

Supporting Information for

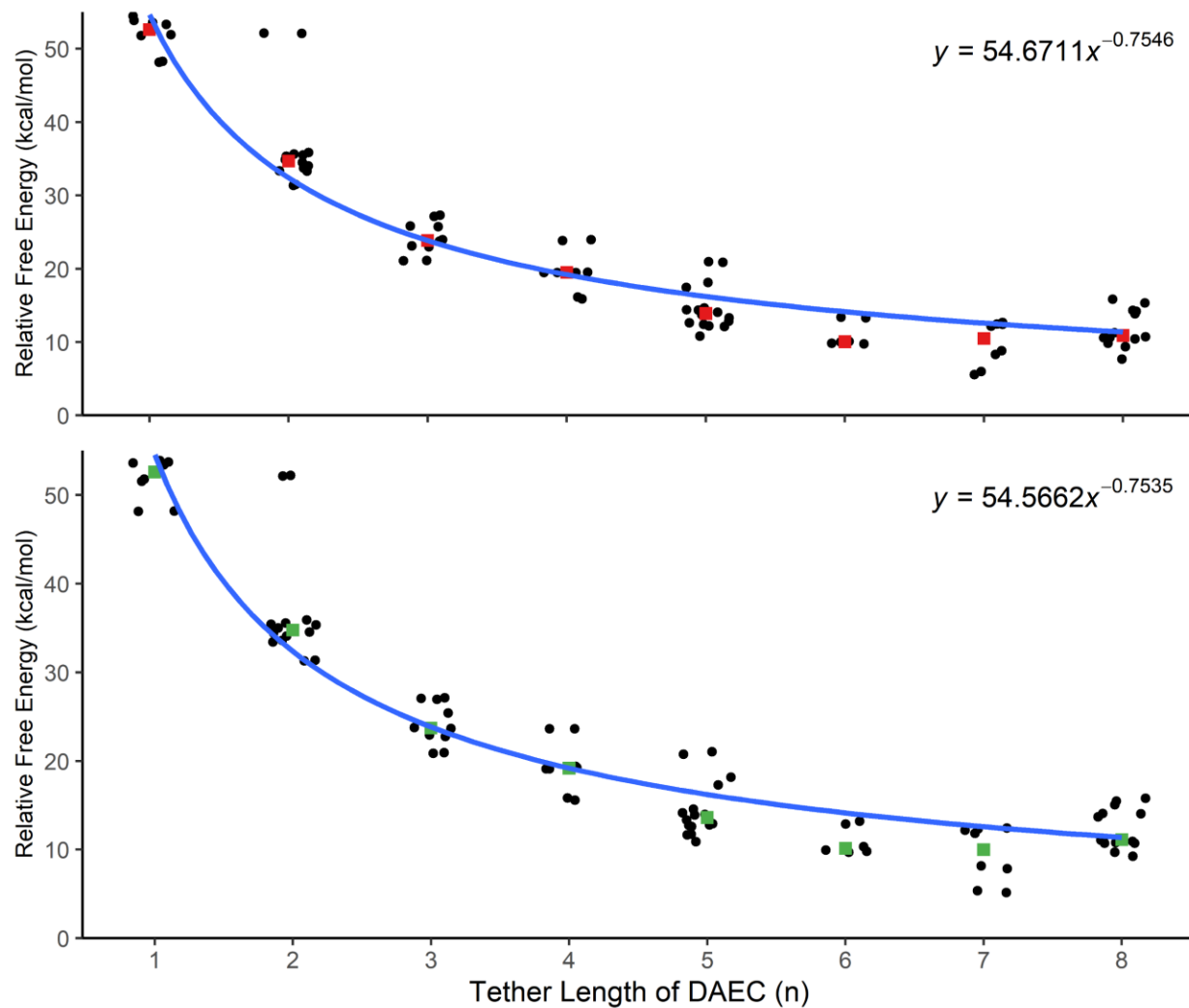
**Computational Insight into the Rope-skipping  
Isomerization of Diarylether Cyclophanes**

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**Figure S1.** Plots of relative activation energies for isomerization between enantiomeric conformations of DAEC of varying tether lengths ( $6 + n$  carbons) within an implicit solvent of benzene (top) and dimethylformamide (bottom). Color squares are used to indicate the median activation energies for each sample of molecule conformations. Blue lines are used to indicate a power law equation fit to the data by minimizing residual sum of squares.

## Cartesian Coordinates of Optimized Stationary Points

### daec[n=1]-1-TS (benzene)

C	-3.010512	-0.036532	0.071993
H	-4.089684	-0.016988	0.200411
C	-2.268187	1.165077	0.150896
C	-0.912108	1.034093	-0.028781
H	-0.284237	1.888556	-0.023644
C	-0.286293	-0.171221	-0.187259
H	0.778064	-0.132785	-0.210930
C	-0.970674	-1.360935	-0.297366
O	-0.276565	-2.560880	-0.517214
C	-2.384153	-1.287946	-0.174977
O	-3.052695	-2.470885	-0.290770
C	-4.466135	-2.464165	-0.172346
H	-4.936619	-1.839869	-0.946385
H	-4.790930	-2.117111	-0.819877
H	-4.781387	-3.503070	-0.308775
C	3.470480	-1.481347	0.873486
H	4.345888	-1.048563	1.355300
C	3.018482	-0.949661	-0.345446
C	3.581018	0.366159	-0.893065
H	3.987501	0.195811	-1.901552
H	4.434589	0.665487	-0.269338
C	2.594564	1.584629	-1.035500
H	1.744877	1.271045	-1.658184
H	3.130369	2.331563	-1.640464
C	1.906555	-1.567840	-0.948258
H	1.526735	-1.190426	-1.895397
C	1.088715	-2.430222	-0.198573
C	1.549438	-2.960748	1.005318
H	0.917770	-3.641095	1.571197
C	2.783710	-2.526111	1.501582
H	3.159702	-2.934238	2.437812
C	2.039570	2.312130	0.226718
H	2.880254	2.723883	0.803434
H	1.555823	1.591020	0.896322
C	1.040913	3.479572	-0.139939
H	0.671599	3.306046	-1.160810
C	-0.213857	3.765075	0.795897
H	1.625002	4.406627	-0.210861
H	-0.183559	3.109677	1.676637
C	-1.649150	3.700951	0.116394
H	-1.513962	3.682486	-0.974854
C	-2.700832	2.589515	0.486048
H	-2.925010	2.655192	1.563408
H	-3.639690	2.853784	-0.023166
H	-2.152921	4.652975	0.330157
H	-0.095362	4.781274	1.192748

Sum of electronic and zero-point Energies= -926.531257

Sum of electronic and thermal Energies= -926.512773

Sum of electronic and thermal Enthalpies= -926.511829

Sum of electronic and thermal Free Energies= -926.576179

### daec[n=1]-1-E1 (benzene)

C	-2.136191	-1.418857	-0.364146
H	-2.769150	-1.485328	-1.244985
C	-2.628222	-0.765697	0.780556
C	-1.824111	-0.715905	1.923924
H	-2.201140	-0.251011	2.832488
C	-0.516420	-1.209123	1.891687
H	0.137355	-1.121935	2.756584
C	-0.002811	-1.761119	0.725327
O	1.334675	-2.116915	0.655839
C	-0.827543	-1.917730	-0.409190
O	-0.253474	-2.509580	-1.488104
C	-1.030605	-2.650388	-2.669266
H	-1.336243	-1.673940	-3.072647

H	-1.922936	-3.268910	-2.495781
H	-0.381487	-3.150811	-3.393569
C	4.103287	0.954133	0.099607
H	4.844258	1.742065	-0.028452
C	2.747268	1.226897	-0.143394
C	2.313398	2.624312	-0.577521
H	3.027395	2.976583	-1.335957
H	2.433982	3.314246	0.273604
C	0.883098	2.758900	-1.139390
H	0.701038	1.927293	-1.835778
H	0.837379	3.669114	-1.753347
C	1.822658	0.189954	0.025076
H	0.772546	0.367095	-0.163801
C	2.229241	-1.081544	0.447446
C	3.580020	-1.350505	0.677773
H	3.882410	-2.344315	0.998185
C	4.508829	-0.322578	0.496876
H	5.564220	-0.522657	0.674234
C	-0.250946	2.812648	-0.085742
H	-0.395072	3.852951	0.243802
H	0.040470	2.253679	0.814283
C	-1.571395	2.231495	-0.616374
H	-1.389083	1.187394	-0.904786
C	-2.757519	2.277043	0.367941
H	-1.858097	2.750433	-1.545278
H	-2.403061	2.031860	1.379483
C	-3.913422	1.319774	-0.023405
H	-3.862280	1.117256	-1.103326
C	-3.953453	-0.031715	0.746035
H	-4.272480	0.164812	1.778740
H	-4.732773	-0.662129	0.293675
H	-4.882862	1.810239	0.141945
H	-3.134947	3.307999	0.425891

Sum of electronic and zero-point Energies= -926.605208

Sum of electronic and thermal Energies= -926.585597

Sum of electronic and thermal Enthalpies= -926.584652

Sum of electronic and thermal Free Energies= -926.652908

### daec[n=1]-1-E2 (benzene)

C	1.847852	1.478110	0.617048
H	2.258003	1.503013	1.622378
C	2.661912	1.027618	-0.436414
C	2.149166	1.050273	-1.738857
H	2.772216	0.740296	-2.575882
C	0.811996	1.397219	-1.965594
H	0.381353	1.353032	-2.963493
C	-0.014265	1.744323	-0.902866
O	-1.367944	1.955489	-1.106010
C	0.515914	1.847374	0.400641
O	-0.346800	2.258706	1.364867
C	0.116925	2.309900	2.706986
H	0.951465	3.016836	2.820220
H	0.426574	1.317831	3.066352
H	-0.732732	2.658427	3.301040
C	-3.956053	-1.035202	0.224368
H	-4.648731	-1.798231	0.577129
C	-2.606656	-1.363439	0.012943
C	-2.113582	-2.783284	0.279308
H	-2.821475	-3.479628	-0.193765
H	-2.188551	-2.987220	1.359823
C	-0.688409	-3.121712	-0.202416
H	-0.565601	-2.745877	-1.228636
H	-0.601097	-4.214342	-0.280098
C	-1.746941	-0.360010	-0.446655
H	-0.704934	-0.582810	-0.634598
C	-2.206811	0.944178	-0.664138

C	-3.550120	1.263255	-0.463627
H	-3.893684	2.279009	-0.641880
C	-4.417442	0.260297	-0.021860
H	-5.467577	0.498446	0.139040
C	0.462793	-2.591610	0.687572
H	0.672476	-3.320012	1.485857
H	0.150185	-1.670739	1.199444
C	1.740309	-2.295547	-0.114645
H	1.499891	-1.533751	-0.868507
C	2.944288	-1.813285	0.719703
H	2.037156	-3.191723	-0.682836
H	2.595327	-1.122091	1.500669
C	4.044535	-1.125149	-0.129381
H	3.974056	-1.482968	-1.166874
C	4.019979	0.430311	-0.127697
H	4.349973	0.782946	0.859375
H	4.767241	0.785847	-0.851477
H	5.039446	-1.429309	0.225031
H	3.374636	-2.672266	1.254318

Sum of electronic and zero-point Energies= -926.605824  
Sum of electronic and thermal Energies= -926.586251  
Sum of electronic and thermal Enthalpies= -926.585307  
Sum of electronic and thermal Free Energies= -926.653115

daec[n=1]-2-TS (benzene)

C	2.894956	0.746900	-0.024241
H	3.919228	1.064391	-0.202214
C	1.850024	1.699526	-0.039207
C	0.590916	1.198044	0.193182
H	-0.261709	1.833552	0.202416
C	0.338675	-0.130982	0.367107
H	-0.690470	-0.380003	0.453223
C	1.318029	-1.097109	0.379580
O	0.967130	-2.449998	0.544058
C	2.648254	-0.638067	0.191705
O	3.619130	-1.595199	0.208815
C	4.967523	-1.196519	0.021415
H	5.298187	-0.497893	0.804237
H	5.123234	-0.735448	-0.965254
H	5.560732	-2.113770	0.085346
C	-2.899055	-2.219142	-0.899749
H	-3.837980	-1.962572	-1.388000
C	-2.610864	-1.689158	0.368549
C	-3.442973	-0.547103	0.961514
H	-4.393413	-0.486951	0.413221
H	-3.703335	-0.786175	2.003190
C	-2.804694	0.901307	1.003583
H	-1.895357	0.873122	1.617866
H	-3.519266	1.510030	1.578313
C	-1.403502	-2.086985	0.976023
H	-1.147081	-1.706981	1.963048
C	-0.383440	-2.660512	0.196731
C	-0.679754	-3.192933	-1.057210
H	0.108687	-3.653576	-1.647389
C	-1.972822	-3.028531	-1.567629
H	-2.221920	-3.444255	-2.542105
C	-2.537022	1.636519	-0.340956
H	-3.478652	1.608580	-0.911183
H	-1.820731	1.076711	-0.953786
C	-2.158294	3.169827	-0.291146
H	-2.912310	3.650349	0.351059
C	-0.777148	3.809371	0.140406
H	-2.360971	3.550830	-1.303478
H	-1.013819	4.877010	0.251852
C	0.459200	3.717274	-0.844923
H	0.185175	3.105721	-1.715823
C	1.850596	3.199619	-0.322964
H	2.606436	3.452368	-1.080427
H	2.135082	3.764480	0.579758
H	0.636069	4.726819	-1.239349

H	-0.497540	3.487155	1.151872
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Sum of electronic and zero-point Energies= -926.525459  
Sum of electronic and thermal Energies= -926.507066  
Sum of electronic and thermal Enthalpies= -926.506121  
Sum of electronic and thermal Free Energies= -926.570149

daec[n=1]-2-E1 (benzene)

C	1.687349	1.789100	0.509059
H	2.150117	1.869147	1.488949
C	2.452341	1.302101	-0.567297
C	1.872569	1.247882	-1.837590
H	2.458641	0.908186	-2.689196
C	0.509908	1.530556	-2.002691
H	0.022166	1.401066	-2.966292
C	-0.267981	1.876735	-0.907250
O	-1.647955	1.927755	-1.013371
C	0.330185	2.081564	0.355723
O	-0.500332	2.489295	1.348903
C	0.034635	2.624780	2.658280
H	0.837280	3.375550	2.692046
H	0.413832	1.666276	3.041203
H	-0.796789	2.958885	3.285517
C	-3.718727	-1.470349	0.244265
H	-4.282114	-2.344145	0.569296
C	-2.339811	-1.582704	-0.001371
C	-1.658085	-2.938885	0.156948
H	-1.805884	-3.288396	1.191234
H	-2.217409	-3.654257	-0.464615
C	-0.161019	-3.068172	-0.201174
H	0.046389	-2.538088	-1.141961
H	0.028300	-4.130086	-0.417196
C	-1.645648	-0.443868	-0.419708
H	-0.584243	-0.508408	-0.620615
C	-2.304734	0.782687	-0.588565
C	-3.676328	0.886218	-0.354514
H	-4.172432	1.843655	-0.491358
C	-4.373678	-0.250456	0.062946
H	-5.443539	-0.178701	0.251759
C	0.837247	-2.639508	0.893156
H	0.600761	-3.206573	1.806223
H	0.696877	-1.579914	1.152557
C	2.313161	-2.898606	0.506742
H	2.367907	-3.863443	-0.019193
C	2.960001	-1.795168	-0.363363
H	2.912674	-3.025803	1.420645
H	3.718810	-2.237046	-1.025537
C	3.621640	-0.674402	0.464924
H	3.022909	-0.484691	1.367466
C	3.800938	0.675660	-0.280745
H	4.413841	1.342073	0.343144
H	4.354195	0.517405	-1.216730
H	4.603217	-1.021693	0.820014
H	2.197012	-1.368406	-1.028271

Sum of electronic and zero-point Energies= -926.605031  
Sum of electronic and thermal Energies= -926.585454  
Sum of electronic and thermal Enthalpies= -926.584510  
Sum of electronic and thermal Free Energies= -926.652877

daec[n=1]-2-E2 (benzene)

C	-1.757518	-1.720725	-0.539557
H	-2.275998	-1.724103	-1.494042
C	-2.447808	-1.293993	0.606817
C	-1.793724	-1.333625	1.844481
H	-2.324194	-1.044058	2.749774
C	-0.433587	-1.644593	1.910388
H	0.111332	-1.591162	2.850263
C	0.273826	-1.939109	0.750984
O	1.655910	-2.023779	0.788619
C	-0.396887	-2.051683	-0.483305
O	0.366177	-2.402412	-1.549970

C	-0.250050	-2.455545	-2.829449
H	-0.636104	-1.471956	-3.134323
H	-1.065688	-3.192400	-2.855719
H	0.536043	-2.764067	-3.524572
C	3.786928	1.480005	0.017087
H	4.367899	2.378125	-0.187998
C	2.384585	1.532433	-0.026818
C	1.686271	2.848387	-0.354369
H	1.739899	3.507147	0.527797
H	2.291589	3.353059	-1.120341
C	0.217799	2.796651	-0.845343
H	0.059834	1.890502	-1.447520
H	0.069840	3.639439	-1.536338
C	1.666602	0.360486	0.234059
H	0.585066	0.382695	0.208154
C	2.326890	-0.841764	0.523449
C	3.722310	-0.888074	0.565507
H	4.219761	-1.828386	0.789356
C	4.441743	0.281543	0.312820
H	5.529786	0.253074	0.339673
C	-0.861475	2.913866	0.250903
H	-0.668732	3.839123	0.814664
H	-0.767356	2.095143	0.979753
C	-2.302862	2.957841	-0.308867
H	-2.302695	3.581303	-1.215522
C	-2.915703	1.574962	-0.630375
H	-2.956465	3.477374	0.407814
H	-3.634319	1.667522	-1.457984
C	-3.631441	0.927375	0.572901
H	-3.079901	1.157005	1.495890
C	-3.796170	-0.615039	0.489131
H	-4.460509	-0.940847	1.301712
H	-4.288058	-0.889057	-0.454669
H	-4.623883	1.387668	0.689030
H	-2.122230	0.910000	-0.996713

Sum of electronic and zero-point Energies= -926.604615  
Sum of electronic and thermal Energies= -926.585023  
Sum of electronic and thermal Enthalpies= -926.584078  
Sum of electronic and thermal Free Energies= -926.652687

#### daec[n=1]-3-TS (benzene)

C	-3.037952	0.373286	-0.075226
H	-4.100506	0.544764	-0.227067
C	-2.139426	1.466822	-0.050870
C	-0.822657	1.134843	0.149343
H	-0.084257	1.889473	0.234168
C	-0.368533	-0.150755	0.220060
H	0.690578	-0.249686	0.252415
C	-1.205798	-1.242754	0.245943
O	-0.683486	-2.536518	0.411649
C	-2.592981	-0.966323	0.102813
O	-3.419931	-2.050563	0.128635
C	-4.815194	-1.843229	-0.019804
H	-5.219907	-1.207041	0.781292
H	-5.272134	-2.835415	0.044552
H	-5.059919	-1.397105	-0.995297
C	3.276932	-1.851275	-0.604069
H	4.230929	-1.508286	-1.001411
C	2.753699	-1.274199	0.566391
C	3.300475	0.026122	1.172660
H	4.299168	-0.148951	1.601418
H	2.659489	0.308488	2.018700
C	3.484634	1.258066	0.205501
H	4.198207	0.939499	-0.567049
H	4.021786	2.018297	0.792904
C	1.544984	-1.801375	1.055999
H	1.118758	-1.389965	1.967695
C	0.712422	-2.565809	0.220049
C	1.231814	-3.128362	-0.943253
H	0.594749	-3.729671	-1.587254

C	2.552214	-2.822022	-1.304082
H	2.975799	-3.265675	-2.203166
C	2.303503	1.963151	-0.550439
H	1.592992	1.212437	-0.911137
H	2.743954	2.386498	-1.465384
C	1.538987	3.134566	0.149640
H	2.253243	3.955352	0.305731
C	0.291592	3.706393	-0.661010
H	1.228712	2.838789	1.162190
H	0.150401	3.104859	-1.569157
C	-1.101439	3.856148	0.089489
H	-0.933061	3.751897	1.171346
C	-2.341651	2.961094	-0.295723
H	-2.582346	3.126034	-1.358600
H	-3.206420	3.349678	0.262946
H	-1.439140	4.891211	-0.052651
H	0.572507	4.704831	-1.019928

Sum of electronic and zero-point Energies= -926.521602  
Sum of electronic and thermal Energies= -926.503127  
Sum of electronic and thermal Enthalpies= -926.502183  
Sum of electronic and thermal Free Energies= -926.566375

#### daec[n=1]-3-E1 (benzene)

C	1.973234	-1.349201	0.608108
H	2.409526	-1.244298	1.597047
C	2.690704	-0.877924	-0.504973
C	2.157545	-1.079042	-1.783789
H	2.715675	-0.762099	-2.662975
C	0.869763	-1.606150	-1.935900
H	0.409350	-1.689947	-2.917957
C	0.113357	-1.939853	-0.818616
O	-1.238168	-2.231433	-0.937920
C	0.686616	-1.880734	0.468712
O	-0.102415	-2.294454	1.493313
C	0.402550	-2.188613	2.817267
H	1.311441	-2.792258	2.953788
H	-0.386973	-2.576040	3.467658
H	0.613053	-1.143999	3.088275
C	-3.756035	0.966696	0.026987
H	-4.424100	1.785305	0.290730
C	-2.466561	1.241300	-0.451635
C	-1.940189	2.655037	-0.622313
H	-2.781318	3.329030	-0.836794
H	-1.289656	2.687054	-1.507366
C	-1.172379	3.243951	0.589745
H	-1.860286	3.288987	1.447204
H	-0.927689	4.288322	0.341250
C	-1.640696	0.163553	-0.790168
H	-0.652033	0.363753	-1.185141
C	-2.065169	-1.158432	-0.630118
C	-3.355686	-1.429270	-0.169445
H	-3.680160	-2.460536	-0.055999
C	-4.192676	-0.357354	0.152023
H	-5.199388	-0.560370	0.513483
C	0.114866	2.530007	1.049171
H	-0.133158	1.519399	1.404151
H	0.486793	3.074179	1.931746
C	1.256534	2.425028	0.020765
H	1.394038	3.391098	-0.490967
C	2.597749	1.998578	0.658739
H	0.988071	1.705256	-0.762893
H	2.399450	1.222145	1.410479
C	3.663745	1.483592	-0.346313
H	3.365087	1.754430	-1.369192
C	3.939531	-0.047080	-0.298022
H	4.391154	-0.293867	0.673036
H	4.689902	-0.286294	-1.064713
H	4.622686	1.990522	-0.169639
H	3.002375	2.852781	1.220308

Sum of electronic and zero-point Energies= -926.604649

Sum of electronic and thermal Energies= -926.585125  
Sum of electronic and thermal Enthalpies= -926.584180  
Sum of electronic and thermal Free Energies= -926.651737

daec[n=1]-3-E2 (benzene)

C	2.191089	-1.376895	-0.408256
H	2.756712	-1.428773	-1.334738
C	2.695157	-0.606634	0.655571
C	1.987138	-0.580028	1.861682
H	2.384911	-0.032918	2.713747
C	0.728039	-1.181326	1.952969
H	0.126115	-1.089008	2.854213
C	0.181951	-1.834682	0.856512
O	-1.150263	-2.223421	0.883780
C	0.942544	-2.005447	-0.319877
O	0.351286	-2.713161	-1.316641
C	1.055986	-2.865033	-2.541323
H	1.234467	-1.895815	-3.029487
H	0.411920	-3.475789	-3.180451
H	2.015119	-3.381995	-2.394539
C	-3.892179	0.769164	-0.123273
H	-4.622173	1.539385	-0.367480
C	-2.555270	0.921022	-0.517965
C	-2.065426	2.130474	-1.294660
H	-2.911692	2.570570	-1.840124
H	-1.351173	1.795479	-2.060024
C	-1.413727	3.262847	-0.458485
H	-2.159326	3.637215	0.258608
H	-1.209902	4.096638	-1.148149
C	-1.646639	-0.092691	-0.192776
H	-0.615665	0.011234	-0.505869
C	-2.042957	-1.226161	0.522339
C	-3.380153	-1.382323	0.899603
H	-3.682965	-2.271284	1.447376
C	-4.294081	-0.378606	0.570075
H	-5.336232	-0.493594	0.863314
C	-0.122283	2.939300	0.319865
H	-0.333018	2.178653	1.085011
H	0.157919	3.849510	0.873141
C	1.089136	2.478597	-0.511539
H	1.222953	3.139622	-1.382966
C	2.399651	2.446341	0.307129
H	0.901286	1.477781	-0.921743
H	2.174600	2.064218	1.312024
C	3.538828	1.598811	-0.323152
H	3.271663	1.334979	-1.356667
C	3.894386	0.293571	0.446360
H	4.321669	0.562742	1.422122
H	4.683707	-0.232392	-0.109657
H	4.459053	2.195002	-0.395455
H	2.744709	3.479393	0.455894

Sum of electronic and zero-point Energies= -926.604519  
Sum of electronic and thermal Energies= -926.584921  
Sum of electronic and thermal Enthalpies= -926.583977  
Sum of electronic and thermal Free Energies= -926.652200

daec[n=1]-4-TS (benzene)

C	-2.505417	1.963852	-0.002251
H	-3.377572	2.606175	0.110543
C	-1.189646	2.466790	0.037160
C	-0.214969	1.511234	-0.117617
H	0.800414	1.807310	-0.137813
C	-0.463189	0.179600	-0.229675
H	0.397096	-0.444452	-0.259287
C	-1.728587	-0.356273	-0.318103
O	-1.839340	-1.752717	-0.529413
C	-2.794117	0.578159	-0.202816
O	-4.125690	0.282120	-0.298209
C	-4.576919	-0.997665	0.144409
H	-4.218772	-1.217222	1.160387

H	-4.260690	-1.800053	-0.530940
H	-5.670193	-0.936454	0.154856
C	1.870956	-3.128100	0.777207
H	2.843266	-3.334352	1.222454
C	1.797201	-2.434336	-0.444648
C	3.030743	-1.766302	-1.066459
H	2.789553	-1.488663	-2.101945
H	3.850321	-2.496896	-1.127432
C	3.626059	-0.486131	-0.352146
H	4.472740	-0.161967	-0.975773
H	4.053834	-0.777593	0.618192
C	0.517202	-2.240308	-0.998952
H	0.419806	-1.719130	-1.948970
C	-0.642263	-2.439233	-0.221177
C	-0.553255	-3.124591	0.986812
H	-1.447216	-3.286860	1.584037
C	0.710256	-3.522136	1.447814
H	0.788092	-4.069366	2.385325
C	2.611940	0.667178	-0.154449
H	1.934686	0.337214	0.639138
H	2.024627	0.719241	-1.078192
C	3.085297	2.113569	0.213279
H	3.552259	2.580865	-0.667026
C	2.043786	3.141493	0.848829
H	3.885323	2.028988	0.963900
H	1.537888	2.641528	1.686665
C	0.973765	3.930384	-0.033000
H	1.225005	4.996696	0.040825
C	-0.575386	3.848149	0.290228
H	-1.071617	4.625990	-0.308370
H	-0.736649	4.138138	1.340805
H	1.110176	3.676261	-1.093885
H	2.677124	3.907376	1.316814

Sum of electronic and zero-point Energies= -926.518587  
Sum of electronic and thermal Energies= -926.500009  
Sum of electronic and thermal Enthalpies= -926.499065  
Sum of electronic and thermal Free Energies= -926.563812

daec[n=1]-4-E1 (benzene)

C	-1.818588	-1.797462	-0.581601
H	-2.342476	-1.949383	-1.523742
C	-2.469148	-1.207656	0.511011
C	-1.757903	-1.086345	1.714603
H	-2.251377	-0.690658	2.600001
C	-0.397627	-1.394832	1.766413
H	0.181804	-1.216204	2.669584
C	0.268873	-1.848015	0.627889
O	1.662103	-1.907060	0.635516
C	-0.459558	-2.131987	-0.540976
O	0.113458	-2.585261	-1.697114
C	0.941540	-3.750412	-1.604475
H	0.398586	-4.575287	-1.121070
H	1.867864	-3.551185	-1.055903
H	1.176887	-4.030117	-2.636329
C	3.437645	1.857076	0.242380
H	3.892222	2.844619	0.180777
C	2.278209	1.576762	-0.496186
C	1.598472	2.619779	-1.366225
H	1.337563	2.164559	-2.333317
H	2.310015	3.427288	-1.586048
C	0.313856	3.253472	-0.765012
H	-0.035130	4.021278	-1.472533
H	0.573987	3.785782	0.162554
C	1.726793	0.292485	-0.400883
H	0.851005	0.044237	-0.988896
C	2.268172	-0.663530	0.460866
C	3.432782	-0.389262	1.180599
H	3.851891	-1.147596	1.837285
C	4.016568	0.874393	1.052856
H	4.923163	1.100916	1.611244

C	-0.825540	2.262153	-0.476644
H	-0.500215	1.566736	0.307191
H	-1.003280	1.647073	-1.371458
C	-2.147364	2.913308	-0.027728
H	-2.628720	3.419038	-0.879622
C	-3.125963	1.915920	0.629498
H	-1.925162	3.702814	0.706844
H	-2.587932	1.430249	1.454719
C	-3.725205	0.834842	-0.305436
H	-4.725922	1.148400	-0.634746
C	-3.836647	-0.581003	0.330970
H	-4.457515	-1.210676	-0.321170
H	-4.357418	-0.511107	1.296260
H	-3.122649	0.743900	-1.219023
H	-3.947882	2.475766	1.098682
Sum of electronic and zero-point Energies= -926.602382			
Sum of electronic and thermal Energies= -926.582563			
Sum of electronic and thermal Enthalpies= -926.581619			
Sum of electronic and thermal Free Energies= -926.650610			

daec[n=1]-4-E2 (benzene)

C	1.640260	-1.700396	-0.638128
H	2.047608	-1.737280	-1.646164
C	2.448985	-1.347072	0.451116
C	1.882329	-1.395407	1.734820
H	2.497391	-1.173541	2.605567
C	0.517071	-1.638523	1.905701
H	0.058904	-1.596854	2.891545
C	-0.302497	-1.834468	0.794409
O	-1.687391	-1.821469	0.930876
C	0.271230	-1.940952	-0.485543
O	-0.481559	-2.147032	-1.610102
C	-1.208471	-3.379187	-1.659061
H	-1.922496	-3.464776	-0.832169
H	-0.519851	-4.236713	-1.638883
H	-1.749194	-3.372927	-2.610729
C	-3.418244	1.803580	-0.235686
H	-3.871282	2.734779	-0.572193
C	-2.160044	1.824265	0.383182
C	-1.384357	3.113015	0.599690
H	-1.044699	3.152657	1.645940
H	-2.062840	3.966262	0.464726
C	-0.148499	3.326290	-0.316504
H	0.263961	4.319344	-0.080217
H	-0.478296	3.372004	-1.365353
C	-1.613161	0.606470	0.809851
H	-0.654923	0.601866	1.314961
C	-2.267250	-0.603973	0.572920
C	-3.531203	-0.619452	-0.020521
H	-4.042610	-1.565210	-0.181085
C	-4.100217	0.594405	-0.413935
H	-5.082722	0.593885	-0.882645
C	0.956019	2.265068	-0.179608
H	0.571868	1.305314	-0.546334
H	1.180923	2.114475	0.887037
C	2.257900	2.586205	-0.937096
H	2.799257	3.400513	-0.430009
C	3.176404	1.357873	-1.116469
H	2.004697	2.967794	-1.938246
H	2.583599	0.581616	-1.618135
C	3.801467	0.779328	0.178932
H	4.828638	1.154769	0.288914
C	3.836813	-0.775838	0.244705
H	4.492201	-1.076743	1.073700
H	4.285789	-1.172392	-0.676625
H	3.254168	1.138377	1.060758
H	3.984296	1.613422	-1.817209
Sum of electronic and zero-point Energies= -926.601512			
Sum of electronic and thermal Energies= -926.581855			
Sum of electronic and thermal Enthalpies= -926.580911			

Sum of electronic and thermal Free Energies= -926.648772

daec[n=2]-1-TS (benzene)

C	-3.043461	0.571912	0.022509
H	-4.121084	0.692522	-0.053590
C	-2.480670	-0.720673	-0.065139
C	-1.105892	-0.796171	0.048785
H	-0.600741	-1.737858	0.026542
C	-0.311403	0.320280	0.175732
H	0.745590	0.153759	0.182588
C	-0.833659	1.594762	0.279043
O	-0.008895	2.712072	0.439194
C	-2.244466	1.723362	0.211177
O	-2.731576	2.991395	0.323849
C	-4.135183	3.183523	0.250661
H	-4.295018	4.259667	0.367837
H	-4.540411	2.862937	-0.720611
H	-4.661840	2.651281	1.056647
C	3.664993	1.370103	-0.941535
H	4.531286	0.895668	-1.400039
C	3.182242	0.889290	0.286208
C	3.720826	-0.398487	0.905670
H	4.195026	-0.168645	1.872280
H	4.520840	-0.790324	0.262385
C	2.680038	-1.531115	1.187692
H	1.884051	-1.121237	1.826103
H	3.195239	-2.275305	1.813813
C	2.082045	1.550276	0.856844
H	1.682945	1.216234	1.811674
C	1.323829	2.449249	0.094131
C	1.813679	2.931701	-1.118706
H	1.223920	3.641180	-1.693769
C	3.024055	2.423339	-1.602264
H	3.421746	2.791036	-2.546270
C	2.019524	-2.289384	0.004083
H	2.799626	-2.772675	-0.604048
H	1.511900	-1.588444	-0.670295
C	1.034165	-3.378054	0.522117
C	0.148062	-4.165960	-0.495834
C	-1.176698	-3.580893	-1.084201
H	-1.535356	-4.328042	-1.806991
H	-0.962792	-2.691147	-1.687447
H	-0.119287	-5.111092	0.001063
H	0.780422	-4.455640	-1.349011
H	0.399262	-2.944312	1.308047
H	1.642703	-4.132124	1.043963
C	-2.334796	-3.298438	-0.066900
H	-3.004747	-4.168824	-0.059130
H	-1.930447	-3.235323	0.953217
C	-3.215967	-2.034408	-0.309523
H	-3.604130	-2.053958	-1.341062
H	-4.102523	-2.102356	0.338467

Sum of electronic and zero-point Energies= -965.844364

Sum of electronic and thermal Energies= -965.824772

Sum of electronic and thermal Enthalpies= -965.823828

Sum of electronic and thermal Free Energies= -965.890590

daec[n=2]-1-E1 (benzene)

C	1.525178	1.969196	0.505537
H	1.999965	2.084706	1.475616
C	2.319375	1.633258	-0.604239
C	1.712111	1.527682	-1.860902
H	2.313995	1.296369	-2.737907
C	0.325477	1.657586	-1.989882
H	-0.165388	1.529303	-2.952059
C	-0.463004	1.901002	-0.871776
O	-1.842379	1.929375	-0.981101
C	0.137056	2.106914	0.388493
O	-0.708768	2.389055	1.412466
C	-0.160942	2.545687	2.714136

H	-1.009985	2.760542	3.369362
H	0.337026	1.627274	3.057033
H	0.549196	3.384131	2.756415
C	-3.974535	-1.420940	0.284184
H	-4.553297	-2.282369	0.615026
C	-2.613203	-1.577469	-0.026334
C	-1.977238	-2.958744	0.098270
H	-2.639092	-3.670391	-0.417005
H	-2.003537	-3.262515	1.157239
C	-0.545313	-3.154936	-0.439967
H	-0.454094	-2.677551	-1.427094
H	-0.403245	-4.230948	-0.619451
C	-1.896500	-0.454419	-0.454601
H	-0.849505	-0.544528	-0.717318
C	-2.517076	0.797851	-0.554524
C	-3.871818	0.945768	-0.254898
H	-4.334998	1.925191	-0.342319
C	-4.592936	-0.175052	0.162883
H	-5.650174	-0.070685	0.401025
C	0.592689	-2.674087	0.479443
H	0.520080	-3.204142	1.442680
H	0.466120	-1.608777	0.712368
C	1.984406	-2.921465	-0.130162
C	3.171062	-2.478466	0.750838
C	3.358824	-0.953193	0.879461
H	4.008189	-0.739841	1.742123
H	2.390416	-0.492978	1.113442
H	4.096801	-2.921208	0.351759
H	3.041250	-2.909066	1.755543
H	2.041909	-2.422704	-1.109776
H	2.087059	-3.997594	-0.338656
C	3.963310	-0.282714	-0.367965
H	5.038402	-0.511655	-0.416345
H	3.518673	-0.710216	-1.277655
C	3.775761	1.256528	-0.422234
H	4.175198	1.709459	0.496292
H	4.372116	1.652831	-1.255831

Sum of electronic and zero-point Energies= -965.896237  
Sum of electronic and thermal Energies= -965.875391  
Sum of electronic and thermal Enthalpies= -965.874447  
Sum of electronic and thermal Free Energies= -965.945554

#### daec[n=2]-1-E2 (benzene)

C	-1.573288	-1.908524	-0.621665
H	-2.091213	-1.942498	-1.576244
C	-2.314015	-1.648539	0.545924
C	-1.650947	-1.638487	1.776728
H	-2.210187	-1.464589	2.693739
C	-0.260711	-1.791522	1.831646
H	0.274398	-1.732748	2.776732
C	0.472412	-1.969522	0.666140
O	1.854325	-2.027249	0.719102
C	-0.185102	-2.074265	-0.578488
O	0.611112	-2.289288	-1.657012
C	0.002783	-2.338742	-2.940302
H	0.817762	-2.512604	-3.648758
H	-0.721741	-3.162573	-3.013541
H	-0.495992	-1.390548	-3.188199
C	4.042346	1.480804	0.195324
H	4.638582	2.382780	0.065091
C	2.647837	1.542624	0.046837
C	1.985158	2.877708	-0.275380
H	2.673929	3.435609	-0.924874
H	1.919827	3.473611	0.649816
C	0.591886	2.846065	-0.944944
H	0.550455	2.013027	-1.662335
H	0.485465	3.761190	-1.545942
C	1.907856	0.364874	0.211405
H	0.831543	0.381977	0.096832
C	2.541424	-0.843762	0.523831

C	3.930160	-0.899762	0.668310
H	4.404298	-1.848225	0.907745
C	4.670958	0.270957	0.501612
H	5.753807	0.236369	0.608985
C	-0.612740	2.770637	0.012229
H	-0.588622	3.643750	0.683737
H	-0.527744	1.891456	0.664382
C	-1.958590	2.744597	-0.733785
C	-3.203048	2.648609	0.173488
C	-3.418404	1.277702	0.846467
H	-4.128636	1.391189	1.679321
H	-2.475647	0.948242	1.302123
H	-4.096690	2.901506	-0.417920
H	-3.129718	3.422616	0.952599
H	-1.956469	1.908865	-1.450363
H	-2.037480	3.657870	-1.343409
C	-3.943767	0.185228	-0.102808
H	-5.009129	0.365516	-0.310021
H	-3.429855	0.252360	-1.072249
C	-3.774513	-1.260382	0.432256
H	-4.262063	-1.350547	1.412916
H	-4.298531	-1.949107	-0.245837

Sum of electronic and zero-point Energies= -965.896242  
Sum of electronic and thermal Energies= -965.875296  
Sum of electronic and thermal Enthalpies= -965.874352  
Sum of electronic and thermal Free Energies= -965.946185

