-1.622050
1	-2.037433	1.638177	-1.704120
1	-0.898397	0.813065	-2.872471
1	-1.094160	-2.453891	-1.103515
1	-0.312203	-1.547061	-2.499186
6	-1.997089	-0.535591	-1.569729
6	-3.231157	-0.733314	-0.854973
6	-4.387820	0.160281	-1.178884
6	-5.454001	-0.303460	-1.965899
6	-4.467583	1.468449	-0.673184
6	-6.547510	0.512227	-2.256348
1	-5.417748	-1.318660	-2.354417
6	-5.552060	2.292888	-0.974544
1	-3.690450	1.819338	-0.003751
6	-6.597786	1.819890	-1.768958
1	-7.359788	0.127578	-2.868069
1	-5.589793	3.301342	-0.569488
1	-7.447259	2.458103	-1.996641
1	-3.506292	-1.791558	-0.853903
6	-3.443725	-1.102045	2.412636
6	-3.316894	-0.780630	3.915042
1	-3.864693	-1.502348	4.531790
1	-2.271233	-0.771443	4.225767
1	-3.736313	0.217418	4.078138
6	-4.944246	-1.129276	2.034368
1	-5.341589	-0.117840	2.163908
1	-5.091512	-1.417727	0.992311
1	-5.505665	-1.821975	2.671827
8	-2.715354	-0.189293	1.663048
1	-2.934747	-0.471851	0.413143
6	-2.875022	-2.476699	2.163022
7	-2.370763	-3.490897	1.898787

TS3A

SCF Energy: -3065.27123525

Sum of electronic and zero-point Energies= -3064.394558

Sum of electronic and thermal Energies= -3064.338897

Sum of electronic and thermal Enthalpies= -3064.337953

Sum of electronic and thermal Free Energies= -3064.486135

Electronic energy in solution by single point calculation = -3063.84503972

6	-0.449704	-3.684921	0.739502

6	-0.184155	-2.311955	0.839783
6	-1.226335	-1.500712	1.301126
6	-2.490563	-1.972408	1.662935
6	-2.726402	-3.340227	1.507726
6	-1.714139	-4.187183	1.050667
6	-3.462425	-0.971528	2.294990
6	-3.283756	0.366742	1.576935
6	-1.989470	0.714048	1.191321
6	-1.650961	1.936420	0.602207
6	-2.669531	2.886739	0.461383
6	-3.978977	2.566581	0.822347
6	-4.287289	1.312518	1.355306
1	0.328694	-4.356558	0.398186
1	-3.698699	-3.752396	1.753092
1	-1.907909	-5.251006	0.949794
1	-2.443951	3.868698	0.064487
1	-4.766432	3.302638	0.691047
1	-5.314231	1.080491	1.612500
8	-0.948366	-0.155650	1.413056
15	0.097810	2.102758	0.075822
15	1.403131	-1.498020	0.349536
6	0.225041	3.751018	-0.724424
6	1.326620	4.574037	-0.446869
6	-0.693552	4.164255	-1.705904
6	1.500611	5.778499	-1.127917
1	2.053889	4.274082	0.297682
6	-0.522010	5.374339	-2.376190
1	-1.551822	3.549047	-1.947522
6	0.578006	6.184967	-2.091822
1	2.362757	6.398619	-0.900607
1	-1.248252	5.679472	-3.124307
1	0.714875	7.124621	-2.619094
6	0.955577	2.317346	1.681383
6	2.351996	2.238028	1.738735
6	0.229858	2.610078	2.847212
6	3.011323	2.468655	2.946416
1	2.931764	1.991131	0.855228
6	0.895915	2.816542	4.052894
1	-0.851392	2.679748	2.816536
6	2.289742	2.749148	4.104775
1	4.093824	2.402630	2.974360
1	0.324405	3.034138	4.951079
1	2.808054	2.910519	5.045955

6	2.310033	-2.911310	-0.406464
6	1.774026	-3.486581	-1.571789
6	3.524840	-3.401963	0.087252
6	2.431345	-4.530431	-2.216789
1	0.844433	-3.110228	-1.977819
6	4.193532	-4.435468	-0.573601
1	3.955812	-2.981414	0.987634
6	3.650237	-5.003982	-1.724844
1	1.998723	-4.962663	-3.114866
1	5.138438	-4.798060	-0.178569
1	4.170872	-5.808975	-2.235960
6	2.256758	-1.235610	1.950839
6	3.573101	-0.745004	1.920514
6	1.647782	-1.486717	3.186828
6	4.277847	-0.561692	3.108638
1	4.033428	-0.478349	0.974557
6	2.347184	-1.265179	4.373508
1	0.631800	-1.864270	3.226926
6	3.667846	-0.816630	4.337773
1	5.298667	-0.192056	3.068963
1	1.861111	-1.456736	5.326320
1	4.214524	-0.657187	5.263196
46	0.855090	0.415999	-1.256330
6	-3.026533	-0.769504	3.773948
1	-3.675828	-0.033091	4.260340
1	-3.098363	-1.716903	4.319348
1	-1.994177	-0.412460	3.837577
6	-4.914275	-1.458450	2.266863
1	-5.011953	-2.401834	2.812769
1	-5.567685	-0.737574	2.767902
1	-5.271432	-1.603399	1.245530
6	-0.549355	0.981970	-2.734647
6	-1.887814	0.585840	-2.308683
6	-2.415650	-0.669561	-2.304007
1	-0.450954	2.039657	-2.970457
1	-2.505437	1.382162	-1.903928
6	-1.595506	-1.873924	-2.691836
1	-0.634195	-1.593412	-3.121871
1	-1.385078	-2.490256	-1.807977
1	-2.129678	-2.509268	-3.408959
6	-3.810583	-0.916512	-1.884204
6	-4.776726	0.109470	-1.838852
6	-4.240288	-2.216898	-1.551914

6	-6.094622	-0.148364	-1.477608
1	-4.499008	1.121015	-2.112655
6	-5.563754	-2.478886	-1.201951
1	-3.529397	-3.034276	-1.553238
6	-6.502735	-1.447539	-1.163335
1	-6.812826	0.667123	-1.459777
1	-5.859347	-3.494978	-0.953899
1	-7.535779	-1.651274	-0.896279
6	2.822610	-0.422443	-3.283358
6	4.052191	-1.298015	-3.320413
1	4.965654	-0.701600	-3.299899
1	4.041740	-1.999977	-2.487574
1	4.026575	-1.872123	-4.258831
6	2.860198	0.856885	-4.090575
1	2.761195	0.576541	-5.151129
1	2.034951	1.514307	-3.818289
1	3.805235	1.384152	-3.957086
8	1.739789	-0.914241	-2.896164
6	3.548013	0.798908	-1.276108
7	4.387528	1.337745	-0.653992
1	-0.120650	0.368832	-3.525012

TS3B

SCF Energy: -3696.07788942

Sum of electronic and zero-point Energies= -3694.987168

Sum of electronic and thermal Energies= -3694.919442

Sum of electronic and thermal Enthalpies= -3694.918498

Sum of electronic and thermal Free Energies= -3695.093295

Electronic energy in solution by single point calculation = -3694.44736336

6	0.426410	0.903728	-3.879141
6	1.002820	0.696361	-2.616662
6	2.004681	-0.273143	-2.522916
6	2.401316	-1.086779	-3.589450
6	1.777952	-0.872137	-4.820215
6	0.814358	0.127632	-4.968282
6	3.522381	-2.101700	-3.340280
6	3.366488	-2.620101	-1.908519
6	2.945820	-1.712208	-0.938652
6	2.808855	-2.025243	0.414898
6	3.125962	-3.326637	0.818608
6	3.540019	-4.265652	-0.126932
6	3.655943	-3.918169	-1.474966
1	-0.349927	1.649607	-3.998176

1	2.045138	-1.481788	-5.676002
1	0.349089	0.288415	-5.935796
1	3.027420	-3.606128	1.861478
1	3.772468	-5.278256	0.187962
1	3.975832	-4.668680	-2.189158
8	2.610524	-0.421888	-1.294598
15	2.119738	-0.720478	1.497541
15	0.386216	1.547123	-1.099142
6	2.185129	-1.499611	3.153929
6	3.215222	-1.238340	4.066935
6	1.163625	-2.399215	3.501459
6	3.220666	-1.865034	5.314285
1	4.009252	-0.546791	3.805615
6	1.181882	-3.031533	4.743597
1	0.351770	-2.598537	2.810096
6	2.207481	-2.762722	5.653543
1	4.019378	-1.651815	6.019265
1	0.387482	-3.725852	5.001055
1	2.214440	-3.249256	6.624817
6	3.438558	0.549359	1.535222
6	3.085546	1.850436	1.917465
6	4.767787	0.271310	1.192545
6	4.046988	2.857137	1.967366
1	2.051456	2.072680	2.159408
6	5.727516	1.283369	1.231650
1	5.049389	-0.733278	0.892684
6	5.369094	2.575762	1.619673
1	3.756609	3.864010	2.247500
1	6.755645	1.061353	0.959342
1	6.116976	3.363262	1.644328
6	-1.215478	2.177673	-1.730473
6	-2.252519	1.235385	-1.854008
6	-1.419132	3.490220	-2.172366
6	-3.466068	1.606105	-2.431112
1	-2.122918	0.206057	-1.523623
6	-2.641794	3.856700	-2.736015
1	-0.625610	4.224193	-2.085918
6	-3.663051	2.915944	-2.873019
1	-4.252696	0.865271	-2.528804
1	-2.793135	4.879635	-3.068091
1	-4.611609	3.203756	-3.317967
6	1.471864	3.008370	-0.919464
6	1.054364	4.050640	-0.076642