#### daec[n=2]-2-TS (benzene)

C	-2.885660	1.156608	0.000075
H	-3.912451	1.501206	-0.091992
C	-2.603928	-0.225868	-0.048848
C	-1.279782	-0.584861	0.084484
H	-1.010899	-1.615773	0.100975
C	-0.263052	0.335516	0.200605
H	0.735594	-0.049818	0.233757
C	-0.508812	1.693464	0.267257
O	0.526718	2.618624	0.421550
C	-1.860112	2.115544	0.172229
O	-2.066709	3.461073	0.246361
C	-3.395712	3.945543	0.142010
H	-3.323660	5.033945	0.228408
H	-4.034385	3.561558	0.951299
H	-3.847636	3.690385	-0.828112
C	3.928123	0.602510	-0.852338
H	4.712974	-0.019525	-1.279769
C	3.329458	0.223908	0.359988
C	3.618344	-1.131285	1.001251
H	4.048274	-0.983131	2.003626
H	4.391430	-1.642175	0.410771
C	2.388311	-2.079521	1.177608
H	1.643869	-1.566180	1.803807
H	2.728500	-2.938623	1.775094
C	2.341930	1.069846	0.891559
H	1.866652	0.821949	1.837776
C	1.785297	2.090325	0.107703
C	2.391514	2.467852	-1.089930
H	1.960244	3.272424	-1.680248
C	3.503776	1.746523	-1.536120
H	3.989841	2.031088	-2.467399
C	1.680431	-2.605071	-0.096460
H	2.376717	-3.230718	-0.675024
H	1.435394	-1.759249	-0.752127
C	0.375124	-3.406986	0.203230
C	-0.642271	-3.454567	-0.980395
C	-2.152652	-3.700754	-0.656488
H	-2.218943	-4.693130	-0.184012
H	-2.658947	-3.811336	-1.627932
H	-0.345946	-4.274391	-1.651745
H	-0.542082	-2.545567	-1.586713
H	-0.100479	-2.971743	1.092921



H	0.632949	-4.434742	0.497708
C	-3.053723	-2.773461	0.234100
H	-3.955357	-3.377790	0.408319
H	-2.600847	-2.647197	1.227660
C	-3.576758	-1.379260	-0.255366
H	-4.519152	-1.174910	0.273690
H	-3.850813	-1.450169	-1.320952

Sum of electronic and zero-point Energies= -965.843760  
Sum of electronic and thermal Energies= -965.824059  
Sum of electronic and thermal Enthalpies= -965.823115  
Sum of electronic and thermal Free Energies= -965.890276

daec[n=2]-2-E1 (benzene)

C	-1.658582	-1.697030	0.535178
H	-2.137398	-1.774203	1.507112
C	-2.430919	-1.312380	-0.573313
C	-1.818993	-1.260374	-1.832048
H	-2.404809	-0.999673	-2.711604
C	-0.448776	-1.507123	-1.966227
H	0.044376	-1.432819	-2.932911
C	0.322783	-1.814375	-0.851666
O	1.691887	-1.985891	-0.972161
C	-0.285851	-1.947717	0.414342
O	0.538195	-2.287937	1.438437
C	-0.013977	-2.385729	2.744144
H	0.818810	-2.659377	3.398298
H	-0.787635	-3.165101	2.799208
H	-0.435956	-1.426914	3.078359
C	4.146965	1.169542	0.213825
H	4.804463	1.976841	0.533972
C	2.806419	1.447234	-0.100719
C	2.282368	2.877502	-0.002988
H	2.909770	3.513142	-0.646129
H	2.456187	3.244701	1.020977
C	0.805849	3.105069	-0.378766
H	0.611684	2.650048	-1.361296
H	0.649054	4.184040	-0.520241
C	1.990235	0.387386	-0.510960
H	0.956362	0.566959	-0.776124
C	2.484229	-0.920043	-0.580202
C	3.819835	-1.189800	-0.279590
H	4.188948	-2.210236	-0.342548
C	4.644226	-0.131980	0.113133
H	5.687155	-0.331308	0.353860
C	-0.216356	2.579601	0.649469
H	-0.240194	3.258669	1.516014
H	0.117750	1.609680	1.041788
C	-1.634544	2.412061	0.077419
C	-2.608745	1.765054	1.073756
C	-4.036055	1.521272	0.546348
H	-4.472694	2.491763	0.262147
H	-4.652975	1.152691	1.381143
H	-2.685162	2.408444	1.964443
H	-2.176984	0.818131	1.424309
H	-1.574211	1.793234	-0.829524
H	-2.026932	3.389736	-0.246199
C	-4.225108	0.562821	-0.648733
H	-5.285147	0.621391	-0.935787
H	-3.661865	0.923833	-1.520394
C	-3.893717	-0.936664	-0.414578
H	-4.481053	-1.521909	-1.137038
H	-4.249913	-1.237117	0.581015

Sum of electronic and zero-point Energies= -965.894501  
Sum of electronic and thermal Energies= -965.873684  
Sum of electronic and thermal Enthalpies= -965.872740  
Sum of electronic and thermal Free Energies= -965.943374

daec[n=2]-2-E2 (benzene)

C	1.735250	-1.701271	0.537942
H	2.271444	-1.794308	1.478372

C	2.433979	-1.267192	-0.604146
C	1.749065	-1.190400	-1.820391
H	2.276723	-0.886553	-2.722281
C	0.377305	-1.462075	-1.879915
H	-0.174161	-1.364408	-2.812313
C	-0.318423	-1.828161	-0.734893
O	-1.687403	-2.033060	-0.790690
C	0.365904	-1.986852	0.489237
O	-0.389784	-2.379281	1.547075
C	0.244189	-2.519719	2.811114
H	-0.540575	-2.839245	3.502745
H	0.667874	-1.566787	3.160218
H	1.035347	-3.282824	2.784424
C	-4.211902	1.221680	-0.145643
H	-4.889870	2.061529	0.000611
C	-2.847608	1.367704	0.153955
C	-2.323524	2.700819	0.681423
H	-2.963319	3.004561	1.523248
H	-2.480310	3.470907	-0.091020
C	-0.852955	2.737744	1.140656
H	-0.664586	1.876937	1.799397
H	-0.710386	3.626975	1.771281
C	-2.004917	0.267685	-0.041388
H	-0.950753	0.344515	0.187631
C	-2.498710	-0.941112	-0.543992
C	-3.857849	-1.085200	-0.830379
H	-4.227621	-2.032386	-1.214892
C	-4.705978	0.005368	-0.623325
H	-5.766996	-0.096589	-0.845176
C	0.189688	2.760168	0.003482
H	0.218575	3.766546	-0.442177
H	-0.124820	2.088059	-0.806043
C	1.600273	2.348871	0.459856
C	2.590799	2.198458	-0.704797
C	4.013108	1.755051	-0.309735
H	4.439054	2.514166	0.365310
H	4.643915	1.774195	-1.212383
H	2.673395	3.163287	-1.229453
H	2.171924	1.493989	-1.435479
H	1.525780	1.393314	0.998844
H	1.987098	3.079964	1.188255
C	4.190899	0.381322	0.371475
H	5.241704	0.318227	0.689967
H	3.598753	0.335979	1.296314
C	3.896839	-0.878297	-0.486677
H	4.446352	-1.719474	-0.038364
H	4.320374	-0.739396	-1.491258

Sum of electronic and zero-point Energies= -965.894296  
Sum of electronic and thermal Energies= -965.873466  
Sum of electronic and thermal Enthalpies= -965.872522  
Sum of electronic and thermal Free Energies= -965.943421

daec[n=2]-3-TS (benzene)

C	3.207489	0.760896	-0.045971
H	4.249041	1.057625	-0.138640
C	2.171290	1.721308	-0.116480
C	0.907505	1.214425	0.015630
H	0.115855	1.901233	0.013248
C	0.583628	-0.109490	0.127050
H	-0.462051	-0.351468	0.127279
C	1.565668	-1.070160	0.232543
O	1.226857	-2.414256	0.413703
C	2.913897	-0.617628	0.151509
O	3.863258	-1.592470	0.259660
C	5.228972	-1.220968	0.175977
H	5.797715	-2.148504	0.292999
H	5.511328	-0.521824	0.977218
H	5.470964	-0.771270	-0.798648
C	-2.754961	-2.685444	-0.793392
H	-3.765460	-2.641780	-1.196616

C	-2.464274	-2.030196	0.414766
C	-3.497457	-1.136372	1.104279
H	-3.560003	-1.427554	2.162888
H	-4.488831	-1.336365	0.674513
C	-3.222495	0.409168	1.082134
H	-2.166263	0.562726	1.332174
H	-3.789021	0.848065	1.917026
C	-1.153854	-2.142383	0.917190
H	-0.891391	-1.655379	1.854192
C	-0.124088	-2.676115	0.123450
C	-0.429103	-3.332428	-1.068103
H	0.373313	-3.754543	-1.667963
C	-1.760468	-3.373359	-1.495711
H	-2.010248	-3.887118	-2.422098
C	-3.591097	1.189273	-0.209214
H	-4.684196	1.160353	-0.331588
H	-3.175803	0.663430	-1.082687
C	-3.117978	2.684008	-0.289131
C	-1.577615	2.715495	-0.217456
C	-0.648593	3.935967	-0.546366
H	-1.133307	4.850983	-0.175996
H	-0.573143	4.057432	-1.636894
H	-1.288976	1.895018	-0.880965
H	-1.339518	2.400648	0.805509
H	-3.572815	3.276284	0.519167
H	-3.488649	3.103028	-1.236090
C	0.816936	3.992183	0.099504
H	0.705064	3.793073	1.176125
H	1.092772	5.053707	0.028455
C	2.131902	3.232596	-0.385568
H	2.270121	3.412880	-1.463957
H	2.970749	3.748476	0.104616

Sum of electronic and zero-point Energies= -965.815040  
Sum of electronic and thermal Energies= -965.795092  
Sum of electronic and thermal Enthalpies= -965.794148  
Sum of electronic and thermal Free Energies= -965.861838

daec[n=2]-3-E1 (benzene)

C	-1.878744	-1.583370	0.643946
H	-2.346368	-1.531033	1.622955
C	-2.644109	-1.267042	-0.491141
C	-2.049933	-1.368636	-1.754091
H	-2.632077	-1.157178	-2.649133
C	-0.693282	-1.687016	-1.873617
H	-0.208904	-1.730455	-2.846596
C	0.078546	-1.916723	-0.740301
O	1.432447	-2.177807	-0.857360
C	-0.520570	-1.905953	0.537637
O	0.299040	-2.187901	1.582804
C	-0.241280	-2.131541	2.896006
H	0.584575	-2.383252	3.567495
H	-1.052644	-2.861054	3.031816
H	-0.610656	-1.124647	3.138775
C	4.161023	0.851362	0.009845
H	4.891418	1.624323	0.245006
C	2.845236	1.217002	-0.316246
C	2.472778	2.694867	-0.392893
H	2.913768	3.106445	-1.314732
H	2.978355	3.223402	-0.429389
C	0.974188	3.050151	-0.378509
H	0.465644	2.512522	-1.189784
H	0.876087	4.117200	-0.628298
C	1.925577	0.201222	-0.608569
H	0.903364	0.449170	-0.869939
C	2.306822	-1.144906	-0.565757
C	3.621022	-1.502112	-0.257973
H	3.896604	-2.553227	-0.232028
C	4.542168	-0.492509	0.026903
H	5.567314	-0.760659	0.276876
C	0.269610	2.786209	0.963199

H	0.690388	3.466328	1.719829
H	0.507282	1.768963	1.306737
C	-1.263749	2.943119	0.935942
C	-1.969231	1.930988	0.013626
C	-3.471002	1.757497	0.301836
H	-3.958368	2.741787	0.223786
H	-3.608587	1.440736	1.348457
H	-1.466558	0.963207	0.114961
H	-1.844486	2.229863	-1.037584
H	-1.535581	3.970935	0.647509
H	-1.636339	2.810287	1.963610
C	-4.219025	0.778661	-0.629990
H	-3.928330	0.976785	-1.672608
H	-5.295482	0.997076	-0.570852
C	-4.055864	-0.736558	-0.336170
H	-4.413469	-0.939872	0.683116
H	-4.729936	-1.280250	-1.014418

Sum of electronic and zero-point Energies= -965.895544  
Sum of electronic and thermal Energies= -965.874647  
Sum of electronic and thermal Enthalpies= -965.873702  
Sum of electronic and thermal Free Energies= -965.944886

daec[n=2]-3-E2 (benzene)

C	-1.989863	-1.674985	-0.470381
H	-2.541586	-1.780483	-1.400415
C	-2.642021	-1.130801	0.650853
C	-1.939765	-1.029077	1.855377
H	-2.434379	-0.633334	2.740181
C	-0.585351	-1.374904	1.915914
H	-0.016448	-1.260494	2.835895
C	0.073211	-1.837786	0.783799
O	1.424175	-2.132738	0.841082
C	-0.637359	-2.030992	-0.420897
O	0.080279	-2.527038	-1.461476
C	-0.581360	-2.715059	-2.704931
H	0.173591	-3.120877	-3.384475
H	-0.959480	-1.765551	-3.110825
H	-1.411280	-3.431001	-2.617272
C	4.238833	0.828103	0.020644
H	4.994393	1.588393	-0.172711
C	2.892211	1.097954	-0.272100
C	2.521551	2.438638	-0.901274
H	2.965262	2.466916	-1.908817
H	3.030480	3.238370	-0.341355
C	1.025587	2.781497	-1.025215
H	0.507051	1.955153	-1.529530
H	0.930219	3.643748	-1.701942
C	1.940488	0.104110	-0.008958
H	0.893520	0.283617	-0.220716
C	2.322544	-1.127369	0.537269
C	3.665672	-1.395327	0.812449
H	3.942071	-2.358404	1.234113
C	4.616776	-0.408163	0.548873
H	5.665009	-0.606116	0.766411
C	0.331620	3.121032	0.306047
H	0.762117	4.056334	0.695604
H	0.566023	2.348431	1.052374
C	-1.201231	3.264191	0.220921
C	-1.914556	1.959690	-0.178012
C	-3.426657	1.949282	0.106642
H	-3.883100	2.820250	-0.388993
H	-3.597924	2.096350	1.185115
H	-1.439778	1.130948	0.358047
H	-1.757608	1.761120	-1.248613
H	-1.468835	4.070716	-0.480295
H	-1.568800	3.586532	1.207396
C	-4.179455	0.685515	-0.364367
H	-3.869122	0.443601	-1.392279
H	-5.252341	0.920779	-0.422770
C	-4.049502	-0.583039	0.519606

H -4.442239 -0.358750 1.521113  
H -4.710699 -1.353109 0.094351  
Sum of electronic and zero-point Energies= -965.895267  
Sum of electronic and thermal Energies= -965.874341  
Sum of electronic and thermal Enthalpies= -965.873397  
Sum of electronic and thermal Free Energies= -965.944870

daec[n=2]-4-TS (benzene)

C -3.111212 0.295044 0.053879  
H -4.175536 0.472608 0.185328  
C -2.212776 1.383336 0.112852  
C -0.877679 1.079806 -0.072098  
H -0.128776 1.840307 -0.070658  
C -0.428258 -0.208541 -0.243341  
H 0.632366 -0.332041 -0.309282  
C -1.281993 -1.292085 -0.309372  
O -0.800524 -2.591664 -0.497521  
C -2.668489 -1.029887 -0.169642  
O -3.490079 -2.114375 -0.250396  
C -4.887073 -1.914594 -0.106060  
H -5.341795 -2.904404 -0.210127  
H -5.286509 -1.250652 -0.886971  
H -5.140303 -1.504176 0.882816  
C 3.122997 -2.324427 0.823496  
H 4.093772 -2.111592 1.268402  
C 2.768770 -1.713013 -0.389859  
C 3.609883 -0.595888 -0.998459  
H 3.838960 -0.835729 -2.047610  
H 4.574962 -0.553721 -0.474632  
C 2.978978 0.840774 -0.997413  
H 2.059340 0.826921 -1.599186  
H 3.683513 1.477819 -1.553914  
C 1.522684 -2.043470 -0.947471  
H 1.220120 -1.604722 -1.895725  
C 0.558785 -2.708684 -0.177036  
C 0.918103 -3.322630 1.022238  
H 0.166208 -3.852430 1.601775  
C 2.229137 -3.171895 1.486734  
H 2.526688 -3.649532 2.418320  
C 2.709169 1.506021 0.375927  
H 3.592298 1.337081 1.011597  
H 1.881468 1.002258 0.892053  
C 2.478041 3.050002 0.354633  
C 1.171887 3.648858 -0.251420  
C -0.049998 3.834656 0.712490  
H 0.095668 4.781641 1.250246  
H -0.042436 3.064370 1.493799  
H 0.877166 3.063919 -1.133306  
H 1.418407 4.641959 -0.653238  
H 3.328588 3.492371 -0.185973  
H 2.573638 3.410988 1.389988  
C -1.452007 3.868761 -0.004268  
H -1.892385 4.863890 0.142443  
H -1.299370 3.774377 -1.089142  
C -2.548640 2.838400 0.415096  
H -3.486053 3.126633 -0.083410  
H -2.747022 2.946909 1.494314

Sum of electronic and zero-point Energies= -965.841413  
Sum of electronic and thermal Energies= -965.821705  
Sum of electronic and thermal Enthalpies= -965.820761  
Sum of electronic and thermal Free Energies= -965.887834

daec[n=2]-4-E1 (benzene)

C -1.762231 -1.993331 -0.487347  
H -2.308133 -2.101628 -1.420647  
C -2.445312 -1.529763 0.651375  
C -1.749476 -1.423669 1.859455  
H -2.267379 -1.090027 2.756370  
C -0.371256 -1.656240 1.901869  
H 0.195522 -1.511715 2.818865

C 0.315403 -2.012772 0.748702  
O 1.695549 -2.116203 0.773402  
C -0.385253 -2.243260 -0.454191  
O 0.364007 -2.642726 -1.514004  
C -0.289149 -2.846939 -2.759408  
H 0.491009 -3.171442 -3.453959  
H -0.744680 -1.919312 -3.135659  
H -1.058905 -3.628892 -2.688968  
C 3.974922 1.300828 0.067617  
H 4.592412 2.182353 -0.099068  
C 2.614448 1.331894 -0.279347  
C 2.054115 2.576949 -0.959338  
H 2.429325 2.579374 -1.995433  
H 2.509096 3.461664 -0.489104  
C 0.527003 2.779151 -1.017641  
H 0.052531 1.904353 -1.484181  
H 0.344199 3.614771 -1.710641  
C 1.839849 0.188184 -0.048101  
H 0.786301 0.188781 -0.302195  
C 2.412527 -0.962515 0.511297  
C 3.770768 -0.992789 0.836561  
H 4.194725 -1.895690 1.268652  
C 4.543737 0.147102 0.610988  
H 5.600878 0.135197 0.870895  
C -0.150658 3.107404 0.324621  
H 0.445483 3.879578 0.835068  
H -0.124841 2.230116 0.985297  
C -1.594070 3.642312 0.192872  
C -2.636472 2.680019 -0.413168  
C -2.943612 1.458612 0.466480  
H -3.413589 1.789699 1.406318  
H -1.996690 0.989660 0.756775  
H -2.288866 2.335798 -1.399140  
H -3.564085 3.241231 -0.603866  
H -1.566874 4.557013 -0.419629  
H -1.941094 3.957994 1.189029  
C -3.830093 0.399690 -0.211772  
H -4.862356 0.769014 -0.303193  
H -3.470102 0.239197 -1.239196  
C -3.848205 -0.974255 0.513271  
H -4.490563 -1.662875 -0.054087  
H -4.301673 -0.862453 1.507728

Sum of electronic and zero-point Energies= -965.894720  
Sum of electronic and thermal Energies= -965.873850  
Sum of electronic and thermal Enthalpies= -965.872906  
Sum of electronic and thermal Free Energies= -965.944430

daec[n=2]-4-E2 (benzene)

C -1.628151 -1.934028 0.615430  
H -2.092066 -1.916192 1.597481  
C -2.421072 -1.669342 -0.514127  
C -1.830966 -1.728212 -1.781566  
H -2.433576 -1.557299 -2.671832  
C -0.450990 -1.922339 -1.909049  
H 0.032178 -1.907083 -2.883506  
C 0.343455 -2.067203 -0.778072  
O 1.722299 -2.116842 -0.887926  
C -0.248629 -2.135202 0.500890  
O 0.599137 -2.343162 1.540920  
C 0.060852 -2.344130 2.855939  
H 0.908046 -2.526023 3.523417  
H -0.682087 -3.143846 2.988549  
H -0.395671 -1.375767 3.106723  
C 3.852679 1.327015 0.105995  
H 4.428519 2.211730 0.373848  
C 2.533434 1.471692 -0.352381  
C 1.961056 2.870027 -0.556864  
H 2.310006 3.229912 -1.538440  
H 2.425005 3.544155 0.178154  
C 0.431469 3.061818 -0.508767

H	-0.050391	2.414165	-1.254369
H	0.228421	4.091425	-0.841434
C	1.813152	0.316138	-0.682643
H	0.794023	0.396340	-1.045145
C	2.396737	-0.951177	-0.556991
C	3.716214	-1.087030	-0.121419
H	4.148216	-2.080323	-0.031252
C	4.436846	0.061998	0.207878
H	5.462549	-0.033249	0.560214
C	-0.213544	2.859857	0.872965
H	0.378657	3.413909	1.617777
H	-0.144625	1.803603	1.167401
C	-1.673384	3.355269	0.973077
C	-2.712596	2.639390	0.085453
C	-2.944439	1.167952	0.459903
H	-3.352914	1.107826	1.481745
H	-1.973805	0.660749	0.495315
H	-2.400242	2.697495	-0.968207
H	-3.663497	3.190828	0.145427
H	-1.689591	4.429341	0.730894
H	-1.995103	3.279837	0.203549
C	-3.863042	0.405363	-0.510315
H	-4.901185	0.753600	-0.402632
H	-3.565132	0.640294	-1.543050
C	-3.829709	-1.139065	-0.340144
H	-4.508711	-1.587948	-1.078563
H	-4.214736	-1.410195	0.652833

Sum of electronic and zero-point Energies= -965.894979  
Sum of electronic and thermal Energies= -965.874173  
Sum of electronic and thermal Enthalpies= -965.873229  
Sum of electronic and thermal Free Energies= -965.944170

#### daec[n=2]-5-TS (benzene)

C	-2.943106	-1.116624	0.049643
H	-3.958161	-1.467497	0.217221
C	-2.678114	0.270164	0.059623
C	-1.367884	0.647981	-0.166827
H	-1.098321	1.681141	-0.214852
C	-0.349970	-0.270137	-0.328334
H	0.645250	0.119285	-0.418529
C	-0.584841	-1.631679	-0.349239
O	0.437653	-2.562102	-0.533568
C	-1.922927	-2.067100	-0.169943
O	-2.118030	-3.415159	-0.207702
C	-3.433542	-3.910489	-0.016342
H	-3.355807	-4.999254	-0.092295
H	-4.123700	-3.543576	-0.790408
H	-3.828329	-3.645843	0.975914
C	4.008188	-0.846499	0.747127
H	4.862024	-0.324634	1.177066
C	3.367371	-0.312999	-0.384894
C	3.678238	1.101042	-0.860946
H	3.423808	1.214623	-1.923698
H	4.758181	1.280919	-0.777286
C	2.927357	2.194779	-0.012753
H	3.612693	3.038393	0.148971
H	2.735640	1.775420	0.984639
C	2.298803	-1.036246	-0.933233
H	1.824142	-0.686033	-1.845819
C	1.715366	-2.094131	-0.217567
C	2.355865	-2.618946	0.903455
H	1.906844	-3.454059	1.435063
C	3.538710	-2.016847	1.348230
H	4.054887	-2.425461	2.214965
C	1.599099	2.748532	-0.597396
H	1.085849	1.964104	-1.168991
H	1.826927	3.537657	-1.330093
C	0.620961	3.292882	0.476439
C	-0.744287	3.817885	-0.079718
C	-2.027281	3.462147	0.762772

H	-2.391869	4.382001	1.237747
H	-1.744608	2.804521	1.595367
H	-0.876050	3.441921	-1.104253
H	-0.684820	4.908612	-0.192651
H	1.117504	4.088501	1.051166
H	0.433978	2.484951	1.197747
C	-3.224310	2.815391	-0.028646
H	-4.106284	3.458127	0.092975
H	-2.998142	2.831166	-1.104569
C	-3.684910	1.374718	0.351399
H	-3.941476	1.355275	1.423619
H	-4.629860	1.174889	-0.175942

Sum of electronic and zero-point Energies= -965.845558  
Sum of electronic and thermal Energies= -965.825674  
Sum of electronic and thermal Enthalpies= -965.824730  
Sum of electronic and thermal Free Energies= -965.892391

#### daec[n=2]-5-E1 (benzene)

C	-1.947244	-1.634659	-0.434260
H	-2.434710	-1.815040	-1.388571
C	-2.695078	-1.072001	0.617709
C	-2.069785	-0.873415	1.851968
H	-2.635504	-0.464305	2.686565
C	-0.712359	-1.177228	2.021755
H	-0.214699	-1.012195	2.974742
C	0.033159	-1.677939	0.963422
O	1.373536	-1.979837	1.129413
C	-0.589971	-1.934845	-0.280202
O	0.209247	-2.457537	-1.245240
C	-0.352639	-2.694445	-2.528607
H	0.460528	-3.098035	-3.138713
H	-0.721651	-1.765220	-2.986309
H	-1.169519	-3.429115	-2.483474
C	4.267090	0.627469	-0.351632
H	5.038751	1.289296	-0.742902
C	3.013028	1.155972	-0.002680
C	2.764694	2.653912	-0.167727
H	2.955731	2.923782	-1.218552
H	3.533823	3.188590	0.410022
C	1.380802	3.184301	0.247388
H	1.434738	4.280373	0.312921
H	1.158746	2.839400	1.268037
C	2.041813	0.280206	0.500339
H	1.067893	0.649839	0.798281
C	2.306776	-1.088270	0.627486
C	3.558267	-1.605321	0.291284
H	3.743866	-2.670551	0.401529
C	4.535472	-0.733731	-0.194912
H	5.514589	-1.126301	-0.464212
C	0.230730	2.779789	-0.696755
H	0.395319	1.750321	-1.041647
H	0.262728	3.402859	-1.603446
C	-1.165072	2.851373	-0.048576
C	-2.204871	1.998111	-0.789495
C	-3.560255	1.853885	-0.067802
H	-4.167654	2.752142	-0.249125
H	-3.394333	1.821506	1.019595
H	-1.772728	0.999615	-0.928793
H	-2.372775	2.396008	-1.802857
H	-1.500787	3.896853	0.034571
H	-1.092227	2.474954	0.983518
C	-4.350746	0.595032	-0.496860
H	-5.429120	0.807907	-0.491529
H	-4.100570	0.346306	-1.539020
C	-4.137973	-0.654104	0.400514
H	-4.593352	-0.455585	1.380504
H	-4.704387	-1.488957	-0.038662

Sum of electronic and zero-point Energies= -965.893053  
Sum of electronic and thermal Energies= -965.872076  
Sum of electronic and thermal Enthalpies= -965.871131

Sum of electronic and thermal Free Energies= -965.942600

daec[n=2]-5-E2 (benzene)

C	-1.961826	-1.411569	0.739327
H	-2.478946	-1.289966	1.686710
C	-2.678935	-1.220904	-0.453849
C	-2.016781	-1.414705	-1.672877
H	-2.556177	-1.296135	-2.610834
C	-0.655339	-1.730176	-1.695633
H	-0.125425	-1.862965	-2.636194
C	0.059033	-1.873718	-0.509795
O	1.402153	-2.206531	-0.553755
C	-0.599313	-1.742255	0.729518
O	0.165762	-1.930893	1.835824
C	-0.444840	-1.778532	3.110010
H	0.345577	-1.967181	3.842046
H	-1.256816	-2.504693	3.259227
H	-0.834706	-0.760220	3.253020
C	4.344560	0.737657	-0.390351
H	5.132800	1.488865	-0.364597
C	3.025143	1.106222	-0.081576
C	2.723399	2.559517	0.278542
H	2.873984	3.182261	-0.618310
H	3.492249	2.892378	0.990845
C	1.333858	2.858216	0.872258
H	1.376484	3.826294	1.391456
H	1.116559	2.113195	1.651820
C	2.033251	0.116552	-0.116201
H	1.007362	0.360353	0.127104
C	2.345536	-1.200833	-0.469315
C	3.661595	-1.562664	-0.766887
H	3.884806	-2.592573	-1.033622
C	4.655073	-0.583165	-0.721262
H	5.683665	-0.855692	-0.951504
C	0.182972	2.882003	-0.155292
H	0.349837	2.098544	-0.906144
H	0.208824	3.830221	-0.713121
C	-1.210053	2.667107	0.468180
C	-2.244308	2.145926	-0.540326
C	-3.595713	1.738067	0.081441
H	-4.209424	2.636652	0.238550
H	-3.425765	1.317303	1.084434
H	-1.808032	1.275400	-1.045438
H	-2.417781	2.893596	-1.330154
H	-1.564317	3.591262	0.950869
H	-1.122392	1.922227	1.274492
C	-4.384310	0.713922	-0.767207
H	-5.463950	0.885959	-0.651992
H	-4.165536	0.876985	-1.832860
C	-4.128906	-0.774675	-0.408512
H	-4.525934	-0.958887	0.599579
H	-4.724827	-1.395755	-1.093103

Sum of electronic and zero-point Energies= -965.892669

Sum of electronic and thermal Energies= -965.871660

Sum of electronic and thermal Enthalpies= -965.870716

Sum of electronic and thermal Free Energies= -965.942370

daec[n=2]-6-TS (benzene)

C	-3.144855	-0.307405	0.057069
H	-4.227801	-0.340188	0.145291
C	-2.475530	0.930731	0.181416
C	-1.100767	0.894799	0.048810
H	-0.517061	1.788733	0.097575
C	-0.410216	-0.280694	-0.132413
H	0.655611	-0.212674	-0.163224
C	-1.033944	-1.502717	-0.267900
O	-0.292090	-2.669141	-0.479465
C	-2.448857	-1.517136	-0.181456
O	-3.044355	-2.734302	-0.327957
C	-4.458477	-2.808249	-0.243273

H	-4.711178	-3.862140	-0.394075
H	-4.945194	-2.205622	-1.024359
H	-4.825290	-2.487725	0.743185
C	3.570290	-1.756708	0.789495
H	4.516219	-1.420228	1.211685
C	3.084077	-1.162752	-0.388877
C	3.748799	0.069097	-0.995973
H	3.420895	0.173491	-2.039865
H	4.837655	-0.080650	-1.026834
C	3.499573	1.437187	-0.267634
H	4.100898	2.184079	-0.808359
H	3.919161	1.386708	0.747819
C	1.883536	-1.658892	-0.920933
H	1.490589	-1.239119	-1.844112
C	1.067832	-2.522078	-0.169626
C	1.559162	-3.107846	0.994384
H	0.927863	-3.785635	1.563585
C	2.840173	-2.754809	1.439220
H	3.237781	-3.214387	2.342170
C	2.027810	1.910898	-0.204980
H	1.514758	1.312937	0.553233
H	1.551821	1.675107	-1.168535
C	1.767445	3.412726	0.093756
C	0.339289	3.929565	-0.288931
C	-0.852085	3.820979	0.732544
H	-0.920438	4.776882	1.268832
H	-0.635948	3.082410	1.513562
H	0.053392	3.431735	-1.226583
H	0.436634	4.991316	-0.554650
H	2.487493	4.006450	-0.489390
H	1.984476	3.633728	1.149797
C	-2.251312	3.527517	0.062228
H	-2.895922	4.402207	0.221555
H	-2.113017	3.463014	-1.026344
C	-3.093357	2.286275	0.503887
H	-4.083609	2.376652	0.033557
H	-3.279742	2.347530	1.588976

Sum of electronic and zero-point Energies= -965.840805

Sum of electronic and thermal Energies= -965.820966

Sum of electronic and thermal Enthalpies= -965.820022

Sum of electronic and thermal Free Energies= -965.887500

daec[n=2]-6-E1 (benzene)

C	-2.080958	-1.746403	-0.385182
H	-2.758327	-1.788866	-1.233772
C	-2.544249	-1.208173	0.828384
C	-1.676354	-1.178973	1.924756
H	-2.021227	-0.786615	2.879373
C	-0.346740	-1.585689	1.784298
H	0.349501	-1.518745	2.617301
C	0.128574	-2.033346	0.556908
O	1.471877	-2.344103	0.402595
C	-0.752125	-2.163606	-0.537075
O	-0.212752	-2.647297	-1.687342
C	-1.059911	-2.783403	-2.819791
H	-0.430733	-3.197659	-3.612959
H	-1.460608	-1.812757	-3.146943
H	-1.893032	-3.473194	-2.621668
C	4.092549	0.899191	0.332769
H	4.783804	1.740447	0.337652
C	2.881303	1.003430	-0.369530
C	2.532561	2.276203	-1.123494
H	2.210090	2.020429	-2.144317
H	3.448941	2.871244	-1.233572
C	1.444879	3.176930	-0.479952
H	1.500451	4.162552	-0.966880
H	1.689261	3.343333	0.579852
C	2.014561	-0.099675	-0.364742
H	1.085835	-0.064588	-0.925394
C	2.331754	-1.257180	0.353639

C	3.546872	-1.360870	1.034452
H	3.779949	-2.274775	1.575101
C	4.425422	-0.275822	1.012636
H	5.373837	-0.344302	1.542560
C	0.012180	2.639108	-0.609933
H	-0.056443	1.674204	-0.093610
H	-0.192552	2.432452	-1.673386
C	-1.081028	3.582293	-0.076440
C	-2.505787	3.012381	-0.250316
C	-2.809314	1.820665	0.680733
H	-3.102211	2.192096	1.674984
H	-1.883426	1.257525	0.838587
H	-2.623932	2.695713	-1.298745
H	-3.245525	3.810905	-0.093137
H	-1.011443	4.546528	-0.602760
H	-0.896864	3.801040	0.987389
C	-3.874918	0.843700	0.153979
H	-4.876410	1.295687	0.209783
H	-3.683646	0.653445	-0.912790
C	-3.896092	-0.523587	0.890392
H	-4.673798	-1.154256	0.436178
H	-4.183559	-0.373678	1.940208

Sum of electronic and zero-point Energies= -965.894557  
Sum of electronic and thermal Energies= -965.873586  
Sum of electronic and thermal Enthalpies= -965.872642  
Sum of electronic and thermal Free Energies= -965.944314

#### daec[n=2]-6-E2 (benzene)

C	-1.645080	-1.875852	0.631048
H	-2.050910	-1.896016	1.638463
C	-2.503793	-1.574935	-0.440083
C	-1.984996	-1.584953	-1.739740
H	-2.636535	-1.382301	-2.587914
C	-0.616279	-1.785854	-1.955001
H	-0.192910	-1.747907	-2.956286
C	0.242550	-1.986079	-0.880381
O	1.609695	-2.088467	-1.078605
C	-0.277430	-2.087514	0.428374
O	0.624673	-2.351616	1.408878
C	0.167441	-2.383769	2.753749
H	1.050859	-2.597604	3.362208
H	-0.578530	-3.176562	2.908941
H	-0.257257	-1.416906	3.060109
C	3.911574	1.131510	0.239939
H	4.523656	1.958256	0.597005
C	2.686287	1.399653	-0.389145
C	2.214199	2.831736	-0.582407
H	1.922719	2.982478	-1.633137
H	3.067704	3.499622	-0.404945
C	1.040012	3.297699	0.319134
H	1.002021	4.396759	0.271050
H	1.260847	3.043248	1.366614
C	1.924142	0.312825	-0.846658
H	0.987144	0.485560	-1.366733
C	2.358365	-1.000673	-0.646149
C	3.586885	-1.259851	-0.035572
H	3.906622	-2.289329	0.102735
C	4.360514	-0.183420	0.400050
H	5.318644	-0.372641	0.881062
C	-0.332475	2.735769	-0.080067
H	-0.310475	1.643174	0.007602
H	-0.507019	2.953237	-1.146583
C	-1.518463	3.287771	0.731003
C	-2.877705	2.713249	0.275129
C	-3.067275	1.224829	0.633112
H	-3.405304	1.134888	1.677356
H	-2.090243	0.731892	0.595675
H	-2.954868	2.838166	-0.816409
H	-3.695044	3.310897	0.704431
H	-1.540080	4.384108	0.635566

H	-1.367290	3.077677	1.801913
C	-4.022203	0.452443	-0.293470
H	-5.064698	0.754726	-0.113469
H	-3.799016	0.723133	-1.336129
C	-3.915435	-1.092081	-0.166287
H	-4.622915	-1.550313	-0.871672
H	-4.227091	-1.402595	0.840897

Sum of electronic and zero-point Energies= -965.895139  
Sum of electronic and thermal Energies= -965.874199  
Sum of electronic and thermal Enthalpies= -965.873255  
Sum of electronic and thermal Free Energies= -965.944597

#### daec[n=2]-7-TS (benzene)

C	0.469725	3.125751	-0.174353
H	0.657394	4.193156	-0.282090
C	1.520620	2.189613	-0.202291
C	1.146893	0.865461	-0.039168
H	1.879486	0.087142	-0.012410
C	-0.163372	0.468648	0.074653
H	-0.337846	-0.586271	0.120487
C	-1.213055	1.373166	0.105474
O	-2.538111	0.937018	0.233390
C	-0.880799	2.743305	-0.010295
O	-1.828937	3.735303	-0.044894
C	-2.659515	3.850441	1.113411
H	-3.300771	4.721019	0.940176
H	-2.053048	4.022927	2.015325
H	-3.283861	2.960938	1.257896
C	-2.362077	-3.035592	-0.948042
H	-2.166476	-4.028314	-1.350383
C	-1.801159	-2.667011	0.285332
C	-0.773174	-3.549494	0.989390
H	-0.628244	-4.462426	0.395552
H	-1.177647	-3.879702	1.958590
C	0.616487	-2.900490	1.292943
H	1.136417	-3.588335	1.976813
H	0.452249	-1.984006	1.878081
C	-2.104216	-1.388513	0.781785
H	-1.697446	-1.065636	1.737165
C	-2.692529	-0.428881	-0.052469
C	-3.256020	-0.800958	-1.271568
H	-3.721174	-0.048492	-1.903401
C	-3.134245	-2.131874	-1.685357
H	-3.570609	-2.441205	-2.633098
C	1.588890	-2.571911	0.127592
H	1.107643	-1.910415	-0.603730
H	1.829533	-3.494983	-0.421842
C	2.907995	-1.944741	0.666544
C	3.977480	-1.409517	-0.339066
C	3.865155	-0.003573	-1.012447
H	2.981749	0.037227	-1.660165
H	4.718234	0.063622	-1.703029
H	4.089145	-2.147898	-1.147745
H	4.936611	-1.423306	0.200794
H	3.409354	-2.725582	1.258263
H	2.661909	-1.160660	1.396976
C	3.916724	1.239249	-0.059317
H	4.952781	1.602213	-0.025659
H	3.684115	0.932186	0.970262
C	3.007427	2.456642	-0.411132
H	3.327929	3.315469	0.196670
H	3.185552	2.754437	-1.457189

Sum of electronic and zero-point Energies= -965.843005  
Sum of electronic and thermal Energies= -965.823177  
Sum of electronic and thermal Enthalpies= -965.822232  
Sum of electronic and thermal Free Energies= -965.889867

#### daec[n=2]-7-E1 (benzene)

C	-1.378768	-2.063389	-0.620040
H	-1.805568	-2.212676	-1.609778

C	-2.204921	-1.819331	0.485555
C	-1.601744	-1.675626	1.744612
H	-2.221319	-1.517658	2.625937
C	-0.211785	-1.675650	1.875566
H	0.262775	-1.513249	2.840803
C	0.597327	-1.824819	0.749760
O	1.973502	-1.703730	0.866156
C	0.014752	-2.068332	-0.506464
O	0.766281	-2.207847	-1.642894
C	1.609705	-3.363707	-1.692705
H	2.127856	-3.318284	-2.655787
H	1.009997	-4.284718	-1.646141
H	2.346222	-3.365682	-0.880889
C	3.752865	1.911385	-0.202971
H	4.242284	2.844282	-0.479374
C	2.366138	1.896147	0.021439
C	1.576860	3.192820	-0.127567
H	1.563989	3.474463	-1.192954
H	2.156419	3.984854	0.368355
C	0.132777	3.234005	0.414632
H	-0.117871	4.286454	0.613690
H	0.091925	2.731140	1.392488
C	1.764036	0.685017	0.382560
H	0.699200	0.643317	0.575572
C	2.525860	-0.483937	0.501598
C	3.904589	-0.462233	0.286760
H	4.479399	-1.378568	0.395057
C	4.509249	0.746187	-0.065788
H	5.584098	0.775267	-0.236021
C	-0.950792	2.658019	-0.515561
H	-0.719872	1.614709	-0.767035
H	-0.929089	3.208159	-1.469855
C	-2.361436	2.756676	0.092031
C	-3.492920	2.203198	-0.798770
C	-3.516254	0.668825	-0.949991
H	-2.505638	0.318917	-1.196593
H	-4.143948	0.399668	-1.812854
H	-3.407691	2.659258	-1.796882
H	-4.461190	2.539073	-0.396227
H	-2.574074	3.814572	0.310532
H	-2.370950	2.245085	1.066794
C	-4.038446	-0.079811	0.289816
H	-5.130952	0.035776	0.348964
H	-3.633387	0.376628	1.204084
C	-3.692788	-1.591781	0.315471
H	-4.240858	-2.063561	1.143000
H	-4.045856	-2.066598	-0.610654

Sum of electronic and zero-point Energies= -965.893865  
Sum of electronic and thermal Energies= -965.872795  
Sum of electronic and thermal Enthalpies= -965.871851  
Sum of electronic and thermal Free Energies= -965.943629

#### daec[n=2]-7-E2 (benzene)

C	-1.495032	-2.085572	0.670548
H	-2.005485	-2.232282	1.620701
C	-2.219409	-1.799411	-0.492147
C	-1.514206	-1.662697	-1.697922
H	-2.053476	-1.477935	-2.624831
C	-0.121103	-1.708305	-1.706836
H	0.439408	-1.546081	-2.624938
C	0.593234	-1.902490	-0.523496
O	1.979199	-1.807763	-0.552279
C	-0.094102	-2.149668	0.679222
O	0.493892	-2.365855	1.889163
C	1.704947	-3.125387	1.961778
H	1.747046	-3.511041	2.986240
H	2.588218	-2.507200	1.770035
H	1.690005	-3.968115	1.258712
C	3.716865	1.977595	-0.413133
H	4.193038	2.956869	-0.389721

C	2.384758	1.844995	0.014247
C	1.644361	3.080774	0.515662
H	1.577247	3.806272	-0.310892
H	2.288885	3.563794	1.265061
C	0.243544	2.896866	1.132011
H	0.033815	3.786665	1.744005
H	0.257940	2.052040	1.836762
C	1.797108	0.575130	-0.022967
H	0.775279	0.437705	0.308996
C	2.518670	-0.531733	-0.489013
C	3.845296	-0.397101	-0.901757
H	4.386354	-1.270188	-1.257750
C	4.436562	0.867565	-0.857715
H	5.469600	0.985407	-1.180259
C	-0.915887	2.723744	0.133983
H	-0.738101	1.849202	-0.505384
H	-0.937489	3.592731	-0.543055
C	-2.278787	2.597115	0.837882
C	-3.484641	2.406485	-0.105052
C	-3.565867	1.029451	-0.793977
H	-2.589226	0.791037	-1.234630
H	-4.268257	1.088976	-1.639147
H	-3.454762	3.191154	-0.876486
H	-4.412135	2.578400	0.462890
H	-2.445331	3.503467	1.440220
H	-2.235428	1.766384	1.558621
C	-4.009307	-0.115697	0.134589
H	-5.089290	-0.029811	0.326250
H	-3.517318	-0.019541	1.112692
C	-3.709041	-1.534308	-0.414499
H	-4.189919	-2.273613	0.241159
H	-4.163135	-1.649453	-1.408751

Sum of electronic and zero-point Energies= -965.893954  
Sum of electronic and thermal Energies= -965.872888  
Sum of electronic and thermal Enthalpies= -965.871944  
Sum of electronic and thermal Free Energies= -965.944086

#### daec[n=3]-1-TS (benzene)

C	2.964639	1.349769	0.042967
H	3.956895	1.718946	-0.202740
C	2.765731	-0.036896	0.191203
C	1.478683	-0.455462	0.498234
H	1.252400	-1.497119	0.634093
C	0.423174	0.432596	0.605727
H	-0.549725	0.013359	0.790699
C	0.596391	1.797733	0.434945
O	-0.452130	2.713472	0.491058
C	1.904852	2.270236	0.168996
O	2.030909	3.618409	0.020476
C	3.318375	4.147545	-0.254084
H	3.187192	5.232100	-0.315920
H	4.033443	3.916199	0.549158
H	3.716047	3.778124	-1.211103
C	-4.007536	0.889195	-0.697377
H	-4.866249	0.344361	-1.086333
C	-3.384655	0.464692	0.488247
C	-3.715093	-0.857890	1.163539
H	-4.763263	-0.876069	1.498229
H	-3.103138	-0.952445	2.070595
C	-3.511491	-2.102481	0.247420
H	-4.296618	-2.063607	-0.520863
H	-3.734115	-2.997560	0.847748
C	-2.308716	1.220524	0.969067
H	-1.858583	0.960772	1.922607
C	-1.709384	2.204545	0.173397
C	-2.327976	2.621898	-1.004325
H	-1.866818	3.400344	-1.606795
C	-3.509471	1.986734	-1.405595
H	-4.006971	2.311295	-2.317673
C	-2.163142	-2.298884	-0.497726

H	-1.804030	-1.329008	-0.868992
H	-2.392150	-2.884218	-1.401174
C	-1.001103	-3.031807	0.217399
C	0.123970	-3.369908	-0.795205
C	1.369358	-4.162041	-0.305188
H	1.040852	-4.932011	0.409847
H	1.756502	-4.717401	-1.173190
C	2.576050	-3.409075	0.319446
H	2.277863	-2.917612	1.252722
H	3.297538	-4.176627	0.635630
H	-0.344447	-3.975475	-1.585838
H	0.442703	-2.445409	-1.296469
H	-1.376268	-3.967809	0.660586
H	-0.618104	-2.432957	1.056487
C	3.307867	-2.414741	-0.635555
H	2.648357	-2.146036	-1.471562
H	4.157124	-2.943922	-1.089449
C	3.844358	-1.092073	-0.015059
H	4.349955	-1.315405	0.938747
H	4.624080	-0.685131	-0.674163

Sum of electronic and zero-point Energies= -1005.142906  
Sum of electronic and thermal Energies= -1005.121798  
Sum of electronic and thermal Enthalpies= -1005.120854  
Sum of electronic and thermal Free Energies= -1005.191276

#### daec[n=3]-1-E1 (benzene)

C	1.716919	-1.804205	0.689266
H	2.213144	-1.661301	1.645113
C	2.475155	-1.716410	-0.493328
C	1.839965	-1.936560	-1.718148
H	2.412442	-1.890373	-2.642399
C	0.459767	-2.173251	-1.769561
H	-0.052112	-2.312426	-2.719133
C	-0.291795	-2.191293	-0.602975
O	-1.662364	-2.373674	-0.653211
C	0.340040	-2.037235	0.651522
O	-0.471969	-2.108053	1.737543
C	0.103107	-1.907613	3.021268
H	-0.722287	-1.996887	3.733413
H	0.861056	-2.670946	3.249223
H	0.552143	-0.907881	3.111606
C	-4.163578	0.933723	-0.205886
H	-4.840070	1.780063	-0.096561
C	-2.838044	1.150752	-0.610474
C	-2.328199	2.551238	-0.895064
H	-3.149041	3.144677	-1.321407
H	-1.548656	2.507476	-1.667620
C	-1.787219	3.314388	0.339200
H	-2.566179	3.317471	1.115729
H	-1.642554	4.365694	0.046057
C	-1.989305	0.044129	-0.754837
H	-0.965602	0.192600	-1.085536
C	-2.452673	-1.249741	-0.494310
C	-3.776752	-1.462245	-0.100848
H	-4.118280	-2.476342	0.090456
C	-4.624445	-0.363027	0.040657
H	-5.657378	-0.521750	0.345755
C	-0.475981	2.791991	0.953696
H	-0.606197	1.749823	1.281086
H	-0.282836	3.373711	1.868541
C	0.758838	2.889014	0.040339
C	2.082558	2.665367	0.793202
C	3.326306	2.589792	-0.117958
H	3.258432	3.386094	-0.874543
H	4.226984	2.814453	0.473750
C	3.517475	1.229091	-0.818985
H	2.552207	0.889010	-1.218689
H	4.177176	1.351314	-1.690985
H	2.212150	3.484149	1.516944
H	2.007766	1.745825	1.393879

H	0.786718	3.882778	-0.435247
H	0.672479	2.163677	-0.781322
C	4.107599	0.145583	0.101546
H	3.646285	0.214885	1.096951
H	5.179558	0.342117	0.252181
C	3.932134	-1.302308	-0.416100
H	4.394386	-1.400056	-1.408144
H	4.481683	-1.981119	0.252911

Sum of electronic and zero-point Energies= -1005.183947  
Sum of electronic and thermal Energies= -1005.161854  
Sum of electronic and thermal Enthalpies= -1005.160910  
Sum of electronic and thermal Free Energies= -1005.234765

#### daec[n=3]-1-E2 (benzene)

C	1.728666	-2.093356	-0.513157
H	2.237000	-2.268983	-1.456913
C	2.471401	-1.612732	0.577308
C	1.820111	-1.409027	1.800369
H	2.381739	-1.061503	2.665406
C	0.442354	-1.609205	1.908150
H	-0.083010	-1.421141	2.841810
C	-0.296506	-2.029404	0.807643
O	-1.667568	-2.182081	0.921274
C	0.347548	-2.313095	-0.413113
O	-0.449430	-2.748280	-1.423017
C	0.148257	-3.016506	-2.684236
H	-0.665720	-3.353921	-3.332265
H	0.604179	-2.114186	-3.117091
H	0.906009	-3.809946	-2.612306
C	-4.202915	0.968686	-0.094612
H	-4.888146	1.774708	-0.352438
C	-2.845538	1.076755	-0.429110
C	-2.314588	2.304885	-1.144928
H	-3.124681	2.733859	-1.750658
H	-1.529571	2.005832	-1.852882
C	-1.773425	3.424550	-0.221174
H	-2.551798	3.675812	0.514137
H	-1.631795	4.325856	-0.837392
C	-1.982446	0.022827	-0.094279
H	-0.930962	0.090877	-0.354537
C	-2.465634	-1.114961	0.559641
C	-3.822653	-1.221782	0.882822
H	-4.179586	-2.117364	1.385199
C	-4.682107	-0.174331	0.553097
H	-5.739076	-0.253401	0.801641
C	-0.459034	3.131836	0.525547
H	-0.583385	2.251972	1.173682
H	-0.264869	3.978536	1.202209
C	0.771356	2.931870	-0.376472
C	2.098939	2.931041	0.402096
C	3.332646	2.579838	-0.456675
H	3.260517	3.116963	-1.414539
H	4.241390	2.961457	0.033333
C	3.506708	1.070281	-0.723597
H	2.529155	0.633237	-0.969760
H	4.136196	0.920215	-1.613517
H	2.239439	3.926185	0.850222
H	2.024763	2.229950	1.247409
H	0.805375	3.733178	-1.132448
H	0.671967	1.992081	-0.938750
C	4.131687	0.308886	0.459522
H	3.712951	0.682929	1.404439
H	5.209775	0.524750	0.499000
C	3.928741	-1.225479	0.415552
H	4.320534	-1.624718	-0.530522
H	4.526175	-1.679806	1.219099

Sum of electronic and zero-point Energies= -1005.183488  
Sum of electronic and thermal Energies= -1005.161358  
Sum of electronic and thermal Enthalpies= -1005.160414  
Sum of electronic and thermal Free Energies= -1005.234517



## daec[n=3]-2-TS (benzene)

C	2.375108	2.145878	-0.089687
H	3.224942	2.800351	0.086119
C	2.571929	0.750512	-0.091455
C	1.454442	-0.041582	-0.314692
H	1.533819	-1.112675	-0.326002
C	0.193523	0.501997	-0.494277
H	-0.629683	-0.178257	-0.629221
C	-0.021736	1.870249	-0.453118
O	-1.293471	2.430436	-0.559654
C	1.098904	2.715702	-0.268229
O	0.838925	4.052676	-0.249027
C	1.926186	4.945818	-0.067256
H	2.671833	4.848044	-0.870109
H	2.418965	4.796483	0.904954
H	1.494690	5.950818	-0.099206
C	-4.018981	-0.264780	1.064088
H	-4.632098	-1.020002	1.553378
C	-3.475856	-0.530555	-0.201644
C	-3.592695	-1.903949	-0.848334
H	-4.156625	-1.829719	-1.790715
H	-4.180745	-2.557880	-0.189815
C	-2.229977	-2.581514	-1.172228
H	-1.692981	-1.954544	-1.899757
H	-2.441111	-3.524976	-1.697387
C	-2.705794	0.472969	-0.810261
H	-2.297360	0.319745	-1.806041
C	-2.317438	1.606428	-0.089234
C	-2.870728	1.872024	1.164278
H	-2.571786	2.767713	1.702825
C	-3.757972	0.944769	1.716943
H	-4.198214	1.138074	2.693385
C	-1.297742	-2.859766	0.026163
H	-1.760764	-3.607217	0.689103
H	-1.200402	-1.946602	0.629594
C	0.116877	-3.334371	-0.386197
C	1.117033	-3.391318	0.791839
C	2.601633	-3.668828	0.432326
H	2.639033	-4.524879	-0.258946
H	3.109196	-4.007254	1.348808
C	3.448829	-2.519792	-0.177884
H	4.397813	-2.958883	-0.518802
H	2.972208	-2.149007	-1.093623
H	0.787480	-4.185079	1.479129
H	1.045485	-2.460023	1.371861
H	0.495576	-2.664531	-1.172001
H	0.053398	-4.328548	-0.855374
C	3.777127	-1.349377	0.797030
H	4.721231	-1.588361	1.305929
H	3.019869	-1.298773	1.591247
C	3.909502	0.070172	0.175272
H	4.497663	0.007408	-0.755120
H	4.501895	0.699544	0.854566

Sum of electronic and zero-point Energies= -1005.152626

Sum of electronic and thermal Energies= -1005.131623

Sum of electronic and thermal Enthalpies= -1005.130679

Sum of electronic and thermal Free Energies= -1005.200722

## daec[n=3]-2-E1 (benzene)

C	1.625519	2.032328	-0.532227
H	2.229873	2.183103	-1.422010
C	2.265992	1.711775	0.675627
C	1.484777	1.535800	1.825235
H	1.961379	1.304738	2.776141
C	0.095006	1.651221	1.761481
H	-0.520486	1.515881	2.648073
C	-0.535196	1.944128	0.555517
O	-1.909630	2.100445	0.508323
C	0.229287	2.149772	-0.610055

O	-0.466562	2.439518	-1.740254
C	0.261247	2.643994	-2.943348
H	0.826079	1.746016	-3.233431
H	0.950019	3.497143	-2.860745
H	-0.488124	2.860239	-3.710248
C	-4.429489	-1.208352	0.341506
H	-5.109716	-2.058333	0.306919
C	-3.083899	-1.383658	-0.022044
C	-2.617418	-2.764552	-0.473245
H	-3.323393	-3.115411	-1.240384
H	-2.735715	-3.467752	0.366837
C	-1.187882	-2.884359	-1.030790
H	-1.005397	-2.062812	-1.739606
H	-1.129121	-3.805973	-1.627856
C	-2.229551	-0.274482	0.027519
H	-1.187027	-0.369642	-0.252865
C	-2.706990	0.975984	0.438746
C	-4.048257	1.146267	0.788954
H	-4.397315	2.127463	1.100491
C	-4.903308	0.044148	0.735142
H	-5.950217	0.166360	1.007704
C	-0.069176	-2.917378	0.026504
H	-0.129315	-3.864418	0.585588
H	-0.223641	-2.121189	0.768343
C	1.328734	-2.756397	-0.588463
C	2.473604	-2.777743	0.437742
C	3.832620	-2.332099	-0.140802
H	4.012608	-2.874900	-1.081257
H	4.640091	-2.636466	0.542621
C	3.936341	-0.814751	-0.397651
H	4.756066	-0.614582	-1.103598
H	3.020949	-0.471528	-0.898614
H	2.568085	-3.793453	0.850081
H	2.207761	-2.131972	1.288409
H	1.349783	-1.807051	-1.143993
H	1.498518	-3.545781	-1.338214
C	4.166730	0.017975	0.876743
H	5.227162	-0.043734	1.162448
H	3.601417	-0.412113	1.715331
C	3.768530	1.507483	0.738673
H	4.244093	1.934966	-0.155384
H	4.171793	2.058862	1.600084

Sum of electronic and zero-point Energies= -1005.182460

Sum of electronic and thermal Energies= -1005.160213

Sum of electronic and thermal Enthalpies= -1005.159269

Sum of electronic and thermal Free Energies= -1005.234322

## daec[n=3]-2-E2 (benzene)

C	1.441186	1.967442	0.605392
H	1.890050	2.042158	1.592018
C	2.280879	1.820053	-0.515044
C	1.699965	1.756735	-1.784270
H	2.330462	1.658122	-2.665672
C	0.306782	1.802109	-1.932172
H	-0.156187	1.742001	-2.914498
C	-0.516201	1.915161	-0.819680
O	-1.887225	1.999141	-0.977485
C	0.051540	2.019638	0.471355
O	-0.827808	2.163195	1.496098
C	-0.315409	2.223189	2.819946
H	0.334373	3.098685	2.963049
H	0.238962	1.309975	3.080374
H	-1.188603	2.312864	3.472449
C	-4.343426	-1.145146	0.211946
H	-5.006597	-1.952594	0.519757
C	-3.008113	-1.433778	-0.116383
C	-2.530019	-2.881538	-0.056295
H	-3.213520	-3.481211	-0.675988
H	-2.672394	-3.255709	0.970102
C	-1.086194	-3.171562	-0.501944

H	-0.895108	-2.670564	-1.462707
H	-1.002483	-4.247911	-0.711110
C	-2.177557	-0.377996	-0.512801
H	-1.144803	-0.561048	-0.787768
C	-2.666106	0.932729	-0.566187
C	-3.996308	1.212236	-0.251464
H	-4.353493	2.237386	-0.304733
C	-4.829655	0.161013	0.136395
H	-5.868766	0.367416	0.387235
C	0.005276	-2.784186	0.512285
H	-0.054257	-3.458324	1.381312
H	-0.182581	-1.773852	0.902392
C	1.416637	-2.826599	-0.091755
C	2.533846	-2.452856	0.896516
C	3.901724	-2.211516	0.224708
H	4.112018	-3.047312	-0.459793
H	4.695074	-2.239383	0.987406
C	3.994574	-0.880391	-0.549140
H	4.829799	-0.926111	-1.263582
H	3.088960	-0.752218	-1.157473
H	2.631685	-3.251482	1.647088
H	2.235054	-1.552252	1.454521
H	1.441285	-2.141659	-0.952251
H	1.616059	-3.829677	-0.501620
C	4.183328	0.351844	0.354379
H	5.235370	0.412926	0.669752
H	3.598259	0.233804	1.277459
C	3.778797	1.689785	-0.309820
H	4.293910	1.792693	-1.275102
H	4.134452	2.516399	0.322676

Sum of electronic and zero-point Energies= -1005.183351  
Sum of electronic and thermal Energies= -1005.161178  
Sum of electronic and thermal Enthalpies= -1005.160234  
Sum of electronic and thermal Free Energies= -1005.234393

#### daec[n=3]-3-TS (benzene)

C	3.155057	1.099003	-0.023248
H	4.187513	1.420161	0.087893
C	2.861226	-0.280486	-0.060006
C	1.529832	-0.631939	-0.208028
H	1.245142	-1.662095	-0.289189
C	0.514040	0.311612	-0.253233
H	-0.499738	-0.050145	-0.295675
C	0.788989	1.669041	-0.232051
O	-0.186868	2.654589	-0.300903
C	2.145277	2.072248	-0.127528
O	2.361778	3.417307	-0.118671
C	3.697262	3.881380	-0.002252
H	4.158077	3.563755	0.944954
H	3.635770	4.973645	-0.022177
H	4.321653	3.540176	-0.841263
C	-4.028533	1.258544	0.538417
H	-4.992319	0.845007	0.831026
C	-3.328155	0.703819	-0.546296
C	-3.782225	-0.570406	-1.241419
H	-3.106549	-0.774820	-2.082631
H	-4.782366	-0.432793	-1.679233
C	-3.861540	-1.815147	-0.310216
H	-4.194017	-2.666774	-0.923172
H	-4.671350	-1.636353	0.411783
C	-2.109742	1.289225	-0.910868
H	-1.578504	0.916166	-1.781653
C	-1.503494	2.255759	-0.097688
C	-2.201818	2.801948	0.978330
H	-1.729703	3.564946	1.591923
C	-3.485594	2.322364	1.263298
H	-4.042642	2.749746	2.094994
C	-2.608530	-2.224514	0.500840
H	-2.949207	-2.908142	1.293672
H	-2.215396	-1.342058	1.026691

C	-1.453516	-2.917673	-0.252047
C	-0.296171	-3.314249	0.696703
C	0.984463	-3.854173	-0.006553
H	0.996619	-3.494318	-1.045284
H	0.912652	-4.946842	-0.093792
C	2.343775	-3.475263	0.681185
H	2.775545	-4.381349	1.125366
H	2.143429	-2.808337	1.530278
H	-0.662489	-4.055835	1.422091
H	-0.033249	-2.429995	1.293349
H	-1.060357	-2.252323	-1.035858
H	-1.833487	-3.809207	-0.775396
C	3.426091	-2.817714	-0.245359
H	3.071472	-2.824139	-1.286078
H	4.324385	-3.449352	-0.239851
C	3.901205	-1.379867	0.103139
H	4.780739	-1.153453	-0.518560
H	4.271703	-1.371509	1.141675

Sum of electronic and zero-point Energies= -1005.145937  
Sum of electronic and thermal Energies= -1005.124796  
Sum of electronic and thermal Enthalpies= -1005.123852  
Sum of electronic and thermal Free Energies= -1005.194324

#### daec[n=3]-3-E1 (benzene)

C	-2.336385	-1.601234	-0.432341
H	-2.955155	-1.780201	-1.307451
C	-2.881669	-0.890730	0.652505
C	-2.087107	-0.683247	1.785369
H	-2.496726	-0.160362	2.646988
C	-0.767824	-1.145730	1.822960
H	-0.144719	-0.991119	2.701039
C	-0.226867	-1.823945	0.737279
O	1.055588	-2.340119	0.810056
C	-1.015949	-2.069531	-0.407384
O	-0.410967	-2.753356	-1.413051
C	-1.164071	-3.027758	-2.586376
H	-2.044439	-3.648713	-2.366300
H	-0.490932	-3.580054	-3.248415
H	-1.485825	-2.103248	-3.087622
C	4.409382	0.022075	0.077061
H	5.303537	0.615133	-0.108707
C	3.177188	0.443663	-0.443434
C	3.077744	1.717564	-1.263135
H	2.296996	1.598931	-2.025851
H	4.019386	1.858017	-1.811771
C	2.810841	3.010007	-0.450093
H	2.861783	3.859104	-1.149054
H	3.635151	3.150825	0.264451
C	2.038891	-0.341432	-0.200154
H	1.077501	-0.041067	-0.606025
C	2.132502	-1.517812	0.549179
C	3.366340	-1.938145	1.057304
H	3.417189	-2.860445	1.630504
C	4.499060	-1.161411	0.815735
H	5.461925	-1.484592	1.207603
C	1.478395	3.063013	0.317540
H	1.446368	4.000413	0.893938
H	1.456542	2.251500	1.059508
C	0.221221	2.961669	-0.559572
C	-1.093876	2.943934	0.243127
C	-2.232756	2.240232	-0.507811
H	-1.891187	1.226975	-0.756611
H	-2.415164	2.739393	-1.472888
C	-3.559132	2.145722	0.271463
H	-4.099643	3.098956	0.182559
H	-3.347486	2.024235	1.344443
H	-1.385335	3.968555	0.521528
H	-0.928705	2.406924	1.189516
H	0.271924	2.038278	-1.153378
H	0.206370	3.784359	-1.291637

C	-4.466957	0.986870	-0.200192
H	-4.298457	0.803867	-1.272015
H	-5.523624	1.275036	-0.106499
C	-4.293892	-0.339636	0.586363
H	-4.962308	-1.091034	0.141432
H	-4.652413	-0.176702	1.612322

Sum of electronic and zero-point Energies= -1005.180862  
Sum of electronic and thermal Energies= -1005.158580  
Sum of electronic and thermal Enthalpies= -1005.157636  
Sum of electronic and thermal Free Energies= -1005.232491

daec[n=3]-3-E2 (benzene)

C	-2.104329	-1.347210	0.726554
H	-2.546845	-1.159548	1.700496
C	-2.897676	-1.184092	-0.422956
C	-2.334144	-1.470047	-1.672047
H	-2.934096	-1.372463	-2.575051
C	-0.996372	-1.869290	-1.772989
H	-0.547842	-2.092692	-2.738432
C	-0.208190	-1.994678	-0.633918
O	1.093670	-2.451167	-0.734895
C	-0.766502	-1.749365	0.639371
O	0.063601	-1.934675	1.698183
C	-0.450295	-1.718268	3.005118
H	-0.776590	-0.677873	3.146367
H	0.377367	-1.930513	3.687945
H	-1.286553	-2.396571	3.227897
C	4.328710	0.111475	-0.147782
H	5.194109	0.757322	-0.006707
C	3.127386	0.655822	-0.625882
C	3.019078	2.134869	-0.950705
H	2.286687	2.276693	-1.756157
H	3.982247	2.481002	-1.351069
C	2.652306	3.049320	0.245573
H	2.691943	4.091534	-0.107004
H	3.435561	2.954750	1.012072
C	2.029814	-0.198914	-0.811547
H	1.095020	0.195043	-1.200391
C	2.130927	-1.561979	-0.519520
C	3.332922	-2.100931	-0.053125
H	3.390119	-3.165145	0.160518
C	4.427170	-1.255074	0.129865
H	5.367190	-1.668077	0.491769
C	1.286736	2.785354	0.902864
H	1.181533	3.458909	1.767444
H	1.275432	1.764079	1.311228
C	0.074030	2.956172	-0.024915
C	-1.270176	2.632959	0.655848
C	-2.346299	2.173280	-0.337532
H	-1.946284	1.314315	-0.891532
H	-2.526191	2.957204	-1.090253
C	-3.687361	1.775865	0.309273
H	-4.262245	2.685425	0.535486
H	-3.498733	1.296659	1.282161
H	-1.621948	3.499496	1.236994
H	-1.114165	1.823361	1.385200
H	0.189170	2.290619	-0.891527
H	0.054449	3.978117	-0.434825
C	-4.539388	0.827969	-0.565005
H	-4.349394	1.040997	-1.627431
H	-5.607820	1.029921	-0.402996
C	-4.325180	-0.685077	-0.295183
H	-4.970319	-1.248058	-0.984811
H	-4.688980	-0.906736	0.718157

Sum of electronic and zero-point Energies= -1005.181371  
Sum of electronic and thermal Energies= -1005.159173  
Sum of electronic and thermal Enthalpies= -1005.158229  
Sum of electronic and thermal Free Energies= -1005.232160

daec[n=3]-4-TS (benzene)

C	3.276579	-0.432431	-0.097935
H	4.359829	-0.489786	-0.028287
C	2.646272	0.825352	0.008967
C	1.262660	0.838399	-0.083193
H	0.713789	1.758461	-0.031314
C	0.526023	-0.324206	-0.224480
H	-0.544673	-0.237072	-0.241606
C	1.127492	-1.565935	-0.321180
O	0.392066	-2.740758	-0.448524
C	2.541869	-1.622580	-0.271368
O	3.091840	-2.864874	-0.375068
C	4.504858	-2.980301	-0.324966
H	4.720812	-4.046970	-0.438462
H	4.988196	-2.425774	-1.142934
H	4.908507	-2.631916	0.637364
C	-3.502887	-2.129771	0.914016
H	-4.482894	-1.902877	1.331496
C	-3.102284	-1.519943	-0.287156
C	-3.947771	-0.442010	-0.946984
H	-5.005713	-0.739260	-0.915844
H	-3.676879	-0.367693	-2.009717
C	-3.846518	0.979394	-0.311079
H	-4.163194	0.927566	0.741191
H	-4.592951	1.606198	-0.822730
C	-1.849053	-1.863401	-0.813257
H	-1.523438	-1.435032	-1.758207
C	-0.947188	-2.637222	-0.069328
C	-1.353215	-3.242682	1.118470
H	-0.648385	-3.853620	1.676761
C	-2.652555	-3.011758	1.584676
H	-2.983176	-3.487102	2.506295
C	-2.468052	1.667651	-0.406220
H	-2.064019	1.512974	-1.419168
H	-1.773388	1.174850	0.283815
C	-2.471484	3.186968	-0.119443
C	-1.125329	3.896663	-0.430009
C	-0.024172	3.812006	0.659682
H	-0.125857	2.867056	1.208183
H	-0.198066	4.592309	1.414866
C	1.426526	3.946483	0.102307
H	1.659362	5.015122	-0.002522
H	1.450991	3.551679	-0.922655
H	-1.325155	4.955817	-0.647586
H	-0.733655	3.475613	-1.368826
H	-2.765520	3.373370	0.925229
H	-3.253156	3.651424	-0.739504
C	2.555194	3.255225	0.940084
H	2.128262	2.837330	1.862965
H	3.271975	4.020705	1.265835
C	3.381942	2.140670	0.232144
H	4.283520	1.950066	0.832403
H	3.750195	2.532210	-0.730787

Sum of electronic and zero-point Energies= -1005.148636  
Sum of electronic and thermal Energies= -1005.127347  
Sum of electronic and thermal Enthalpies= -1005.126403  
Sum of electronic and thermal Free Energies= -1005.197627

daec[n=3]-4-E1 (benzene)

C	1.920111	-1.756758	-0.724913
H	2.490515	-1.741352	-1.649305
C	2.569726	-1.429150	0.475998
C	1.834845	-1.465182	1.667992
H	2.318206	-1.236123	2.615521
C	0.474181	-1.776634	1.648935
H	-0.109038	-1.793958	2.566981
C	-0.171905	-2.068778	0.450604
O	-1.519542	-2.398147	0.455188
C	0.556129	-2.082300	-0.754894
O	-0.145869	-2.390371	-1.878531
C	0.551049	-2.431914	-3.116319

H	-0.193885	-2.711978	-3.866769
H	0.975484	-1.451499	-3.377331
H	1.352571	-3.184383	-3.104079
C	-4.292813	0.709718	0.634087
H	-5.024047	1.513787	0.700503
C	-3.186225	0.849212	-0.217750
C	-2.990982	2.111571	-1.037662
H	-3.954946	2.632351	-1.114704
H	-2.703077	1.841947	-2.064963
C	-1.942315	3.106651	-0.479019
H	-2.180114	3.331032	0.571785
H	-2.052425	4.053917	-1.028832
C	-2.263576	-0.204806	-0.291915
H	-1.419428	-0.142679	-0.971088
C	-2.424740	-1.350438	0.491821
C	-3.536771	-1.490921	1.325948
H	-3.649381	-2.397077	1.915915
C	-4.470859	-0.455113	1.385806
H	-5.339922	-0.554209	2.033828
C	-0.487475	2.629374	-0.591724
H	-0.271909	2.387196	-1.645863
H	-0.370101	1.693897	-0.032047
C	0.546134	3.651179	-0.093454
C	2.009818	3.222652	-0.314485
C	2.419986	1.944654	0.434187
H	1.786620	1.110437	0.113999
H	2.224072	2.079300	1.510255
C	3.898975	1.572214	0.238151
H	4.514829	2.437977	0.527412
H	4.099713	1.409589	-0.833277
H	2.670566	4.048189	-0.006880
H	2.184047	3.082807	-1.393805
H	0.380565	3.843100	0.978628
H	0.379520	4.612790	-0.603384
C	4.391624	0.349670	1.039844
H	4.034392	0.426972	2.077582
H	5.488995	0.395749	1.098546
C	4.039276	-1.046561	0.472489
H	4.599246	-1.791116	1.059311
H	4.427055	-1.118563	-0.553554

Sum of electronic and zero-point Energies= -1005.182538  
Sum of electronic and thermal Energies= -1005.160202  
Sum of electronic and thermal Enthalpies= -1005.159258  
Sum of electronic and thermal Free Energies= -1005.234230

daec[n=3]-4-E2 (benzene)

C	1.804144	-1.806294	0.445938
H	2.305730	-1.874220	1.406763
C	2.547752	-1.434621	-0.689771
C	1.898858	-1.379897	-1.926320
H	2.457973	-1.110146	-2.820158
C	0.527789	-1.652484	-2.025850
H	0.013919	-1.605731	-2.983368
C	-0.209089	-1.972803	-0.893646
O	-1.562333	-2.250430	-0.986304
C	0.434551	-2.069925	0.361847
O	-0.358710	-2.417504	1.408427
C	0.225119	-2.482013	2.702000
H	-0.587782	-2.753842	3.381488
H	1.010919	-3.249554	2.753880
H	0.641934	-1.511135	3.006481
C	-4.263967	0.626784	0.359235
H	-4.981911	1.363260	0.716862
C	-3.143057	1.050745	-0.369944
C	-2.918654	2.523138	-0.665097
H	-3.867743	3.056601	-0.520245
H	-2.654729	2.648204	-1.726189
C	-1.832914	3.220077	0.193490
H	-2.045440	3.045573	1.259089
H	-1.927312	4.305207	0.034233

C	-2.239054	0.078674	-0.826456
H	-1.377385	0.371583	-1.418789
C	-2.437017	-1.272689	-0.534691
C	-3.562570	-1.691030	0.178303
H	-3.697782	-2.749153	0.386040
C	-4.474797	-0.731350	0.618312
H	-5.354832	-1.045162	1.177085
C	-0.393689	2.792048	-0.126800
H	-0.209558	2.935498	-1.204550
H	-0.286651	1.717403	0.061838
C	0.678625	3.554025	0.667105
C	2.124257	3.203115	0.263889
C	2.506773	1.732323	0.491190
H	1.846135	1.085593	-0.095854
H	2.326236	1.473962	1.547556
C	3.971196	1.418130	0.143782
H	4.617434	2.107385	0.709339
H	4.154455	1.642353	-0.919376
H	2.815918	3.847757	0.828494
H	2.273103	3.456718	-0.798142
H	0.542857	3.358835	1.742930
H	0.527723	4.636518	0.533579
C	4.432121	-0.022525	0.447469
H	4.092699	-0.307723	1.454803
H	5.530999	-0.030197	0.493028
C	4.028007	-1.116774	-0.569255
H	4.565673	-2.037148	-0.291477
H	4.409464	-0.834908	-1.560704

Sum of electronic and zero-point Energies= -1005.183155  
Sum of electronic and thermal Energies= -1005.160854  
Sum of electronic and thermal Enthalpies= -1005.159909  
Sum of electronic and thermal Free Energies= -1005.234483

daec[n=3]-5-TS (benzene)

C	2.109827	2.592475	-0.192856
H	2.795064	3.427071	-0.053625
C	2.568145	1.268257	-0.215999
C	1.601022	0.286951	-0.390946
H	1.894297	-0.742085	-0.435578
C	0.256867	0.575170	-0.482047
H	-0.420730	-0.257232	-0.553726
C	-0.212056	1.885939	-0.462039
O	-1.572635	2.185759	-0.574596
C	0.742380	2.919623	-0.329018
O	0.438736	4.255363	-0.356334
C	-0.600851	4.731367	0.501754
H	-0.510683	4.302249	1.510182
H	-1.594984	4.510399	0.099403
H	-0.463408	5.816550	0.562311
C	-3.890132	-1.032275	0.723183
H	-4.411310	-1.894490	1.135916
C	-3.120729	-1.172005	-0.444615
C	-2.828417	-2.528183	-1.069575
H	-2.228618	-2.378122	-1.977142
H	-3.762622	-3.008504	-1.397592
C	-2.114368	-3.535545	-0.119806
H	-1.975021	-4.472394	-0.680439
H	-2.818398	-3.778410	0.689049
C	-2.501315	-0.027299	-0.961622
H	-1.949616	-0.091739	-1.895366
C	-2.450125	1.158975	-0.218278
C	-3.210549	1.292017	0.941877
H	-3.179700	2.220498	1.506254
C	-3.967856	0.198454	1.379550
H	-4.574984	0.294397	2.277725
C	-0.774113	-3.137967	0.548950
H	-0.621196	-3.834792	1.387463
H	-0.878420	-2.145292	1.010692
C	0.504596	-3.159604	-0.316481
C	1.786889	-2.882361	0.511774

C	3.063818	-2.634644	-0.335801
H	2.801845	-2.120735	-1.271311
H	3.457323	-3.609259	-0.661675
C	4.241055	-1.892422	0.357367
H	5.082215	-1.890602	-0.353238
H	4.572507	-2.523667	1.196662
H	1.966543	-3.727167	1.193649
H	1.595713	-2.019758	1.163939
H	0.425666	-2.413040	-1.120992
H	0.595371	-4.134459	-0.820708
C	4.113655	-0.453046	0.945607
H	3.296842	-0.417495	1.679136
H	5.033359	-0.316428	1.531912
C	3.996526	0.794993	0.004161
H	4.585879	1.614135	0.437193
H	4.472652	0.568179	-0.963506

Sum of electronic and zero-point Energies= -1005.141364  
Sum of electronic and thermal Energies= -1005.120028  
Sum of electronic and thermal Enthalpies= -1005.119084  
Sum of electronic and thermal Free Energies= -1005.190537