6	2.741005	3.068747	-1.505890
6	1.883375	5.146570	0.151354
1	0.070511	4.016585	0.378977
6	3.575982	4.159335	-1.259848
1	3.079553	2.265230	-2.150865
6	3.149105	5.202820	-0.438171
1	1.538626	5.956026	0.789296
1	4.561802	4.192601	-1.714636
1	3.799107	6.053829	-0.255371
46	0.041860	0.233756	0.917038
6	4.880058	-1.354409	-3.435108
1	5.706617	-2.043936	-3.230905
1	5.011614	-0.933900	-4.438174
1	4.928292	-0.536616	-2.709633
6	3.501541	-3.241341	-4.366669
1	3.648045	-2.854171	-5.379003
1	4.318067	-3.944241	-4.178079
1	2.554977	-3.790334	-4.336848
1	-2.633779	0.545491	3.584822
6	-1.308852	-0.827139	1.776233
7	-1.902344	-1.850590	1.855327
13	-3.240270	-2.543119	0.628391
8	-3.232771	-4.241723	0.964346
8	-4.709016	-1.654905	0.948397
8	-2.587373	-2.057066	-0.944687
6	-3.959582	-5.320111	0.434372
6	-5.277726	-0.600839	0.216350
6	-1.690518	-2.830438	-1.714499
6	-6.397609	0.027381	1.048393
1	-6.014303	0.349372	2.022573
1	-6.839444	0.893664	0.539751
1	-7.186338	-0.712056	1.229111
6	-5.793087	-1.078974	-1.145635
1	-4.966934	-1.502450	-1.724327
1	-6.555084	-1.854762	-1.005982
1	-6.244440	-0.254542	-1.713952
6	-4.929148	-4.887867	-0.671846
1	-4.378273	-4.441083	-1.509337
1	-5.502615	-5.740924	-1.055391
1	-5.632436	-4.140395	-0.290639
6	-2.982791	-6.389166	-0.064683
1	-2.389018	-5.997867	-0.899912
1	-2.293268	-6.669376	0.738515

1	-3.510713	-7.289087	-0.404690
6	-0.298575	-2.852595	-1.078716
1	0.060949	-1.825369	-0.946811
1	-0.331511	-3.321011	-0.090114
1	0.423522	-3.399002	-1.697186
6	-1.643207	-2.273797	-3.138323
1	-1.237763	-1.256998	-3.143151
1	-1.008671	-2.892402	-3.784948
1	-2.651484	-2.241618	-3.565142
1	-4.521067	0.182085	0.022426
1	-4.558351	-5.765241	1.247474
1	-2.051067	-3.871263	-1.771259
6	-2.017141	0.873211	1.458049
6	-2.875987	1.089621	2.676564
6	-1.938252	2.191025	2.262840
1	-2.550436	0.910565	0.518084
1	-3.940953	1.198139	2.497455
6	-2.507116	3.409575	1.594484
6	-1.909975	4.669280	1.756761
6	-3.659277	3.332758	0.793305
6	-2.430531	5.804217	1.130625
1	-1.033180	4.776728	2.385756
6	-4.183143	4.463596	0.176298
1	-4.153734	2.380395	0.636290
6	-3.569863	5.708159	0.335722
1	-1.943555	6.765026	1.275376
1	-5.071093	4.367534	-0.441023
1	-3.978512	6.589244	-0.150678
6	-0.741154	2.412501	3.172578
1	0.099666	2.858720	2.631270
1	-1.005955	3.080921	4.001200
1	-0.398973	1.465304	3.596285

TS3

SCF Energy: -2275.41788656

Sum of electronic and zero-point Energies= -2274.466383

Sum of electronic and thermal Energies= -2274.411395

Sum of electronic and thermal Enthalpies= -2274.410451

Sum of electronic and thermal Free Energies= -2274.553912

Electronic energy in solution by single point calculation = -2274.23752015

46	0.553878	-0.767656	0.004418
15	-1.614061	-1.644698	-0.476317
6	-3.114076	-0.564361	-0.188166

6	-3.118696	0.765956	0.302274
6	-4.364591	-1.162799	-0.445831
6	-4.356531	1.367401	0.603675
6	-1.951425	1.701357	0.448890
6	-5.576929	-0.537040	-0.177226
1	-4.396216	-2.152817	-0.870046
6	-5.574525	0.736714	0.383570
1	-4.341277	2.377579	0.999363
6	-1.253803	1.818510	1.668874
6	-1.706581	2.627717	-0.594154
1	-6.509219	-1.048602	-0.397939
1	-6.504331	1.242922	0.626042
6	-0.282150	2.817074	1.799864
6	-0.723920	3.605719	-0.414353
6	0.010674	3.710420	0.768636
1	0.264340	2.904920	2.734301
1	-0.529853	4.307929	-1.219124
6	-1.737424	-2.160731	-2.327349
6	-1.951693	-3.155786	0.667257
6	-3.300872	-3.892015	0.549086
1	-3.242217	-4.776626	1.195972
1	-4.134163	-3.286415	0.911251
1	-3.529281	-4.245129	-0.456043
6	-0.821850	-4.168201	0.405215
1	-0.976083	-4.699291	-0.539590
1	0.170297	-3.712982	0.366233
1	-0.828949	-4.920009	1.205045
6	-2.118308	-0.894271	-3.115100
1	-1.488426	-0.042502	-2.856842
1	-1.994112	-1.089032	-4.187478
1	-3.158813	-0.605865	-2.940414
6	-0.352767	-2.662861	-2.774944
1	0.443158	-1.942250	-2.608277
1	-0.046748	-3.566964	-2.247964
1	-0.393545	-2.893627	-3.847451
6	-1.610338	0.948292	2.864183
1	-2.045781	0.025726	2.476123
6	-2.527243	2.634798	-1.882566
1	-3.030896	1.668534	-1.968579
6	1.077904	4.777907	0.939248
1	1.540838	4.620575	1.922630
6	-2.681796	1.641834	3.727919
1	-2.945538	1.012948	4.586451

1	-2.306410	2.598681	4.109869
1	-3.594813	1.838351	3.159175
6	-0.404894	0.563057	3.732362
1	-0.710972	-0.180917	4.476670
1	0.397824	0.128804	3.133616
1	-0.009948	1.425650	4.281933
6	0.458416	6.186322	0.933749
1	-0.309441	6.282138	1.708859
1	1.225611	6.948746	1.111618
1	-0.012300	6.403427	-0.032302
6	2.184860	4.658838	-0.122694
1	2.651320	3.668749	-0.102881
1	1.783495	4.818204	-1.130364
1	2.963765	5.410816	0.048277
6	-1.685189	2.832506	-3.154779
1	-2.319513	2.711895	-4.039888
1	-1.249981	3.836869	-3.201893
1	-0.866581	2.111758	-3.226152
6	-3.615139	3.724301	-1.816770
1	-3.159750	4.715202	-1.704437
1	-4.212626	3.726653	-2.735995
1	-4.291604	3.566513	-0.972920
6	-2.743263	-3.270049	-2.682762
1	-2.480025	-4.224149	-2.221574
1	-3.777678	-3.025490	-2.433431
1	-2.705623	-3.417884	-3.769401
6	-1.882921	-2.630129	2.113220
1	-2.713152	-1.946320	2.318004
1	-1.986050	-3.482805	2.797820
1	-0.938562	-2.137246	2.334336
6	0.766373	0.522356	-1.613538
6	2.267722	0.919939	0.202313
1	0.623242	0.120123	-2.612772
1	0.111663	1.348904	-1.362746
1	3.225456	0.816069	0.699024
1	1.491425	1.465971	0.728848
6	2.127863	0.582679	-1.128252
6	3.264154	0.073868	-1.991399
6	4.627362	0.191293	-1.351545
6	5.263261	-0.939518	-0.825159
6	5.256522	1.438635	-1.237180
6	6.501984	-0.819050	-0.190915
1	4.770478	-1.902789	-0.916214

6	6.492291	1.559551	-0.602310
1	4.770153	2.321518	-1.647593
6	7.118252	0.427696	-0.073880
1	6.987363	-1.705083	0.210193
1	6.967957	2.533576	-0.522794
1	8.082214	0.518359	0.419669
1	3.056333	-0.973812	-2.245307
6	2.094160	-2.478917	2.251630
6	3.508104	-1.995028	2.097267
1	4.155163	-2.795968	1.734500
1	3.566523	-1.152356	1.414867
1	3.866181	-1.688084	3.092322
6	1.911342	-3.873583	2.788409
1	2.620055	-4.086810	3.596692
1	0.885240	-4.031308	3.123736
1	2.130654	-4.554007	1.956993
8	1.111956	-1.756936	2.057330
1	3.232359	0.653746	-2.924713
6	2.291116	-3.047050	-0.506117
7	2.714523	-3.043814	-1.605473

TS4A

SCF Energy: -2872.10231274

Sum of electronic and zero-point Energies= -2871.312895

Sum of electronic and thermal Energies= -2871.263622

Sum of electronic and thermal Enthalpies= -2871.262678

Sum of electronic and thermal Free Energies= -2871.397076

Electronic energy in solution by single point calculation = -2870.77156872

6	-3.330583	1.079090	0.806862
6	-2.080032	0.443353	0.860006
6	-1.054814	1.127329	1.522083
6	-1.221352	2.356701	2.165461
6	-2.476716	2.960266	2.078245
6	-3.518103	2.328114	1.396788
6	-0.028607	2.897147	2.962541
6	1.225152	2.614485	2.133187
6	1.266949	1.400226	1.448202
6	2.335388	0.995461	0.641790
6	3.440120	1.852509	0.557824
6	3.437164	3.070233	1.241337
6	2.339074	3.450190	2.017466
1	-4.153484	0.597834	0.292445
1	-2.646578	3.927780	2.536112