#### daec[n=3]-5-E1 (benzene)

C	1.932613	1.811819	-0.618258
H	2.478456	1.978628	-1.544960
C	2.579872	1.282594	0.505084
C	1.827736	1.111472	1.679365
H	2.307403	0.734497	2.580783
C	0.465874	1.407488	1.705730
H	-0.123033	1.256453	2.607804
C	-0.174530	1.890414	0.562876
O	-1.534915	2.163421	0.602520
C	0.565491	2.119228	-0.608273
O	-0.014864	2.553320	-1.771266
C	-0.573595	3.871558	-1.740396
H	0.200074	4.616444	-1.502166
H	-1.392956	3.949125	-1.016803
H	-0.956878	4.059851	-2.748367
C	-4.270124	-0.958869	0.198655
H	-5.002570	-1.758804	0.102060
C	-2.992686	-1.116965	-0.358585
C	-2.606101	-2.390357	-1.086864
H	-1.950248	-2.141259	-1.931666
H	-3.509424	-2.838921	-1.522662
C	-1.921799	-3.466593	-0.205970
H	-1.793733	-4.368988	-0.823446
H	-2.611930	-3.744639	0.604244
C	-2.069144	-0.069039	-0.229159
H	-1.082618	-0.161593	-0.672185
C	-2.411195	1.100504	0.453486
C	-3.688470	1.259317	0.998644
H	-3.936001	2.181056	1.519264
C	-4.612654	0.222504	0.863372
H	-5.610021	0.337961	1.284009
C	-0.565583	-3.082838	0.412751
H	-0.241855	-3.909568	1.063909
H	-0.698131	-2.213945	1.073562
C	0.551425	-2.776040	-0.596985
C	1.893102	-2.422748	0.066993
C	2.914071	-1.844677	-0.924586
H	2.497884	-0.928674	-1.366934
H	3.038212	-2.551195	-1.760477
C	4.310429	-1.555902	-0.343431
H	4.963744	-1.218235	-1.163342
H	4.743927	-2.504488	0.010791
H	2.311245	-3.317894	0.555070
H	1.709497	-1.694146	0.868800
H	0.249140	-1.936223	-1.239131
H	0.688025	-3.635274	-1.273165
C	4.418059	-0.537678	0.809350
H	3.823061	-0.874200	1.669661

H	5.463226	-0.548718	1.151105
C	4.057769	0.932691	0.476313
H	4.572783	1.573947	1.207676
H	4.477591	1.197576	-0.504150

Sum of electronic and zero-point Energies= -1005.180013  
Sum of electronic and thermal Energies= -1005.157640  
Sum of electronic and thermal Enthalpies= -1005.156696  
Sum of electronic and thermal Free Energies= -1005.231663

#### daec[n=3]-5-E2 (benzene)

C	1.772481	1.601391	0.699760
H	2.183722	1.555355	1.706278
C	2.591688	1.396849	-0.422272
C	2.006808	1.508110	-1.690885
H	2.620357	1.376535	-2.580467
C	0.638323	1.762287	-1.834808
H	0.180019	1.825306	-2.819225
C	-0.168760	1.912127	-0.709550
O	-1.526979	2.148570	-0.852393
C	0.405867	1.852747	0.574572
O	-0.357442	1.967724	1.707817
C	-0.875515	3.276793	1.966394
H	-1.506583	3.634017	1.143822
H	-0.057356	3.992559	2.135989
H	-1.476460	3.191855	2.877289
C	-4.241951	-0.927835	-0.100137
H	-4.970324	-1.714182	0.091543
C	-2.933051	-1.269689	-0.469945
C	-2.509273	-2.720243	-0.604823
H	-1.822048	-2.820211	-1.455780
H	-3.391865	-3.325755	-0.852696
C	-1.852965	-3.336092	0.657035
H	-1.704225	-4.409438	0.462148
H	-2.568607	-3.271435	1.489806
C	-2.015724	-0.238253	-0.720548
H	-1.002545	-0.479188	-1.026550
C	-2.394744	1.099460	-0.589756
C	-3.704019	1.436918	-0.236264
H	-3.984762	2.484230	-0.157932
C	-4.621056	0.413715	0.006967
H	-5.643054	0.667393	0.282988
C	-0.517453	-2.716167	1.106090
H	-0.208313	-3.212781	2.038844
H	-0.673352	-1.659423	1.366453
C	0.625988	-2.816958	0.084191
C	1.948975	-2.213962	0.587093
C	2.980508	-2.021881	-0.535065
H	2.559597	-1.341893	-1.289180
H	3.131105	-2.984163	-1.049631
C	4.360944	-1.509921	-0.083893
H	5.026228	-1.485975	-0.961414
H	4.800141	-2.251264	0.602123
H	2.370861	-2.854844	1.377882
H	1.738219	-1.244584	1.059254
H	0.338869	-2.300647	-0.843369
H	0.782650	-3.870672	-0.197588
C	4.429952	-0.135965	0.612524
H	3.813737	-0.141074	1.522229
H	5.465001	-0.002097	0.959048
C	4.071634	1.101399	-0.248310
H	4.541521	1.978726	0.222094
H	4.540877	1.004316	-1.237570

Sum of electronic and zero-point Energies= -1005.180211  
Sum of electronic and thermal Energies= -1005.157860  
Sum of electronic and thermal Enthalpies= -1005.156916  
Sum of electronic and thermal Free Energies= -1005.231544

#### daec[n=4]-1-TS (benzene)

C	-0.120014	3.340209	-0.104315
H	-0.078168	4.389861	-0.383374

C	1.057369	2.569481	-0.171556
C	0.965186	1.229758	0.189105
H	1.831994	0.586661	0.163099
C	-0.245184	0.662380	0.572295
H	-0.252445	-0.386226	0.821167
C	-1.419141	1.401987	0.594072
O	-2.661980	0.858023	0.906983
C	-1.352429	2.778694	0.269305
O	-2.529896	3.459836	0.319904
C	-2.520932	4.841268	-0.004539
H	-3.554427	5.180944	0.112511
H	-2.200577	5.014252	-1.042674
H	-1.873994	5.415019	0.675271
C	-3.200497	-2.888074	-0.854728
H	-3.275240	-3.831227	-1.394052
C	-2.270893	-2.750737	0.186074
C	-1.165449	-3.759386	0.438288
H	-1.528940	-4.793358	0.360019
H	-0.781315	-3.633471	1.460300
C	-0.012463	-3.539751	-0.587475
H	0.083297	-2.463944	-0.786304
H	-0.322657	-3.985218	-1.542757
C	-2.222118	-1.530693	0.874094
H	-1.572017	-1.434018	1.737917
C	-2.914645	-0.413520	0.400393
C	-3.841701	-0.552595	-0.634781
H	-4.392811	0.318936	-0.978679
C	-4.007765	-1.807661	-1.228435
H	-4.733808	-1.927900	-2.030480
C	1.364538	-4.103161	-0.168253
H	1.214822	-5.019241	0.422827
H	1.913183	-4.417657	-1.068585
C	3.914328	-1.164044	0.632317
C	2.263102	-3.130105	0.629546
H	3.053049	-3.715493	1.124626
H	1.681677	-2.670679	1.445224
C	4.691065	-0.033839	-0.112181
H	4.713495	-0.250596	-1.190742
C	2.941701	-2.022150	-0.205105
H	2.181768	-1.386991	-0.682335
H	3.502090	-2.490800	-1.029560
H	5.738310	-0.087874	0.212877
C	4.196817	1.426860	0.116629
H	5.064492	2.064662	0.336716
H	3.587085	1.458740	1.028852
H	4.647933	-1.851964	1.078316
H	3.372420	-0.729483	1.486159
C	3.424990	2.076505	-1.063099
H	2.919167	1.303798	-1.658081
H	4.153817	2.539426	-1.742704
C	2.381787	3.145109	-0.658194
H	2.182841	3.798085	-1.520456
H	2.814041	3.803667	0.113057

Sum of electronic and zero-point Energies= -1044.434652  
Sum of electronic and thermal Energies= -1044.411859  
Sum of electronic and thermal Enthalpies= -1044.410915  
Sum of electronic and thermal Free Energies= -1044.486222

#### daec[n=4]-1-E1 (benzene)

C	-1.334466	2.377699	0.693693
H	-1.868534	2.350835	1.639308
C	-2.070630	2.391550	-0.505873
C	-1.378872	2.451977	-1.718630
H	-1.930197	2.475953	-2.656454
C	0.021194	2.447917	-1.739486
H	0.569611	2.470546	-2.678512
C	0.740274	2.380601	-0.554081
O	2.123821	2.355766	-0.577332
C	0.063948	2.366990	0.686289
O	0.852046	2.323761	1.791171

C	0.223626	2.267924	3.064408
H	1.036785	2.231269	3.795024
H	-0.398232	1.367171	3.169903
H	-0.390560	3.160434	3.252216
C	4.166154	-1.272804	-0.314161
H	4.724538	-2.205504	-0.252541
C	2.778696	-1.302823	-0.501134
C	2.007747	-2.605983	-0.587008
H	2.672565	-3.413525	-0.924947
H	1.225506	-2.506092	-1.351967
C	1.362730	-3.011226	0.757112
H	0.814740	-2.150846	1.165052
H	2.165100	-3.221298	1.479272
C	2.079638	-0.088675	-0.584462
H	1.005142	-0.100109	-0.744068
C	2.752436	1.130405	-0.475980
C	4.139979	1.157199	-0.291718
H	4.646532	2.115954	-0.214621
C	4.836181	-0.047857	-0.213113
H	5.915557	-0.031505	-0.072052
C	0.430914	-4.235266	0.676525
H	0.990458	-5.085753	0.257033
H	0.161549	-4.528738	1.702949
C	-3.148014	-2.861309	-0.335288
C	-0.867954	-4.048842	-0.134208
H	-1.412279	-5.005911	-0.131865
H	-0.629788	-3.846889	-1.189551
C	-3.993350	-1.638949	0.077436
H	-3.984461	-1.555874	1.176167
C	-1.795603	-2.943481	0.393474
H	-1.284747	-1.973522	0.321253
H	-1.980793	-3.105894	1.467739
H	-5.044331	-1.803560	-0.203092
C	-3.505842	-0.317270	-0.541609
H	-3.749410	-0.309073	-1.615866
H	-2.410614	-0.268297	-0.483542
H	-3.714456	-3.783649	-0.137236
H	-2.981127	-2.836580	-1.424052
C	-4.084105	0.935780	0.130620
H	-3.834142	0.909641	1.202131
H	-5.183156	0.920924	0.076198
C	-3.583202	2.270161	-0.473451
H	-4.017465	3.098730	0.105980
H	-3.969611	2.372628	-1.496694

Sum of electronic and zero-point Energies= -1044.471037  
Sum of electronic and thermal Energies= -1044.447458  
Sum of electronic and thermal Enthalpies= -1044.446514  
Sum of electronic and thermal Free Energies= -1044.524375

#### daec[n=4]-1-E2 (benzene)

C	-1.177832	2.563937	-0.650974
H	-1.641341	2.696563	-1.624397
C	-2.002018	2.439733	0.479902
C	-1.403009	2.289747	1.736442
H	-2.020241	2.213443	2.629615
C	-0.012595	2.198846	1.850088
H	0.464483	2.050954	2.816314
C	0.794185	2.273212	0.720059
O	2.168067	2.166059	0.847529
C	0.217133	2.491990	-0.547955
O	1.083652	2.585718	-1.589249
C	0.551582	2.762919	-2.895039
H	1.415861	2.806200	-3.563984
H	-0.016247	3.700897	-2.976629
H	-0.090777	1.920075	-3.188556
C	4.113751	-1.407782	-0.074158
H	4.647020	-2.327667	-0.308349
C	2.718326	-1.365847	-0.178946
C	1.904833	-2.579134	-0.588385
H	2.551655	-3.308267	-1.096309

H	1.150837	-2.267692	-1.324820
C	1.202640	-3.267329	0.602982
H	0.668008	-2.509247	1.191404
H	1.972957	-3.674469	1.273989
C	2.051486	-0.168461	0.124191
H	0.968928	-0.125780	0.046037
C	2.764427	0.964620	0.520398
C	4.160394	0.920040	0.622180
H	4.698563	1.813379	0.929052
C	4.823889	-0.268808	0.324445
H	5.909227	-0.306925	0.400531
C	0.235641	-4.400107	0.209494
H	0.785102	-5.155663	-0.373352
H	-0.088713	-4.907831	1.130956
C	-3.242947	-2.679118	-0.600804
C	-1.018532	-3.980248	-0.584073
H	-1.597127	-4.888556	-0.813216
H	-0.726226	-3.562547	-1.559521
C	-4.063298	-1.535496	0.030321
H	-4.112637	-1.690931	1.119908
C	-1.928060	-2.976119	0.140865
H	-1.380252	-2.037281	0.300196
H	-2.165765	-3.358703	1.146586
H	-5.102137	-1.584855	-0.328827
C	-3.493357	-0.137329	-0.263342
H	-3.642264	0.095696	-1.330026
H	-2.406858	-0.146507	-0.107064
H	-3.850774	-3.596037	-0.625661
H	-3.026399	-2.431797	-1.652556
C	-4.098947	0.978780	0.599053
H	-3.945732	0.730779	1.660075
H	-5.188438	1.022140	0.449294
C	-3.510338	2.384715	0.323161
H	-3.986332	3.101489	1.007980
H	-3.782246	2.698338	-0.694344

Sum of electronic and zero-point Energies= -1044.471085  
Sum of electronic and thermal Energies= -1044.447504  
Sum of electronic and thermal Enthalpies= -1044.446560  
Sum of electronic and thermal Free Energies= -1044.524227

#### daec[n=4]-2-TS (benzene)

C	2.907448	1.812307	0.030219
H	3.853357	2.305635	0.237935
C	2.884922	0.409554	-0.111541
C	1.656082	-0.178990	-0.383141
H	1.568610	-1.242424	-0.536441
C	0.486065	0.569671	-0.460429
H	-0.438170	0.037189	-0.616279
C	0.499223	1.949258	-0.319667
O	-0.627190	2.755740	-0.391251
C	1.743309	2.587417	-0.084111
O	1.700101	3.943475	0.033216
C	2.913629	4.633424	0.287005
H	3.644575	4.483216	-0.521240
H	3.363189	4.328726	1.243759
H	2.648279	5.693739	0.337662
C	-4.255354	0.895837	0.498586
H	-5.164646	0.376982	0.797440
C	-3.498459	0.416676	-0.582975
C	-3.803825	-0.906899	-1.263972
H	-3.098500	-1.051391	-2.093357
H	-4.807851	-0.888603	-1.713913
C	-3.752276	-2.124869	-0.299855
H	-3.964850	-3.031054	-0.887146
H	-4.594233	-2.022474	0.399586
C	-2.353805	1.131083	-0.956145
H	-1.800026	0.824022	-1.837771
C	-1.866300	2.174670	-0.160352
C	-2.620287	2.645294	0.915136
H	-2.240718	3.469737	1.513206

C	-3.835681	2.020709	1.213584
H	-4.435322	2.387852	2.044466
C	-2.476160	-2.346595	0.547930
H	-2.140847	-1.386675	0.965892
H	-2.776092	-2.952226	1.416641
C	0.953422	-4.346540	0.480995
C	-1.279299	-3.069064	-0.109167
H	-0.850967	-2.459777	-0.919466
H	-1.635286	-3.998435	-0.581957
C	2.095451	-3.699459	-0.331101
H	1.665981	-3.121203	-1.162849
C	-0.198980	-3.420712	0.940314
H	-0.709670	-3.922757	1.776188
H	0.209258	-2.491486	1.364846
H	2.682788	-4.496096	-0.812215
C	3.058453	-2.809493	0.489777
H	3.666511	-3.458124	1.136751
H	2.481165	-2.177854	1.176130
H	0.523424	-5.171151	-0.108048
H	1.391233	-4.818211	1.374310
C	3.993284	-1.919101	-0.384033
H	4.998837	-2.360268	-0.404813
H	3.645449	-1.933239	-1.427174
C	4.135376	-0.443556	0.058209
H	4.449529	-0.413229	1.114646
H	4.964278	0.012118	-0.504101

Sum of electronic and zero-point Energies= -1044.441719  
Sum of electronic and thermal Energies= -1044.419145  
Sum of electronic and thermal Enthalpies= -1044.418200  
Sum of electronic and thermal Free Energies= -1044.492382

#### daec[n=4]-2-E1 (benzene)

C	-1.175516	-2.630097	-0.502932
H	-1.571953	-2.953984	-1.461486
C	-2.073899	-2.272667	0.518794
C	-1.562106	-1.884411	1.760843
H	-2.240911	-1.625146	2.570683
C	-0.180551	-1.780266	1.955907
H	0.230325	-1.444060	2.905119
C	0.699052	-2.078829	0.923839
O	2.061183	-1.949529	1.126869
C	0.208374	-2.547717	-0.314264
O	1.146000	-2.858149	-1.246147
C	0.705346	-3.296380	-2.524138
H	0.109016	-2.525443	-3.033253
H	0.119417	-4.224083	-2.453699
H	1.614230	-3.487804	-3.101661
C	4.116342	1.418536	-0.219148
H	4.680805	2.283201	-0.564879
C	2.750048	1.314783	-0.519172
C	2.050147	2.400483	-1.316336
H	1.191279	1.970544	-1.849043
H	2.739723	2.764289	-2.091013
C	1.586930	3.621247	-0.483369
H	1.337745	4.435600	-1.180978
H	2.440467	3.978377	0.110935
C	2.043956	0.187859	-0.073173
H	0.986850	0.093221	-0.302658
C	2.692739	-0.817709	0.652185
C	4.056310	-0.711025	0.944656
H	4.541550	-1.505923	1.505450
C	4.758473	0.411593	0.507075
H	5.820690	0.496699	0.729888
C	0.387189	3.389090	0.452529
H	0.593025	2.536430	1.116796
H	0.294930	4.267142	1.110152
C	-3.531843	2.957322	0.055941
C	-0.958743	3.173065	-0.261633
H	-0.922653	2.248110	-0.854880
H	-1.120766	3.990208	-0.983535

C	-3.780207	1.635421	-0.696991
H	-3.076482	1.548046	-1.538741
C	-2.146721	3.121755	0.713047
H	-2.156925	4.054347	1.298158
H	-1.981452	2.316937	1.444450
H	-4.783128	1.677238	-1.149563
C	-3.666498	0.380611	0.180628
H	-4.359294	0.462718	1.033833
H	-2.659277	0.336930	0.613148
H	-3.694470	3.793932	-0.641320
H	-4.299494	3.064175	0.838167
C	-3.939026	-0.930401	-0.572363
H	-5.002577	-0.988543	-0.848115
H	-3.376007	-0.929868	-1.518147
C	-3.559190	-2.204961	0.224393
H	-4.125170	-2.228947	1.166066
H	-3.870576	-3.086712	-0.353566

Sum of electronic and zero-point Energies= -1044.470416  
Sum of electronic and thermal Energies= -1044.446923  
Sum of electronic and thermal Enthalpies= -1044.445979  
Sum of electronic and thermal Free Energies= -1044.523441

#### daec[n=4]-2-E2 (benzene)

C	-1.500112	-2.103431	0.755273
H	-2.072836	-1.900044	1.655485
C	-2.184300	-2.268791	-0.461705
C	-1.447888	-2.564986	-1.614160
H	-1.960506	-2.718913	-2.561983
C	-0.051422	-2.628870	-1.565566
H	0.534498	-2.834747	-2.458548
C	0.620813	-2.399620	-0.370986
O	2.003016	-2.436917	-0.327827
C	-0.102948	-2.160927	0.816304
O	0.638903	-1.981408	1.939404
C	-0.038484	-1.697861	3.155748
H	-0.710811	-2.518150	3.445721
H	-0.611250	-0.761188	3.091706
H	0.743709	-1.589520	3.912603
C	4.198421	1.107185	-0.372483
H	4.800764	2.014138	-0.395031
C	2.857240	1.151980	-0.783152
C	2.239127	2.452765	-1.263940
H	1.345986	2.234721	-1.864429
H	2.949365	2.947873	-1.941690
C	1.880955	3.455492	-0.140531
H	1.680525	4.433055	-0.605326
H	2.767766	3.595884	0.494377
C	2.104795	-0.030839	-0.757841
H	1.070270	-0.016712	-1.088682
C	2.681437	-1.233108	-0.331716
C	4.018918	-1.273207	0.071628
H	4.447330	-2.218353	0.395282
C	4.768974	-0.096900	0.048450
H	5.812027	-0.123094	0.359192
C	0.684482	3.076878	0.750436
H	0.838632	2.071778	1.171171
H	0.671216	3.764847	1.609892
C	-3.264095	3.039678	0.419677
C	-0.688046	3.140109	0.057055
H	-0.742652	2.380159	-0.735398
H	-0.795008	4.113989	-0.447950
C	-3.634993	1.936767	-0.591351
H	-2.978649	2.000220	-1.472433
C	-1.855416	2.955747	1.040445
H	-1.779768	3.731482	1.818087
H	-1.736745	1.997594	1.568287
H	-4.652693	2.135171	-0.961804
C	-3.565305	0.513275	-0.020112
H	-4.182252	0.450468	0.891338
H	-2.535138	0.308549	0.296183

H	-3.377978	4.018896	-0.070785
H	-4.001371	3.025626	1.237561
C	-4.006457	-0.577462	-1.007612
H	-5.089707	-0.501420	-1.184873
H	-3.521838	-0.407011	-1.980764
C	-3.677352	-2.020057	-0.543171
H	-4.144856	-2.203426	0.434801
H	-4.133439	-2.728166	-1.248753

Sum of electronic and zero-point Energies= -1044.470389  
Sum of electronic and thermal Energies= -1044.446894  
Sum of electronic and thermal Enthalpies= -1044.445950  
Sum of electronic and thermal Free Energies= -1044.523416

#### daec[n=4]-3-TS (benzene)

C	2.718556	2.048329	-0.086400
H	3.624915	2.635872	0.035890
C	2.818370	0.644212	-0.168802
C	1.636727	-0.066982	-0.328485
H	1.648987	-1.140093	-0.427959
C	0.396335	0.564041	-0.353018
H	-0.483969	-0.055871	-0.419154
C	0.290382	1.944512	-0.277681
O	-0.906908	2.641825	-0.304951
C	1.481040	2.705522	-0.155063
O	1.314481	4.055718	-0.093092
C	2.469571	4.867787	0.044609
H	3.156811	4.746148	-0.805747
H	3.008505	4.654473	0.979655
H	2.106927	5.899849	0.067601
C	-4.362821	0.486309	0.606185
H	-5.232013	-0.099049	0.901802
C	-3.579306	0.073199	-0.483904
C	-3.814290	-1.251738	-1.188565
H	-3.145563	-1.318019	-2.057118
H	-4.839307	-1.297123	-1.585762
C	-3.618340	-2.491477	-0.272342
H	-3.806243	-3.390754	-0.878589
H	-4.412530	-2.473315	0.487949
C	-2.487713	0.868367	-0.853526
H	-1.909456	0.603782	-1.733654
C	-2.083869	1.949073	-0.059946
C	-2.865216	2.354231	1.022531
H	-2.550496	3.207032	1.618480
C	-4.024409	1.633672	1.327851
H	-4.644936	1.949048	2.164640
C	-2.270620	-2.643341	0.467769
H	-2.037394	-1.705964	0.993484
H	-2.417532	-3.394677	1.258818
C	1.463290	-3.718558	-0.292108
C	-1.050822	-3.075706	-0.368931
H	-0.841828	-2.332107	-1.153505
H	-1.284290	-4.013797	-0.897511
C	2.780628	-3.757487	0.521973
H	3.524719	-4.331008	-0.052354
C	0.213869	-3.272468	0.494941
H	0.002253	-4.020382	1.275380
H	0.420515	-2.335581	1.031320
H	2.601040	-4.338050	1.439895
C	3.409360	-2.399754	0.918554
H	4.176890	-2.588612	1.683422
H	2.654991	-1.777479	1.415476
H	1.279587	-4.728121	-0.690117
H	1.591687	-3.080948	-1.179819
C	4.069536	-1.620624	-0.248999
H	3.547067	-1.831900	-1.192605
H	5.089719	-2.003978	-0.391183
C	4.151592	-0.087267	-0.066226
H	4.847008	0.319418	-0.816340
H	4.612248	0.137747	0.909456

Sum of electronic and zero-point Energies= -1044.448087



Sum of electronic and thermal Energies= -1044.425773  
Sum of electronic and thermal Enthalpies= -1044.424829  
Sum of electronic and thermal Free Energies= -1044.497892

daec[n=4]-3-E1 (benzene)

C	1.526379	2.216928	-0.669619
H	1.952843	2.396357	-1.652892
C	2.388805	1.906550	0.397736
C	1.838862	1.702423	1.667631
H	2.488323	1.487315	2.513466
C	0.453561	1.760513	1.857355
H	0.012893	1.592248	2.837316
C	-0.394044	2.040344	0.792597
O	-1.752833	2.154402	1.022207
C	0.141315	2.299149	-0.488124
O	-0.758430	2.604747	-1.458761
C	-0.273780	2.859882	-2.770086
H	0.239784	1.982959	-3.190169
H	0.405436	3.724330	-2.788819
H	-1.157555	3.083046	-3.374534
C	-4.470044	-0.838020	0.012483
H	-5.204132	-1.601299	-0.240827
C	-3.133714	-1.004864	-0.377343
C	-2.702880	-2.245153	-1.138169
H	-1.921359	-1.978808	-1.862466
H	-3.555118	-2.608031	-1.728967
C	-2.207997	-3.414752	-0.250173
H	-2.117767	-4.308851	-0.886203
H	-2.988539	-3.642045	0.490382
C	-2.202890	-0.005630	-0.049429
H	-1.165385	-0.116808	-0.350181
C	-2.604716	1.135018	0.651841
C	-3.941472	1.298629	1.032665
H	-4.231006	2.196575	1.572726
C	-4.866060	0.306987	0.710195
H	-5.907236	0.431639	1.002705
C	-0.874503	-3.182974	0.481982
H	-0.942866	-2.265067	1.083816
H	-0.725691	-4.002832	1.201125
C	2.879319	-2.642283	-0.599297
C	0.356099	-3.101601	-0.435818
H	0.197004	-2.335610	-1.209838
H	0.472727	-4.054920	-0.975944
C	4.172918	-2.208288	0.118844
H	5.021178	-2.315187	-0.575120
C	1.652094	-2.768404	0.317901
H	1.845283	-3.539244	1.081162
H	1.498997	-1.829039	0.868204
H	4.368544	-2.909655	0.944463
C	4.158317	-0.773007	0.680373
H	5.003390	-0.650302	1.374765
H	3.253274	-0.631311	1.284982
H	3.058192	-3.610803	-1.090949
H	2.649984	-1.935280	-1.411197
C	4.241047	0.330392	-0.387895
H	3.579352	0.094011	-1.233135
H	5.261891	0.358993	-0.797286
C	3.873465	1.741632	0.136495
H	4.197606	2.486932	-0.603213
H	4.439575	1.946673	1.056194

Sum of electronic and zero-point Energies= -1044.470400  
Sum of electronic and thermal Energies= -1044.446958  
Sum of electronic and thermal Enthalpies= -1044.446014  
Sum of electronic and thermal Free Energies= -1044.523186

daec[n=4]-3-E2 (benzene)

C	1.721358	1.917360	0.611401
H	2.280084	1.829804	1.538432
C	2.417453	1.876086	-0.609845
C	1.696419	2.032467	-1.799313

H	2.218131	2.020638	-2.754543
C	0.308046	2.199580	-1.773250
H	-0.260249	2.329140	-2.691605
C	-0.377290	2.205383	-0.563931
O	-1.741378	2.431846	-0.533490
C	0.329778	2.071988	0.650352
O	-0.420277	2.110765	1.781666
C	0.237707	1.959501	3.031913
H	0.962416	2.767349	3.208909
H	0.747697	0.988128	3.106173
H	-0.549602	2.011027	3.789460
C	-4.482829	-0.682507	-0.151381
H	-5.225595	-1.474021	-0.063845
C	-3.196308	-0.987335	-0.619550
C	-2.831452	-2.411001	-0.997215
H	-2.055311	-2.397093	-1.773856
H	-3.709339	-2.891768	-1.451006
C	-2.365663	-3.293977	0.186921
H	-2.300090	-4.333946	-0.168301
H	-3.149523	-3.281612	0.958169
C	-2.256712	0.049059	-0.735946
H	-1.260022	-0.163915	-1.113100
C	-2.600479	1.360099	-0.390632
C	-3.886370	1.659120	0.069932
H	-4.130716	2.686622	0.326923
C	-4.820919	0.630805	0.186942
H	-5.824362	0.858299	0.542667
C	-1.026407	-2.894561	0.829780
H	-1.072821	-1.840869	1.142401
H	-0.897202	-3.478062	1.754222
C	2.746987	-2.773206	-0.306899
C	0.206749	-3.105871	-0.063292
H	0.079396	-2.565378	-1.013200
H	0.287677	-4.171715	-0.330740
C	4.049480	-2.226370	0.311447
H	4.901158	-2.526808	-0.318381
C	1.510890	-2.634180	0.596109
H	1.676717	-3.196154	1.529402
H	1.383664	-1.583339	0.893284
H	4.207459	-2.714808	1.285304
C	4.082618	-0.698096	0.509104
H	4.904550	-0.439807	1.193977
H	3.161951	-0.382422	1.016181
H	2.892659	-3.836366	-0.552078
H	2.550451	-2.270253	-1.266036
C	4.259138	0.108073	-0.789163
H	3.638736	-0.316234	-1.590845
H	5.301743	0.015242	-1.127816
C	3.910712	1.612431	-0.650714
H	4.343345	2.152580	-1.503744
H	4.392793	2.015763	0.251566

Sum of electronic and zero-point Energies= -1044.470360  
Sum of electronic and thermal Energies= -1044.446831  
Sum of electronic and thermal Enthalpies= -1044.445886  
Sum of electronic and thermal Free Energies= -1044.523572

daec[n=4]-4-TS (benzene)

C	-1.087030	-3.251371	0.017568
H	-1.297329	-4.315461	-0.052248
C	0.252054	-2.813466	-0.044823
C	0.472183	-1.446146	0.059803
H	1.472359	-1.043910	0.065173
C	-0.576871	-0.541117	0.169154
H	-0.334816	0.508139	0.189033
C	-1.896033	-0.961144	0.242853
O	-2.980442	-0.104634	0.379347
C	-2.156204	-2.353164	0.175339
O	-3.466471	-2.714910	0.260854
C	-3.788168	-4.095114	0.195125
H	-4.877052	-4.151708	0.286947

H	-3.327266	-4.660286	1.018684
H	-3.484212	-4.539352	-0.764368
C	-2.209610	3.854869	-0.695598
H	-1.951065	4.848452	-1.058699
C	-1.472795	3.282431	0.350276
C	-0.159224	3.867471	0.843779
H	-0.030531	3.647494	1.913376
H	-0.143465	4.960450	0.736278
C	1.015655	3.230892	0.046089
H	1.004926	3.628713	-0.979805
H	0.807131	2.160011	-0.054410
C	-1.846904	2.009366	0.807910
H	-1.323653	1.572184	1.653806
C	-2.780955	1.243344	0.104020
C	-3.516865	1.819083	-0.934968
H	-4.260678	1.222487	-1.456915
C	-3.251882	3.141984	-1.299487
H	-3.826018	3.600382	-2.102565
C	2.419780	3.393449	0.651089
H	2.711026	4.454417	0.631757
H	2.392927	3.104750	1.713944
C	4.543194	0.208148	-0.472703
C	3.512732	2.559695	-0.062982
H	4.493689	2.876027	0.323153
H	3.517041	2.804745	-1.136863
C	4.545011	-1.289584	-0.076423
H	4.410849	-1.346942	1.014513
C	3.381283	1.033314	0.119648
H	2.436476	0.697885	-0.325313
H	3.308842	0.815227	1.975555
H	5.549012	-1.694467	-0.266404
C	3.490084	-2.199631	-0.772223
H	3.971308	-2.764540	-1.583473
H	2.740426	-1.578045	-1.273010
H	5.491251	0.648738	-0.127416
H	4.548036	0.305537	-1.569709
C	2.802350	-3.201674	0.195729
H	3.486588	-4.045869	0.362292
H	2.677833	-2.726276	1.179137
C	1.425855	-3.768348	-0.235485
H	1.232514	-4.689574	0.333091
H	1.473302	-4.082576	-1.291297

Sum of electronic and zero-point Energies= -1044.441261  
Sum of electronic and thermal Energies= -1044.418512  
Sum of electronic and thermal Enthalpies= -1044.417568  
Sum of electronic and thermal Free Energies= -1044.492563

#### daec[n=4]-4-E1 (benzene)

C	-0.930352	-2.378125	0.774285
H	-1.408074	-2.355771	1.749550
C	-1.724534	-2.594503	-0.365344
C	-1.100484	-2.648895	-1.616877
H	-1.691451	-2.833544	-2.512174
C	0.280479	-2.452295	-1.731255
H	0.774483	-2.482864	-2.699802
C	1.054657	-2.207273	-0.602675
O	2.424263	-2.050053	-0.722251
C	0.452656	-2.188389	0.674440
O	1.288358	-1.975733	1.723607
C	0.728525	-1.908232	3.027719
H	1.568778	-1.719259	3.701941
H	0.244480	-2.854460	3.309395
H	0.003064	-1.086556	3.114607
C	4.166231	1.685360	-0.087845
H	4.642399	2.649077	0.084899
C	2.817886	1.634399	-0.461873
C	1.987341	2.892947	-0.646824
H	1.653107	2.948658	-1.694821
H	2.614828	3.779065	-0.478821
C	0.741606	2.944460	0.261432

H	1.057466	3.022277	1.312472
H	0.220254	1.982724	0.180050
C	2.226701	0.379323	-0.679618
H	1.186389	0.314602	-0.986699
C	2.960779	-0.794248	-0.506235
C	4.311406	-0.739666	-0.144529
H	4.866421	-1.665935	-0.019680
C	4.904849	0.504953	0.059379
H	5.953820	0.555896	0.346171
C	-0.239363	4.083064	-0.071934
H	0.171337	5.038537	0.286134
H	-0.327022	4.182200	-1.165619
C	-3.764318	2.358138	0.448282
C	-1.647659	3.863578	0.519458
H	-2.215273	4.805323	0.479252
H	-1.557341	3.607969	1.587270
C	-4.376893	1.086376	-0.175046
H	-4.362041	1.184934	-1.272212
C	-2.434507	2.761680	-0.209464
H	-1.799917	1.869959	-0.296514
H	-2.631426	3.086692	-1.243456
H	-5.437366	1.007238	0.106813
C	-3.645331	-0.204681	0.234408
H	-3.863324	-0.420546	1.292820
H	-2.560893	-0.044492	0.179138
H	-4.478713	3.191125	0.368929
H	-3.608707	2.192980	1.526413
C	-3.998546	-1.427283	-0.622876
H	-5.077761	-1.632998	-0.556361
H	-3.794218	-1.196109	-1.679259
C	-3.231986	-2.716230	-0.235950
H	-3.589813	-3.536362	-0.874472
H	-3.489309	-2.990821	0.796843

Sum of electronic and zero-point Energies= -1044.470423  
Sum of electronic and thermal Energies= -1044.446791  
Sum of electronic and thermal Enthalpies= -1044.445847  
Sum of electronic and thermal Free Energies= -1044.523633

#### daec[n=4]-4-E2 (benzene)

C	-0.906120	-2.716691	-0.503341
H	-1.424982	-3.045040	-1.399735
C	-1.648901	-2.501706	0.671783
C	-0.974148	-2.097012	1.828187
H	-1.527670	-1.938001	2.751388
C	0.407775	-1.882540	1.805315
H	0.939821	-1.560613	2.697730
C	1.131140	-2.070529	0.633816
O	2.503858	-1.887351	0.626606
C	0.477958	-2.504943	-0.539528
O	1.266136	-2.673926	-1.632797
C	0.655407	-3.107503	-2.840267
H	1.464046	-3.176505	-3.573638
H	-0.095136	-2.387169	-3.196927
H	0.186918	-4.095553	-2.724768
C	4.134414	1.919263	0.146808
H	4.582383	2.905763	0.040319
C	2.788725	1.728047	-0.188653
C	1.928639	2.862525	-0.719897
H	1.631484	2.628481	-1.754495
H	2.526314	3.782816	-0.776000
C	0.649501	3.111851	0.104649
H	0.923446	3.464280	1.110093
H	0.145607	2.149471	0.256824
C	2.231960	0.446855	-0.041298
H	1.192230	0.274526	-0.303038
C	3.000111	-0.612852	0.443083
C	4.349226	-0.420075	0.766055
H	4.931639	-1.259723	1.137040
C	4.906214	0.847840	0.612439
H	5.952939	1.005474	0.866766

C	-0.335891	4.102609	-0.542974
H	0.028499	5.130292	-0.399220
H	-0.357203	3.939159	-1.632271
C	-3.845288	2.411850	0.156333
C	-1.773191	3.973269	0.003547
H	-2.358851	4.859255	-0.284035
H	-1.744828	3.970720	1.104753
C	-4.387086	1.012060	-0.201666
H	-4.294756	0.863152	-1.289486
C	-2.485202	2.705864	-0.497207
H	-1.825091	1.842518	-0.340384
H	-2.621830	2.779990	-1.587910
H	-5.463564	0.961005	0.019170
C	-3.663216	-0.128691	0.536730
H	-3.970038	-0.124400	1.594783
H	-2.582333	0.062579	0.539880
H	-4.571021	3.180091	-0.149715
H	-3.756145	2.496200	1.251053
C	-3.907063	-1.519319	-0.064245
H	-4.983280	-1.749474	-0.054946
H	-3.605415	-1.509718	-1.122856
C	-3.158030	-2.663123	0.662154
H	-3.426140	-3.614477	0.180051
H	-3.518606	-2.727189	1.698170

Sum of electronic and zero-point Energies= -1044.469833  
Sum of electronic and thermal Energies= -1044.446150  
Sum of electronic and thermal Enthalpies= -1044.445206  
Sum of electronic and thermal Free Energies= -1044.523569

#### daec[n=5]-1-TS (benzene)

C	2.901044	1.986167	-0.249376
H	3.829137	2.527277	-0.087664
C	2.960142	0.611710	-0.542632
C	1.753371	-0.056997	-0.746854
H	1.745705	-1.109185	-1.007260
C	0.528247	0.601176	-0.625921
H	-0.380748	0.029364	-0.749154
C	0.471138	1.962262	-0.342697
O	-0.684337	2.710695	-0.225778
C	1.682467	2.671495	-0.159708
O	1.558203	3.999465	0.112888
C	2.742017	4.756092	0.311742
H	3.385344	4.748546	-0.580514
H	2.410824	5.780714	0.505905
H	3.317114	4.393856	1.176799
C	-4.389229	1.009374	0.660432
H	-5.346013	0.565362	0.929899
C	-3.694195	0.541181	-0.465573
C	-4.186323	-0.649366	-1.268597
H	-3.511687	-0.806628	-2.120307
H	-5.176912	-0.436868	-1.697773
C	-4.301211	-1.955126	-0.439326
H	-5.136328	-1.840641	0.266827
C	-3.058719	-2.376956	0.368622
H	-3.361964	-3.187992	1.048315
H	-2.754561	-1.543984	1.018590
C	-1.838288	-2.861413	-0.433374
H	-1.530725	-2.097491	-1.163919
H	-2.116808	-3.749650	-1.022882
H	-4.594953	-2.767091	-1.121824
C	-2.477411	1.150089	-0.801273
H	-1.966530	0.849446	-1.710726
C	-1.908973	2.121273	0.031455
C	-2.604422	2.578791	1.153088
H	-2.155230	3.346723	1.777413
C	-3.855956	2.032958	1.447360
H	-4.406528	2.392610	2.314689
C	1.743559	-4.131345	0.728051
C	-0.648921	-3.199123	0.484487
H	-0.331154	-2.281410	1.001625

H	-0.995172	-3.883236	1.275873
C	2.609906	-2.906692	1.099363
H	3.092046	-3.086561	2.071945
C	0.556246	-3.846354	-0.219298
H	0.886644	-3.214301	-1.058244
H	0.228315	-4.793665	-0.673803
H	1.971754	-2.024540	1.244389
C	3.716202	-2.590808	0.073680
H	3.293563	-2.560345	-0.940599
H	4.413708	-3.441253	0.064657
H	2.392674	-4.896471	0.275201
H	1.345017	-4.586863	1.647167
C	4.513566	-1.284499	0.351578
H	4.306755	-0.933795	1.373087
H	5.587626	-1.515713	0.327560
C	4.292563	-0.111186	-0.638131
H	4.429969	-0.494382	-1.661710
H	5.097265	0.620667	-0.483037

Sum of electronic and zero-point Energies= -1083.737061  
Sum of electronic and thermal Energies= -1083.712976  
Sum of electronic and thermal Enthalpies= -1083.712032  
Sum of electronic and thermal Free Energies= -1083.790409

#### daec[n=5]-1-E1 (benzene)

C	1.133811	2.466397	-0.760917
H	1.591080	2.595567	-1.737859
C	1.961438	2.419701	0.372969
C	1.367300	2.264679	1.631940
H	1.984462	2.240806	2.527796
C	-0.018539	2.142533	1.750330
H	-0.491997	2.027247	2.722681
C	-0.832559	2.183265	0.622729
O	-2.205284	2.167268	0.786837
C	-0.260445	2.360712	-0.653438
O	-1.130662	2.411167	-1.695719
C	-0.606256	2.587118	-3.004821
H	0.057934	1.758607	-3.290574
H	-1.472825	2.599437	-3.672107
H	-0.063833	3.538842	-3.098598
C	-4.588840	-1.184143	0.141585
H	-5.240090	-2.041211	-0.022597
C	-3.244814	-1.250901	-0.253079
C	-2.707613	-2.513578	-0.901086
H	-1.955405	-2.250836	-1.656804
H	-3.529489	-2.997719	-1.446054
C	-2.114084	-3.552193	0.084405
H	-2.833089	-3.707186	0.901678
C	-0.737044	-3.204466	0.677343
H	-0.509679	-3.930124	1.473236
H	-0.781118	-2.221478	1.169429
C	0.407157	-3.218038	-0.348210
H	0.205893	-2.480897	-1.140230
H	0.431271	-4.198341	-0.850957
H	-2.036321	-4.515388	-0.442926
C	-2.419538	-0.133663	-0.042981
H	-1.378178	-0.164170	-0.350217
C	-2.937203	1.025046	0.544282
C	-4.281261	1.086937	0.929807
H	-4.658856	2.001651	1.379767
C	-5.099295	-0.022441	0.727091
H	-6.145731	0.022539	1.023819
C	4.307137	-2.547878	-0.290748
C	1.789485	-2.921177	0.252097
H	1.737285	-1.978534	0.816627
H	2.050505	-3.701068	0.985268
C	4.471056	-1.268933	0.552100
H	5.535287	-1.158701	0.812329
C	2.887473	-2.827353	-0.818657
H	2.607674	-2.048724	-1.544234
H	2.910923	-3.768413	-1.389731

H	3.942020	-1.388460	1.509525
C	3.975661	0.018867	-0.122064
H	2.898232	-0.065145	-0.317998
H	4.456546	0.136761	-1.106553
H	4.990332	-2.498229	-1.152871
H	4.643683	-3.405899	0.311506
C	4.230916	1.274015	0.725421
H	3.947563	1.070413	1.768703
H	5.308198	1.496396	0.742481
C	3.471041	2.528302	0.239649
H	3.732842	2.733422	-0.807861
H	3.822528	3.394513	0.819892

Sum of electronic and zero-point Energies= -1083.755237

Sum of electronic and thermal Energies= -1083.730421

Sum of electronic and thermal Enthalpies= -1083.729477

Sum of electronic and thermal Free Energies= -1083.810166

daec[n=5]-1-E2 (benzene)

C	1.223721	2.304270	0.636953
H	1.718652	2.309713	1.603716
C	2.002813	2.394721	-0.532425
C	1.353185	2.410045	-1.769503
H	1.935112	2.481717	-2.686263
C	-0.044214	2.338039	-1.842519
H	-0.558886	2.364189	-0.530318
C	-0.805483	2.240872	-0.685341
O	-2.185038	2.276859	-0.758272
C	-0.170087	2.223421	0.577546
O	-0.994604	2.140162	1.653594
C	-0.410155	2.091577	2.947681
H	0.155205	3.007938	3.170907
H	-1.246046	2.005374	3.647843
H	0.248811	1.218671	3.061262
C	-4.569088	-1.061055	-0.045269
H	-5.222568	-1.916119	0.121175
C	-3.270965	-1.267913	-0.536467
C	-2.787653	-2.674655	-0.836501
H	-2.043451	-2.645758	-1.643214
H	-3.634919	-3.257141	-1.224347
C	-2.207192	-3.435577	0.381353
H	-2.931308	-3.375772	1.206760
C	-0.832816	-2.955164	0.878589
H	-0.611882	-3.466556	1.828178
H	-0.879008	-1.881784	1.116321
C	0.320359	-3.214599	-0.103381
H	0.144234	-2.664044	-1.039678
H	0.330555	-4.281404	-0.379218
H	-2.133763	-4.500891	0.113805
C	-2.446981	-0.152936	-0.756206
H	-1.444104	-0.285791	-1.154928
C	-2.918923	1.137007	-0.492111
C	-4.215294	1.337254	-0.010266
H	-4.557649	2.351080	0.180419
C	-5.034297	0.230781	0.212292
H	-6.046065	0.379409	0.585620
C	4.235167	-2.626537	-0.094562
C	1.699308	-2.818718	0.445234
H	1.652954	-1.779663	0.803576
H	1.935690	-3.434951	1.327638
C	4.413484	-1.231762	0.534078
H	5.470306	-1.109148	0.817736
C	2.817561	-2.957715	-0.599174
H	2.576212	-2.319616	-1.462420
H	2.821322	-3.988761	-0.985343
H	3.845941	-1.180588	1.475590
C	3.986568	-0.058584	-0.359833
H	2.928986	-0.172926	-0.632384
H	4.549192	-0.084055	-1.306816
H	4.935596	-2.734059	-0.937226
H	4.538072	-3.381293	0.647636

C	4.178308	1.306791	0.315742
H	3.774690	1.261592	1.338479
H	5.251955	1.519693	0.426734
C	3.516733	2.482711	-0.434553
H	3.936267	2.552764	-1.447748
H	3.792680	3.418360	0.075787

Sum of electronic and zero-point Energies= -1083.755803

Sum of electronic and thermal Energies= -1083.731022

Sum of electronic and thermal Enthalpies= -1083.730078

Sum of electronic and thermal Free Energies= -1083.810510

daec[n=5]-2-TS (benzene)

C	-2.970803	-1.918318	-0.188733
H	-3.923706	-2.393783	0.026377
C	-2.951779	-0.542867	-0.482838
C	-1.714389	0.042878	-0.754923
H	-1.645448	1.093738	-1.012108
C	-0.534856	-0.701402	-0.705995
H	0.404994	-0.200086	-0.894259
C	-0.555607	-2.060560	-0.410166
O	0.563464	-2.873635	-0.358712
C	-1.798433	-2.685642	-0.156868
O	-1.750423	-4.017349	0.121926
C	-2.971723	-4.690605	0.384083
H	-3.479261	-4.284628	1.271748
H	-2.701586	-5.734109	0.572248
H	-3.654928	-4.645158	-0.476829
C	4.231691	-1.254834	0.792688
H	5.173969	-0.821060	1.124319
C	3.667001	-0.840853	-0.423511
C	4.269978	0.296673	-1.224381
H	3.859798	0.284681	-2.243859
H	5.356379	0.158587	-1.320820
C	4.013063	1.685564	-0.583341
H	4.523578	1.721201	0.390934
C	2.532710	2.050214	-0.376796
H	2.052805	1.269579	0.229942
H	2.014184	2.049937	-1.348121
C	2.342514	3.405026	0.328023
H	2.667831	4.220535	-0.337498
H	3.020576	3.437194	1.194892
H	4.498566	2.448455	-1.210684
C	2.466488	-1.432884	-0.838662
H	2.042703	-1.169211	-1.803830
C	1.788925	-2.329720	-0.006485
C	2.354656	-2.736569	1.203449
H	1.820217	-3.449883	1.825465
C	3.590767	-2.209687	1.585958
H	4.043880	-2.529410	2.522544
C	-1.515854	4.379157	0.348244
C	0.916283	3.693308	0.837701
H	0.587590	2.853312	1.468948
H	0.963634	4.568368	1.504631
C	-2.360538	3.205368	0.908026
H	-2.812666	3.492078	1.868648
C	-0.143243	3.982853	-0.239871
H	-0.261164	3.115091	-0.906848
H	0.222083	4.804832	-0.875022
H	-1.709879	2.348514	1.132931
C	-3.490198	2.753517	-0.037773
H	-3.081623	2.583470	-1.043718
H	-4.189186	3.594341	-0.156635
H	-2.100136	4.899401	-0.425437
H	-1.344469	5.125457	1.138106
C	-4.274645	1.497998	0.441889
H	-5.330425	1.770362	0.577289
H	-3.916514	1.192921	1.435459
C	-4.239164	0.265165	-0.497667
H	-5.067900	-0.401574	-0.222783
H	-4.455283	0.602030	-1.524051

Sum of electronic and zero-point Energies= -1083.736308  
 Sum of electronic and thermal Energies= -1083.712189  
 Sum of electronic and thermal Enthalpies= -1083.711245  
 Sum of electronic and thermal Free Energies= -1083.790044

daec[n=5]-2-E1 (benzene)

C	-0.752422	-2.700471	-0.702625
H	-1.172393	-2.973438	-1.666588
C	-1.611169	-2.594364	0.403495
C	-1.065392	-2.250830	1.647086
H	-1.705052	-2.178093	2.524126
C	0.301948	-1.998203	1.773226
H	0.737660	-1.731206	2.733411
C	1.145411	-2.094249	0.670857
O	2.507032	-1.915939	0.842363
C	0.624869	-2.464110	-0.585168
O	1.521756	-2.549702	-1.602697
C	1.047810	-2.923670	-2.889178
H	0.592694	-3.924445	-2.877296
H	1.928821	-2.936762	-3.537321
H	0.321630	-2.197054	-3.281715
C	4.370444	1.760014	0.242924
H	4.884402	2.708601	0.096372
C	3.112855	1.556629	-0.342779
C	2.474562	2.648297	-1.182168
H	2.015003	2.202916	-2.077227
H	3.269630	3.313877	-1.544649
C	1.410732	3.512928	-0.463025
H	1.823542	3.884543	0.486907
C	0.070556	2.807217	-0.211607
H	0.216918	1.953028	0.465312
H	-0.285315	2.386933	-1.164269
C	-1.003180	3.736470	0.376505
H	-1.136559	4.605233	-0.288272
H	-0.637423	4.140568	1.332920
H	1.227434	4.401395	-1.086621
C	2.468301	0.323792	-0.149565
H	1.500966	0.142564	-0.607606
C	3.072545	-0.678495	0.614425
C	4.332735	-0.473056	1.187508
H	4.784289	-1.271230	1.771322
C	4.973867	0.749523	0.997460
H	5.954031	0.914765	1.441404
C	-4.514619	2.081762	-0.465696
C	-2.369837	3.065403	0.610630
H	-2.229727	2.190508	1.263078
H	-3.013889	3.761296	1.170864
C	-4.609502	0.800046	0.383400
H	-5.670918	0.518545	0.465121
C	-3.098259	2.649231	-0.678054
H	-2.492887	1.916833	-1.229376
H	-3.176108	3.528322	-1.337027
H	-4.278173	1.010406	1.411400
C	-3.813004	-0.395208	-0.160807
H	-2.744757	-0.142116	-0.195226
H	-4.113390	-0.597379	-1.201862
H	-4.961290	1.886010	-1.453040
H	-5.142709	2.856191	0.001581
C	-3.997275	-1.666660	0.679414
H	-5.047652	-1.990957	0.631083
H	-3.803080	-1.432188	1.736570
C	-3.101371	-2.849131	0.250878
H	-3.380380	-3.728927	0.850536
H	-3.319237	-3.110802	-0.794047

Sum of electronic and zero-point Energies= -1083.755194  
 Sum of electronic and thermal Energies= -1083.730322  
 Sum of electronic and thermal Enthalpies= -1083.729378  
 Sum of electronic and thermal Free Energies= -1083.810486

daec[n=5]-2-E2 (benzene)

C	-1.687968	-2.059431	0.531294
H	-2.209887	-2.062813	1.483253
C	-2.428933	-1.935802	-0.658877
C	-1.741683	-1.957434	-1.876744
H	-2.293263	-1.869086	-2.810843
C	-0.349935	-2.113633	-1.911014
H	0.185973	-2.159303	-2.856430
C	0.374822	-2.236618	-0.732503
O	1.728017	-2.519141	-0.769823
C	-0.297086	-2.202492	0.510751
O	0.489171	-2.338311	1.610575
C	-0.128453	-2.298810	2.889095
H	-0.644944	-1.343229	3.059837
H	0.683460	-2.403623	3.614563
H	-0.839943	-3.126988	3.020931
C	4.646627	0.296539	0.180378
H	5.436715	1.009056	0.412782
C	3.537907	0.715384	-0.570089
C	3.440326	2.148576	-1.059763
H	2.962566	2.164984	-2.050310
H	4.456486	2.542092	-1.199910
C	2.668297	3.111576	-0.126780
H	3.127017	3.097228	0.873502
C	1.170410	2.802939	-0.017227
H	1.033505	1.808588	0.431825
H	0.753002	2.736621	-1.032876
C	0.374848	3.831671	0.801425
H	0.435762	4.819468	0.317018
H	0.849360	3.946889	1.788097
H	2.801155	4.133751	-0.513248
C	2.535325	-0.221659	-0.868883
H	1.674201	0.070843	-1.464962
C	2.646720	-1.542151	-0.425602
C	3.757319	-1.955460	0.314325
H	3.819443	-2.990052	0.641139
C	4.754405	-1.027602	0.614413
H	5.623918	-1.341065	1.189588
C	-3.328065	2.793323	-0.152031
C	-1.100168	3.437887	1.004054
H	-1.125751	2.431219	1.445779
H	-1.558776	4.106991	1.748297
C	-3.252115	1.268746	0.032203
H	-2.765043	1.033497	0.989406
C	-1.950525	3.468860	-0.278703
H	-1.407035	2.979726	-1.099844
H	-2.084830	4.516922	-0.587743
H	-2.601842	0.846197	-0.746395
C	-4.623973	0.580980	-0.006986
H	-5.069021	0.707799	-1.007028
H	-5.300031	1.102292	0.689014
H	-3.912143	3.013776	-1.059102
H	-3.889097	3.239022	0.685231
C	-4.630820	-0.913214	0.363365
H	-5.679405	-1.232839	0.452117
H	-4.198363	-1.041798	1.366826
C	-3.949682	-1.879502	-0.632071
H	-4.314552	-2.893859	-0.404391
H	-4.311731	-1.658713	-1.646325

Sum of electronic and zero-point Energies= -1083.751773  
 Sum of electronic and thermal Energies= -1083.726807  
 Sum of electronic and thermal Enthalpies= -1083.725863  
 Sum of electronic and thermal Free Energies= -1083.807232

daec[n=5]-3-TS (benzene)

C	1.681574	2.835138	0.225592
H	2.251155	3.656734	0.651202
C	2.291539	1.570996	0.121381
C	1.537720	0.534898	-0.433541
H	1.948797	-0.457948	-0.534823
C	0.223229	0.739985	-0.843995

H	-0.327171	-0.089977	-1.266347
C	-0.397916	1.971788	-0.684603
O	-1.728339	2.184531	-1.025736
C	0.347827	3.049723	-0.158959
O	-0.310600	4.235391	-0.044269
C	0.400723	5.349862	0.472335
H	0.733053	5.177632	1.506786
H	-0.304921	6.185921	0.457300
H	1.270849	5.601757	-0.151336
C	-4.402820	-0.493559	0.744352
H	-5.075982	-1.190215	1.241597
C	-3.628001	-0.928425	-0.343051
C	-3.619306	-2.378532	-0.791663
H	-3.042899	-2.461757	-1.722593
H	-4.641770	-2.704775	-1.033600
C	-3.053916	-3.359721	0.268012
H	-3.736170	-3.358266	1.130568
C	-1.629792	-3.090750	0.794547
H	-1.475847	-3.740503	1.669902
H	-1.570671	-2.060563	1.174524
C	-0.469674	-3.333794	-0.187504
H	-0.548617	-2.649642	-1.046370
H	-0.546335	-4.351493	-0.602960
H	-3.103156	-4.376065	-0.151922
C	-2.793253	0.001596	-0.975177
H	-2.237559	-0.294694	-1.859908
C	-2.645006	1.296703	-0.468235
C	-3.416825	1.722756	0.612804
H	-3.296708	2.736811	0.984992
C	-4.312557	0.823994	1.200316
H	-4.925158	1.148948	2.039393
C	3.491228	-3.263950	0.222072
C	0.907106	-3.157424	0.482918
H	0.954260	-2.154426	0.930778
H	0.985532	-3.866285	1.322841
C	3.938823	-1.850755	0.658965
H	4.768158	-1.949203	1.375997
C	2.106672	-3.370246	-0.458239
H	2.023805	-4.371754	-0.907796
H	2.045249	-2.664750	-1.301275
C	3.124047	-1.370190	1.217339
C	4.399008	-0.948657	-0.502001
H	3.666106	-0.979303	-1.317454
H	5.316920	-1.379079	-0.931321
H	4.250923	-3.677921	-0.458848
H	3.490210	-3.921931	1.104524
C	4.707527	0.523950	-1.38646
H	4.913343	1.069062	-1.071517
H	5.646049	0.545834	0.436053
C	3.678834	1.329451	0.695852
H	3.562434	0.835657	1.673317
H	4.137116	2.302865	0.919808

Sum of electronic and zero-point Energies= -1083.735222

Sum of electronic and thermal Energies= -1083.711478

Sum of electronic and thermal Enthalpies= -1083.710534

Sum of electronic and thermal Free Energies= -1083.787310

daec[n=5]-3-E1 (benzene)

C	1.719111	2.544037	-0.096496
H	2.422483	3.062288	-0.741907
C	2.214092	1.688573	0.904513
C	1.299066	1.037998	1.737958
H	1.657409	0.386614	2.532627
C	-0.077360	1.230819	1.576673
H	-0.787495	0.734956	2.234228
C	-0.559113	2.063711	0.572412
O	-1.905124	2.334269	0.426617
C	0.344980	2.737569	-0.278374
O	-0.210477	3.540585	-1.223693
C	0.658875	4.243288	-2.099584

H	1.314951	4.935727	-1.552022
H	0.008341	4.816793	-2.766419
H	1.274246	3.556301	-2.698897
C	-4.750945	-0.679263	0.033326
H	-5.516861	-1.445938	-0.073388
C	-3.468656	-0.904021	-0.492549
C	-3.144260	-2.212720	-1.187535
H	-2.358809	-2.048619	-1.937026
H	-4.032060	-2.547710	-1.741709
C	-2.720307	-3.354022	-0.229096
H	-3.494471	-3.461997	0.544374
C	-1.350205	-3.178938	0.449601
H	-1.257661	-3.932433	1.246587
H	-1.311791	-2.201885	0.953233
C	-0.149362	-3.316348	-0.499235
H	-0.243253	-2.601496	-1.330733
H	-0.166532	-4.317196	-0.960045
H	-2.720754	-4.296572	-0.797777
C	-2.498867	0.099450	-0.354881
H	-1.504700	-0.043281	-0.770856
C	-2.804715	1.295334	0.305477
C	-4.084358	1.515346	0.822207
H	-4.299978	2.456497	1.321565
C	-5.053809	0.521659	0.678467
H	-6.053828	0.688131	1.074923
C	3.781511	-3.024294	-0.139267
C	1.206417	-3.092183	0.187172
H	1.213236	-2.088070	0.635720
H	1.318319	-3.801417	1.023229
C	4.054139	-1.615314	0.422889
H	5.071173	-1.606771	0.845953
C	2.395423	-3.245410	-0.773334
H	2.372612	-4.257609	-1.206065
H	2.263786	-2.557397	-1.621898
H	3.377371	-1.416856	1.265508
C	3.934451	-0.488742	-0.615579
H	2.889580	-0.392750	-0.941461
H	4.507298	-0.769912	-1.513280
H	4.548155	-3.253245	-0.895960
H	3.925802	-3.758598	0.668551
C	4.439395	0.884669	-0.140783
H	4.373540	1.590469	-0.981963
H	5.508989	0.812735	0.109363
C	3.708736	1.489620	1.080017
H	3.879715	0.857647	1.960986
H	4.180561	2.457862	1.307166

Sum of electronic and zero-point Energies= -1083.754696

Sum of electronic and thermal Energies= -1083.729948

Sum of electronic and thermal Enthalpies= -1083.729004

Sum of electronic and thermal Free Energies= -1083.809722

daec[n=5]-3-E2 (benzene)

C	1.337407	1.828950	0.965616
H	1.792772	1.524525	1.903619
C	2.171278	2.179679	-0.110148
C	1.578179	2.596086	-1.308015
H	2.198224	2.886794	-2.153557
C	0.185984	2.646607	-1.429969
H	-0.285509	2.974221	-2.353739
C	-0.633118	2.294060	-0.362464
O	-2.000656	2.456476	-0.474866
C	-0.057721	1.888272	0.860979
O	-0.927795	1.588686	1.860164
C	-0.401643	1.193439	3.119903
H	0.187615	0.268715	3.041755
H	-1.270180	1.012558	3.759537
H	0.217544	1.985444	3.565161
C	-4.656218	-0.750108	-0.430913
H	-5.374029	-1.568976	-0.425968
C	-3.319338	-1.003331	-0.772928

C	-2.870371	-2.412446	-1.109746
H	-2.054232	-2.376197	-1.843680
H	-3.700588	-2.938796	-1.600579
C	-2.430951	-3.250838	0.117461
H	-3.229333	-3.203934	0.871963
C	-1.097676	-2.832772	0.763186
H	-1.004306	-3.342315	1.734424
H	-1.121485	-1.756316	0.988096
C	0.141181	-3.159158	-0.085491
H	0.036780	-2.717335	-1.088009
H	0.192519	-4.248660	-0.242142
H	-2.362524	-4.304744	-0.193146
C	-2.411281	0.066696	-0.785689
H	-1.375185	-0.101410	-1.068776
C	-2.832851	1.355670	-0.446227
C	-4.167476	1.604036	-0.112934
H	-4.470724	2.617267	0.138081
C	-5.073497	0.544164	-0.109455
H	-6.115017	0.731228	0.146258
C	4.036945	-2.529481	0.213894
C	1.461308	-2.668185	0.527050
H	1.403591	-1.578070	0.662369
H	1.583941	-3.096109	1.535286
C	4.203857	-1.001346	0.327582
H	5.214833	-0.795874	0.713724
C	2.684484	-3.024731	-0.331245
H	2.735372	-4.119458	-0.436756
H	2.533928	-2.635880	-1.349397
H	3.509056	-0.609341	1.083516
C	4.008326	-0.245997	-0.996585
H	2.958050	-0.314612	-1.311790
H	4.593760	-0.747428	-1.783173
H	4.834411	-2.920508	-0.437021
H	4.209774	-2.976921	1.205153
C	4.426147	1.234198	-0.965395
H	4.297227	1.654843	-1.973259
H	5.502457	1.303752	-0.745279
C	3.680875	2.127555	0.051676
H	3.918745	1.799412	1.071830
H	4.087158	3.146716	-0.037722

Sum of electronic and zero-point Energies= -1083.755499  
Sum of electronic and thermal Energies= -1083.730716  
Sum of electronic and thermal Enthalpies= -1083.729772  
Sum of electronic and thermal Free Energies= -1083.810283

daec[n=5]-4-TS (benzene)

C	2.008923	2.869176	0.026208
H	2.685008	3.652035	-0.306575
C	2.511966	1.566467	0.198045
C	1.618484	0.581121	0.615647
H	1.949094	-0.437408	0.766603
C	0.273889	0.869051	0.836997
H	-0.379529	0.067190	1.148842
C	-0.231853	2.147778	0.637723
O	-1.566657	2.483244	0.823229
C	0.655073	3.174271	0.238069
O	0.103184	4.406035	0.062029
C	0.953544	5.470881	-0.334706
H	0.312202	6.354953	-0.400108
H	1.410230	5.283780	-1.317964
H	1.746989	5.655105	0.404469
C	-4.397746	-0.061747	-0.901806
H	-5.103558	-0.727498	-1.396160
C	-3.646384	-0.525791	0.188249
C	-3.634864	-1.984070	0.605694
H	-4.654847	-2.375301	0.726662
H	-3.151443	-2.066670	1.588620
C	-2.868562	-2.861651	-0.427202
H	-3.570545	-3.164020	-1.216267
C	-2.184463	-4.111621	0.168695

H	-2.103036	-4.882800	-0.612042
H	-2.830514	-4.542258	0.948615
C	-0.774403	-3.863944	0.750697
H	-0.480175	-4.741681	1.345966
H	-0.805855	-3.019848	1.458257
H	-2.113488	-2.242708	-0.928364
C	-2.765591	0.364712	0.816481
H	-2.241365	0.046092	1.711679
C	-2.529624	1.636857	0.287051
C	-3.278314	2.093299	-0.799745
H	-3.095359	3.091853	-1.188103
C	-4.231362	1.245037	-1.370737
H	-4.824902	1.596801	-2.212693
C	2.744560	-3.073700	-0.875574
C	0.304110	-3.602019	-0.316691
H	0.322413	-4.451133	-1.018669
H	0.024445	-2.723284	-0.916547
C	4.175682	-2.724106	-0.410586
H	4.848328	-2.795110	-1.279531
C	1.723494	-3.379025	0.237233
H	2.048479	-4.269944	0.797661
H	1.699090	-2.558269	0.968993
H	4.517927	-3.495592	0.296263
C	4.365786	-1.336942	0.240382
H	5.374623	-1.291456	0.677780
H	3.683405	-1.237005	1.093248
H	2.352192	-2.261492	-1.505232
H	2.803980	-3.952315	-1.535964
C	4.208774	-0.149802	-0.738316
H	3.387985	-0.341312	-1.441894
H	5.120357	-0.098670	-1.351173
C	3.971913	1.237705	-0.086227
H	4.377522	2.017056	-0.745715
H	4.559935	1.305061	0.843795

Sum of electronic and zero-point Energies= -1083.734100  
Sum of electronic and thermal Energies= -1083.709997  
Sum of electronic and thermal Enthalpies= -1083.709053  
Sum of electronic and thermal Free Energies= -1083.787447

daec[n=5]-4-E1 (benzene)

C	-1.279847	2.272224	0.815628
H	-1.760819	2.173058	1.784810
C	-2.082307	2.430322	-0.330263
C	-1.457193	2.580109	-1.570995
H	-2.057649	2.711992	-2.468839
C	-0.059730	2.566737	-1.669632
H	0.436873	2.689826	-2.629395
C	0.725300	2.405628	-0.535628
O	2.102079	2.487854	-0.633772
C	0.115193	2.259314	0.731211
O	0.961094	2.123665	1.784994
C	0.401244	1.958409	3.080425
H	1.251764	1.860077	3.761039
H	-0.217608	1.051499	3.141133
H	-0.199248	2.830983	3.375626
C	4.554205	-0.867340	-0.319621
H	5.218939	-1.726805	-0.249387
C	3.185384	-1.064135	-0.540159
C	2.589489	-2.452311	-0.663367
H	3.366446	-3.166302	-0.970760
H	1.841205	-2.444150	-1.467565
C	1.932128	-2.954282	0.642409
H	2.721629	-3.132663	1.386546
C	1.093827	-4.235027	0.462206
H	0.880950	-4.665700	1.452619
H	1.699163	-4.985008	-0.069631
C	-0.236787	-4.030166	-0.289244
H	-0.631088	-5.009673	-0.598388
H	-0.050335	-3.480062	-1.223941
H	1.305616	-2.153415	1.059123

C	2.344399	0.056295	-0.634806
H	1.281602	-0.080142	-0.819748
C	2.864477	1.345109	-0.506426
C	4.233880	1.539207	-0.290085
H	4.617107	2.552384	-0.199001
C	5.069807	0.428061	-0.198429
H	6.135717	0.573857	-0.031801
C	-3.616040	-2.142501	0.482653
C	-1.315861	-3.293830	0.523027
H	-1.686448	-3.958288	1.319755
H	-0.873596	-2.427040	1.036497
C	-4.640238	-1.376114	-0.378584
H	-5.573365	-1.243932	0.190201
C	-2.489558	-2.797661	-0.333251
H	-2.907257	-3.633666	-0.916583
H	-2.100495	-2.080880	-1.072359
H	-4.904009	-1.996263	-1.248681
C	-4.156355	0.005923	-0.863454
H	-4.776335	0.330960	-1.712756
H	-3.131380	-0.074274	-1.253154
H	-3.176785	-1.460270	1.226644
H	-4.134067	-2.921234	1.062124
C	-4.212885	1.090157	0.223627
H	-3.711432	0.736453	1.135995
H	-5.264122	1.259458	0.501697
C	-3.593872	2.443878	-0.192185
H	-3.876257	3.196958	0.558504
H	-4.042069	2.772066	-1.140446

Sum of electronic and zero-point Energies= -1083.755429  
Sum of electronic and thermal Energies= -1083.730509  
Sum of electronic and thermal Enthalpies= -1083.729565  
Sum of electronic and thermal Free Energies= -1083.810769

#### daec[n=5]-4-E2 (benzene)

C	-1.302607	2.526560	-0.593052
H	-1.804948	2.685046	-1.543022
C	-2.079129	2.358763	0.565577
C	-1.426999	2.172249	1.790831
H	-2.008393	2.054812	2.703506
C	-0.031671	2.143033	1.854355
H	0.485794	2.006845	2.801317
C	0.731172	2.304315	0.702578
O	2.110012	2.362583	0.799231
C	0.098157	2.505071	-0.541640
O	0.920745	2.664620	-1.610520
C	0.332665	2.863608	-2.888825
H	1.168265	2.959466	-3.588068
H	-0.270496	3.782486	-2.917945
H	-0.290797	2.007847	-3.185817
C	4.554058	-0.899113	-0.070690
H	5.216424	-1.734523	-0.291366
C	3.169088	-1.058777	-0.195981
C	2.553187	-2.378270	-0.617574
H	3.312787	-3.004207	-1.106455
H	1.782957	-2.179025	-1.375162
C	1.926695	-3.166439	0.554690
H	2.733226	-3.499094	1.223928
C	1.093712	-4.386079	0.114467
H	0.869087	-4.999751	1.000335
H	1.709395	-5.018829	-0.543247
C	-0.226484	-4.047071	-0.605874
H	-0.626113	-4.962191	-1.068055
H	-0.023814	-3.361327	-1.442239
H	1.305490	-2.486342	1.153617
C	2.329448	0.030654	0.089055
H	1.252220	-0.080852	-0.003655
C	2.868315	1.254679	0.487313
C	4.255088	1.412444	0.608503
H	4.652617	2.376012	0.917279
C	5.088045	0.331624	0.329050

H	6.166270	0.450702	0.420861
C	-3.603550	-2.266203	0.397311
C	-1.309756	-3.433517	0.297843
H	-1.695323	-4.207601	0.980191
H	-0.869624	-2.657997	0.941924
C	-4.599255	-1.365514	-0.361602
H	-5.552657	-1.322957	0.186653
C	-2.467924	-2.803792	-0.488972
H	-2.882550	-3.538686	-1.197373
H	-2.062831	-1.987665	-1.106908
H	-4.830659	-1.833144	-1.330585
C	-4.095018	0.074341	-0.591748
H	-4.648969	0.528565	-1.427398
H	-3.041214	0.051040	-0.905265
H	-3.173795	-1.707251	1.242762
H	-4.140382	-3.116739	0.843068
C	-4.249213	0.977547	0.641690
H	-3.831528	0.480557	1.529102
H	-5.321868	1.114955	0.845458
C	-3.595444	2.372283	0.500619
H	-3.976662	3.014601	1.307279
H	-3.923463	2.833235	-0.441949

Sum of electronic and zero-point Energies= -1083.754900  
Sum of electronic and thermal Energies= -1083.729992  
Sum of electronic and thermal Enthalpies= -1083.729048  
Sum of electronic and thermal Free Energies= -1083.810307

#### daec[n=5]-5-TS (benzene)

C	-1.275555	3.054958	-0.480036
H	-1.681952	3.941516	-0.963855
C	-2.067350	1.909351	-0.306386
C	-1.469150	0.815779	0.331895
H	-2.022487	-0.096710	0.497299
C	-0.141179	0.849357	0.741202
H	0.280705	-0.024489	1.220198
C	0.657812	1.964600	0.496909
O	2.013535	1.983757	0.814258
C	0.074239	3.096969	-0.100601
O	0.800734	4.219852	-0.406365
C	1.328422	4.943096	0.709433
H	1.832510	5.820471	0.290648
H	2.049886	4.343841	1.276955
H	0.519950	5.276298	1.377338
C	4.183050	-1.189199	-0.823270
H	4.723254	-2.013960	-1.285340
C	3.394573	-1.423043	0.315185
C	3.184647	-2.819906	0.871292
H	2.615436	-2.750196	1.807708
H	4.153250	-3.270716	1.134164
C	2.469330	-3.785644	-0.108795
H	3.135255	-3.955042	-0.967406
C	1.096310	-3.347809	-0.656954
H	0.835928	-4.034804	-1.476858
H	1.189233	-2.354463	-1.119302
C	-0.075257	-3.332557	0.341074
H	0.117694	-2.603525	1.143130
H	-0.150121	-4.314270	0.835855
H	2.370147	-4.761342	0.390974
C	2.735433	-0.333463	0.898201
H	2.172534	-0.475776	1.816183
C	2.766921	0.928411	0.297506
C	3.546460	1.154932	-0.835921
H	3.560652	2.144726	-1.284806
C	4.272916	0.089958	-1.377709
H	4.891585	0.255957	-2.257684
C	-3.983805	-2.691832	-0.072714
C	-1.416772	-2.999644	-0.340931
H	-1.316385	-2.037114	-0.862872
H	-1.610980	-3.748472	-1.125509
C	-4.214485	-1.262851	-0.614045



H	-5.053407	-1.285637	-1.326173
C	-2.623934	-2.958052	0.613437
H	-2.446501	-2.210451	1.402031
H	-2.689012	-3.924792	1.136056
H	-3.339393	-0.954070	-1.201906
C	-4.524810	-0.219191	0.475682
H	-3.798946	-0.300986	1.294062
H	-5.493835	-0.473547	0.932156
H	-4.789834	-2.932632	0.637535
H	-4.093631	-3.405836	-0.903188
C	-4.610363	1.252331	0.003582
H	-4.730730	1.889246	0.093192
H	-5.535923	1.371921	-0.579894
C	-3.473829	1.830696	-0.877776
H	-3.429914	1.251424	-1.813233
H	-3.780852	2.841067	-1.181163

Sum of electronic and zero-point Energies= -1083.733579

Sum of electronic and thermal Energies= -1083.709678

Sum of electronic and thermal Enthalpies= -1083.708733

Sum of electronic and thermal Free Energies= -1083.785961

daec[n=5]-5-E1 (benzene)

C	1.307815	1.775346	0.940775
H	1.723012	1.430741	1.886021
C	2.150454	2.206639	-0.093144
C	1.553530	2.659187	-1.280361
H	2.175981	3.015245	-2.099361
C	0.165799	2.659477	-1.432005
H	-0.298810	3.008127	-2.351522
C	-0.659227	2.219287	-0.395619
O	-2.029604	2.318094	-0.547660
C	-0.083830	1.782215	0.810834
O	-0.856295	1.317064	1.846114
C	-1.549054	2.328829	2.584591
H	-2.139887	1.804075	3.341758
H	-2.217955	2.915164	1.942191
H	-0.837166	3.005164	3.080652
C	-4.567445	-0.983439	-1.773866
H	-5.254313	-1.828255	-0.465039
C	-3.213386	-1.197694	-0.778277
C	-2.706038	-2.599803	-1.054198
H	-1.877565	-2.560106	-1.773866
H	-3.506855	-3.174184	-1.539990
C	-2.260226	-3.374967	0.212007
H	-3.073108	-3.327328	0.950868
C	-0.952767	-2.889984	0.863934
H	-0.853200	-3.375693	1.846629
H	-1.017797	-1.811462	1.068472
C	0.306750	-3.190323	0.036333
H	0.202354	-2.765741	-0.973787
H	0.392859	-4.279930	-0.104973
H	-2.151854	-4.436707	-0.058134
C	-2.344224	-0.096522	-0.802658
H	-1.294986	-0.235959	-1.049754
C	-2.821724	1.184192	-0.511306
C	-4.172711	1.394725	-0.221844
H	-4.521935	2.403914	-0.018066
C	-5.040539	0.302748	-0.208995
H	-6.094852	0.459306	0.012085
C	4.176141	-2.428138	0.353402
C	1.604417	-2.651625	0.656490
H	1.511057	-1.562965	0.780867
H	1.730486	-3.064288	1.670397
C	4.289290	-0.893032	0.433241
H	5.290417	-0.643429	0.819071
C	2.844835	-2.981212	-0.187977
H	2.687119	-2.617854	-1.214578
H	2.934898	-4.075332	-0.272193
H	3.577380	-0.509266	1.177161
C	4.074740	-0.174531	-0.908492

H	3.029242	-0.287153	-1.227177
H	4.681680	-0.671872	-1.681265
H	4.990832	-2.806013	-0.283959
H	4.357755	-2.846423	1.355668
C	4.440242	1.319650	-0.907736
H	4.300758	1.714718	-1.924744
H	5.512166	1.431976	-0.684086
C	3.657812	2.207267	0.086825
H	3.893377	1.903511	1.114816
H	4.032181	3.237009	-0.016939

Sum of electronic and zero-point Energies= -1083.752607

Sum of electronic and thermal Energies= -1083.727626

Sum of electronic and thermal Enthalpies= -1083.726682

Sum of electronic and thermal Free Energies= -1083.807809

daec[n=5]-5-E2 (benzene)