1	-4.488053	2.811735	1.330013
1	4.291737	1.571970	-0.052121
1	4.297444	3.729103	1.168658
1	2.353388	4.406094	2.529544
8	0.195528	0.535677	1.525823
15	2.105369	-0.559678	-0.312573
15	-1.703128	-1.132964	-0.026198
6	3.683412	-0.665850	-1.252166
6	4.702734	-1.571235	-0.929609
6	3.849704	0.170241	-2.369096
6	5.860497	-1.637654	-1.707319
1	4.591624	-2.224970	-0.071547
6	5.011348	0.112993	-3.136039
1	3.068825	0.876421	-2.632792
6	6.019899	-0.796790	-2.808803
1	6.640510	-2.347979	-1.447500
1	5.125531	0.771147	-3.992826
1	6.921801	-0.850949	-3.411671
6	2.301696	-1.853372	0.968428
6	1.810524	-3.134509	0.684230
6	2.940060	-1.615840	2.192331
6	1.975423	-4.168481	1.603554
1	1.287632	-3.308560	-0.252116
6	3.086215	-2.648259	3.118894
1	3.322250	-0.625316	2.418886
6	2.608617	-3.926139	2.823411
1	1.583427	-5.154709	1.378604
1	3.575868	-2.454880	4.069533
1	2.720961	-4.729499	3.546119
6	-3.376061	-1.643116	-0.597584
6	-3.676417	-1.658668	-1.963118
6	-4.369667	-2.005944	0.328763
6	-4.954992	-2.018396	-2.398248
1	-2.904558	-1.427741	-2.684441
6	-5.643948	-2.358284	-0.106933
1	-4.139924	-2.010162	1.390017
6	-5.939569	-2.362844	-1.474289
1	-5.170829	-2.039005	-3.462594
1	-6.405766	-2.634008	0.617149
1	-6.932592	-2.644343	-1.813945
6	-1.439927	-2.382492	1.299406
6	-1.560052	-3.731227	0.924122
6	-1.111430	-2.072816	2.622938

6	-1.376036	-4.744737	1.860339
1	-1.813801	-3.983344	-0.101989
6	-0.910383	-3.092362	3.555321
1	-1.018969	-1.040416	2.935415
6	-1.047659	-4.427960	3.180861
1	-1.485458	-5.782683	1.557854
1	-0.650424	-2.837110	4.578841
1	-0.896450	-5.218175	3.910893
46	0.053413	-0.746220	-1.536326
6	0.074993	2.086905	4.283994
1	0.931760	2.434020	4.872213
1	-0.835839	2.217197	4.878503
1	0.207866	1.019700	4.084668
6	-0.182929	4.382247	3.306455
1	-1.067036	4.538054	3.932140
1	0.678437	4.734991	3.881839
1	-0.281926	4.992686	2.405787
6	0.341587	0.159361	-3.713363
6	0.229748	1.368971	-2.871944
6	-0.921826	2.024539	-2.543085
1	1.359556	-0.118846	-3.972619
1	1.169547	1.750785	-2.487540
6	-2.260635	1.554275	-3.059637
1	-2.176662	0.623533	-3.619554
1	-2.960773	1.377108	-2.235060
1	-2.717520	2.303744	-3.719416
6	-0.909150	3.234138	-1.693335
6	0.258658	3.712536	-1.062258
6	-2.089710	3.979407	-1.502774
6	0.254113	4.897188	-0.336159
1	1.186109	3.155287	-1.125819
6	-2.098410	5.156900	-0.758211
1	-3.017508	3.641159	-1.947376
6	-0.923261	5.634356	-0.181490
1	1.176805	5.236643	0.123509
1	-3.028754	5.705443	-0.637748
1	-0.922489	6.561991	0.384304
6	-0.539514	-1.495282	-3.301108
7	-0.944568	-2.361470	-3.988590
1	-0.286312	0.187425	-4.597880

TS4B

SCF Energy: -3502.13862834

Sum of electronic and zero-point Energies= -3501.131742

Sum of electronic and thermal Energies= -3501.067166

Sum of electronic and thermal Enthalpies= -3501.066222

Sum of electronic and thermal Free Energies= -3501.235830

Electronic energy in solution by single point calculation = -3500.67135723

6	-3.400809	1.060665	2.930995
6	-2.835485	0.425141	1.815665
6	-2.454277	-0.914393	1.958594
6	-2.527458	-1.610674	3.169873
6	-3.064503	-0.930811	4.265446
6	-3.517310	0.384995	4.143026
6	-2.062570	-3.069808	3.187917
6	-0.892752	-3.201600	2.208223
6	-0.938427	-2.445993	1.037056
6	0.008014	-2.539842	0.011140
6	1.056298	-3.451347	0.181677
6	1.148498	-4.203745	1.352450
6	0.185959	-4.080369	2.355625
1	-3.718723	2.094291	2.855513
1	-3.138148	-1.427998	5.226034
1	-3.947316	0.889203	5.002997
1	1.810217	-3.553734	-0.588630
1	1.979910	-4.888854	1.483577
1	0.278714	-4.678695	3.254839
8	-1.965044	-1.542031	0.839363
15	-0.177111	-1.399944	-1.415266
15	-2.410327	1.317213	0.266720
6	1.162545	-1.903921	-2.551967
6	0.901710	-2.422341	-3.828665
6	2.493164	-1.693238	-2.152812
6	1.957990	-2.723219	-4.690085
1	-0.120788	-2.591464	-4.149383
6	3.542959	-1.999783	-3.015696
1	2.737312	-1.291261	-1.178781
6	3.278557	-2.512873	-4.287509
1	1.745954	-3.125598	-5.677055
1	4.557357	-1.816911	-2.675788
1	4.096531	-2.747047	-4.963383
6	-1.710129	-1.995425	-2.222132
6	-2.420118	-1.103643	-3.035985
6	-2.193360	-3.299146	-2.047977
6	-3.593398	-1.508325	-3.670910
1	-2.057661	-0.086997	-3.154420

6	-3.373968	-3.698870	-2.673292
1	-1.647608	-3.997506	-1.421284
6	-4.075362	-2.804631	-3.485216
1	-4.140736	-0.803866	-4.287915
1	-3.745081	-4.709754	-2.528274
1	-4.996696	-3.116958	-3.968896
6	-2.493312	3.065517	0.846407
6	-1.467712	3.491246	1.713094
6	-3.458839	3.992003	0.433103
6	-1.413034	4.812897	2.152794
1	-0.717333	2.777927	2.043692
6	-3.393095	5.319155	0.865722
1	-4.259392	3.680358	-0.228505
6	-2.372987	5.733619	1.722373
1	-0.616001	5.124215	2.821714
1	-4.144720	6.028689	0.531636
1	-2.323948	6.766623	2.053452
6	-3.867407	1.145618	-0.823805
6	-3.845770	1.826034	-2.053139
6	-4.955399	0.324683	-0.512044
6	-4.916392	1.713820	-2.936723
1	-2.987085	2.441732	-2.311697
6	-6.013341	0.191252	-1.413342
1	-4.974698	-0.210210	0.432051
6	-6.001845	0.891686	-2.619311
1	-4.897848	2.255218	-3.878483
1	-6.850197	-0.456127	-1.167504
1	-6.830899	0.793211	-3.314253
46	-0.287321	0.855341	-0.749650
6	-3.226185	-3.952948	2.661466
1	-2.918042	-5.003759	2.630852
1	-4.099479	-3.860702	3.316817
1	-3.519479	-3.652068	1.651065
6	-1.679062	-3.529041	4.600750
1	-2.535157	-3.459616	5.277980
1	-1.370354	-4.578052	4.593567
1	-0.860204	-2.928168	5.009166
6	1.005682	3.358819	-1.197386
6	1.733705	3.414139	-2.517141
1	2.755920	3.049016	-2.420095
1	1.207859	2.826169	-3.273618
1	1.753054	4.463308	-2.846741
6	1.710451	3.946810	0.003571

1	1.791851	5.032711	-0.156284
1	1.144543	3.781383	0.923264
1	2.708449	3.528606	0.135055
8	-0.274100	3.822261	-1.387685
1	-0.722634	3.895553	-0.525040
6	1.597475	1.320757	-0.829577
7	2.704561	1.072042	-0.510013
13	4.126537	0.654554	0.696092
8	4.791610	-0.764984	-0.089176
8	5.099242	2.104413	0.729546
8	3.338554	0.405221	2.235207
6	5.616485	-1.784911	0.422260
6	5.705873	2.655416	-0.416122
6	2.228469	-0.429630	2.458635
6	6.985002	1.894316	-0.780437
1	6.751131	0.842088	-0.968699
1	7.463507	2.315741	-1.673844
1	7.696148	1.946272	0.052975
6	5.983128	4.137634	-0.159230
1	5.052902	4.661929	0.086770
1	6.664474	4.244646	0.692766
1	6.436545	4.619774	-1.034231
6	6.347687	-1.355548	1.698965
1	5.626321	-1.132675	2.493857
1	7.025440	-2.141754	2.054267
1	6.936074	-0.450538	1.512556
6	4.787389	-3.054259	0.647203
1	4.004283	-2.863227	1.389443
1	4.302732	-3.356636	-0.287506
1	5.410425	-3.885590	1.000631
6	0.975973	0.419877	2.704597
1	1.157052	1.111126	3.536964
1	0.738780	1.005683	1.809122
1	0.105479	-0.201877	2.943659
6	2.508860	-1.348373	3.650550
1	2.711022	-0.745529	4.543688
1	1.657974	-2.010573	3.851315
1	3.390118	-1.967914	3.454903
1	5.016783	2.586982	-1.281596
1	6.379354	-2.013655	-0.341699
1	2.029950	-1.068759	1.580338