C	1.535112	2.751886	-0.183368
H	2.137510	3.348946	-0.865193
C	2.138234	1.972745	0.809357
C	1.304112	1.229563	1.658797
H	1.737799	0.625838	2.453631
C	-0.080985	1.276226	1.512499
H	-0.727259	0.719217	2.186957
C	-0.671635	2.053084	0.511766
O	-2.050116	2.178583	0.439604
C	0.143720	2.805896	-0.356964
O	-0.294864	3.646044	-1.336603
C	-1.491021	3.353456	-2.062615
H	-1.422014	3.942010	-2.983960
H	-2.387511	3.648067	-1.507939
H	-1.554717	2.288640	-2.323577
C	-4.580999	-1.117941	0.158956
H	-5.267809	-1.959358	0.081789
C	-3.293352	-1.223064	-0.389844
C	-2.851095	-2.504915	-1.069508
H	-2.104219	-2.275515	-1.840995
H	-3.712055	-2.940186	-1.595470
C	-2.289215	-3.577809	-0.102890
H	-3.029669	-3.749715	0.691696
C	-0.928541	-3.250782	0.537341
H	-0.740151	-3.976756	1.342848
H	-0.979024	-2.266604	1.025802
C	0.257634	-3.280749	-0.439160
H	0.070820	-2.595466	-1.279934
H	0.333985	-4.286486	-0.882910
H	-2.206516	-4.525864	-0.656015
C	-2.426726	-0.124343	-0.289176
H	-1.428708	-0.178865	-0.716283
C	-2.840320	1.046584	0.356430
C	-4.124855	1.147312	0.897203
H	-4.424103	2.070541	1.386804
C	-4.990780	0.058091	0.791421
H	-5.994215	0.130096	1.206950
C	4.144784	-2.579204	-0.177629
C	1.598075	-2.904496	0.210021
H	1.510444	-1.896981	0.642043
H	1.801655	-3.582688	1.054469
C	4.286209	-1.139220	0.353518
H	5.304676	-1.022132	0.756486
C	2.775117	-2.951236	-0.775986
H	2.555144	-2.294611	-1.631103
H	2.846839	-3.967627	-1.193295
H	3.608327	-0.991867	1.205794
C	4.037558	-0.050553	-0.702425
H	2.982840	-0.064099	-1.009981
H	4.619430	-0.291720	-1.605885
H	4.914448	-2.744776	-0.947612
H	4.379261	-3.279558	0.639160
C	4.412443	1.375253	-0.262782
H	4.259864	2.054650	-1.114080

H	5.488318	1.414308	-0.033114
C	3.647694	1.929334	0.961423
H	3.897115	1.336068	1.850712
H	4.022328	2.944779	1.159881

Sum of electronic and zero-point Energies= -1083.752098  
Sum of electronic and thermal Energies= -1083.727213  
Sum of electronic and thermal Enthalpies= -1083.726269  
Sum of electronic and thermal Free Energies= -1083.807154

daec[n=5]-6-TS (benzene)

C	1.903451	2.924777	0.092175
H	2.597797	3.711684	-0.189602
C	2.409925	1.642906	0.375809
C	1.492896	0.653256	0.726846
H	1.824431	-0.347293	0.970855
C	0.124201	0.909692	0.759424
H	-0.547835	0.098896	1.003351
C	-0.378729	2.168664	0.454920
O	-1.729930	2.481633	0.450347
C	0.528806	3.204285	0.132743
O	-0.024336	4.416672	-0.146511
C	0.844093	5.488217	-0.479912
H	1.415759	5.279857	-1.396508
H	1.542296	5.716636	0.338875
H	0.196663	6.353594	-0.650875
C	-4.341989	-0.520442	-0.810006
H	-4.993254	-1.314069	-1.173413
C	-3.701397	-0.660353	0.431132
C	-3.784697	-1.948752	1.227314
H	-4.831530	-2.273047	1.317332
H	-3.425068	-1.766260	2.249505
C	-2.973819	-3.114411	0.601617
H	-3.080831	-3.990716	1.259087
C	-1.480107	-2.835582	0.351423
H	-1.001534	-2.506177	1.286509
H	-1.387200	-1.997380	-0.353483
C	-0.737623	-4.059802	-0.222749
H	-1.401155	-4.552013	-0.950688
H	-0.570027	-4.800205	0.575226
H	-3.439608	-3.394414	-0.355295
C	-2.890766	0.389212	0.883442
H	-2.432118	0.329069	1.866655
C	-2.623396	1.490825	0.064252
C	-3.262628	1.624575	-1.169136
H	-3.055975	2.497162	-1.783409
C	-4.142346	0.622505	-1.588485
H	-4.652880	0.722815	-2.544543
C	3.023950	-3.008180	-0.936108
C	0.590567	-3.759134	-0.946729
H	0.900623	-4.669047	-1.483947
H	0.399259	-3.003804	-1.725595
C	4.308988	-2.607742	-0.179911
H	5.145076	-2.624654	-0.896649
C	1.773244	-3.288980	-0.080316
H	2.006267	-4.058506	0.673332
H	1.487473	-2.388098	0.478724
H	4.537338	-3.386675	0.564013
C	4.302050	-1.240240	0.533797
H	5.223463	-1.155083	1.130108
H	3.487059	-1.221222	1.266896
H	3.249725	-3.915730	-1.517437
H	2.776043	-2.238311	-1.681925
C	4.225670	-0.021984	-0.412313
H	3.484933	-0.198199	-1.203165
H	5.195559	0.065297	-0.923751
C	3.897168	1.335554	0.266663
H	4.363384	1.361093	1.265133
H	4.374923	2.145148	-0.301354

Sum of electronic and zero-point Energies= -1083.738569  
Sum of electronic and thermal Energies= -1083.714569

Sum of electronic and thermal Enthalpies= -1083.713625  
Sum of electronic and thermal Free Energies= -1083.791382

daec[n=5]-6-E1 (benzene)

C	-1.343094	2.027137	0.772669
H	-1.882414	1.798018	1.687287
C	-2.071681	2.347691	-0.388747
C	-1.367633	2.663916	-1.553492
H	-1.909559	2.919556	-2.461904
C	0.033766	2.664661	-1.561859
H	0.589927	2.924556	-2.459704
C	0.745668	2.345288	-0.413172
O	2.123632	2.454777	-0.400686
C	0.054048	2.020209	0.776771
O	0.830354	1.736534	1.854959
C	0.189143	1.389779	3.074309
H	-0.428048	0.486271	2.964373
H	-0.433485	2.213500	3.452439
H	0.994463	1.190927	3.787181
C	4.604276	-0.882143	-0.158811
H	5.278482	-1.735418	-0.102459
C	3.359883	-1.024205	-0.789820
C	2.947908	-2.354749	-1.391230
H	3.852124	-2.897877	-1.698763
H	2.366613	-2.176775	-2.307836
C	2.122735	-3.273518	-0.459301
H	2.012996	-4.246201	-0.963227
C	0.730281	-2.733003	-0.106536
H	0.230497	-2.418969	-1.034669
H	0.829413	-1.825895	0.507590
C	-0.153875	-3.754365	0.625893
H	0.392136	-4.147608	1.497410
H	-0.329406	-4.617584	-0.035928
H	2.691934	-3.466840	0.462460
C	2.509418	0.090539	-0.861927
H	1.547564	0.010556	-1.362176
C	2.897050	1.313077	-0.307735
C	4.142627	1.452588	0.311047
H	4.422475	2.417084	0.726763
C	4.990671	0.348006	0.381325
H	5.962677	0.448698	0.861117
C	-3.774717	-2.163374	0.470763
C	-1.507858	-3.197195	1.102886
H	-2.057941	-3.998629	1.620228
H	-1.329568	-2.415849	1.859377
C	-4.616542	-1.449744	-0.606043
H	-5.649037	-1.341295	-0.239020
C	-2.388451	-2.615319	-0.013543
H	-2.512116	-3.364316	-0.812791
H	-1.868208	-1.764593	-0.472575
H	-4.678536	-2.100982	-1.491478
C	-4.096923	-0.065479	-1.042543
H	-4.641974	0.248811	-1.945816
H	-3.042486	-0.139563	-1.342235
H	-4.331864	-3.041985	0.830193
H	-3.657262	-1.508254	1.347387
C	-4.251231	1.027367	0.025641
H	-3.836795	0.681435	0.982794
H	-5.322179	1.203614	0.207673
C	-3.590165	2.372434	-0.346772
H	-3.971193	2.708572	-1.321227
H	-3.912964	3.129007	0.384720

Sum of electronic and zero-point Energies= -1083.756069  
Sum of electronic and thermal Energies= -1083.731200  
Sum of electronic and thermal Enthalpies= -1083.730256  
Sum of electronic and thermal Free Energies= -1083.810808

daec[n=5]-6-E2 (benzene)

C	-1.145085	2.630977	-0.519965
H	-1.588045	3.005363	-1.438470

C	-1.991011	2.258502	0.537329
C	-1.414990	1.781842	1.722230
H	-2.048212	1.499955	2.561241
C	-0.027804	1.681084	1.844702
H	0.430364	1.327841	2.765817
C	0.805088	2.056882	0.794964
O	2.176768	2.057942	0.979369
C	0.250354	2.541098	-0.406498
O	1.136178	2.888199	-1.376679
C	0.627507	3.399708	-2.601018
H	0.056767	4.326671	-2.446073
H	-0.005556	2.663339	-3.117131
H	1.503878	3.615950	-3.218798
C	4.582004	-1.215906	0.064505
H	5.234270	-2.058027	-0.161140
C	3.297413	-1.166467	-0.494323
C	2.813005	-2.278725	-1.405900
H	3.687276	-2.771385	-1.852782
H	2.242168	-1.845349	-2.240574
C	1.939013	-3.360688	-0.726999
H	1.799276	-4.177676	-1.451646
C	0.562721	-2.863035	-0.265075
H	0.093428	-2.318700	-1.097699
H	0.684834	-2.131135	0.546454
C	-0.377454	-3.985254	0.201496
H	0.128595	-4.584823	0.973849
H	-0.566658	-4.671438	-0.639624
H	2.486258	-3.793753	0.123797
C	2.472347	-0.068252	-0.199265
H	1.478593	-0.005464	-0.632654
C	2.925427	0.950421	0.642818
C	4.212949	0.900210	1.190121
H	4.544674	1.709553	1.835671
C	5.033996	-0.186347	0.895670
H	6.036282	-0.230036	1.318300
C	-3.914011	-2.208492	0.332108
C	-1.721639	-3.486176	0.764522
H	-2.313561	-4.354228	1.093960
H	-1.532327	-2.886589	1.669109
C	-4.687484	-1.256473	-0.602458
H	-5.723591	-1.160823	-0.242354
C	-2.551009	-2.650120	-0.222024
H	-2.707380	-3.224845	-1.149706
H	-1.974224	-1.761644	-0.509377
H	-4.756484	-1.722289	-1.597546
C	-4.081773	0.153712	-0.751649
H	-4.548268	0.652820	-1.614895
H	-3.012664	0.076468	-0.993509
H	-4.531281	-3.099946	0.521197
H	-3.769626	-1.732437	1.313844
C	-4.264912	1.046838	0.484584
H	-3.951044	0.509467	1.390106
H	-5.336231	1.261583	0.615458
C	-3.499834	2.387256	0.413082
H	-3.748906	2.900204	-0.526628
H	-3.865075	3.036686	1.222531

Sum of electronic and zero-point Energies= -1083.755172  
Sum of electronic and thermal Energies= -1083.730227  
Sum of electronic and thermal Enthalpies= -1083.729283  
Sum of electronic and thermal Free Energies= -1083.810706

#### daec[n=5]-7-TS (benzene)

C	-3.106500	1.864256	0.103131
H	-3.940771	2.526000	-0.113466
C	-1.812571	2.410640	0.192748
C	-0.764174	1.533634	0.465327
H	0.249833	1.895237	0.565915
C	-0.981455	0.165199	0.607337
H	-0.127496	-0.471131	0.786369
C	-2.255409	-0.380262	0.498816

O	-2.538717	-1.734446	0.614558
C	-3.344724	0.489904	0.258983
O	-4.569107	-0.098418	0.170146
C	-5.695679	0.731472	-0.065859
H	-5.624519	1.251049	-1.033020
H	-6.560416	0.061243	-0.082620
H	-5.829974	1.473200	0.735253
C	0.371763	-4.318641	-0.896075
H	1.144685	-4.939157	-1.347189
C	0.669158	-3.552138	0.238777
C	2.084129	-3.363541	0.749291
H	2.682138	-4.276361	0.622735
H	2.061728	-3.143264	1.826222
C	2.763988	-2.185032	-0.001668
H	3.028914	-2.520900	-1.015765
C	4.003797	-1.610385	0.698843
H	4.680945	-2.434211	0.972951
H	3.698708	-1.145202	1.648841
C	4.806062	-0.605148	-0.153653
H	5.157518	-1.129011	-1.056228
H	5.714242	-0.328530	0.404252
H	2.023427	-1.385475	-0.138950
C	-0.352766	-2.779265	0.808692
H	-0.160085	-2.234623	1.728429
C	-1.584099	-2.637301	0.165447
C	-1.879103	-3.405209	-0.964141
H	-2.851283	-3.301627	-1.439116
C	-0.904296	-4.269757	-1.468415
H	-1.128390	-4.877137	-2.343431
C	3.431803	3.114153	0.048870
C	4.100845	0.693729	-0.602813
H	4.784244	1.207078	-1.297256
H	3.206431	0.451932	-1.194858
C	2.126345	3.293031	-0.774702
H	1.689323	2.310117	-0.999051
C	3.739772	1.677257	0.526948
H	4.586907	1.729122	1.228909
H	2.889554	1.292118	1.111499
H	2.353840	3.736560	-1.754603
C	1.062660	4.168509	-0.078732
H	1.473924	5.180884	0.045550
H	0.904705	3.800991	0.944910
H	4.292983	3.469819	-0.535757
H	3.388762	3.766982	0.933441
C	-0.296321	4.249646	-0.836363
H	-0.265808	3.598472	-1.721391
H	-0.425424	5.269615	-1.223111
C	-1.564319	3.897566	-0.016089
H	-1.509923	4.409367	0.958782
H	-2.439558	4.325864	-0.524103

Sum of electronic and zero-point Energies= -1083.728331  
Sum of electronic and thermal Energies= -1083.704217  
Sum of electronic and thermal Enthalpies= -1083.703272  
Sum of electronic and thermal Free Energies= -1083.781811

#### daec[n=5]-7-E1 (benzene)

C	-1.301093	2.375824	0.664995
H	-1.797932	2.388994	1.630650
C	-2.080532	2.389271	-0.506956
C	-1.429168	2.399485	-1.744044
H	-2.012047	2.418354	-2.662870
C	-0.030093	2.395879	-1.814269
H	0.484420	2.414470	-2.772370
C	0.731974	2.374802	-0.653875
O	2.111200	2.454331	-0.723305
C	0.095697	2.362590	0.608183
O	0.921631	2.348730	1.686089
C	0.339222	2.299435	2.980886
H	-0.276352	1.398050	3.113552
H	1.177810	2.269195	3.682522

H	-0.270033	3.191782	3.185205
C	4.508126	-0.889696	-0.061845
H	5.156374	-1.747718	0.108046
C	3.180337	-1.091225	-0.457459
C	2.614149	-2.482748	-0.669465
H	3.415516	-3.226840	-0.562665
H	2.252460	-2.568513	-1.706188
C	1.450876	-2.832015	0.280749
H	1.820465	-2.857713	1.317266
C	0.771318	-4.163127	-0.068477
H	1.509593	-4.976837	0.000196
H	0.455385	-4.136707	-1.122208
C	-0.434102	-4.520040	0.822143
H	-0.085308	-4.659529	1.857121
H	-0.824958	-5.497766	0.500193
H	0.712381	-2.020412	0.243614
C	2.361014	0.028910	-0.672056
H	1.330861	-0.104957	-0.992041
C	2.860331	1.318325	-0.487871
C	4.190996	1.517395	-0.102035
H	4.558373	2.531710	0.031454
C	5.006622	0.407457	0.108055
H	6.041599	0.554238	0.412129
C	-3.453226	-2.314344	-0.519911
C	-1.589860	-3.500005	-0.830365
H	-2.374219	-3.876117	1.505894
H	-1.242643	-2.557009	1.274456
C	-3.182452	-0.862763	-0.090122
H	-2.409532	-0.428288	-0.739658
C	-2.214594	-3.228211	-0.547883
H	-2.497810	-4.190422	-1.002954
H	-1.463451	-2.786531	-1.219821
H	-2.769240	-0.846058	0.929224
C	-4.452551	0.002455	-0.124547
H	-5.236124	-0.519215	0.447095
H	-4.828898	0.060689	-1.158560
H	-4.211851	-2.753377	0.148202
H	-3.905284	-2.305947	-1.523977
C	-4.329039	1.426904	0.448502
H	-3.867644	1.381868	1.446445
H	-5.346646	1.811171	0.610863
C	-3.595789	2.471005	-0.424336
H	-4.008680	2.434826	-1.442348
H	-3.858203	3.466720	-0.033105

Sum of electronic and zero-point Energies= -1083.753972  
Sum of electronic and thermal Energies= -1083.729008  
Sum of electronic and thermal Enthalpies= -1083.728064  
Sum of electronic and thermal Free Energies= -1083.809587

daec[n=5]-7-E2 (benzene)

C	0.002623	2.850677	-0.698134
H	-0.408004	3.131865	-1.663727
C	-0.788005	3.020773	0.449954
C	-0.250720	2.673564	1.695846
H	-0.836541	2.816373	2.601752
C	1.030904	2.125878	1.784654
H	1.453083	1.833572	2.743479
C	1.796777	1.932287	0.640132
O	3.068409	1.397310	0.751676
C	1.296947	2.318326	-0.619894
O	2.122679	2.113229	-1.678693
C	1.660206	2.473595	-2.973271
H	1.441595	3.549129	-3.039789
H	2.477088	2.229402	-3.658378
H	0.766000	1.900827	-3.258748
C	3.721589	-2.673876	0.139565
H	3.918440	-3.734364	-0.008104
C	2.453106	-2.156087	-0.148360
C	1.340487	-3.033986	-0.691660
H	1.715877	-4.058775	-0.819796

H	1.068752	-2.682073	-1.699671
C	0.062952	-3.063635	0.172071
H	0.301422	-3.483906	1.160910
C	-1.064637	-3.875354	-0.481154
H	-0.706170	-4.901239	-0.657979
H	-1.277545	-3.459336	-1.477688
C	-2.367374	-3.954202	0.335527
H	-2.144993	-4.395327	1.319581
H	-3.044229	-4.662868	-0.166685
H	-0.275759	-2.034471	0.353653
C	2.220249	-0.786326	0.050601
H	1.240996	-0.370927	-0.166649
C	3.235407	0.046770	0.523022
C	4.506321	-0.472341	0.800413
H	5.283442	0.194397	1.165695
C	4.738193	-1.832376	0.607114
H	5.722754	-2.242482	0.825364
C	-4.710293	-0.914248	-0.577966
C	-3.129050	-2.630665	0.549225
H	-4.026633	-2.857054	1.145850
H	-2.528249	-1.946616	1.165332
C	-4.448727	0.285080	0.351553
H	-4.173112	-0.073131	1.354996
C	-3.561513	-1.926897	-0.750593
H	-3.897152	-2.689044	-1.471403
H	-2.696140	-1.435876	-1.218721
H	-5.398984	0.826463	0.480346
C	-3.383953	1.278456	-0.140016
H	-3.622637	1.590333	-1.169902
H	-2.402501	0.786217	-0.189275
H	-5.590529	-1.456735	-0.199081
H	-4.996054	-0.534153	-1.571359
C	-3.289080	2.522424	0.756253
H	-3.104382	2.208000	1.794317
H	-4.262657	3.035553	0.763780
C	-2.207749	3.545229	0.340408
H	-2.398048	3.876979	-0.689892
H	-2.315797	4.436568	0.976167

Sum of electronic and zero-point Energies= -1083.755312  
Sum of electronic and thermal Energies= -1083.730398  
Sum of electronic and thermal Enthalpies= -1083.729454  
Sum of electronic and thermal Free Energies= -1083.810658

daec[n=5]-8-TS (benzene)

C	1.301276	-3.295791	0.219787
H	1.504898	-4.357959	0.326919
C	-0.041188	-2.862227	0.162301
C	-0.236560	-1.489015	0.019392
H	-1.216596	-1.052696	0.029978
C	0.820271	-0.597214	-0.099464
H	0.588232	0.445700	-0.260017
C	2.135530	-1.013755	0.024183
O	3.212207	-0.144903	0.002390
C	2.383879	-2.399405	0.175731
O	3.694942	-2.760202	0.262923
C	4.003966	-4.137070	0.409601
H	5.095603	-4.193726	0.458269
H	3.650719	-4.727563	-0.448808
H	3.579823	-4.553639	1.335251
C	2.276051	3.863585	-0.683499
H	2.004474	4.893905	-0.908790
C	1.690044	3.216821	0.419439
C	0.623372	3.912889	1.249411
H	0.967637	4.931780	1.477614
H	0.514565	3.401442	2.216082
C	-0.775194	4.036004	0.576756
H	-1.316019	4.842511	1.094378
C	-1.670062	2.779208	0.596357
H	-1.798430	2.451305	1.640402
H	-1.167767	1.953109	0.073772

C	-3.060754	3.040005	-0.028458
H	-2.946133	3.203990	-1.111571
H	-3.441556	3.990000	0.377504
H	-0.644119	4.378923	-0.460499
C	2.083477	1.903122	0.701397
H	1.665024	1.388527	1.562602
C	2.935655	1.207251	-0.169303
C	3.515482	1.856419	-1.257436
H	4.185122	1.305649	-1.912991
C	3.198487	3.198962	-1.492442
H	3.653272	3.716679	-2.334897
C	-4.925937	-0.486947	-0.107284
C	-4.143936	1.962426	0.218189
H	-4.216543	1.779128	1.302315
H	-5.118638	2.376924	-0.081741
C	-4.597939	-1.921499	-0.613968
H	-4.765064	-1.992628	-1.699602
C	-3.917678	0.619735	-0.499790
H	-2.900565	0.290434	-0.262897
H	-3.938933	0.774977	-1.590479
H	-5.296803	-2.628568	-0.142338
C	-3.138600	-2.252894	-0.277371
H	-2.969306	-1.933213	0.763239
H	-2.550811	-1.588378	-0.907717
H	-5.932519	-0.200103	-0.446708
H	-4.977895	-0.525755	0.992550
C	-2.525535	-3.655724	-0.442082
H	-3.221080	-4.429794	-0.084076
H	-2.350549	-3.865707	-1.507469
C	-1.200148	-3.842919	0.362102
H	-0.830694	-4.861010	0.174573
H	-1.470287	-3.825207	1.431349

Sum of electronic and zero-point Energies= -1083.724372  
 Sum of electronic and thermal Energies= -1083.700344  
 Sum of electronic and thermal Enthalpies= -1083.699400  
 Sum of electronic and thermal Free Energies= -1083.777033

daec[n=5]-8-E1 (benzene)

C	1.529501	-2.345166	0.474279
H	2.093366	-2.351549	1.402363
C	2.224557	-2.298672	-0.749208
C	1.488680	-2.312512	-1.936948
H	2.005261	-2.281320	-2.894278
C	0.088624	-2.363072	-1.909309
H	-0.490485	-2.387740	-2.829668
C	-0.591197	-2.386064	-0.698653
O	-1.966999	-2.519573	-0.670385
C	0.133353	-2.384567	0.515550
O	-0.613335	-2.432718	1.649677
C	0.059108	-2.408131	2.900795
H	-0.726891	-2.439323	3.660861
H	0.647072	-1.487538	3.026567
H	0.716207	-3.281207	3.024605
C	-4.491381	0.639646	0.326535
H	-5.186347	1.442578	0.568188
C	-3.414949	0.895850	-0.537500
C	-3.247227	2.276960	-1.145588
H	-4.247789	2.696674	-1.318792
H	-2.775465	2.190105	-2.135060
C	-2.439965	3.289131	-0.297082
H	-2.661037	4.299639	-0.673025
C	-0.921061	3.074687	-0.333306
H	-0.586101	3.113494	-1.382942
H	-0.685212	2.063587	0.025524
C	-0.138870	4.120270	0.480591
H	-0.331470	3.967112	1.554239
H	-0.531051	5.121382	0.243040
H	-2.800133	3.262903	0.742399
C	-2.537233	-0.155100	-0.846904
H	-1.705653	0.009892	-1.528304

C	-2.746417	-1.430778	-0.312098
C	-3.824577	-1.680858	0.538869
H	-3.962657	-2.683136	0.935364
C	-4.693220	-0.636490	0.856912
H	-5.537221	-0.822431	1.518873
C	3.591015	2.804542	0.266877
C	1.379116	4.121048	0.221478
H	1.556395	4.338069	-0.844268
H	1.837531	4.952105	0.779601
C	4.282741	1.459419	0.560492
H	4.071250	1.171634	1.603023
C	2.087876	2.810361	0.589320
H	1.599766	1.981595	0.061013
H	1.947466	2.609024	1.663934
H	5.374046	1.587966	0.498192
C	3.848611	0.320305	-0.375920
H	4.201361	0.531005	-1.398108
H	2.753528	0.294955	-0.434938
H	4.086327	3.599537	0.845070
H	3.737572	3.064910	-0.793693
C	4.336981	-1.066566	0.062706
H	5.434421	-1.119353	0.004433
H	4.086061	-1.215386	1.123721
C	3.742977	-2.227037	-0.766225
H	4.159958	-3.173242	-0.387868
H	4.080343	-2.140851	-1.808386

Sum of electronic and zero-point Energies= -1083.754758  
 Sum of electronic and thermal Energies= -1083.729769  
 Sum of electronic and thermal Enthalpies= -1083.728824  
 Sum of electronic and thermal Free Energies= -1083.810308

daec[n=5]-8-E2 (benzene)

C	1.584281	-2.418988	-0.855761
H	2.112961	-2.455770	-1.803981
C	2.327147	-2.276397	0.326955
C	1.641932	-2.231771	1.547957
H	2.193725	-2.134806	2.480899
C	0.248326	-2.309358	1.579294
H	-0.292210	-2.281228	2.522849
C	-0.483971	-2.435697	0.401887
O	-1.859941	-2.593137	0.457657
C	0.184634	-2.503058	-0.836057
O	-0.601596	-2.630777	-1.939878
C	0.032687	-2.740255	-3.206881
H	-0.775962	-2.857907	-3.934171
H	0.692122	-3.618723	-3.254269
H	0.610277	-1.837174	-3.452374
C	-4.393372	0.689384	0.870516
H	-5.084156	1.524783	0.975488
C	-3.431539	0.712971	-0.153282
C	-3.375282	1.888809	-1.111752
H	-4.405004	2.204110	-1.331136
H	-2.942106	1.564585	-2.068783
C	-2.591759	3.120989	-0.599293
H	-2.860183	3.982452	-1.229501
C	-1.066693	2.952728	-0.616783
H	-0.747748	2.731547	-1.648744
H	-0.789135	2.075704	-0.016456
C	-0.313646	4.196062	-0.113395
H	-0.508763	4.328964	0.962504
H	-0.728736	5.087920	-0.608270
H	-2.929714	3.368442	0.418377
C	-2.559255	-0.377507	-0.280947
H	-1.827279	-0.404428	-1.083845
C	-2.655239	-1.466423	0.593677
C	-3.620520	-1.487881	1.602105
H	-3.682257	-2.351732	2.259180
C	-4.488414	-0.401656	1.735331
H	-5.245710	-0.411511	2.517266
C	3.454047	2.985640	0.057917

C	1.205761	4.166112	-0.361857
H	1.387616	4.097544	-1.446641
H	1.638432	5.127173	-0.043225
C	4.179853	1.782626	0.690556
H	3.950143	1.753819	1.767726
C	1.943669	3.019454	0.342954
H	1.494014	2.065809	0.038552
H	1.782864	3.095836	1.430589
H	5.267729	1.932990	0.616885
C	3.808434	0.431914	0.058448
H	4.163581	0.406604	-0.984514
H	2.716258	0.342098	0.007851
H	3.910001	3.917239	0.426549
H	3.620002	2.977894	-1.031482
C	4.354989	-0.783844	0.818008
H	5.454975	-0.787918	0.787408
H	4.080522	-0.696398	1.879801
C	3.839168	-2.137253	0.277146
H	4.303114	-2.945947	0.861432
H	4.181502	-2.270263	-0.758651

Sum of electronic and zero-point Energies= -1083.754323

Sum of electronic and thermal Energies= -1083.729252

Sum of electronic and thermal Enthalpies= -1083.728307

Sum of electronic and thermal Free Energies= -1083.810447

daec[n=6]-1-TS (benzene)

C	-1.611477	-3.348818	0.042372
H	-2.195317	-4.243087	-0.159263
C	-2.284320	-2.119569	0.191501
C	-1.511429	-0.990760	0.453253
H	-1.973142	-0.022181	0.606189
C	-0.116906	-1.065591	0.532890
H	0.438495	-0.153476	0.701656
C	0.545348	-2.277072	0.382717
O	1.913591	-2.459469	0.471066
C	-0.219980	-3.446402	0.142919
O	0.488075	-4.601721	0.014841
C	-0.228789	-5.803289	-0.221159
H	-0.924827	-6.030160	0.599859
H	0.525935	-6.593347	-0.279670
H	-0.785726	-5.766825	-1.169227
C	4.620719	0.485667	-0.722831
H	5.316783	1.246679	-1.071937
C	3.718770	0.786036	0.308735
C	3.569057	2.192031	0.856954
H	4.537457	2.596233	1.184916
H	2.929519	2.158177	1.749164
C	2.946650	3.152198	-0.195054
H	3.748754	3.529050	-0.844430
C	2.166536	4.338231	0.407861
H	2.127434	5.153686	-0.330073
H	2.723210	4.738337	1.268958
C	0.722476	4.007286	0.842030
H	0.336559	4.844233	1.443715
C	-0.244486	3.752188	-0.328196
H	0.107149	2.896879	-0.924171
H	-0.222058	4.620669	-1.005845
H	0.724700	3.133350	1.512972
H	2.280995	2.578530	-0.852712
C	2.849919	-0.220434	0.753376
H	2.202573	-0.025390	1.602517
C	2.797198	-1.458589	0.104547
C	3.695777	-1.750073	-0.925022
H	3.653243	-2.724937	-1.403636
C	4.620490	-0.779454	-1.316842
H	5.328764	-1.004696	-2.112092
C	-4.119925	3.016315	-0.735992
C	-1.698016	3.488800	0.101023
H	-1.715239	2.650889	0.814357
H	-2.080874	4.362428	0.652770

C	-4.472824	1.805653	0.149823
H	-5.516323	1.905792	0.485926
C	-2.627808	3.189294	-1.088665
H	-2.260336	2.296488	-1.616659
H	-2.544208	4.014756	-1.812377
H	-3.865894	1.838561	1.067323
C	-4.293995	0.430762	-0.518363
H	-3.304821	0.375491	-0.988095
H	-5.016362	0.324472	-1.342207
H	-4.695594	2.953606	-1.672512
H	-4.466688	3.931142	-0.230883
C	-4.469810	-0.741585	0.473281
H	-5.543512	-0.924039	0.622303
H	-4.081215	-0.450498	1.460360
C	-3.802169	-2.066311	0.056347
H	-4.232070	-2.882148	0.656382
H	-4.076729	-2.298238	-0.985855

Sum of electronic and zero-point Energies= -1123.023407

Sum of electronic and thermal Energies= -1122.998088

Sum of electronic and thermal Enthalpies= -1122.997144

Sum of electronic and thermal Free Energies= -1123.078469

daec[n=6]-1-E1 (benzene)

C	-0.979735	2.521561	0.790056
H	-1.590585	2.376753	1.676454
C	-1.602303	2.917857	-0.406466
C	-0.808003	3.127173	-1.539788
H	-1.267625	3.447096	-2.473183
C	0.575987	2.937211	-1.481873
H	1.204425	3.109067	-2.352796
C	1.184238	2.537885	-0.297092
O	2.562641	2.448621	-0.228672
C	0.405572	2.326307	0.860688
O	1.085043	1.947745	1.973977
C	0.346020	1.698395	3.161683
H	-0.175047	2.601258	3.511261
H	1.082578	1.395481	3.911365
H	-0.382934	0.886900	3.022028
C	4.591135	-1.187652	-0.389605
H	5.149453	-2.121009	-0.442027
C	3.212985	-1.186576	-0.643086
C	2.469021	-2.470267	-0.952653
H	3.112580	-3.142465	-1.538598
H	1.604422	-2.236090	-1.587473
C	1.993942	-3.214989	0.314865
H	2.878324	-3.537489	0.883106
C	1.105996	-4.440479	0.024842
H	0.995955	-5.023227	0.952367
H	1.631002	-5.098560	-0.684655
C	-0.297084	-4.123778	-0.529621
H	-0.761359	-5.061289	-0.871285
C	-1.236884	-3.443011	0.477557
H	-0.738958	-2.567774	0.920595
H	-1.432541	-4.133388	1.313690
H	-0.209579	-3.493465	-1.427468
H	1.462871	-2.508225	0.967532
C	2.510600	0.027022	-0.581001
H	1.443549	0.043735	-0.788359
C	3.176106	1.214735	-0.267942
C	4.552672	1.210095	-0.014626
H	5.050053	2.147352	0.221807
C	5.250960	0.005491	-0.078070
H	6.322578	-0.001123	0.113721
C	-4.797583	-1.730191	0.307770
C	-2.567496	-2.981635	-0.134582
H	-2.351166	-2.276922	-0.951395
H	-3.081566	-3.837194	-0.601177
C	-4.620347	-0.552215	-0.670146
H	-5.618449	-0.241440	-1.015846
C	-3.501970	-2.323378	0.891758

H	-2.949130	-1.539028	1.430500
H	-3.773338	-3.070173	1.653659
H	-4.085075	-0.887381	-1.571071
C	-3.894379	0.665958	-0.078273
H	-2.861747	0.393550	0.178732
H	-4.379693	0.954975	0.868580
H	-5.434299	-1.398420	1.142676
H	-5.359816	-2.528285	-0.201440
C	-3.877167	1.876354	-1.021734
H	-4.912845	2.185480	-1.229002
H	-3.444166	1.583869	-1.990297
C	-3.106594	3.102701	-0.476364
H	-3.327523	3.963592	-1.122580
H	-3.495956	3.355467	0.520346

Sum of electronic and zero-point Energies= -1123.042035

Sum of electronic and thermal Energies= -1123.015721

Sum of electronic and thermal Enthalpies= -1123.014777

Sum of electronic and thermal Free Energies= -1123.099771

daec[n=6]-1-E2 (benzene)

C	-0.479286	2.992007	-0.628111
H	-0.806194	3.322915	-1.610239
C	-1.418041	2.941050	0.419100
C	-0.988657	2.536877	1.686657
H	-1.694990	2.502426	2.513638
C	0.346137	2.173531	1.901930
H	0.691852	1.859015	2.883978
C	1.265367	2.217139	0.861673
O	2.595736	1.938722	1.115323
C	0.859176	2.641404	-0.423659
O	1.830755	2.676200	-1.371921
C	1.473591	3.077908	-2.687260
H	0.726400	2.402110	-3.127827
H	2.395367	3.026733	-3.273729
H	1.089871	4.108185	-2.705084
C	4.416858	-1.601595	-0.116982
H	4.918754	-2.515370	-0.431158
C	3.029283	-1.483276	-0.268464
C	2.194271	-2.619387	-0.824736
H	2.795303	-3.215061	-1.526753
H	1.363916	-2.197438	-1.406353
C	1.634792	-3.552138	-0.272544
H	2.478825	-4.048877	0.772586
C	0.658247	-4.623591	-0.249316
H	0.460786	-5.341562	0.561562
H	1.154258	-5.197909	-1.047076
C	-0.688332	-4.093821	-0.780759
H	-1.226952	-4.924883	-1.261049
C	-1.595348	-3.467294	0.289881
H	-1.037152	-2.706697	0.855492
H	-1.878803	-4.239675	1.022687
H	-0.509891	-3.358139	-1.579489
H	1.147890	-2.943125	1.046626
C	2.399672	-0.295618	0.135813
H	1.323068	-0.192175	0.025874
C	3.146499	0.753575	0.675539
C	4.532744	0.631667	0.827473
H	5.093902	1.462482	1.247706
C	5.158083	-0.548568	0.429756
H	6.236627	-0.645331	0.541828
C	-4.979870	-1.419751	0.262013
C	-2.858637	-2.809384	-0.284524
H	-2.552175	-2.030998	-0.999302
H	-3.432267	-3.547147	-0.868289
C	-4.662487	-0.149284	-0.550776
H	-5.613017	0.275907	-0.908687
C	-3.763904	-2.199566	0.796765
H	-3.161471	-1.544791	1.443918
H	-4.128157	-3.007033	1.450282
H	-4.096929	-0.415111	-1.456533

C	-3.892897	0.931448	0.224172
H	-2.918673	0.538775	0.545093
H	-4.441248	1.177685	1.148122
H	-5.616848	-1.139775	1.115405
H	-5.589635	-2.091943	-0.361562
C	-3.673039	2.214783	-0.588416
H	-4.648827	2.638622	-0.870191
H	-3.162565	1.968062	-1.532006
C	-2.865669	3.307448	0.151225
H	-2.899898	4.228363	-0.448732
H	-3.364371	3.539010	1.102837

Sum of electronic and zero-point Energies= -1123.042232

Sum of electronic and thermal Energies= -1123.015976

Sum of electronic and thermal Enthalpies= -1123.015032

Sum of electronic and thermal Free Energies= -1123.099681

daec[n=6]-2-TS (benzene)

C	-2.173019	2.938706	0.026626
H	-2.897516	3.709076	-0.224195
C	-2.637981	1.641205	0.320937
C	-1.688840	0.673263	0.641768
H	-1.988311	-0.336201	0.900951
C	-0.320284	0.967759	0.640507
H	0.383371	0.175483	0.860359
C	0.134854	2.245847	0.346167
O	1.459051	2.640865	0.339610
C	-0.812147	3.256795	0.043798
O	-0.298871	4.488000	-0.226705
C	-1.203648	5.533620	-0.545253
H	-1.780975	5.309882	-1.454613
H	-0.585188	6.418765	-0.722029
H	-1.897457	5.738533	0.283436
C	4.592156	0.049611	-0.594293
H	5.410729	-0.614412	-0.865936
C	3.812215	-0.231056	0.538666
C	4.038622	-1.479676	1.374370
H	3.275022	-1.518700	2.162039
H	5.005545	-1.409679	1.895830
C	4.031059	-2.806029	0.573862
H	4.940394	-2.849664	-0.042925
C	2.822224	-3.047268	-0.348872
H	3.019892	-3.959634	-0.932383
H	2.765078	-2.230486	-1.082709
C	1.453608	-3.194182	0.335701
H	1.245642	-2.308319	0.954805
C	0.316885	-3.369766	-0.685642
H	0.524259	-4.253487	-1.309950
H	0.327680	-2.508261	-1.371749
H	1.473177	-4.051839	1.027048
H	4.119798	-3.633139	1.294435
C	2.779610	0.656347	0.874521
H	2.208461	0.492250	1.783872
C	2.476987	1.747342	0.051606
C	3.254389	2.015684	-1.077036
H	3.011213	2.876650	-1.694166
C	4.322761	1.170165	-1.383512
H	4.938007	1.378335	-2.256949
C	-3.632510	-3.699507	-0.618066
C	-1.088922	-3.498602	-0.077717
H	-1.142049	-4.401816	0.551166
H	-1.263679	-2.648413	0.598138
C	-4.135937	-2.573945	0.305928
H	-3.492630	-2.523277	1.197490
C	-2.192325	-3.548940	-1.148886
H	-1.988460	-4.393279	-1.825445
H	-2.120157	-2.646851	-1.774450
H	-5.134217	-2.847723	0.681005
C	-4.204224	-1.177549	-0.335332
H	-4.942189	-1.179264	-1.152328
H	-3.242400	-0.944300	-0.807020

H	-3.711894	-4.653891	-0.074659
H	-4.311652	-3.786878	-1.480401
C	-4.562746	-0.070338	0.680083
H	-4.115884	-0.307263	1.657042
H	-5.649251	-0.072408	0.847047
C	-4.134658	1.352066	0.274515
H	-4.505851	1.566673	-0.740756
H	-4.648719	2.073298	0.928092

Sum of electronic and zero-point Energies= -1123.027566  
Sum of electronic and thermal Energies= -1123.002301  
Sum of electronic and thermal Enthalpies= -1123.001357  
Sum of electronic and thermal Free Energies= -1123.082230

daec[n=6]-2-E1 (benzene)

C	1.338965	2.195574	0.738125
H	1.972433	1.968172	1.590484
C	1.940609	2.593920	-0.469148
C	1.117274	2.909415	-1.556073
H	1.560511	3.230514	-2.496959
C	-0.274801	2.838230	-1.438500
H	-0.923327	3.110707	-2.268090
C	-0.862612	2.446396	-0.240851
O	-2.234228	2.520728	-0.085906
C	-0.053024	2.111643	0.866189
O	-0.712692	1.747880	1.996206
C	0.052847	1.425180	3.148890
H	0.712611	0.563822	2.969708
H	-0.673457	1.166014	3.924547
H	0.654204	2.281121	3.487823
C	-4.794014	-0.755484	-0.288471
H	-5.496693	-1.584586	-0.355652
C	-3.502013	-0.895933	-0.817537
C	-3.090621	-2.195920	-1.485253
H	-2.187821	-2.030162	-2.086952
H	-3.877949	-2.491236	-2.194006
C	-2.863893	-3.377628	-0.512132
H	-3.777601	-3.521291	0.082541
C	-1.665432	-3.229975	0.440472
H	-1.700352	-4.049199	1.174900
H	-1.770870	-2.299375	1.017898
C	-0.297231	-3.242205	-0.256696
H	-0.253265	-2.431669	-0.999106
C	0.885428	-3.077410	0.707976
H	0.926010	-3.932569	1.400971
H	0.710248	-2.187930	1.334155
H	-0.183159	-4.179044	-0.825439
H	-2.740027	-4.294106	-1.109360
C	-2.614216	0.188478	-0.735313
H	-1.613719	0.105288	-1.152931
C	-3.019303	1.388703	-0.141124
C	-4.308335	1.522568	0.383914
H	-4.597885	2.467002	0.837465
C	-5.189083	0.444540	0.307041
H	-6.195159	0.545764	0.710446
C	4.730933	-2.266071	0.241983
C	2.233000	-2.916608	-0.010316
H	2.459010	-3.824868	-0.591433
C	2.132927	-2.105734	-0.746332
C	4.684610	-1.077784	-0.740041
H	4.097145	-1.353341	-1.628411
C	3.399554	-2.606785	0.938984
H	3.562704	-3.465634	1.607828
H	3.110608	-1.772114	1.595291
H	5.705694	-0.890361	-1.106448
C	4.110305	0.218208	-0.149137
H	4.674428	0.492455	0.757502
H	3.076345	0.043341	0.176091
H	5.094824	-3.152250	-0.300468
H	5.482786	-2.057929	1.018917
C	4.129205	1.397104	-1.131057

H	3.639921	1.101513	-2.071516
H	5.171299	1.638935	-1.389031
C	3.450891	2.680928	-0.594915
H	3.889078	2.934352	0.381378
H	3.699592	3.511055	-1.270258

Sum of electronic and zero-point Energies= -1123.040979  
Sum of electronic and thermal Energies= -1123.014779  
Sum of electronic and thermal Enthalpies= -1123.013835  
Sum of electronic and thermal Free Energies= -1123.097765

daec[n=6]-2-E2 (benzene)

C	0.866156	2.794519	-0.592219
H	1.158531	3.189700	-1.561452
C	1.861624	2.559760	0.373932
C	1.476497	2.073003	1.627474
H	2.226517	1.898706	2.396130
C	0.129925	1.815720	1.906478
H	-0.181827	1.448402	2.881482
C	-0.848842	2.050480	0.948049
O	-2.176667	1.916861	1.305654
C	-0.486055	2.556678	-0.320144
O	-1.509574	2.786585	-1.183222
C	-1.202198	3.291168	-2.475539
H	-0.718441	4.276934	-2.419901
H	-2.161588	3.389647	-2.991320
H	-0.558305	2.599682	-3.037970
C	-4.730271	-1.048072	-0.115205
H	-5.424169	-1.806599	-0.474233
C	-3.384334	-1.099246	-0.506608
C	-2.897221	-2.217677	-1.409254
H	-2.013309	-1.882937	-1.967528
H	-3.671848	-2.425719	-2.160749
C	-2.581087	-3.544656	-0.675268
H	-3.472379	-3.848549	-0.107391
C	-1.370314	-3.507245	0.273060
H	-1.344266	-4.447990	0.843862
H	-1.511848	-2.707197	1.014714
C	-0.020469	-3.313033	-0.433302
H	-0.048416	-2.393631	-1.036970
C	1.174034	-3.220887	0.527021
H	1.290459	-4.169849	1.073821
H	0.959359	-2.455138	1.289216
H	0.140991	-4.136173	-1.147825
H	-2.419725	-4.324840	-1.435108
C	-2.504412	-0.106977	-0.044966
H	-1.458664	-0.129184	-0.340135
C	-2.969333	0.916307	0.787036
C	-4.313250	0.962024	1.173662
H	-4.649111	1.769877	1.818863
C	-5.186335	-0.024727	0.719515
H	-6.233704	0.010809	1.014222
C	4.945127	-2.088812	0.108587
C	2.486092	-2.855924	-0.182749
H	2.752447	-3.643085	-0.906261
H	2.309279	-1.948084	-0.777684
C	4.790873	-0.776583	-0.686916
H	4.171676	-0.956603	-1.578304
C	3.660732	-2.617481	0.777220
H	3.898821	-3.555490	1.301660
H	3.342009	-1.913691	1.560315
H	5.780643	-0.482230	-1.068720
C	4.185938	0.388171	0.110630
H	4.814800	0.598429	0.991118
H	3.204246	0.092698	0.502996
H	5.345743	-2.859616	-0.567828
H	5.707896	-1.946616	0.889706
C	4.020956	1.671201	-0.714738
H	3.452609	1.445845	-1.630242
H	5.008813	2.025524	-1.045973
C	3.318406	2.824480	0.041107



H 3.871002 3.031810 0.968461  
H 3.388260 3.734449 -0.571605  
Sum of electronic and zero-point Energies= -1123.041254  
Sum of electronic and thermal Energies= -1123.015069  
Sum of electronic and thermal Enthalpies= -1123.014125  
Sum of electronic and thermal Free Energies= -1123.097922

daec[n=6]-3-TS (benzene)

C -3.045481 -2.090505 0.136456  
H -3.977771 -2.611969 -0.064122  
C -3.068355 -0.687432 0.261656  
C -1.861352 -0.039277 0.514512  
H -1.825404 1.037869 0.633968  
C -0.663266 -0.755076 0.625483  
H 0.256315 -0.211652 0.801778  
C -0.643342 -2.138045 0.500936  
O 0.484345 -2.928573 0.633191  
C -1.860311 -2.822263 0.257414  
O -1.768795 -4.175592 0.146551  
C -2.959003 -4.908419 -0.098487  
H -2.657449 -5.959259 -0.143109  
H -3.422091 -4.625792 -1.055511  
H -3.691771 -4.777998 0.711471  
C 4.196572 -1.775476 -0.886733  
H 5.158684 -1.485937 -1.306334  
C 3.650358 -1.038782 0.175317  
C 4.303149 0.234147 0.679294  
H 5.347258 0.050085 0.970640  
H 3.783236 0.558575 1.590003  
C 4.263111 1.369864 -0.380968  
H 3.391814 1.223013 -1.031389  
C 4.223637 2.794081 0.206645  
H 4.485322 3.508407 -0.588861  
H 5.008184 2.893879 0.972492  
C 2.869082 3.214402 0.814434  
H 2.995867 4.192889 1.302372  
C 1.715347 3.305078 -0.198848  
H 1.568430 2.327030 -0.679645  
H 1.993682 3.999249 -1.007776  
H 2.587266 2.516475 1.618437  
H 5.139088 1.273544 -1.037281  
C 2.420191 -1.447110 0.710368  
H 2.015795 -0.930009 1.575813  
C 1.709488 -2.508395 0.140186  
C 2.256737 -3.233728 -0.920598  
H 1.694708 -4.065404 -1.337376  
C 3.510952 -2.871310 -1.417095  
H 3.947536 -3.438280 -2.237321  
C -2.156314 4.038394 0.055753  
C 0.377915 3.747082 0.417126  
H 0.464308 4.777981 0.795300  
H 0.163769 3.121033 1.298498  
C -3.379820 3.758599 -0.842724  
H -3.204911 4.217128 -1.828088  
C -0.803318 3.646024 -0.562323  
H -0.851054 2.614541 -0.940661  
H -0.609882 4.279540 -1.442442  
H -4.255406 4.276312 -0.421043  
C -3.732803 2.269764 -1.041421  
H -2.844078 1.721047 -1.378710  
H -4.459493 2.184856 -1.863398  
H -2.136336 5.111341 0.300049  
H -2.278924 3.521321 1.019691  
C -4.332545 1.590284 0.205860  
H -5.354676 1.969100 0.351631  
H -3.781057 1.884844 1.109346  
C -4.395218 0.053141 0.137852  
H -4.883203 -0.247306 -0.803080  
H -5.064634 -0.303384 0.936161  
Sum of electronic and zero-point Energies= -1123.026279

Sum of electronic and thermal Energies= -1123.000885  
Sum of electronic and thermal Enthalpies= -1122.999941  
Sum of electronic and thermal Free Energies= -1123.081567

daec[n=6]-3-E1 (benzene)

C 1.744746 -2.337152 0.550673  
H 2.395707 -2.303507 1.419209  
C 2.316410 -2.259634 -0.731470  
C 1.473036 -2.331966 -1.846864  
H 1.895184 -2.285992 -2.849095  
C 0.092946 -2.488000 -1.687125  
H -0.564709 -2.573275 -2.549365  
C -0.465633 -2.560681 -0.415406  
O -1.811440 -2.834293 -0.249357  
C 0.360840 -2.476007 0.724957  
O -0.269356 -2.554229 1.925200  
C 0.518766 -2.475192 3.104761  
H -0.186411 -2.547460 3.937835  
H 1.057619 -1.518662 3.168950  
H 1.238318 -3.304278 3.167895  
C -4.781846 0.086140 -0.351750  
H -5.581164 0.824573 -0.388873  
C -3.453248 0.489554 -0.538328  
C -3.096730 1.947613 -0.750281  
H -3.866993 2.436378 -1.364670  
H -2.161894 2.002909 -1.322646  
C -2.939237 2.728357 0.573373  
H -2.279874 2.161314 1.244285  
C -2.407113 4.164944 0.406825  
H -2.386306 4.638903 1.400283  
H -3.123059 4.748750 -0.192171  
C -1.010924 4.289182 -0.236299  
H -0.742110 5.355456 -0.284564  
C 0.095091 3.516381 0.496223  
H -0.202338 2.462794 0.597243  
H 0.193325 3.899195 1.524748  
H -1.053101 3.947937 -1.281587  
H -3.914449 2.766460 1.079993  
C -2.435208 -0.477177 -0.498462  
H -1.401292 -0.178935 -0.651778  
C -2.744635 -1.821647 -0.277097  
C -4.073681 -2.219987 -0.087125  
H -4.290524 -3.271824 0.081185  
C -5.083606 -1.260718 -0.125831  
H -6.118120 -1.568754 0.015910  
C 3.817547 2.507621 -0.291761  
C 1.461718 3.554830 -0.203433  
H 1.851352 4.584751 -0.221018  
H 1.332771 3.260219 -1.257234  
C 4.821789 1.532715 0.353610  
H 5.026421 1.870323 1.381433  
C 2.481045 2.614535 0.456019  
H 2.023770 1.617276 0.532810  
H 2.667755 2.941516 1.491741  
H 5.780732 1.601858 -0.183136  
C 4.383760 0.055656 0.402734  
H 3.413574 -0.025911 0.911074  
H 5.098601 -0.498699 1.030730  
H 4.283219 3.503655 -0.345012  
H 3.625927 2.212099 -1.334347  
C 4.310788 -0.633953 -0.967687  
H 5.314510 -0.624887 -1.419174  
H 3.662108 -0.067607 -1.650548  
C 3.814830 -2.100853 -0.915516  
H 4.347691 -2.630036 -0.112000  
H 4.101423 -2.595741 -1.853303  
Sum of electronic and zero-point Energies= -1123.039846  
Sum of electronic and thermal Energies= -1123.013618  
Sum of electronic and thermal Enthalpies= -1123.012674  
Sum of electronic and thermal Free Energies= -1123.097530

## daec[n=6]-3-E2 (benzene)

C	-1.315793	2.550628	-0.811659
H	-1.688526	2.659798	-1.826561
C	-2.241415	2.425200	0.240816
C	-1.756402	2.309596	1.547701
H	-2.451563	2.231234	2.380926
C	-0.378705	2.303950	1.795895
H	0.009033	2.221152	2.808607
C	0.529893	2.428193	0.751604
O	1.876218	2.540875	1.043027
C	0.062873	2.566192	-0.575052
O	1.017858	2.716885	-1.529116
C	0.605967	2.846084	-2.882901
H	1.527059	2.940242	-3.465063
H	-0.010966	3.743607	-1.635848
H	0.051583	1.959931	-3.223961
C	4.704574	-0.338906	0.006982
H	5.465369	-1.071618	-0.257461
C	3.349306	-0.654244	-0.157139
C	2.910147	-2.015561	-0.659234
H	3.657169	-2.415278	-1.360187
H	1.980316	-1.897283	-1.230595
C	2.688731	-3.036447	0.478830
H	2.055310	-2.577430	1.249931
C	2.073788	-4.374793	0.025403
H	2.005549	-5.034369	0.904175
H	2.764419	-4.871942	-0.673220
C	0.685421	-4.280757	-0.639569
H	0.353523	-5.297290	-0.900426
C	-0.387016	-3.599116	0.222258
H	-0.026876	-2.609359	0.537409
H	-0.533669	-4.172953	1.151253
H	0.769610	-3.743743	-1.596388
H	3.653261	-3.235084	0.968203
C	2.381918	0.304985	0.181670
H	1.326363	0.074495	0.060449
C	2.765641	1.556349	0.667804
C	4.120284	1.867051	0.833539
H	4.395451	2.848335	1.211845
C	5.081501	0.913784	0.501839
H	6.136244	1.153963	0.624324
C	-4.019681	-2.212761	-0.395182
C	-1.735971	-3.406209	-0.486276
H	-2.188087	-4.383936	-0.715521
H	-1.562629	-2.916385	-1.458002
C	-4.983622	-1.326000	0.417227
H	-5.236774	-1.849527	1.352092
C	-2.712553	-2.551866	0.335279
H	-2.198374	-1.621604	0.617633
H	-2.946185	-3.066026	1.281462
H	-5.929133	-1.226993	-0.138486
C	-4.464373	0.081283	0.771873
H	-3.510636	0.001196	1.310696
H	-5.169647	0.543189	1.480165
H	-4.541145	-3.146684	-0.655465
H	-3.782527	-1.727256	-1.354028
C	-4.301040	1.023623	-0.429784
H	-5.284123	1.167005	-0.903634
H	-3.656458	0.565123	-1.193148
C	-3.727444	2.415746	-0.066881
H	-4.283515	2.818644	0.791700
H	-3.918216	3.098748	-0.906426

Sum of electronic and zero-point Energies= -1123.040688

Sum of electronic and thermal Energies= -1123.014478

Sum of electronic and thermal Enthalpies= -1123.013534

Sum of electronic and thermal Free Energies= -1123.097627

## daec[n=7]-1-TS (benzene)

C	-3.328693	2.102969	-0.008793
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H	-4.140638	2.814087	0.117532
C	-2.001980	2.571683	0.056868
C	-0.981293	1.637942	-0.118891
H	0.058992	1.938551	-0.109734
C	-1.261892	0.284679	-0.324587
H	-0.436135	-0.406250	-0.429433
C	-2.570797	-0.176301	-0.382822
O	-2.936581	-1.491386	-0.610591
C	-3.627966	0.753349	-0.230123
O	-4.886589	0.240284	-0.306896
C	-5.981967	1.129372	-0.154919
H	-5.988901	1.904526	-0.935337
H	-5.982354	1.610580	0.834406
H	-6.880927	0.513525	-0.253989
C	-0.594477	-4.634480	0.820865
H	0.010312	-5.444301	1.226320
C	-0.058609	-3.798672	-0.169746
C	1.397451	-3.897404	-0.579956
H	1.529755	-3.472474	-1.584126
H	1.713550	-4.949048	-0.634827
C	2.297768	-3.151850	0.435796
H	1.911346	-2.131564	0.570059
C	3.794577	-3.102026	0.082318
H	4.139013	-4.118289	-0.164525
H	4.350356	-2.812607	0.985755
C	4.194032	-2.158776	-1.069800
H	3.700310	-2.479881	-1.999406
C	3.912085	-0.655845	-0.860366
H	2.827214	-0.477297	-0.849805
H	4.291006	-0.120667	-1.745273
H	5.273057	-2.286601	-1.247638
H	2.180909	-3.641445	1.413328
C	-0.863620	-2.775623	-0.691634
H	-0.488566	-2.160782	-1.505061
C	-2.132892	-2.526630	-0.159110
C	-2.660228	-3.362718	0.828272
H	-3.657160	-3.163234	1.212520
C	-1.891631	-4.429362	1.298645
H	-2.299982	-5.090546	2.060767
C	3.275399	2.220533	0.259703
C	4.547636	-0.046511	0.403333
H	3.998833	-0.386874	1.294342
H	5.571677	-0.436853	0.513243
C	2.172532	4.526397	-0.140892
H	2.412777	5.599168	-0.185200
H	2.019637	4.213444	-1.185680
C	4.621508	1.493525	0.414225
H	5.294776	1.825143	-0.392464
C	0.854681	4.328536	0.637513
H	0.841371	4.985655	1.520351
H	5.097776	1.812557	1.354377
H	0.816466	3.310357	1.039006
C	-0.397572	4.601721	-0.224570
H	-0.242301	4.188434	-1.231768
H	-0.498587	5.688216	-0.361087
H	2.561440	1.822288	0.996527
C	3.388305	3.751976	0.404320
H	4.280849	4.090425	-0.144202
H	3.566188	4.012290	1.459518
C	-1.730064	4.047827	0.327281
H	-2.558925	4.630033	-0.099275
H	2.853746	1.990059	-0.730440
H	-1.775278	4.232319	1.413529

Sum of electronic and zero-point Energies= -1162.307117

Sum of electronic and thermal Energies= -1162.280513

Sum of electronic and thermal Enthalpies= -1162.279569

Sum of electronic and thermal Free Energies= -1162.363865

## daec[n=7]-1-E1 (benzene)

C	-2.095514	2.927571	-0.261261
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H	-2.158199	3.760042	-0.956716
C	-1.308356	3.067976	0.895793
C	-1.240327	1.996375	1.791281
H	-0.646783	2.084761	2.699133
C	-1.942010	0.811764	1.541420
H	-1.901042	-0.015615	2.245967
C	-2.711312	0.677869	0.389809
O	-3.497295	-0.430398	0.149229
C	-2.794706	1.746226	-0.530707
O	-3.574318	1.533306	-1.623719
C	-3.696305	2.582525	-2.572624
H	-2.724816	2.843854	-3.017424
H	-4.146766	3.482128	-2.128240
H	-4.357669	2.199618	-3.355433
C	-2.075403	-4.339228	0.276242
H	-1.732902	-5.372471	0.298715
C	-1.196427	-3.329001	-0.140993
C	0.228721	-3.664481	-0.536314
H	0.505579	-3.095379	-1.434356
H	0.282344	-4.727190	-0.813042
C	1.252057	-3.388079	0.587450
H	1.299787	-2.305233	0.772843
C	2.659474	-3.950603	0.315791
H	2.588124	-5.046932	0.241894
H	3.285937	-3.752972	1.197684
C	3.375511	-3.433785	-0.947146
H	2.805788	-3.736587	-1.838053
C	3.620450	-1.915312	-1.014631
H	2.656412	-1.387245	-1.020526
H	4.091904	-1.686556	-1.983512
H	4.344211	-3.951676	-1.024097
H	0.877384	-3.834987	1.519716
C	-1.653715	-2.002309	-0.169064
H	-0.993788	-1.204426	-0.502166
C	-2.963909	-1.700049	0.216812
C	-3.837611	-2.712500	0.627467
H	-4.853152	-2.450147	0.912748
C	-3.385421	-4.030975	0.652476
H	-4.061066	-4.823832	0.968307
C	3.729462	1.093931	-0.131575
C	4.507740	-1.360029	0.111210
H	3.995233	-1.473723	1.078457
H	5.421968	-1.970511	0.179545
C	3.019503	3.565985	-0.390153
H	3.428400	4.588247	-0.372306
H	2.661863	3.401038	-1.419262
C	4.911791	0.115072	-0.064295
H	5.521806	0.221872	-0.975548
C	1.823924	3.481007	0.569888
H	2.173336	3.620854	1.605996
H	5.567058	0.400332	0.773462
H	1.390857	2.473083	0.527985
C	0.725328	4.507029	0.262703
H	0.439320	4.428549	-0.797427
H	1.123380	5.524089	0.398050
H	3.043929	0.883180	0.702863
C	4.154790	2.570375	-0.091228
H	4.961881	2.731730	-0.822695
H	4.591706	2.794675	0.894912
C	-0.541511	4.354739	1.136588
H	-1.202008	5.212515	0.943411
H	3.152455	0.913733	-1.051103
H	-0.256906	4.415354	2.196507

Sum of electronic and zero-point Energies= -1162.324373  
Sum of electronic and thermal Energies= -1162.296830  
Sum of electronic and thermal Enthalpies= -1162.295886  
Sum of electronic and thermal Free Energies= -1162.383647

daec[n=7]-1-E2 (benzene)

C	0.593891	2.841662	0.934991
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H	1.079645	2.754403	1.902709
C	1.334973	3.333240	-0.153082
C	0.700500	3.459025	-1.394493
H	1.249973	3.847913	-2.249860
C	-0.641669	3.098551	-1.544793
H	-1.149771	3.206607	-2.500327
C	-1.371193	2.616607	-0.462768
O	-2.727689	2.402921	-0.610526
C	-0.754529	2.487849	0.800666
O	-1.546000	2.033274	1.806809
C	-0.972079	1.868917	3.096081
H	-0.612344	2.824702	3.503583
H	-0.145870	1.143570	3.081826
H	-1.775773	1.486553	3.731831
C	-4.554981	-1.327421	-0.363133
H	-5.062143	-2.289268	-0.308559
C	-3.170011	-1.287330	-0.574366
C	-2.377972	-2.575233	-0.696539
H	-1.676559	-2.501293	-1.539284
H	-3.068738	-3.395286	-0.939541
C	-1.603241	-2.938093	0.590118
H	-0.793208	-2.209689	0.740402
C	-1.047840	-4.374222	0.614311
H	-1.896607	-5.075428	0.594437
H	-0.552372	-4.535977	1.582748
C	-0.085647	-4.761784	-0.524986
H	-0.624384	-4.725821	-1.483356
C	1.193229	-3.914673	-0.651152
H	0.922513	-2.874612	-0.881559
H	1.759533	-4.275887	-1.524167
H	0.200260	-5.815819	-0.384125
H	-2.277164	-2.817431	1.450454
C	-2.529399	-0.039086	-0.647771
H	-1.457481	0.015138	-0.825049
C	-3.267581	1.138442	-0.503591
C	-4.651181	1.092899	-0.297672
H	-5.199782	2.025787	-0.196010
C	-5.287372	-0.143992	-0.229437
H	-6.363591	-0.185609	-0.070964
C	3.390521	-1.783666	-0.012069
C	2.109770	-3.948463	0.582462
H	1.601412	-3.474135	1.435630
H	2.278489	-4.996728	0.875302
C	4.726697	0.331689	-0.652406
H	5.749550	0.739206	-0.659602
H	4.429160	0.242238	-1.709519
C	3.475096	-3.267352	0.377082
H	4.042182	-3.810796	-0.395527
C	3.789826	1.329904	0.043566
H	4.078712	1.427524	1.103042
H	4.059379	-3.364015	1.305466
H	2.764886	0.936099	0.041402
C	3.790505	2.715807	-0.614149
H	3.562084	2.609776	-1.685484
H	4.800501	3.149379	-0.557742
H	2.709875	-1.270202	0.683662
C	4.753160	-1.072892	-0.023546
H	5.474798	-1.690150	-0.580826
H	5.140524	-1.010690	1.005925
C	2.794193	3.716168	0.014768
H	2.960333	4.702621	-0.441655
H	2.932913	-1.689756	-1.008267
H	3.022584	3.828193	1.084186

Sum of electronic and zero-point Energies= -1162.325017  
Sum of electronic and thermal Energies= -1162.297486  
Sum of electronic and thermal Enthalpies= -1162.296542  
Sum of electronic and thermal Free Energies= -1162.384015

daec[n=7]-2-TS (benzene)

C	1.774241	3.278380	0.375101
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H	2.433606	4.142009	0.349602
C	2.343698	1.991812	0.453651
C	1.477135	0.902217	0.482490
H	1.865859	-0.106240	0.565709
C	0.089092	1.071131	0.401606
H	-0.551930	0.197163	0.385675
C	-0.466669	2.341020	0.323083
O	-1.816318	2.617101	0.244994
C	0.391312	3.469463	0.322238
O	-0.224929	4.681063	0.248222
C	0.587875	5.843929	0.239893
H	-0.103682	6.690032	0.184202
H	1.257008	5.867618	-0.633058
H	1.187385	5.928063	1.158386
C	-4.653857	-0.171699	-0.995804
H	-5.408698	-0.878247	-1.335846
C	-3.966486	-0.410757	0.205597
C	-4.237212	-1.657648	1.031171
H	-5.265720	-1.618625	1.421550
H	-3.581473	-1.652801	1.911543
C	-4.076364	-2.991423	0.262913
H	-4.333132	-3.811056	0.951133
C	-2.691120	-3.256297	-0.354535
H	-2.424895	-2.421207	-1.019254
H	-2.768715	-4.142772	-1.002460
C	-1.555420	-3.484064	0.654305
H	-1.806492	-4.340407	1.300727
C	-0.191570	-3.726741	-0.013620
H	0.031018	-2.880138	-0.680201
H	-0.250928	-4.615724	-0.661861
H	-1.470096	-2.615736	1.325270
H	-4.827182	-3.028479	-0.539258
C	-3.016139	0.529966	0.628768
H	-2.499654	0.390596	1.575476
C	-2.723216	1.650682	-0.157207
C	-3.406196	1.876800	-1.353151
H	-3.169676	2.760567	-1.939913
C	-4.381663	0.964011	-1.760455
H	-4.926212	1.137400	-2.686798
C	2.817531	-2.852870	-0.458663
C	0.950754	-3.902983	0.998101
H	0.957674	-3.035023	1.677470
H	0.737558	-4.777919	1.631616
C	4.848195	-1.514618	-1.380977
H	5.943072	-1.455666	-1.278198
H	4.659028	-1.782880	-2.431885
C	2.359535	-4.054701	0.393817
H	2.415943	-4.977507	-0.203815
C	4.242747	-0.117518	-1.132633
H	3.173810	-0.132961	-1.379990
H	3.067237	-4.192992	1.225640
H	4.699722	0.584596	-1.847188
C	4.439481	0.436128	0.288948
H	5.517262	0.478838	0.507404
H	4.017988	-0.257098	1.030324
H	2.348706	-1.943166	-0.060941
C	4.341848	-2.658485	-0.478487
H	4.822891	-3.592911	-0.807021
H	4.686991	-2.496355	0.554079
C	3.859416	1.845711	0.521969
H	4.201272	2.196803	1.508884
H	2.442619	-2.952668	-1.488209
H	4.310134	2.540893	-0.203241

Sum of electronic and zero-point Energies= -1162.314176  
Sum of electronic and thermal Energies= -1162.287673  
Sum of electronic and thermal Enthalpies= -1162.286728  
Sum of electronic and thermal Free Energies= -1162.370422

daec[n=7]-2-E2 (benzene)

C	-2.101501	2.581253	-0.493583
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H	-2.886995	2.914740	-1.166140
C	-2.464736	2.013444	0.742593
C	-1.444019	1.596232	1.600212
H	-1.688513	1.172107	2.571913
C	-0.096366	1.727722	1.235988
H	0.686203	1.398073	1.913660
C	0.251783	2.293347	0.013677
O	1.545187	2.506213	-0.410556
C	-0.764644	2.730602	-0.868743
O	-0.338656	3.277836	-2.040173
C	-1.319334	3.738276	-2.956631
H	-0.764395	4.133447	-3.812809
H	-1.935060	4.541034	-2.524789
H	-1.974257	2.922427	-3.297101
C	4.797514	0.429705	1.151339
H	5.673581	-0.090676	1.535838
C	4.104314	-0.102449	0.050939
C	4.559691	-1.390236	-0.610099
H	5.646820	-1.345203	-0.768877
H	4.109071	-1.461023	-1.608193
C	4.251549	-2.678165	0.190822
H	4.677277	-3.528294	-0.363805
C	2.765015	-2.947022	0.478073
H	2.361376	-2.127448	1.091005
H	2.692292	-3.852788	1.099576
C	1.878180	-3.118403	-0.764444
H	2.274009	-3.927461	-1.399012
C	0.408420	-3.399062	-0.414609
H	0.094927	-2.686427	0.361500
H	0.317935	-4.400255	0.036645
H	1.922462	-2.205514	-1.376018
H	4.792168	-2.636591	1.147922
C	2.989159	0.596572	-0.429779
H	2.435423	0.232295	-1.292265
C	2.587131	1.795247	0.165260
C	3.284395	2.325450	1.251147
H	2.969065	3.270475	1.686340
C	4.392738	1.627944	1.742498
H	4.950569	2.032215	2.585116
C	-2.581314	-2.654792	-0.171556
C	-0.537428	-3.279485	-1.619024
H	-0.434154	-2.267416	-2.042080
H	-0.213876	-3.973065	-2.410741
C	-4.676020	-2.046346	1.209262
H	-5.774997	-2.011815	1.147249
H	-4.441634	-2.751600	2.021724
C	-2.024244	-3.530551	-1.306493
H	-2.179712	-4.591287	-1.053530
C	-4.142793	-0.660669	1.616970
H	-3.048010	-0.701493	1.689507
H	-2.605782	-3.351242	-2.224211
H	-4.502616	-0.435280	2.633163
C	-4.552277	0.495531	0.693974
H	-5.648762	0.592144	0.709543
H	-4.277713	0.273467	-0.347306
H	-2.200912	-1.629095	-0.288284
C	-4.116493	-2.624262	-0.105786
H	-4.507521	-3.646998	-0.222269
H	-4.502625	-2.058492	-0.967183
C	-3.933165	1.858736	1.094018
H	-4.500307	2.658341	0.597588
H	-2.187236	-3.012992	0.791259
H	-4.073683	2.007581	2.174761

Sum of electronic and zero-point Energies= -1162.320417  
Sum of electronic and thermal Energies= -1162.292896  
Sum of electronic and thermal Enthalpies= -1162.291952  
Sum of electronic and thermal Free Energies= -1162.379267

daec[n=7]-2-E1 (benzene)

C	-1.247095	2.548939	0.363317
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H	-1.802195	2.686384	1.286219
C	-1.952685	2.491598	-0.853561
C	-1.224974	2.346402	-2.039453
H	-1.746956	2.307910	-2.993846
C	0.173834	2.289160	-2.016878
H	0.747353	2.225301	-2.938874
C	0.864765	2.363911	-0.812976
O	2.240097	2.498402	-0.812737
C	0.149840	2.479242	0.400592
O	0.905108	2.551194	1.527789
C	0.241335	2.670069	2.778213
H	1.032053	2.683306	3.533910
H	-0.424423	1.815425	2.966418
H	-0.335925	3.603826	2.842935
C	4.947068	-0.438394	0.355666
H	5.697006	-1.179475	0.628200
C	3.835661	-0.827735	-0.409387
C	3.709257	-2.266138	-0.880254
H	4.666625	-2.566870	-1.330244
H	2.966180	-2.324484	-1.685842
C	3.364811	-3.289521	0.227874
H	3.533091	-4.300612	-0.173494
C	1.932221	-3.201045	0.779968
H	1.735234	-2.173802	1.122159
H	1.859578	-3.838357	1.674471
C	0.847010	-3.621082	-0.222474
H	1.026804	-4.659495	-0.544065
C	-0.580618	-3.487410	0.325344
H	-0.698366	-2.478836	0.746835
H	-0.728344	-4.187465	1.163336
H	0.926697	-3.007099	-1.131901
H	4.079487	-3.166111	1.054273
C	2.887970	0.144896	-0.764220
H	2.026281	-0.125199	-1.371182
C	3.066874	1.477842	-0.377666
C	4.176057	1.858519	0.379955
H	4.288006	2.901652	0.663321
C	5.112354	0.891259	0.746896
H	5.981655	1.180917	1.334737
C	-3.343032	-2.093132	0.319312
C	-1.654973	-3.720475	-0.747251
H	-1.451509	-3.045932	-1.594570
H	-1.559559	-4.742568	-1.145288
C	-5.099762	-0.384950	1.133479
H	-6.154411	-0.101392	0.993365
H	-4.990104	-0.622241	2.203072
C	-3.103708	-3.488817	-0.283177
H	-3.394804	-4.258257	0.448844
C	-4.202790	0.828560	0.823950
H	-3.161815	0.585510	1.075521
H	-3.768844	-3.629772	-1.149198
H	-4.492951	1.648750	1.499663
C	-4.274507	1.337266	-0.622337
H	-5.325805	1.542759	-0.876807
H	-3.936653	0.557019	-1.319085
H	-2.750603	-1.355729	-0.242615
C	-4.815780	-1.659958	0.316200
H	-5.439424	-2.473346	0.718259
H	-5.143153	-1.521013	-0.725366
C	-3.465179	2.630442	-0.884719
H	-3.754109	3.020792	-1.869938
H	-2.956837	-2.065055	1.349176
H	-3.774621	3.390106	-0.151297

Sum of electronic and zero-point Energies= -1162.320463  
Sum of electronic and thermal Energies= -1162.292921  
Sum of electronic and thermal Enthalpies= -1162.291977  
Sum of electronic and thermal Free Energies= -1162.379953

daec[n=7]-3-TS (benzene)

C	-1.694852	-3.573981	0.213292
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H	-2.039476	-4.589603	0.401352
C	-0.327032	-3.261531	0.271430
C	0.030435	-1.935324	0.006778
H	1.070528	-1.632143	0.002354
C	-0.926159	-0.958101	-0.267403
H	-0.596959	0.058947	-0.437011
C	-2.282755	-1.276295	-0.302415
O	-3.291180	-0.366784	-0.580226
C	-2.669683	-2.612118	-0.068829
O	-3.989994	-2.987436	-0.042528
C	-4.661476	-2.972637	-1.304766
H	-5.678671	-3.329958	-1.112378
H	-4.170036	-3.650752	-2.018776
H	-4.705025	-1.962723	-1.729845
C	-3.081746	3.540411	0.871863
H	-3.030068	4.549686	1.277448
C	-2.169124	3.143182	-0.117039
C	-1.017422	4.037540	-0.530941
H	-1.366439	5.065532	-0.706278
H	-0.598042	3.680393	-1.481287
C	0.083812	4.061669	0.557362
H	-0.332984	4.547027	1.451134
C	1.380775	4.784008	0.145769
H	1.911505	5.098127	1.057306
H	1.121143	5.713035	-0.384914
C	2.362193	3.967422	-0.718432
H	3.155209	4.648742	-1.063248
C	3.022880	2.778503	0.005781
H	2.281235	1.986754	0.184548
H	3.361905	3.107169	1.001458
H	1.861271	3.609203	-1.631407
H	0.310735	3.030154	0.860667
C	-2.271911	1.846644	-0.640418
H	-1.617812	1.542361	-1.452800
C	-3.195674	0.938801	-0.113901
C	-4.097487	1.337156	0.874480
H	-4.816682	0.617916	1.257541
C	-4.047293	2.650160	1.348431
H	-4.753175	2.972866	2.111391
C	4.192311	-0.327189	-0.202839
C	4.228685	2.207696	-0.760129
H	3.916522	1.916155	-1.775944
H	4.961187	3.018389	-0.894039
C	4.354708	-2.893618	0.041926
H	4.155001	-2.924593	-1.040652
H	5.094301	-3.685700	0.229237
C	4.936488	1.013522	-0.088387
H	5.123735	1.247104	0.971808
C	3.053039	-3.217271	0.807821
H	2.535612	-2.284325	1.056586
H	5.928892	0.894749	-0.549701
H	3.297119	-3.676854	1.777556
C	2.109662	-4.152419	0.024503
H	2.588067	-5.139887	-0.052082
H	2.012876	-3.787237	-1.008583
H	3.212125	-0.251738	0.289970
C	4.978736	-1.522170	0.368951
H	5.998561	-1.495853	-0.044627
H	5.091025	-1.408811	1.458810
C	0.694723	-4.337936	0.618164
H	0.773422	-4.421959	1.714694
H	3.984390	-0.520903	-1.267682
H	0.293395	-5.304244	0.283115

Sum of electronic and zero-point Energies= -1162.307221  
Sum of electronic and thermal Energies= -1162.280125  
Sum of electronic and thermal Enthalpies= -1162.279181  
Sum of electronic and thermal Free Energies= -1162.365296

daec[n=7]-3-E1 (benzene)

C	0.196450	-3.706037	-0.192444
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H	0.637204	-4.462007	-0.839984
C	0.874646	-3.258637	0.950075
C	0.245085	-2.293317	1.747803
H	0.738261	-1.932562	2.648747
C	-1.016939	-1.795255	1.417390
H	-1.503650	-1.061881	2.055422
C	-1.675685	-2.245681	0.271043
O	-2.963720	-1.861587	-0.046107
C	-1.063350	-3.216174	-0.546342
O	-1.683287	-3.760952	-1.641003
C	-1.983886	-2.868574	-2.716914
H	-2.335593	-3.498502	-3.540619
H	-1.083648	-2.324443	-3.039366
H	-2.769017	-2.152470	-2.449364
C	-4.352395	2.050604	0.283216
H	-4.744364	3.064098	0.352297
C	-3.022523	1.849189	-0.117413
C	-2.117014	3.026907	-0.418451
H	-2.713338	3.845812	-0.846421
H	-1.386084	2.738892	-1.185679
C	-1.379016	3.549980	0.833586
H	-2.124705	3.766488	1.612293
C	-0.544162	4.820780	0.591545
H	-0.159572	5.170097	1.562222
H	-1.213734	5.616071	0.228648
C	0.638025	4.690235	-0.386984
H	1.079632	5.689668	-0.522006
C	1.741997	3.720105	0.061158
H	1.333249	2.702645	0.134125
H	2.070113	3.989459	1.078365
H	0.273011	4.391864	-1.381589
H	-0.746549	2.747954	1.240179
C	-2.536753	0.537142	-0.209759
H	-1.513002	0.357712	-0.530349
C	-3.365132	-0.546010	0.103133
C	-4.688851	-0.341394	0.500454
H	-5.313385	-1.201318	0.728272
C	-5.176150	0.963710	0.584861
H	-6.207681	1.131509	0.888842
C	3.784125	1.290451	-0.553376
C	2.960066	3.724009	-0.876482
H	2.636451	3.459729	-1.896181
H	3.348500	4.752101	-0.941294
C	4.701053	-1.119939	-0.324828
H	4.442698	-1.322991	-1.376545
H	5.638713	-1.664545	-0.133829
C	4.107142	2.789072	-0.451878
H	4.406768	3.029009	0.580997
C	3.600150	-1.688178	0.583456
H	2.652997	-1.167318	0.390139
H	4.986792	3.003533	-1.078248
H	3.854052	-1.479593	1.635705
C	3.385848	-3.196893	0.404088
H	4.320015	-3.730016	0.637472
H	3.166440	-3.411347	-0.652991
H	2.912879	1.058110	0.073646
C	4.961012	0.387534	-0.151758
H	5.841413	0.663868	-0.752420
H	5.234373	0.591416	0.895998
C	2.257083	-3.786191	1.281780
H	2.480366	-3.581645	2.338535
H	3.486245	1.056029	-1.588547
H	2.265248	-4.879746	1.168669