TS4

SCF Energy: -2082.25013524

Sum of electronic and zero-point Energies= -2081.395094

Sum of electronic and thermal Energies= -2081.347034

Sum of electronic and thermal Enthalpies= -2081.346089

Sum of electronic and thermal Free Energies= -2081.475198

Electronic energy in solution by single point calculation = -2081.16405434

46	-0.076314	-0.640645	-0.276040
15	-2.284647	-1.306724	-0.087643
6	-3.264126	0.196621	0.362919
6	-2.608719	1.444172	0.518550
6	-4.662133	0.148800	0.507829
6	-3.384456	2.576198	0.825479
6	-1.128475	1.717769	0.363424
6	-5.412378	1.281878	0.809159
1	-5.176307	-0.794663	0.378445
6	-4.766599	2.506215	0.972714
1	-2.878751	3.530244	0.939463
6	-0.307626	1.847699	1.521743
6	-0.628556	2.191224	-0.879286
1	-6.491056	1.207436	0.912453
1	-5.333307	3.402798	1.206734
6	0.967211	2.399016	1.398129
6	0.661508	2.737111	-0.945618
6	1.482334	2.849417	0.176127
1	1.583898	2.496666	2.287164
1	1.015840	3.100639	-1.902669
6	-3.067654	-2.006166	-1.687796
6	-2.519566	-2.555775	1.337805
6	-3.958600	-2.724837	1.850935
1	-3.956810	-3.479539	2.647811
1	-4.343404	-1.796053	2.281380
1	-4.654671	-3.065522	1.082494
6	-1.940407	-3.914092	0.897742
1	-2.558667	-4.409432	0.145149
1	-0.921301	-3.817804	0.512409
1	-1.905292	-4.574812	1.773384
6	-3.383244	-0.826944	-2.621424
1	-2.485495	-0.249454	-2.841346
1	-3.764053	-1.219630	-3.572583
1	-4.139748	-0.155180	-2.205700
6	-1.984080	-2.869221	-2.368542
1	-1.077512	-2.286795	-2.554673
1	-1.694232	-3.734344	-1.769903

1	-2.370701	-3.234498	-3.328976
6	-0.814660	1.470409	2.904951
1	-1.722150	0.876452	2.772749
6	-1.499298	2.226622	-2.125848
1	-2.389844	1.629334	-1.923521
6	2.883191	3.446657	0.132289
1	2.938687	4.167803	0.961162
6	-1.203812	2.726243	3.706179
1	-1.574662	2.447665	4.699501
1	-0.338686	3.386048	3.839393
1	-1.988187	3.295489	3.197915
6	0.200071	0.621765	3.687883
1	-0.260266	0.225754	4.599957
1	0.558639	-0.219363	3.088576
1	1.069860	1.214903	3.991554
6	3.192733	4.203171	-1.164193
1	2.448387	4.979671	-1.372583
1	4.173729	4.684391	-1.091775
1	3.226185	3.520151	-2.021281
6	3.958475	2.370794	0.385981
1	3.770338	1.817490	1.311241
1	3.983713	1.648666	-0.435085
1	4.949814	2.831957	0.463723
6	-0.794218	1.622577	-3.349762
1	-1.488348	1.555868	-4.195246
1	0.054132	2.236548	-3.672196
1	-0.414916	0.619035	-3.129719
6	-1.971174	3.663159	-2.413231
1	-1.118846	4.326211	-2.601185
1	-2.620019	3.684742	-3.296594
1	-2.534496	4.068888	-1.566647
6	-4.348199	-2.838721	-1.513675
1	-4.190737	-3.733784	-0.909662
1	-5.166073	-2.261176	-1.073688
1	-4.685363	-3.170230	-2.504257
6	-1.663927	-2.040901	2.506456
1	-2.027454	-1.079516	2.876996
1	-1.717547	-2.759200	3.334477
1	-0.617801	-1.931947	2.212433
6	2.764392	0.127255	-2.653340
6	2.176844	-0.572998	-0.353536
1	3.346338	0.040413	-3.566805
1	2.009511	0.905934	-2.619439

1	2.755094	-0.802071	0.538443
1	1.799228	0.452903	-0.238664
6	2.958680	-0.702853	-1.618277
6	4.012725	-1.791553	-1.652945
6	4.990174	-1.645189	-0.503690
6	4.875145	-2.447664	0.637791
6	5.975857	-0.650878	-0.534653
6	5.731253	-2.259358	1.725179
1	4.096875	-3.205617	0.671398
6	6.833004	-0.462115	0.548933
1	6.062074	-0.015922	-1.413464
6	6.711961	-1.267071	1.684424
1	5.630276	-2.889543	2.604856
1	7.594505	0.312370	0.508505
1	7.378399	-1.121356	2.530243
1	3.513883	-2.763723	-1.581653
1	4.540736	-1.749854	-2.612148
6	1.174173	-2.148157	-0.254414
7	1.494250	-3.282366	-0.184345

TS5A

SCF Energy: -2678.13458569

Sum of electronic and zero-point Energies= -2677.428590

Sum of electronic and thermal Energies= -2677.383192

Sum of electronic and thermal Enthalpies= -2677.382248

Sum of electronic and thermal Free Energies= -2677.509317

Electronic energy in solution by single point calculation = -2676.96230161

6	-3.152234	2.271087	-1.240388
6	-2.006029	1.727751	-0.642363
6	-0.839725	2.501699	-0.676729
6	-0.758099	3.756885	-1.288388
6	-1.917775	4.253661	-1.887843
6	-3.105472	3.520125	-1.856898
6	0.577753	4.502275	-1.201067
6	1.691900	3.459171	-1.322782
6	1.484137	2.226925	-0.702781
6	2.430325	1.196696	-0.680048
6	3.659531	1.435666	-1.306877
6	3.898436	2.654832	-1.942248
6	2.924161	3.655387	-1.954745
1	-4.075612	1.704128	-1.241166
1	-1.901959	5.219236	-2.381007
1	-3.999530	3.923329	-2.323033

1	4.417455	0.660172	-1.309977
1	4.851474	2.827270	-2.433378
1	3.132159	4.593259	-2.457806
8	0.281356	1.973184	-0.071701
15	1.925641	-0.405824	0.057894
15	-1.933743	0.015664	0.042132
6	3.473088	-1.387799	-0.057984
6	4.448729	-1.391061	0.949237
6	3.675262	-2.155122	-1.216368
6	5.609274	-2.151100	0.800351
1	4.299596	-0.802365	1.848581
6	4.843095	-2.903708	-1.364649
1	2.915736	-2.177117	-1.991379
6	5.809986	-2.906055	-0.357117
1	6.357438	-2.151810	1.588516
1	4.989619	-3.493207	-2.265339
1	6.714620	-3.497182	-0.470780
6	1.813259	-0.009121	1.847832
6	1.113851	-0.901974	2.672024
6	2.385820	1.135828	2.416173
6	1.005730	-0.666885	4.040202
1	0.637842	-1.771985	2.228121
6	2.263961	1.379092	3.785160
1	2.926265	1.836769	1.787670
6	1.577979	0.477173	4.599367
1	0.449145	-1.359051	4.663556
1	2.707876	2.273136	4.214899
1	1.479323	0.669881	5.663964
6	-3.594627	-0.630619	-0.412400
6	-3.681099	-1.421445	-1.567691
6	-4.759936	-0.355416	0.317881
6	-4.912336	-1.924120	-1.989441
1	-2.774588	-1.652538	-2.122602
6	-5.989053	-0.864571	-0.101343
1	-4.702961	0.253713	1.214556
6	-6.067215	-1.648326	-1.255481
1	-4.964022	-2.540999	-2.881771
1	-6.886288	-0.649049	0.472442
1	-7.025188	-2.047032	-1.577390
6	-2.075201	0.251422	1.859421
6	-2.481442	-0.842303	2.641865
6	-1.707530	1.441304	2.497982
6	-2.543723	-0.736648	4.029333

1	-2.768785	-1.772257	2.159727
6	-1.755867	1.539350	3.888951
1	-1.383211	2.293874	1.912952
6	-2.179693	0.456418	4.658242
1	-2.875234	-1.586636	4.619795
1	-1.460519	2.467231	4.370291
1	-2.221209	0.537876	5.740723
46	-0.101979	-1.311488	-0.721842
6	0.678269	5.151064	0.206242
1	1.636922	5.670314	0.314904
1	-0.132466	5.874069	0.349246
1	0.608205	4.393782	0.992777
6	0.696152	5.598895	-2.266322
1	-0.091932	6.347107	-2.140398
1	1.649689	6.126353	-2.170789
1	0.626725	5.186512	-3.277995
6	-0.631175	-3.976806	-1.034138
6	-1.573026	-3.760524	0.134897
1	-1.074187	-3.255684	0.965599
1	-2.463122	-3.205319	-0.157018
1	-1.892068	-4.757514	0.483235
6	0.623895	-4.741099	-0.637365
1	0.319270	-5.668014	-0.128850
1	1.229491	-4.992224	-1.509193
1	1.234749	-4.145611	0.046246
8	-1.344493	-4.503110	-2.076389
1	-0.755290	-4.486812	-2.857104
6	0.386593	-2.593107	-2.140767
7	0.791809	-2.882103	-3.213912

TS5

SCF Energy: -1888.29844449

Sum of electronic and zero-point Energies= -1887.514467

Sum of electronic and thermal Energies= -1887.469723

Sum of electronic and thermal Enthalpies= -1887.468778

Sum of electronic and thermal Free Energies= -1887.589507

Electronic energy in solution by single point calculation = -1887.38226623

46	0.322848	-1.222880	0.333407
6	2.037408	-3.087329	-0.726171
6	1.741726	-2.404952	-2.044090
1	0.672686	-2.363710	-2.244397
1	2.158940	-1.396991	-2.071862
1	2.232337	-2.997301	-2.833757

6	1.242064	-4.343033	-0.425716
1	1.504431	-5.101079	-1.179624
1	1.484588	-4.734764	0.564373
1	0.170138	-4.141644	-0.465963
8	3.397665	-3.253094	-0.658002
1	3.624259	-3.506145	0.256941
6	1.912892	-2.112230	1.063299
7	2.615954	-2.408237	1.964768
15	-1.920177	-0.628638	-0.171528
6	-2.271516	1.184394	0.019416
6	-1.222319	2.128828	0.169572
6	-3.597494	1.653044	0.047361
6	-1.556171	3.482666	0.343762
6	0.242053	1.794000	0.194215
6	-3.907102	2.999530	0.217074
1	-4.411243	0.949088	-0.062732
6	-2.875498	3.924011	0.366783
1	-0.748751	4.195303	0.476374
6	0.833972	1.351663	1.404838
6	1.055196	2.027939	-0.938221
1	-4.945058	3.319255	0.235487
1	-3.093732	4.978834	0.506948
6	2.208818	1.078423	1.424795
6	2.424478	1.751951	-0.858184
6	3.018120	1.255920	0.303269
1	2.658954	0.702750	2.336855
1	3.045677	1.930859	-1.730363
6	-2.493474	-1.002403	-1.955222
6	-3.064949	-1.532116	1.080839
6	-4.539520	-1.722752	0.691251
1	-5.050087	-2.250926	1.506951
1	-5.070041	-0.779447	0.542072
1	-4.656466	-2.331128	-0.208611
6	-2.445551	-2.928078	1.310062
1	-2.462551	-3.542265	0.405618
1	-1.404541	-2.848121	1.639468
1	-3.020050	-3.454582	2.083624
6	-1.456683	-0.310821	-2.854833
1	-0.436888	-0.590128	-2.584686
1	-1.629541	-0.587628	-3.902824
1	-1.537255	0.775851	-2.778582
6	-2.414304	-2.522859	-2.175309
1	-1.454396	-2.927470	-1.839603

1	-3.209589	-3.058506	-1.649696
1	-2.520803	-2.742230	-3.245342
6	0.045814	1.339975	2.710208
1	-1.014626	1.259250	2.460190
6	0.505351	2.646557	-2.218139
1	-0.582684	2.530374	-2.210478
6	4.502580	0.944532	0.364078
1	4.695067	0.482893	1.340731
6	0.237379	2.687293	3.433435
1	-0.347008	2.713041	4.360953
1	1.292251	2.839784	3.689710
1	-0.082595	3.524889	2.805452
6	0.397389	0.175043	3.645236
1	-0.279473	0.173486	4.507760
1	0.321275	-0.788485	3.133007
1	1.419209	0.252952	4.030907
6	5.338424	2.233583	0.274579
1	5.061822	2.940279	1.064763
1	6.407741	2.011129	0.370047
1	5.184693	2.733279	-0.689615
6	4.923778	-0.065124	-0.715419
1	4.365682	-1.000903	-0.624725
1	4.756745	0.338009	-1.722021
1	5.992479	-0.294462	-0.626628
6	1.046018	1.982734	-3.495953
1	0.493593	2.343314	-4.371156
1	2.102110	2.225283	-3.657481
1	0.956081	0.894229	-3.457611
6	0.804910	4.157748	-2.257541
1	1.886470	4.334138	-2.230573
1	0.408997	4.607324	-3.176139
1	0.359969	4.678857	-1.405306
6	-3.880014	-0.487114	-2.372416
1	-4.694017	-0.915678	-1.786115
1	-3.939071	0.601993	-2.303856
1	-4.053749	-0.758660	-3.422041
6	-2.995035	-0.764877	2.412395
1	-3.434111	0.233821	2.340336
1	-3.547632	-1.325021	3.177359
1	-1.964046	-0.665400	2.757175

TS6A

SCF Energy: -2678.13620702

Sum of electronic and zero-point Energies= -2677.434036

Sum of electronic and thermal Energies= -2677.388674

Sum of electronic and thermal Enthalpies= -2677.387730

Sum of electronic and thermal Free Energies= -2677.514619

Electronic energy in solution by single point calculation = -2676.97190686

6	-3.943337	0.014315	-1.415143
6	-2.726257	0.266243	-0.765592
6	-2.227798	1.572704	-0.828452
6	-2.852234	2.612393	-1.523480
6	-4.054428	2.315777	-2.170793
6	-4.598758	1.031552	-2.107618
6	-2.189313	3.993983	-1.479048
6	-0.674036	3.773358	-1.517433
6	-0.170309	2.680631	-0.812257
6	1.189262	2.373101	-0.712495
6	2.093925	3.231229	-1.348875
6	1.625976	4.333552	-2.066177
6	0.257240	4.600203	-2.154257
1	-4.365258	-0.983371	-1.397110
1	-4.574511	3.086891	-2.728179
1	-5.536906	0.819553	-2.611609
1	3.157022	3.023342	-1.293309
1	2.333036	4.990172	-2.564236
1	-0.080415	5.460407	-2.721813
8	-1.040409	1.819245	-0.171887
15	1.628918	0.809855	0.140235
15	-1.686395	-1.061050	-0.015524
6	3.451482	0.740500	-0.029128
6	4.322579	1.484949	0.780327
6	3.977259	-0.117915	-1.007463
6	5.701581	1.375073	0.606295
1	3.920552	2.139857	1.547716
6	5.359134	-0.231914	-1.172036
1	3.307949	-0.721640	-1.615164
6	6.219889	0.515991	-0.367483
1	6.372758	1.952426	1.236530
1	5.750863	-0.928602	-1.906493
1	7.295480	0.422277	-0.489638
6	1.384206	1.222754	1.909847
6	1.424685	0.165657	2.829952
6	1.172052	2.526324	2.374549
6	1.279257	0.411726	4.192598
1	1.558800	-0.850584	2.470713

6	1.010858	2.768936	3.739809
1	1.135320	3.351466	1.670316
6	1.070070	1.714236	4.650801
1	1.306725	-0.415625	4.894759
1	0.844531	3.783993	4.090501
1	0.945374	1.903975	5.713263
6	-2.756831	-2.541956	-0.247345
6	-2.466774	-3.447411	-1.274307
6	-3.884833	-2.761926	0.558847
6	-3.288292	-4.553712	-1.496760
1	-1.588089	-3.281601	-1.890927
6	-4.701239	-3.870655	0.341003
1	-4.120141	-2.066127	1.358080
6	-4.404574	-4.768626	-0.687719
1	-3.050372	-5.249652	-2.296183
1	-5.568422	-4.034710	0.974623
1	-5.039839	-5.634079	-0.854023
6	-1.814071	-0.810917	1.800376
6	-1.407819	-1.872563	2.625239
6	-2.256057	0.378037	2.388752
6	-1.467540	-1.753840	4.010709
1	-1.057759	-2.797903	2.175431
6	-2.296026	0.501525	3.778737
1	-2.572507	1.207986	1.768540
6	-1.910628	-0.562936	4.591721
1	-1.162262	-2.587348	4.637400
1	-2.630578	1.433930	4.224084
1	-1.947184	-0.464256	5.672856
46	0.462005	-1.165155	-0.707468
6	-2.545431	4.659376	-0.122076
1	-2.062082	5.639445	-0.043791
1	-3.629595	4.793682	-0.038835
1	-2.208578	4.043551	0.717096
6	-2.667949	4.898806	-2.620778
1	-3.747107	5.065909	-2.555636
1	-2.192181	5.881744	-2.557055
1	-2.440937	4.465613	-3.600161
6	2.516207	-3.522743	-1.196435
6	2.677762	-3.254715	0.314390
1	3.230419	-4.061963	0.808608
1	3.207736	-2.313263	0.476248
1	1.678164	-3.179107	0.758683
6	1.813026	-4.872555	-1.435912

1	0.814740	-4.829387	-0.985422
1	1.706951	-5.050496	-2.509295
1	2.365434	-5.705375	-0.987554
8	1.852865	-2.482398	-1.876772
1	0.416132	-2.544535	-1.500742
6	3.879125	-3.570441	-1.796665
7	4.944395	-3.569287	-2.259354

TS6B

SCF Energy: -2872.07936979

Sum of electronic and zero-point Energies= -2871.289247

Sum of electronic and thermal Energies= -2871.240636

Sum of electronic and thermal Enthalpies= -2871.239692

Sum of electronic and thermal Free Energies= -2871.372315

Electronic energy in solution by single point calculation = -2870.74090255

6	0.225148	-4.026492	-0.934069
6	-0.209942	-2.780714	-0.458047
6	-1.585181	-2.614948	-0.269780
6	-2.538286	-3.592095	-0.575944
6	-2.065548	-4.808518	-1.073086
6	-0.695669	-5.027503	-1.237663
6	-4.007716	-3.266645	-0.286467
6	-4.217647	-1.781040	-0.593414
6	-3.180090	-0.908624	-0.267971
6	-3.243137	0.477460	-0.427400
6	-4.431168	1.016433	-0.934154
6	-5.488370	0.172926	-1.280419
6	-5.383257	-1.210467	-1.115971
1	1.283353	-4.202773	-1.086104
1	-2.764191	-5.597019	-1.330201
1	-0.345218	-5.984048	-1.613591
1	-4.517387	2.088815	-1.070491
1	-6.403804	0.596823	-1.682190
1	-6.219218	-1.843068	-1.393661
8	-1.996480	-1.405649	0.241749
15	-1.720976	1.430292	-0.048228
15	0.918541	-1.344704	-0.182582
6	-2.308290	3.161481	-0.207058
6	-2.851279	3.871783	0.873975
6	-2.230679	3.774764	-1.467030
6	-3.311251	5.176354	0.696219
1	-2.912644	3.407191	1.852362
6	-2.699819	5.077690	-1.639296

1	-1.778854	3.252070	-2.302840
6	-3.239020	5.780715	-0.560760
1	-3.726223	5.720334	1.540486
1	-2.628031	5.544111	-2.617604
1	-3.596271	6.797968	-0.696311
6	-1.553859	1.211114	1.768280
6	-0.308580	1.484615	2.349660
6	-2.611556	0.794847	2.587042
6	-0.127593	1.362823	3.725455
1	0.524267	1.772911	1.715788
6	-2.425156	0.657272	3.962978
1	-3.580504	0.577876	2.148324
6	-1.184474	0.944044	4.534536
1	0.846355	1.563419	4.158656
1	-3.250792	0.327772	4.588037
1	-1.038885	0.832822	5.605353
6	2.450921	-1.997020	-0.966529
6	2.554434	-1.869939	-2.361724
6	3.490911	-2.616400	-0.263627
6	3.680158	-2.339543	-3.036871
1	1.745661	-1.401181	-2.917520
6	4.617857	-3.085917	-0.940124
1	3.426110	-2.726083	0.812898
6	4.719522	-2.943379	-2.324729
1	3.747246	-2.228387	-4.115297
1	5.418490	-3.562554	-0.381259
1	5.601091	-3.303546	-2.847365
6	1.293508	-1.408154	1.610551
6	2.392383	-0.669233	2.078571
6	0.494741	-2.102233	2.525560
6	2.704579	-0.657707	3.435532
1	3.010569	-0.112443	1.383595
6	0.797184	-2.067814	3.887595
1	-0.361905	-2.669767	2.178846
6	1.906409	-1.356263	4.345011
1	3.569718	-0.095537	3.774353
1	0.165364	-2.603554	4.590385
1	2.143985	-1.340078	5.405119
46	0.311478	0.833609	-1.126405
6	-4.259586	-3.482538	1.230648
1	-5.295490	-3.228526	1.481103
1	-4.078273	-4.529013	1.499943
1	-3.597291	-2.851794	1.831221

6	-4.963425	-4.160301	-1.086163
1	-4.816929	-5.213080	-0.827458
1	-6.003748	-3.919349	-0.849085
1	-4.816486	-4.042700	-2.164575
1	2.765958	3.447997	-2.953605
6	0.529520	2.104424	-2.610060
7	0.203632	2.779420	-3.519816
6	2.240072	1.500308	-1.972596
6	3.175447	2.557369	-2.488200
6	2.993505	2.406809	-0.990995
1	2.641258	0.504977	-2.115252
1	4.099723	2.195933	-2.934218
6	4.066240	1.770476	-0.157234
6	4.312974	2.205843	1.155533
6	4.836296	0.696970	-0.638761
6	5.277184	1.590266	1.956017
1	3.744068	3.031540	1.566081
6	5.795553	0.079200	0.159440
1	4.676357	0.316664	-1.642369
6	6.020845	0.517832	1.465764
1	5.443087	1.953940	2.966917
1	6.358763	-0.757574	-0.241890
1	6.766450	0.032533	2.089015
6	2.209566	3.534217	-0.334730
1	1.707878	3.201774	0.580233
1	2.875049	4.367576	-0.078253
1	1.440035	3.909105	-1.011051

TS6

SCF Energy: -1988.77010553

Sum of electronic and zero-point Energies= -1987.924298

Sum of electronic and thermal Energies= -1987.878639

Sum of electronic and thermal Enthalpies= -1987.877695

Sum of electronic and thermal Free Energies= -1988.000606

Electronic energy in solution by single point calculation = -1987.72605525

46	-0.536080	-0.829148	-0.256384
15	-1.056069	1.460962	-0.053598
6	0.423674	2.547168	0.258572
6	1.744813	2.037617	0.323690
6	0.240831	3.927807	0.468180
6	2.801130	2.931942	0.582866
6	2.186869	0.604131	0.189821
6	1.297019	4.795533	0.725991

1	-0.756734	4.339437	0.426842
6	2.594798	4.292428	0.780767
1	3.806892	2.527207	0.639278
6	2.285295	-0.197069	1.350803
6	2.760541	0.149079	-1.019183
1	1.103670	5.852900	0.882760
1	3.437249	4.948083	0.981724
6	2.936771	-1.430712	1.273354
6	3.386832	-1.100280	-1.050352
6	3.490486	-1.907209	0.084954
1	3.032130	-2.035113	2.171480
1	3.824517	-1.443302	-1.983096
6	-1.756771	2.108977	-1.717586
6	-2.293634	1.871117	1.359481
6	-3.082751	3.186131	1.246672
1	-3.770003	3.249272	2.100308
1	-2.446033	4.072934	1.287816
1	-3.690163	3.236309	0.341036
6	-3.293348	0.699895	1.423414
1	-3.899030	0.605338	0.520717
1	-2.774991	-0.248385	1.571356
1	-3.975921	0.860374	2.268519
6	-0.836964	1.514310	-2.797137
1	-0.791487	0.422320	-2.719186
1	-1.219197	1.776174	-3.792607
1	0.178797	1.906583	-2.716566
6	-3.162202	1.522292	-1.920639
1	-3.175362	0.446545	-1.741231
1	-3.910817	1.982456	-1.271263
1	-3.475595	1.699068	-2.958097
6	1.788221	0.294518	2.701338
1	1.156316	1.166114	2.523472
6	2.774524	1.006604	-2.276127
1	2.081462	1.837844	-2.119357
6	4.216969	-3.240907	0.045304
1	4.149525	-3.676630	1.051224
6	2.969126	0.759111	3.572365
1	2.610802	1.141155	4.535694
1	3.659440	-0.069180	3.770949
1	3.532869	1.556837	3.077483
6	0.936128	-0.750828	3.436299
1	0.521594	-0.321003	4.355725
1	0.109134	-1.092073	2.806103

1	1.527697	-1.627012	3.725751
6	5.708315	-3.048910	-0.281162
1	6.182976	-2.366467	0.432021
1	6.239879	-4.007136	-0.248422
1	5.838985	-2.627578	-1.284799
6	3.561816	-4.229284	-0.933849
1	2.514548	-4.408393	-0.671773
1	3.589436	-3.844102	-1.959934
1	4.090754	-5.189495	-0.923353
6	2.311307	0.229203	-3.519128
1	2.177479	0.910579	-4.367161
1	3.048844	-0.523959	-3.818291
1	1.363431	-0.284007	-3.334673
6	4.168854	1.615991	-2.509746
1	4.921131	0.828233	-2.633500
1	4.173413	2.235450	-3.414559
1	4.473749	2.243263	-1.666432
6	-1.796515	3.631446	-1.917700
1	-2.417439	4.143221	-1.179147
1	-0.796214	4.071018	-1.894144
1	-2.225579	3.841776	-2.906243
6	-1.503919	1.880424	2.678438
1	-0.771045	2.691247	2.721471
1	-2.205093	2.012299	3.512393
1	-0.986238	0.931732	2.829557
6	0.062080	-3.436138	0.920092
6	0.155717	-2.875607	-0.503650
1	-0.098169	-4.509372	1.055623
1	0.860163	-3.049826	1.553001
1	-0.260143	-3.485719	-1.300745
1	1.107293	-2.397885	-0.758956
6	-1.115415	-2.581933	0.717372
6	-2.409458	-2.924365	0.934004
1	-2.578376	-3.632258	1.750984
6	-3.621411	-2.468156	0.260415
6	-4.852645	-2.507459	0.941480
6	-3.622385	-2.029637	-1.077255
6	-6.030764	-2.088459	0.328738
1	-4.872089	-2.856366	1.971361
6	-4.803751	-1.625697	-1.695142
1	-2.682953	-2.011066	-1.620663
6	-6.012788	-1.641383	-0.994939
1	-6.965585	-2.113629	0.882607

1	-4.781982	-1.296846	-2.731032
1	-6.931570	-1.322712	-1.479258

TS7B

SCF Energy: -3696.060339

Sum of electronic and zero-point Energies= -3694.971788

Sum of electronic and thermal Energies= -3694.903044

Sum of electronic and thermal Enthalpies= -3694.902100

Sum of electronic and thermal Free Energies= -3695.081346

Electronic energy in solution by single point calculation = -3694.41506164

6	-2.604334	3.644386	-2.201540
6	-2.402814	2.566385	-1.326257
6	-2.671221	2.787608	0.032730
6	-3.108679	4.017002	0.538621
6	-3.286478	5.064709	-0.367163
6	-3.042536	4.878011	-1.727699
6	-3.409773	4.105829	2.036024
6	-2.372946	3.249107	2.763990
6	-1.996201	2.045939	2.161598
6	-1.159825	1.108700	2.780914
6	-0.657931	1.421080	4.050523
6	-0.982780	2.632378	4.658392
6	-1.836293	3.535291	4.022531
1	-2.388542	3.524167	-3.256001
1	-3.617333	6.034839	-0.014376
1	-3.186037	5.701430	-2.420831
1	-0.001187	0.717955	4.550321
1	-0.576522	2.871261	5.636452
1	-2.089539	4.465256	4.518926
8	-2.479870	1.730906	0.904972
15	-0.718763	-0.430390	1.891189
15	-1.619537	0.986137	-1.863773
6	0.507283	-1.232722	2.988674
6	0.166640	-2.201480	3.943075
6	1.856271	-0.892607	2.802424
6	1.168420	-2.834225	4.682079
1	-0.873273	-2.471034	4.097312
6	2.854101	-1.523381	3.541805
1	2.144795	-0.154724	2.064099
6	2.510186	-2.501834	4.478053
1	0.898893	-3.590820	5.414171
1	3.885864	-1.255675	3.339635
1	3.285688	-3.008637	5.045983

6	-2.234266	-1.460741	2.043078
6	-2.182674	-2.794633	1.607859
6	-3.459470	-0.947429	2.487742
6	-3.325318	-3.588825	1.593405
1	-1.243149	-3.219809	1.282310
6	-4.605858	-1.745159	2.478606
1	-3.522831	0.072559	2.849013
6	-4.545509	-3.063462	2.025927
1	-3.257979	-4.613644	1.239512
1	-5.547527	-1.331881	2.830003
1	-5.440640	-3.678983	2.014809
6	-0.983170	1.381247	-3.537582
6	0.404591	1.543776	-3.668616
6	-1.798441	1.536674	-4.671014
6	0.966690	1.858335	-4.906971
1	1.041866	1.421179	-2.798354
6	-1.234459	1.843485	-5.908760
1	-2.873601	1.410560	-4.583908
6	0.148844	2.005132	-6.027811
1	2.042348	1.981105	-4.989457
1	-1.873726	1.957847	-6.779862
1	0.585964	2.243291	-6.993442
6	-2.995295	-0.192980	-2.150437
6	-2.968442	-1.089933	-3.231523
6	-3.945679	-0.392795	-1.134351
6	-3.880750	-2.145713	-3.302694
1	-2.232437	-0.967949	-4.019112
6	-4.848859	-1.449872	-1.206841
1	-3.951149	0.253370	-0.264101
6	-4.820828	-2.332688	-2.289675
1	-3.849592	-2.823200	-4.152249
1	-5.561335	-1.595976	-0.401665
1	-5.523111	-3.159746	-2.339662
46	-0.016927	-0.028912	-0.279214
6	-4.808160	3.477671	2.286634
1	-5.041299	3.488305	3.357102
1	-5.578815	4.043512	1.751787
1	-4.841028	2.441160	1.937534
6	-3.419061	5.554305	2.539962
1	-4.190657	6.136645	2.028383
1	-3.656254	5.588700	3.607128
1	-2.451953	6.042223	2.382169
1	1.763820	-1.489566	-1.682947

6	1.472983	1.371887	-0.018737
7	2.624146	1.605706	-0.013547
13	4.274072	0.597887	-0.033185
8	4.719549	0.295484	1.629252
8	3.719338	-0.894115	-0.799947
8	5.421805	1.571328	-0.918558
6	5.378483	1.167427	2.523682
6	4.512478	-2.015193	-1.137200
6	5.099735	2.547900	-1.881741
6	5.204714	-2.607872	0.094757
1	4.470298	-2.826023	0.876928
1	5.736577	-3.533129	-0.160507
1	5.922293	-1.894337	0.513517
6	5.515718	-1.672802	-2.242756
1	4.989402	-1.279398	-3.118683
1	6.213408	-0.900850	-1.900177
1	6.088188	-2.558259	-2.546336
6	6.874518	1.233070	2.203611
1	7.018537	1.652881	1.202265
1	7.413791	1.852924	2.931392
1	7.305612	0.225825	2.219138
6	4.742044	2.561555	2.530131
1	4.876795	3.043954	1.554746
1	3.667537	2.489411	2.729578
1	5.198702	3.201640	3.295308
6	4.534748	1.906830	-3.156299
1	5.278354	1.237696	-3.603981
1	3.645107	1.310665	-2.923514
1	4.261385	2.671486	-3.895578
6	6.352917	3.371241	-2.179138
1	7.136484	2.723259	-2.589607
1	6.146794	4.172066	-2.900114
1	6.733875	3.820214	-1.255918
1	3.825808	-2.781737	-1.537170
1	5.259616	0.740083	3.534079
1	4.328062	3.228265	-1.480231
6	-0.342244	-1.905008	-1.037643
6	0.724503	-1.614515	-1.982263
6	0.304368	-3.129907	-0.627372
1	-1.336310	-2.023292	-1.451950
1	0.504195	-1.592190	-3.047451
6	-0.344085	-4.419122	-0.919079
6	0.032849	-5.577485	-0.207062

6	-1.403459	-4.534268	-1.845765
6	-0.633790	-6.785933	-0.395011
1	0.835381	-5.526909	0.518923
6	-2.060378	-5.743285	-2.036331
1	-1.712357	-3.676905	-2.430622
6	-1.684230	-6.876345	-1.308820
1	-0.330540	-7.658516	0.176263
1	-2.871475	-5.801139	-2.756511
1	-2.202085	-7.819497	-1.456783
6	1.513479	-3.116994	0.261626
1	1.200025	-3.315290	1.295391
1	2.239136	-3.884733	-0.020720
1	2.010345	-2.145965	0.264897

TS7

SCF Energy: -1888.28660242

Sum of electronic and zero-point Energies= -1887.506334

Sum of electronic and thermal Energies= -1887.462027

Sum of electronic and thermal Enthalpies= -1887.461083

Sum of electronic and thermal Free Energies= -1887.579929

Electronic energy in solution by single point calculation = -1887.36091657

46	0.569796	-0.927170	0.617153
6	2.921778	-2.694441	-0.619052
6	3.204086	-4.144549	-1.049290
1	4.063642	-4.201256	-1.725730
1	3.397935	-4.763333	-0.169828
1	2.317646	-4.530297	-1.562066
6	2.653844	-1.802716	-1.845012
1	1.802209	-2.212004	-2.396012
1	2.404734	-0.786900	-1.520537
1	3.522512	-1.761071	-2.512021
8	1.842747	-2.736231	0.278581
1	2.030601	-1.393313	0.998974
15	-1.743209	-1.032599	-0.122199
6	-2.611380	0.604313	-0.108137
6	-1.872779	1.811409	0.029589
6	-4.009289	0.686710	-0.215447
6	-2.571143	3.027357	0.078442
6	-0.379170	1.841187	0.139089
6	-4.684547	1.904765	-0.171135
1	-4.587115	-0.221113	-0.334360
6	-3.959144	3.084325	-0.019452
1	-2.003380	3.943194	0.203875

6	0.224588	1.314682	1.338712
6	0.425969	2.341909	-0.885099
1	-5.767478	1.927844	-0.252475
1	-4.467317	4.043319	0.024739
6	1.632242	1.208597	1.384824
6	1.836418	2.282618	-0.749666
6	2.455697	1.698412	0.336000
1	2.111513	0.905249	2.309557
1	2.447005	2.689955	-1.547298
6	-1.847604	-1.562697	-1.945273
6	-2.751067	-2.223036	0.986651
6	-4.001238	-2.875976	0.375907
1	-4.466711	-3.520606	1.132899
1	-4.756414	-2.150368	0.063312
1	-3.757574	-3.508560	-0.480901
6	-1.767827	-3.344207	1.390479
1	-1.422853	-3.925264	0.531945
1	-0.879441	-2.939659	1.885633
1	-2.269647	-4.031521	2.084122
6	-0.942613	-0.563196	-2.686349
1	0.062006	-0.533446	-2.257704
1	-0.863527	-0.852128	-3.742400
1	-1.359305	0.446428	-2.645931
6	-1.241943	-2.972571	-2.064666
1	-0.282932	-3.044161	-1.541026
1	-1.908650	-3.741073	-1.662265
1	-1.075172	-3.207170	-3.124129
6	-0.586947	1.264114	2.633837
1	-1.610361	0.981747	2.376364
6	-0.143465	2.984793	-2.145067
1	-1.200157	2.708935	-2.220254
6	3.962721	1.625158	0.503075
1	4.180560	0.699592	1.048515
6	-0.642853	2.680190	3.239023
1	-1.248688	2.684671	4.152636
1	0.364328	3.030037	3.494365
1	-1.081733	3.394970	2.536203
6	-0.068177	0.259752	3.669980
1	-0.758077	0.209032	4.519906
1	0.029635	-0.742904	3.237914
1	0.912248	0.549191	4.064064
6	4.457503	2.806487	1.360466
1	3.948754	2.837132	2.330533

1	5.534873	2.725113	1.544274
1	4.266587	3.759182	0.851505
6	4.730023	1.556736	-0.821913
1	4.361065	0.742193	-1.452651
1	4.651850	2.493263	-1.387707
1	5.791444	1.374282	-0.626944
6	0.556263	2.520775	-3.435601
1	0.004189	2.882389	-4.310536
1	1.574035	2.919516	-3.507682
1	0.619621	1.431702	-3.496244
6	-0.066211	4.520890	-2.046339
1	0.976259	4.847393	-1.953650
1	-0.488553	4.988272	-2.943764
1	-0.609869	4.899707	-1.175846
6	-3.235508	-1.512227	-2.600606
1	-3.944917	-2.210103	-2.153540
1	-3.663148	-0.506643	-2.553825
1	-3.136890	-1.778553	-3.661244
6	-3.153161	-1.463640	2.263494
1	-3.869452	-0.662081	2.064953
1	-3.617310	-2.167703	2.965696
1	-2.282150	-1.030573	2.760190
6	4.131378	-2.155281	0.078898
7	5.037208	-1.703959	0.649931

TS8

SCF Energy: -2275.39253974

Sum of electronic and zero-point Energies= -2274.440485

Sum of electronic and thermal Energies= -2274.387091

Sum of electronic and thermal Enthalpies= -2274.386147

Sum of electronic and thermal Free Energies= -2274.525824

Electronic energy in solution by single point calculation = -2274.21799073

46	-0.368716	-0.526923	0.105735
15	1.463193	-1.760291	-0.524053
6	3.149149	-1.010590	-0.301560
6	3.395731	0.320163	0.123366
6	4.261725	-1.838276	-0.553624
6	4.727851	0.710527	0.356091
6	2.391716	1.426632	0.279968
6	5.572040	-1.419486	-0.348905
1	4.104960	-2.841826	-0.917010
6	5.808070	-0.135632	0.135281
1	4.902349	1.723720	0.702422

6	2.260172	2.367788	-0.768783
6	1.738889	1.652835	1.508841
1	6.394916	-2.096365	-0.558958
1	6.820006	0.210984	0.323432
6	1.443123	3.482819	-0.573516
6	0.904429	2.769671	1.642633
6	0.734636	3.695466	0.613146
1	1.345062	4.211090	-1.373906
1	0.392492	2.920732	2.584814
6	1.447245	-3.288260	0.641901
6	1.385131	-2.314226	-2.355590
6	2.173685	-3.582226	-2.724424
1	2.037171	-3.771991	-3.796607
1	3.247496	-3.478898	-2.554898
1	1.815868	-4.466392	-2.192303
6	-0.093846	-2.553622	-2.725884
1	-0.502533	-3.434827	-2.226897
1	-0.729761	-1.706507	-2.467000
1	-0.163391	-2.723369	-3.807788
6	1.300427	-2.734130	2.072174
1	0.400912	-2.125861	2.200091
1	1.231151	-3.579112	2.769675
1	2.174686	-2.143773	2.359214
6	0.194738	-4.114385	0.302541
1	-0.691985	-3.482999	0.225658
1	0.306734	-4.673437	-0.630335
1	0.020641	-4.842801	1.104071
6	3.016748	2.229314	-2.086475
1	3.367419	1.196823	-2.167590
6	2.036747	0.788923	2.725449
1	2.401823	-0.173853	2.360714
6	-0.177003	4.910951	0.722351
1	0.410891	5.776544	0.382436
6	4.256172	3.143622	-2.104374
1	4.796188	3.043066	-3.053372
1	3.961154	4.193248	-1.990971
1	4.947263	2.899048	-1.293133
6	2.142057	2.520745	-3.318262
1	2.683184	2.254996	-4.233373
1	1.205681	1.956520	-3.298273
1	1.885439	3.583347	-3.389085
6	-0.655490	5.205738	2.147830
1	0.183245	5.314515	2.844157

1	-1.233597	6.135638	2.165012
1	-1.308003	4.407948	2.522019
6	-1.382770	4.775903	-0.229627
1	-1.062878	4.595224	-1.260942
1	-2.022491	3.939490	0.070225
1	-1.987387	5.689992	-0.215295
6	0.824181	0.521913	3.626936
1	1.101827	-0.192237	4.411264
1	0.489330	1.435635	4.131679
1	-0.024181	0.104468	3.080082
6	3.176421	1.427695	3.543943
1	2.877421	2.417044	3.909448
1	3.421206	0.803933	4.411791
1	4.084325	1.549223	2.945232
6	2.671755	-4.218192	0.633575
1	2.901723	-4.629211	-0.351585
1	3.562077	-3.722018	1.025408
1	2.452966	-5.065391	1.295973
6	1.933618	-1.139826	-3.184814
1	3.010702	-1.016389	-3.043030
1	1.749506	-1.330671	-4.249193
1	1.450596	-0.197553	-2.924408
6	-2.122008	1.039062	0.468326
6	-0.693084	0.769656	-1.455970
1	-3.111334	1.196367	0.899760
1	-1.466710	1.858173	0.770599
1	-0.512784	0.414788	-2.469345
1	-0.071751	1.620935	-1.186993
6	-2.098433	0.829057	-1.015303
6	-3.103859	0.505236	-1.885684
6	-4.548667	0.424991	-1.709779
6	-5.227598	0.379181	-0.472486
6	-5.344124	0.371042	-2.877809
6	-6.617280	0.303359	-0.413033
1	-4.685709	0.367613	0.459876
6	-6.730493	0.295180	-2.817583
1	-4.849813	0.398171	-3.846354
6	-7.380667	0.264383	-1.580191
1	-7.095936	0.262266	0.561486
1	-7.307425	0.259125	-3.738191
1	-8.463965	0.201149	-1.529201
1	-2.782378	0.329034	-2.912463
6	-2.863751	-1.854341	2.161519

6	-3.330550	-2.408758	0.798390
1	-4.310179	-2.891254	0.882210
1	-3.400041	-1.616771	0.050627
1	-2.607119	-3.149954	0.450487
6	-2.624000	-3.000208	3.158432
1	-1.821702	-3.634315	2.768903
1	-2.312334	-2.595730	4.124904
1	-3.524167	-3.608883	3.296852
8	-1.692418	-1.079055	2.076934
1	-1.909060	-0.059514	1.342732
6	-3.958479	-0.984647	2.692726
7	-4.799076	-0.279136	3.073754

TS9

SCF Energy: -2712.31553376

Sum of electronic and zero-point Energies= -2711.230466

Sum of electronic and thermal Energies= -2711.167147

Sum of electronic and thermal Enthalpies= -2711.166203

Sum of electronic and thermal Free Energies= -2711.328738

Electronic energy in solution by single point calculation = -2711.10643905

46	0.991267	-0.839087	-0.154866
6	-1.180496	-2.884837	-0.377301
6	0.039612	-3.732905	-0.062934
1	0.878186	-3.497095	-0.719087
1	0.339274	-3.605013	0.978230
1	-0.250401	-4.784627	-0.205058
6	-1.575003	-2.861369	-1.849124
1	-1.773523	-3.896310	-2.159450
1	-2.483577	-2.275779	-1.999508
1	-0.771971	-2.451005	-2.466482
8	-2.162974	-3.218261	0.473976
1	-3.028675	-2.716319	0.250421
6	-0.974672	-1.024422	-0.092827
7	-1.941501	-0.342242	0.038515
13	-3.821588	-0.105087	0.224006
8	-4.443143	0.873146	-1.070673
8	-4.259806	-1.826908	-0.003120
8	-4.113337	0.530153	1.813690
6	-4.618202	0.435353	-2.401867
6	-5.462918	-2.473619	0.410243
6	-3.269382	0.319486	2.930287
6	-5.664609	-3.707508	-0.466906
1	-4.789918	-4.364864	-0.409710

1	-6.546063	-4.277524	-0.151550
1	-5.799341	-3.405723	-1.512304
6	-6.651933	-1.516648	0.345203
1	-6.493554	-0.658183	1.006970
1	-6.790489	-1.147422	-0.677232
1	-7.572300	-2.022953	0.659240
6	-5.814281	1.168720	-3.006718
1	-5.632040	2.249798	-2.997333
1	-5.997844	0.852996	-4.041030
1	-6.714389	0.973279	-2.414672
6	-3.338681	0.672321	-3.213565
1	-3.121669	1.745944	-3.268326
1	-2.485116	0.180844	-2.735355
1	-3.437459	0.288330	-4.236630
6	-3.270586	-1.151199	3.359864
1	-4.291164	-1.466129	3.609465
1	-2.898487	-1.796453	2.557805
1	-2.635777	-1.305764	4.241587
6	-3.725458	1.234323	4.066247
1	-4.752686	0.985725	4.357234
1	-3.078082	1.127666	4.945433
1	-3.709702	2.281018	3.745718
1	-5.336747	-2.798214	1.455119
1	-4.834178	-0.646927	-2.416995
1	-2.235711	0.591181	2.661919
15	3.359290	-1.084911	0.004363
6	3.981219	0.648502	0.104705
6	3.057481	1.719033	0.048604
6	5.355895	0.943257	0.165365
6	3.558415	3.034557	0.047196
6	1.544083	1.646815	-0.024054
6	5.830126	2.250978	0.168501
1	6.071451	0.132571	0.206208
6	4.921241	3.306731	0.105895
1	2.846941	3.852992	-0.005858
6	0.905175	1.774392	-1.298719
6	0.795426	1.985260	1.141359
1	6.898366	2.441977	0.214376
1	5.269455	4.335582	0.100459
6	-0.401870	2.249072	-1.365812
6	-0.509568	2.461092	1.010501
6	-1.119148	2.649223	-0.233642
1	-0.867514	2.354969	-2.340512

1	-1.052372	2.733841	1.907712
6	3.869311	-1.925989	1.644954
6	4.318358	-1.897374	-1.447590
6	5.752397	-2.366781	-1.152186
1	6.169702	-2.814536	-2.063419
1	6.411197	-1.541292	-0.871348
1	5.797891	-3.126041	-0.369360
6	3.477464	-3.104315	-1.911533
1	3.377099	-3.871243	-1.140080
1	2.473177	-2.785265	-2.206906
1	3.957456	-3.568289	-2.782813
6	2.888934	-1.398534	2.706431
1	1.848192	-1.571476	2.414627
1	3.071870	-1.911132	3.659587
1	3.019775	-0.328044	2.874147
6	3.647506	-3.444083	1.517832
1	2.640645	-3.673426	1.157932
1	4.369016	-3.925268	0.853683
1	3.758969	-3.902927	2.508238
6	1.662762	1.533306	-2.594497
1	2.660028	1.178582	-2.330824
6	1.419096	1.938125	2.528134
1	2.402432	1.470712	2.431922
6	-2.454648	3.356269	-0.409350
1	-3.104837	2.689005	-0.986075
6	1.847029	2.840745	-3.383868
1	2.439088	2.662630	-4.289336
1	0.882652	3.262379	-3.687693
1	2.366359	3.591074	-2.778178
6	0.985008	0.451775	-3.450561
1	1.558109	0.261419	-4.366115
1	0.905381	-0.485088	-2.884328
1	-0.028207	0.748173	-3.742445
6	-2.252757	4.653223	-1.219401
1	-1.784951	4.464738	-2.191400
1	-3.217946	5.140373	-1.398503
1	-1.613126	5.356903	-0.671759
6	-3.185345	3.663000	0.900433
1	-3.421724	2.748364	1.448901
1	-2.601792	4.334779	1.543813
1	-4.134959	4.161430	0.678750
6	0.580909	1.093544	3.501780
1	1.119654	0.949355	4.445719

1	-0.370396	1.582860	3.735177
1	0.351059	0.111855	3.077854
6	1.644689	3.352315	3.092199
1	0.695959	3.892300	3.185953
1	2.103989	3.300312	4.086479
1	2.303818	3.937012	2.442761
6	5.295596	-1.640496	2.140003
1	6.067339	-1.975801	1.444607
1	5.443644	-0.575009	2.333987
1	5.454022	-2.172456	3.087068
6	4.369416	-0.898106	-2.615626
1	4.930632	0.006347	-2.366837
1	4.860934	-1.377959	-3.471396
1	3.366963	-0.608697	-2.933364

TS

SCF Energy: -286.515865

Sum of electronic and zero-point Energies= -286.413255

Sum of electronic and thermal Energies= -286.405893

Sum of electronic and thermal Enthalpies= -286.404948

Sum of electronic and thermal Free Energies= -286.444168

Electronic energy in solution by single point calculation =-286.419561046

6	-0.658949	-0.003321	0.170382
6	-0.413835	-1.474725	0.188470
1	-0.453535	-1.884455	-0.821680
1	0.537324	-1.729634	0.649172
1	-1.250270	-1.904984	0.766031
6	-1.815866	0.539884	-0.585927
1	-2.154273	1.484126	-0.155467
1	-1.437978	0.734433	-1.597923
1	-2.632128	-0.183988	-0.661464
8	-0.116977	0.802582	1.016012
1	0.864527	0.532900	1.093204
6	1.531518	0.204331	-0.975823
7	2.229277	0.133419	-0.026083