Sum of electronic and zero-point Energies= -1162.324213  
Sum of electronic and thermal Energies= -1162.296249  
Sum of electronic and thermal Enthalpies= -1162.295305  
Sum of electronic and thermal Free Energies= -1162.384650

daec[n=7]-3-E2 (benzene)

C	0.049509	-2.826392	1.042884
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H	0.471737	-2.768828	2.044413
C	0.746234	-3.470298	0.011177
C	0.146491	-3.521235	-1.256910
H	0.656195	-4.025072	-2.076546
C	-1.100924	-2.939067	-1.484846
H	-1.571286	-2.981717	-2.464520
C	-1.783105	-2.302809	-0.446610
O	-3.064115	-1.838557	-0.681048
C	-1.207544	-2.250106	0.835121
O	-1.833608	-1.609514	1.874913
C	-2.948085	-2.312216	2.434864
H	-3.347989	-1.669555	3.225520
H	-2.626454	-3.269754	2.870837
H	-3.728903	-2.498216	1.686895
C	-4.148349	2.181334	-0.652589
H	-4.461630	3.224063	-0.658259
C	-2.781393	1.869770	-0.668427
C	-1.744583	2.975749	-0.649937
H	-2.166334	3.872251	-1.127316
H	-0.876914	2.679284	-1.254684
C	-1.282795	3.340856	0.778576
H	-2.173272	3.485590	1.407123
C	-0.423165	4.615706	0.860562
H	-0.192783	4.807881	1.919968
H	-1.032284	5.469504	0.524779
C	0.891751	4.613136	0.060176
H	1.357468	5.605253	0.166241
C	1.906897	3.541858	0.484947
H	1.480294	2.543358	0.316034
H	2.084630	3.616601	1.570114
H	0.675928	4.501022	-1.013346
H	-0.746792	2.485346	1.213360
C	-2.390093	0.521473	-0.668695
H	-1.334497	0.261621	-0.689758
C	-3.355411	-0.488035	-0.643021
C	-4.718686	-0.173461	-0.629558
H	-5.447764	-0.979920	-0.623202
C	-5.106914	1.164835	-0.635369
H	-6.166202	1.415462	-0.629675
C	3.945665	1.179010	-0.338855
C	3.248389	3.667115	-0.254725
H	3.069168	3.630278	-1.341449
H	3.668043	4.664741	-0.052949
C	4.744126	-1.273207	-0.524447
H	4.586106	-1.234078	-1.614242
H	5.638983	-1.896196	-0.371434
C	4.296318	2.603175	0.117793
H	4.451615	2.610370	1.208633
C	3.541080	-1.963408	0.136275
H	2.636064	-1.357783	-0.006119
H	5.262386	2.888788	-0.326502
H	3.706120	-2.014736	1.224846
C	3.288397	-3.376113	-0.405641
H	4.191408	-3.989219	-0.264134
H	3.121116	-3.325543	-1.492319
H	2.995375	0.870046	0.116759
C	5.034219	0.147065	-0.007118
H	5.989402	0.489280	-0.434619
H	5.186093	0.113836	1.083695
C	2.100649	-4.108739	0.257110
H	2.278877	-4.175834	1.339397
H	3.774532	1.183349	-1.427880
H	2.081280	-5.142891	-0.116983

Sum of electronic and zero-point Energies= -1162.324887  
Sum of electronic and thermal Energies= -1162.296937  
Sum of electronic and thermal Enthalpies= -1162.295993  
Sum of electronic and thermal Free Energies= -1162.385143

daec[n=7]-4-TS (benzene)

C	0.358164	3.497192	0.266823
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H	0.553180	4.459385	0.733014
C	1.416235	2.575163	0.151432
C	1.146938	1.339539	-0.438666
H	1.928213	0.597785	-0.549493
C	-0.134393	1.031642	-0.905453
H	-0.321466	0.071609	-1.376712
C	-1.178351	1.936611	-0.773774
O	-2.452350	1.658039	-1.248419
C	-0.934230	3.194700	-0.178535
O	-2.006924	4.025917	-0.071631
C	-1.805410	5.306776	0.507489
H	-2.780433	5.802307	0.480397
H	-1.082006	5.902789	-0.067727
H	-1.466922	5.232923	1.551469
C	-4.620868	-1.335561	0.689991
H	-5.196319	-2.107243	1.199259
C	-3.694399	-1.700584	-0.300553
C	-3.437778	-3.158303	-0.636354
H	-2.821227	-3.218693	-1.542994
H	-4.390103	-3.652497	-0.879037
C	-2.767783	-3.953596	0.510687
H	-3.431880	-3.918287	1.386335
C	-1.368846	-3.472429	0.937502
H	-1.129826	-3.933660	1.907820
H	-1.395680	-2.388150	1.120301
C	-0.227777	-3.799832	-0.040123
H	-0.176151	-4.891597	-0.180390
C	1.133624	-3.282235	0.452564
H	1.288970	-3.618214	1.490340
H	1.102089	-2.183127	0.496637
H	-0.439452	-3.376915	-1.034193
H	-2.715620	-5.011866	0.212379
C	-2.985621	-0.683267	-0.953142
H	-2.293080	-0.931859	-1.753247
C	-3.160372	0.655862	-0.591850
C	-4.078409	1.012000	0.396242
H	-4.199679	2.060772	0.653228
C	-4.814832	0.005641	1.027649
H	-5.540935	0.271268	1.793951
C	3.950051	-1.720123	-0.379209
C	2.333912	-3.743326	-0.391014
H	2.172781	-3.480147	-1.448768
H	2.380270	-4.842337	-0.357902
C	5.606383	0.286169	-0.235612
H	6.414204	0.673263	0.404981
H	6.068705	0.087099	-1.214789
C	3.683038	-3.163882	0.083121
H	4.504465	-3.803236	-0.273250
C	4.547961	1.390199	-0.428639
H	3.821829	1.069488	-1.186291
H	3.722624	-3.210182	1.183189
H	5.048626	2.270302	-0.861173
C	3.826843	1.829185	0.858218
H	4.588106	2.177775	1.572149
H	3.338035	0.970582	1.339539
H	3.041006	-1.120980	-0.235035
C	5.120286	-1.051113	0.359842
H	5.977217	-1.742572	0.374090
H	4.837462	-0.910602	1.413966
C	2.793679	2.962127	0.678386
H	2.650305	3.459284	1.648882
H	4.143796	-1.722489	-1.463738
H	3.224809	3.735042	0.021074

Sum of electronic and zero-point Energies= -1162.313006  
Sum of electronic and thermal Energies= -1162.286404  
Sum of electronic and thermal Enthalpies= -1162.285460  
Sum of electronic and thermal Free Energies= -1162.369299

daec[n=7]-4-E1 (benzene)

C	0.891540	2.173690	1.082698
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H	1.320343	1.880474	2.037203
C	1.729522	2.752006	0.110488
C	1.166478	3.143578	-1.107291
H	1.792051	3.595908	-1.874213
C	-0.205549	2.990814	-1.338286
H	-0.658961	3.326053	-2.268215
C	-1.034805	2.452712	-0.360962
O	-2.399853	2.520999	-0.552220
C	-0.482640	2.023951	0.869062
O	-1.362868	1.523720	1.775668
C	-0.863733	1.078366	3.029439
H	-1.733060	0.706190	3.578891
H	-0.402214	1.900323	3.595538
H	-0.135822	0.263267	2.908366
C	-5.046547	-0.686136	-0.562570
H	-5.766555	-1.502870	-0.582240
C	-3.697866	-0.947527	-0.850756
C	-3.263290	-2.367544	-1.161519
H	-2.358222	-2.354940	-1.783671
H	-4.045102	-2.846783	-1.766899
C	-3.019734	-3.236981	0.098646
H	-3.853588	-3.078654	0.796694
C	-1.682603	-2.964143	0.810637
H	-1.731321	-3.354151	1.838344
H	-1.535877	-1.877704	0.907576
C	-0.477224	-3.596347	0.096712
H	-0.552667	-4.692843	0.173468
C	0.883012	-3.133515	0.633839
H	0.924738	-3.281023	1.724945
H	0.971626	-2.048855	0.471781
H	-0.519295	-3.369412	-0.979634
H	-3.059270	-4.297747	-0.192099
C	-2.782518	0.116784	-0.835444
H	-1.735866	-0.056012	-1.076499
C	-3.215717	1.410106	-0.525683
C	-4.560727	1.664350	-0.242349
H	-4.867838	2.681745	-0.014046
C	-5.471753	0.609577	-0.263757
H	-6.521310	0.802530	-0.048683
C	3.686293	-1.930083	-0.527662
C	2.069025	-3.863865	-0.018585
H	1.914982	-3.907440	-1.108737
H	2.072083	-4.908823	0.326204
C	5.330709	-0.010880	-1.059260
H	6.315432	0.383980	-0.764249
H	5.435641	-0.332626	-2.106974
C	3.441241	-3.225049	0.262188
H	4.235190	-3.946082	0.014973
C	4.301028	1.133736	-1.003649
H	3.334523	0.791890	-1.399137
H	3.539318	-3.025433	1.341519
H	4.637833	1.929726	-1.686054
C	4.101497	1.736814	0.393381
H	5.082654	2.019022	0.805722
H	3.688859	0.981903	1.078023
H	2.860023	-1.228399	-0.347943
C	5.017749	-1.244999	-0.192608
H	5.837157	-1.970101	-0.315542
H	5.024564	-0.966699	0.872172
C	3.197170	2.988975	0.419028
H	3.275152	3.446991	1.416020
H	3.657297	-2.160126	-1.605115
H	3.595925	3.728614	-0.289507

Sum of electronic and zero-point Energies= -1162.323589  
Sum of electronic and thermal Energies= -1162.296058  
Sum of electronic and thermal Enthalpies= -1162.295114  
Sum of electronic and thermal Free Energies= -1162.383360

daec[n=7]-4-E2 (benzene)

C	1.654144	2.868019	0.040982
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H	2.461737	3.423526	-0.426852
C	1.940456	2.071829	1.164466
C	0.889942	1.369332	1.761155
H	1.076335	0.756277	2.641515
C	-0.414076	1.458559	1.258018
H	-1.225926	0.925825	1.745305
C	-0.687309	2.247411	0.143296
O	-1.944410	2.440530	-0.384072
C	0.360328	2.964222	-0.479449
O	0.007457	3.715364	-1.558263
C	1.022878	4.458756	-2.214198
H	0.525974	4.976676	-3.039989
H	1.808968	3.804735	-2.619922
H	1.479422	5.202849	-1.544985
C	-5.128043	-0.125882	0.383600
H	-5.983029	-0.776793	0.560883
C	-4.038493	-0.606100	-0.363443
C	-4.043881	-2.024975	-0.899569
H	-3.346245	-2.102118	-1.743773
H	-5.041391	-2.248402	-1.303669
C	-3.703591	-3.099094	0.162743
H	-4.386901	-2.971663	1.014794
C	-2.251768	-3.079793	0.671493
H	-2.190242	-3.690742	1.584702
H	-1.985365	-2.056850	0.976410
C	-1.215849	-3.601662	-0.336673
H	-1.422713	-4.663096	-0.548045
C	0.231595	-3.445286	0.150120
H	0.336273	-3.910417	1.143564
H	0.440879	-2.374887	0.294418
H	-1.323365	-3.077273	-1.298272
H	-3.925602	-4.089527	-0.262902
C	-2.956379	0.254010	-0.592556
H	-2.105071	-0.075008	-1.184820
C	-2.966097	1.556602	-0.081535
C	-4.049946	2.028222	0.658583
H	-4.037605	3.048806	1.032431
C	-5.134730	1.176000	0.885236
H	-5.990776	1.535132	1.453400
C	3.219254	-2.373045	-0.665552
C	1.270356	-4.063070	-0.799167
H	1.109104	-3.682111	-1.820467
H	1.095685	-5.148546	-0.851319
C	5.217375	-0.731421	-0.513183
H	6.215208	-0.636506	-0.057053
H	5.381751	-0.728616	-1.601965
C	2.731640	-3.804167	-0.387665
H	3.389024	-4.508820	-0.919401
C	4.380251	0.509366	-0.149633
H	3.426103	0.485695	-0.693525
H	2.850414	-4.031856	0.683995
H	4.912206	1.401193	-0.517218
C	4.107500	0.681068	1.350825
H	5.063744	0.675846	1.896942
H	3.533513	-0.176376	1.729915
H	2.507591	-1.650493	-0.242583
C	4.622240	-2.093114	-0.107519
H	5.309767	-2.882855	-0.448405
H	4.594776	-2.177301	0.989443
C	3.353679	1.982071	1.711113
H	3.319696	2.066625	2.806972
H	3.215177	-2.199900	-1.753986
H	3.937653	2.842675	1.354216

Sum of electronic and zero-point Energies= -1162.323777  
Sum of electronic and thermal Energies= -1162.296303  
Sum of electronic and thermal Enthalpies= -1162.295359  
Sum of electronic and thermal Free Energies= -1162.382555

daec[n=8]-1-TS (benzene)

C	-4.019956	1.201183	0.057995
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H	-4.946360	1.694660	0.339934
C	-2.901549	1.994892	-0.266380
C	-1.726780	1.338440	-0.627976
H	-0.841063	1.895834	-0.912382
C	-1.651172	-0.059823	-0.642235
H	-0.709927	-0.527557	-0.900661
C	-2.754637	-0.838868	-0.319432
O	-2.790724	-2.220783	-0.335388
C	-3.968328	-0.194977	0.029453
O	-5.012032	-1.016394	0.326896
C	-6.251839	-0.421114	0.676078
H	-6.649618	0.199669	-0.140230
H	-6.169299	0.188655	1.588095
H	-6.939065	-1.251999	0.862007
C	0.503142	-4.582709	0.656966
H	1.354312	-5.199168	0.941944
C	0.593301	-3.750525	-0.468665
C	1.894614	-3.582270	-1.227579
H	1.695022	-3.067855	-2.177973
H	2.328980	-4.559005	-1.485511
C	2.926659	-2.766787	-0.410373
H	2.406784	-1.935009	0.084228
C	4.086052	-2.215867	-1.254587
H	3.701924	-1.419497	-1.909955
H	4.455088	-3.004658	-1.928298
C	5.281725	-1.697779	-0.430799
H	6.032018	-1.285096	-1.122967
C	4.977498	-0.655452	0.661903
H	5.905574	-0.485335	1.229479
H	4.264200	-1.077887	1.385460
H	5.763327	-2.561133	0.054216
H	3.318966	-3.400065	0.399634
C	-0.524104	-2.983288	-0.828068
H	-0.492227	-2.387587	-1.735644
C	-1.671458	-2.975685	-0.027936
C	-1.752886	-3.803995	1.094360
H	-2.661386	-3.796853	1.690873
C	-0.666868	-4.619237	1.419902
H	-0.728454	-5.273841	2.287370
C	2.437680	3.248031	0.362105
C	4.452631	0.706706	0.178159
H	5.158063	1.132196	-0.554039
H	3.499744	0.575659	-0.354743
C	0.660061	4.879179	-0.577074
H	0.517169	5.942863	-0.822038
H	0.748674	4.359989	-1.545089
C	4.271408	1.692945	1.345603
H	5.222213	1.751854	1.897927
H	3.538538	1.277108	2.055574
C	-0.590149	4.360679	0.154729
H	-0.794842	4.995157	1.031136
H	-0.394152	3.359297	0.555306
C	-1.836599	4.324312	-0.751836
H	-1.560531	3.927277	-1.740102
H	-2.173231	5.355584	-0.931986
C	1.986069	4.708990	0.186796
H	2.772001	5.257095	-0.355550
H	1.911460	5.188726	1.175674
C	-3.027230	3.513616	-0.206989
H	1.725017	2.709961	1.005007
C	3.845172	3.122556	0.966525
H	3.893876	3.745335	1.873394
H	4.580859	3.551825	0.267636
H	-3.221571	3.813907	0.835667
H	-3.931452	3.803860	-0.762802
H	2.406663	2.744525	-0.616513

Sum of electronic and zero-point Energies= -1201.597466  
Sum of electronic and thermal Energies= -1201.569337  
Sum of electronic and thermal Enthalpies= -1201.568393  
Sum of electronic and thermal Free Energies= -1201.656580



## daec[n=8]-1-E1 (benzene)

C	-2.218191	2.778655	-0.485155
H	-2.350936	3.278169	-1.440991
C	-1.383969	3.370752	0.481040
C	-1.233002	2.735304	1.717250
H	-0.601927	3.181041	2.483374
C	-1.891294	1.528478	1.980473
H	-1.787063	1.028832	2.940850
C	-2.711410	0.947903	1.021233
O	-3.437947	-0.181435	1.347661
C	-2.890802	1.578989	-0.230437
O	-3.730145	0.953932	-1.096224
C	-3.933232	1.536272	-2.376426
H	-2.994453	1.600072	-2.945482
H	-4.381955	2.537092	-2.298736
H	-4.626298	0.870529	-2.898593
C	-2.626990	-3.963309	-0.196493
H	-2.441147	-4.962044	-0.588427
C	-1.714744	-2.933278	-0.462279
C	-0.451286	-3.202095	-1.255633
H	-0.198215	-2.316563	-1.856680
H	-0.634303	-4.019492	-1.967770
C	0.762828	-3.567838	-0.375142
H	0.938978	-2.751911	0.339917
C	2.029181	-3.836546	-1.201250
H	2.258154	-2.948775	-1.809678
H	1.818127	-4.642465	-1.921090
C	3.268583	-4.237574	-0.378797
H	4.088142	-4.464273	-1.078358
C	3.765404	-3.201384	0.647225
H	4.638517	-3.623806	1.168260
H	3.000684	-3.050657	1.424005
H	3.054564	-5.178860	0.150718
H	0.517974	-4.454749	0.228956
C	-1.971452	-1.648962	0.043412
H	-1.272014	-0.839991	-0.153179
C	-3.123479	-1.404384	0.794959
C	-4.031188	-2.436499	1.060018
H	-4.921185	-2.219368	1.645240
C	-3.774570	-3.712152	0.561916
H	-4.480684	-4.516317	0.761495
C	3.813905	1.330396	0.046510
C	4.148048	-1.838673	0.050791
H	4.895577	-1.982432	-0.746551
H	3.268224	-1.395775	-0.435059
C	2.956925	3.543706	-0.976848
H	3.309278	4.535326	-1.300761
H	2.648112	3.017936	-1.894701
C	4.702069	-0.857374	1.095359
H	5.608584	-1.290143	1.545898
H	3.974675	-0.758032	1.917150
C	1.734319	3.720284	-0.063536
H	2.041514	4.240831	0.858300
H	1.361133	2.737133	0.252074
C	0.590836	4.499426	-0.726616
H	0.302337	3.998558	-1.663503
H	0.947670	5.500783	-1.011730
C	4.132685	2.784021	-0.335763
H	4.979562	2.790954	-1.039387
H	4.477406	3.328866	0.557642
C	-0.662954	4.667260	0.163315
H	3.036068	1.312894	0.824385
C	5.033897	0.544842	0.553019
H	5.521353	1.122960	1.353354
H	5.777642	0.461379	-0.255566
H	-0.371910	5.160003	1.101651
H	-1.358123	5.352135	-0.343336
H	3.379966	0.822863	-0.828057

Sum of electronic and zero-point Energies= -1201.612652

Sum of electronic and thermal Energies= -1201.583696

Sum of electronic and thermal Enthalpies= -1201.582752

Sum of electronic and thermal Free Energies= -1201.673462

## daec[n=8]-1-E2 (benzene)

C	-0.200296	3.008074	0.908129
H	0.521196	3.008836	1.720015
C	0.065993	3.777731	-0.238063
C	-0.877802	3.792268	-1.271364
H	-0.697219	4.390027	-2.162935
C	-2.061437	3.055623	-1.162531
H	-2.810975	3.075663	-1.950477
C	-2.317553	2.295704	-0.026716
O	-3.542740	1.672554	0.120673
C	-1.379785	2.262603	1.027603
O	-1.717332	1.501062	2.100350
C	-0.801196	1.419450	3.183307
H	-0.633778	2.402337	3.646965
H	0.163077	0.996015	2.866790
H	-1.265021	0.751342	3.914649
C	-4.128631	-2.408926	-0.459514
H	-4.318542	-3.469042	-0.620149
C	-2.907733	-1.853094	-0.866936
C	-1.839911	-2.720978	-1.503165
H	-1.195682	-2.101694	-2.143502
H	-2.316694	-3.459692	-2.163974
C	-0.958034	-3.467265	-0.479435
H	-0.483205	-2.729393	0.182601
C	0.105855	-4.346775	-1.152551
H	0.747565	-3.716308	-1.786133
H	-0.396061	-5.044262	-1.840903
C	0.976534	-5.170292	-0.184749
H	1.654491	-5.800067	-0.781536
C	1.811793	-4.364828	0.828133
H	2.368917	-5.075436	1.458166
H	1.143162	-3.821634	1.512986
H	0.329125	-5.866081	0.371127
H	-1.598183	-4.088044	0.165797
C	-2.682150	-0.482791	-0.663427
H	-1.745781	-0.033902	-0.986083
C	-3.663885	0.312159	-0.064736
C	-4.880691	-0.246891	0.341238
H	-5.628946	0.394125	0.800438
C	-5.104161	-1.607820	0.140640
H	-6.051449	-2.045610	0.450757
C	3.902897	-0.384982	0.013357
C	2.799243	-3.370210	0.199936
H	3.451485	-3.899399	-0.513908
H	2.241984	-2.629965	-0.389915
C	4.178635	1.909506	-1.147630
H	4.950745	2.638323	-1.439106
H	3.757105	1.522337	-2.088976
C	3.667490	-2.646456	1.240563
H	4.260134	-3.392864	1.791611
H	3.011688	-2.171087	1.987995
C	3.074159	2.635176	-0.363994
H	3.478484	2.973243	0.604540
H	2.264683	1.931434	-0.129070
C	2.490838	3.840910	-1.112412
H	2.119049	3.519255	-2.097055
H	3.293895	4.567380	-1.308983
C	4.852598	0.755611	-0.383149
H	5.662682	0.346925	-1.006799
H	5.339333	1.153238	0.521864
C	1.353775	4.571026	-0.358560
H	3.141890	-0.006600	0.712428
C	4.616714	-1.580607	0.663826
H	5.260586	-1.209969	1.476561
H	5.294112	-2.046532	-0.069469
H	1.711641	4.849223	0.643282

H 1.140923 5.512449 -0.883687  
H 3.354609 -0.717045 -0.880898  
Sum of electronic and zero-point Energies= -1201.612304  
Sum of electronic and thermal Energies= -1201.583321  
Sum of electronic and thermal Enthalpies= -1201.582377  
Sum of electronic and thermal Free Energies= -1201.673478

daec[n=8]-2-TS (benzene)

C -1.911653 -3.341482 -0.353817  
H -2.301790 -4.298702 -0.689935  
C -0.543876 -3.063448 -0.542949  
C -0.062958 -1.830306 -0.106504  
H 0.983135 -1.571532 -0.218760  
C -0.913199 -0.896776 0.492663  
H -0.502030 0.046394 0.830254  
C -2.267701 -1.158148 0.648976  
O -3.151367 -0.267845 1.242183  
C -2.779436 -2.408043 0.225667  
O -4.113643 -2.600783 0.411908  
C -4.672371 -3.842470 0.010966  
H -4.561222 -4.009236 -1.070696  
H -5.736818 -3.783155 0.257050  
H -4.223128 -4.685433 0.556209  
C -3.537556 3.559553 -0.391902  
H -3.647229 4.545924 -0.840171  
C -2.357453 3.232089 0.292281  
C -1.155785 4.155910 0.320692  
H -0.469473 3.817420 1.108218  
H -1.452345 5.180084 0.587368  
C -0.410479 4.178683 -1.043635  
H -0.558755 3.214746 -1.550411  
C 1.103977 4.447601 -0.945737  
H 1.297141 5.266507 -0.234789  
H 1.464221 4.804021 -1.922608  
C 1.920747 3.203712 -0.552535  
H 1.583088 2.830569 0.425567  
C 3.437831 3.448184 -0.521667  
H 3.734340 3.933503 -1.464538  
H 3.675773 4.169143 0.276794  
H 1.702060 2.401302 -1.275556  
H -0.882098 4.931831 -1.689929  
C -2.255623 1.962591 0.876633  
H -1.377575 1.718838 1.466239  
C -3.262361 1.008950 0.705102  
C -4.433812 1.338874 0.020243  
H -5.211244 0.587768 -0.091527  
C -4.570378 2.624689 -0.509966  
H -5.483887 2.892050 -1.038226  
C 5.151721 -0.876234 0.434487  
C 4.299759 2.184215 -0.334860  
H 4.101562 1.488017 -1.164458  
H 5.358499 2.472434 -0.429234  
C 3.974106 -3.132567 -0.008575  
H 4.668753 -3.639367 0.677897  
H 4.450048 -3.172723 -1.001433  
C 4.103756 1.468213 1.011632  
H 3.094011 1.036582 1.065152  
H 4.149460 2.220233 1.815254  
C 2.636023 -3.902434 -0.042438  
H 2.024128 -3.588688 0.815584  
H 2.824339 -4.976151 0.103796  
C 1.838645 -3.729083 -1.351830  
H 2.291989 -4.369179 -2.122105  
H 1.941378 -2.702695 -1.731237  
C 3.833364 -1.669710 0.450099  
H 3.089965 -1.152254 -0.173090  
H 3.422657 -1.670569 1.472359  
C 0.343727 -4.084803 -1.245934  
H 5.964744 -1.530093 0.786532  
C 5.150122 0.381424 1.326448

H 6.151625 0.838062 1.290447  
H 5.004426 0.057715 2.368861  
H -0.053502 -4.237242 -2.261485  
H 0.238381 -5.060470 -0.745572  
H 5.410618 -0.611730 -0.601783  
Sum of electronic and zero-point Energies= -1201.591987  
Sum of electronic and thermal Energies= -1201.563932  
Sum of electronic and thermal Enthalpies= -1201.562988  
Sum of electronic and thermal Free Energies= -1201.650950

daec[n=8]-2-E1 (benzene)

C 0.875949 -2.693847 1.213424  
H 0.591220 -2.698949 2.262070  
C 0.074247 -3.390133 0.290320  
C 0.459708 -3.404478 -1.054005  
H -0.129694 -3.955188 -1.783992  
C 1.605957 -2.716545 -1.470429  
H 1.914351 -2.718504 -2.513363  
C 2.388691 -2.024467 -0.554101  
O 3.563699 -1.433311 -0.979236  
C 2.035433 -2.022300 0.814223  
O 2.877213 -1.355889 1.646171  
C 2.553881 -1.296973 3.028452  
H 1.588815 -0.797735 3.197427  
H 3.349843 -0.709068 3.494306  
H 2.531204 -2.298556 3.481531  
C 4.125381 2.696817 -0.932325  
H 4.298430 3.771774 -0.930137  
C 2.826678 2.201300 -0.761818  
C 1.643495 3.119791 -0.531430  
H 0.783671 2.736325 -1.096919  
H 1.859708 4.119392 -0.933720  
C 1.260361 3.248430 0.961469  
H 1.248396 2.246653 1.416347  
C -0.100128 3.927060 1.206623  
H -0.145863 4.876871 0.650273  
H -0.176950 4.195479 2.271327  
C -1.300522 3.046362 0.826288  
H -1.215478 2.751772 -0.228052  
C -2.666223 3.709839 1.058327  
H -2.741994 4.015309 2.113377  
H -2.725283 4.638586 0.468441  
H -1.252922 2.110298 1.406607  
H 2.054178 3.805815 1.479272  
C 2.621859 0.812942 -0.774500  
H 1.616639 0.415359 -0.658008  
C 3.697816 -0.060876 -0.935250  
C 4.994597 0.436359 -1.109749  
H 5.816804 -0.262544 -1.241235  
C 5.197751 1.815232 -1.109360  
H 6.204278 2.206630 -1.246750  
C -5.304004 0.213924 -0.560891  
C -3.868813 2.811480 0.710633  
H -3.814069 1.892052 1.313633  
H -4.794681 3.321379 1.019448  
C -4.381975 -2.180061 -0.590594  
H -5.080585 -2.507826 -1.374688  
H -4.919442 -2.314248 0.361843  
C -3.972032 2.455433 -0.780885  
H -3.067651 1.919901 -1.100103  
H -3.986563 3.390212 -1.363260  
C -3.134222 -3.087646 -0.600201  
H -2.414790 -2.713206 -1.343665  
H -3.418754 -4.097224 -0.933466  
C -2.456514 -3.215295 0.772961  
H -3.180907 -3.660066 1.471733  
H -2.214485 -2.220334 1.174953  
C -4.082043 -0.687565 -0.809858  
H -3.250318 -0.374312 -0.161748  
H -3.725441 -0.551947 -1.843339

C	-1.178361	-4.091568	0.779416
H	-6.197700	-0.272238	-0.982227
C	-5.207421	1.625302	-1.171652
H	-6.118182	2.185787	-0.908733
H	-5.218985	1.528030	-2.268437
H	-1.003471	-4.441503	1.806128
H	-1.361225	-4.991557	0.174847
H	-5.486664	0.279864	0.522268
Sum of electronic and zero-point Energies= -1201.607355			
Sum of electronic and thermal Energies= -1201.578455			
Sum of electronic and thermal Enthalpies= -1201.577511			
Sum of electronic and thermal Free Energies= -1201.668016			

daec[n=8]-2-E2 (benzene)

C	0.818045	-3.268841	0.006735
H	0.331151	-3.988612	-0.644526
C	0.294834	-3.052320	1.292514
C	0.944303	-2.142630	2.136089
H	0.566363	-1.972632	3.142631
C	2.085075	-1.461890	1.705250
H	2.600718	-0.765889	2.363061
C	2.585632	-1.665940	0.422516
O	3.751409	-1.054854	-0.001288
C	1.951889	-2.578801	-0.445720
O	2.509643	-2.721152	-1.676310
C	1.911858	-3.637931	-2.581673
H	1.931624	-4.665801	-2.191181
H	2.513760	-3.589241	-3.493825
H	0.874884	-3.357935	-2.818444
C	4.041812	3.074502	-0.493457
H	4.145861	4.150132	-0.626082
C	2.765781	2.506119	-0.395507
C	1.507843	3.350534	-0.431663
H	0.747103	2.824443	-1.023841
H	1.706323	4.298178	-0.951560
C	0.942619	3.655226	0.975477
H	0.943518	2.730492	1.571507
C	-0.480611	4.243501	0.966674
H	-0.525884	5.093426	0.267118
H	-0.700623	4.657917	1.962247
C	-1.563408	3.215327	0.603834
H	-1.330660	2.772160	-0.373574
C	-2.989067	3.786112	0.574989
H	-3.212561	4.242363	1.551706
H	-3.039575	4.604411	-0.161145
H	-1.523061	2.386322	1.329118
H	1.629230	4.345405	1.486476
C	2.650608	1.116873	-0.229654
H	1.665061	0.663721	-0.163100
C	3.791017	0.314665	-0.149725
C	5.065811	0.885762	-0.252172
H	5.940108	0.242192	-0.195873
C	5.180539	2.263679	-0.426591
H	6.169779	2.710539	-0.509165
C	-5.172909	-0.130106	-0.727609
C	-4.076722	2.744214	0.249917
H	-4.033955	1.938167	0.998470
H	-5.065762	3.214004	0.366925
C	-4.098182	-2.410521	-0.248566
H	-4.673503	-2.921308	-1.035011
H	-4.736006	-2.433353	0.649484
C	-3.972000	2.152892	-1.164806
H	-3.002148	1.652245	-1.288601
H	-3.975295	2.980994	-1.891059
C	-2.799941	-3.195422	0.033141
H	-2.025895	-2.890432	-0.687030
H	-2.975075	-4.267751	-0.142765
C	-2.281115	-3.027681	1.469720
H	-3.049835	-3.411283	2.157279
H	-2.159066	-1.961517	1.710785

C	-3.873789	-0.953588	-0.687500
H	-3.147272	-0.469787	-0.018265
H	-3.406899	-0.957984	-1.685435
C	-0.953804	-3.769631	1.768494
H	-5.975011	-0.749479	-1.158432
C	-5.093153	1.171302	-1.548861
H	-6.063769	1.687629	-1.485347
H	-4.962702	0.903191	-2.608920
H	-0.875954	-3.912548	2.854781
H	-1.000977	-4.776448	1.328455
H	-5.490196	0.089680	0.302854
Sum of electronic and zero-point Energies= -1201.606691			
Sum of electronic and thermal Energies= -1201.577689			
Sum of electronic and thermal Enthalpies= -1201.576745			
Sum of electronic and thermal Free Energies= -1201.668586			

daec[n=8]-3-TS (benzene)

C	-2.477861	-3.149240	0.786607
H	-2.983241	-4.096863	0.967853
C	-1.075296	-3.088800	0.723339
C	-0.505016	-1.830791	0.508613
H	0.572538	-1.708401	0.480214
C	-1.290841	-0.691257	0.319686
H	-0.805246	0.258827	0.127892
C	-2.681232	-0.768155	0.375270
O	-3.526300	0.315987	0.213409
C	-3.282279	-2.019063	0.632677
O	-4.641052	-2.150643	0.789027
C	-5.419313	-2.023246	-0.402107
H	-6.453782	-2.239334	-0.114719
H	-5.097219	-2.749432	-1.163654
H	-5.363974	-1.009283	-0.816044
C	-2.022993	3.684446	-1.713604
H	-1.612903	4.547166	-2.237236
C	-1.630616	3.438947	-0.384748
C	-0.604239	4.373864	0.245836
H	-1.068953	5.364536	0.360961
H	0.183487	4.524747	-0.506690
C	0.058316	3.971802	1.588882
H	-0.313344	4.630979	2.384105
C	1.599530	4.030478	1.557086
H	1.978281	4.142743	2.583939
H	1.923493	4.934019	1.016859
C	2.256775	2.782821	0.939144
H	1.803165	2.561338	-0.038634
C	3.784283	2.917303	0.793541
H	4.170125	3.477783	1.659353
H	4.014029	3.535742	-0.088254
H	2.023858	1.919584	1.583201
H	-0.232887	2.957425	1.888353
C	-2.181189	2.329931	0.268287
H	-1.940089	2.107383	1.303111
C	-3.027532	1.451169	-0.418051
C	-3.409076	1.698234	-1.734290
H	-4.071498	1.004206	-2.244917
C	-2.912086	2.838344	-2.373359
H	-3.201957	3.049629	-3.400884
C	4.963094	-1.566456	-1.634000
C	4.564320	1.592337	0.717967
H	4.389019	1.028692	1.648613
H	5.640114	1.827606	0.710658
C	3.213522	-3.039991	-0.409772
H	4.015608	-3.743932	-0.136488
H	3.146987	-2.327093	0.425452
C	4.259031	0.673991	-0.477630
H	4.389375	1.232472	-1.418670
H	3.204060	0.364735	-0.449278
C	1.871206	-3.786731	-0.520752
H	1.990448	-4.683279	-1.147320
H	1.158956	-3.147334	-1.058219

C	1.277894	-4.185648	0.849408
H	1.552253	-3.431794	1.602055
H	1.742065	-5.122003	1.189741
C	3.596076	-2.275860	-1.686855
H	3.601562	-2.971382	-2.540294
H	2.805171	-1.542602	-1.906974
C	-0.251101	-4.363472	0.870600
H	5.752430	-2.331186	-1.565126
C	5.174488	-0.563263	-0.483529
H	5.074988	-1.084388	0.480484
H	6.219477	-0.218660	-0.522836
H	-0.545979	-5.067202	0.075582
H	-0.535350	-4.856641	1.812438
H	5.126552	-1.051718	-2.593586

Sum of electronic and zero-point Energies= -1201.587991

Sum of electronic and thermal Energies= -1201.559548

Sum of electronic and thermal Enthalpies= -1201.558604

Sum of electronic and thermal Free Energies= -1201.648784

daec[n=8]-3-E1 (benzene)

C	-3.892982	-0.388377	-0.036225
H	-4.671867	-0.127826	0.677731
C	-3.612348	0.448572	-1.122195
C	-2.610196	0.049973	-2.021610
H	-2.386471	0.662872	-2.892967
C	-1.862062	-1.102125	-1.787916
H	-1.058559	-1.393737	-2.460538
C	-2.104044	-1.888944	-0.659873
O	-1.295478	-2.995263	-0.416988
C	-3.160570	-1.557482	0.203598
O	-3.445533	-2.274504	1.339530
C	-3.838098	-3.638218	1.139957
H	-4.071227	-4.032558	2.134176
H	-3.034451	-4.229806	0.687911
H	-4.736729	-3.692955	0.508428
C	2.287377	-2.349197	1.626074
H	3.223481	-2.200626	2.161813
C	2.309731	-2.896896	0.335741
C	3.611392	-3.278702	-0.339955
H	3.484306	-4.267610	-0.804037
H	4.395285	-3.396105	0.421625
C	4.128834	-2.312876	-1.434409
H	4.919230	-2.853307	-1.975123
C	4.715283	-0.967628	-0.953072
H	5.485328	-0.658281	-1.676309
H	5.252572	-1.124429	-0.004056
C	3.732363	0.207713	-0.800629
H	2.958475	-0.030775	-0.059589
C	4.462902	1.507319	-0.418164
H	5.336107	1.616440	-1.080673
H	4.872382	1.409225	0.600108
H	3.207345	0.356218	-1.758076
H	3.332058	-2.130702	-2.171151
C	1.088174	-3.092348	-0.328423
H	1.061716	-3.525177	-1.326728
C	-0.114814	-2.739891	0.281412
C	-0.135228	-2.195044	1.569506
H	-1.083665	-1.952262	2.039109
C	1.076749	-2.001192	2.233151
H	1.075313	-1.585215	2.339065
C	0.795348	4.661967	1.512576
C	3.638529	2.803565	-0.512600
H	3.211176	2.885511	-1.525049
H	4.330461	3.654444	-0.411596
C	-1.328203	3.936709	0.211557
H	-1.653575	4.983584	0.100747
H	-0.713558	3.714607	-0.673436
C	2.516474	2.972180	0.524888
H	2.932714	2.831891	1.535840
H	1.762425	2.183338	0.392917

C	-2.542871	2.996785	0.204298
H	-3.232091	3.265142	1.020523
H	-2.188742	1.981719	0.430567
C	-3.302792	2.973175	-1.131468
H	-2.574804	2.913807	-1.954203
H	-3.847839	3.917816	-1.275739
C	-0.473480	3.790601	1.480283
H	-1.090118	4.041418	2.357257
H	-0.197967	2.732444	1.603561
C	-4.296758	1.794121	-1.272357
H	0.501284	5.719507	1.422672
C	1.857034	4.359763	0.437656
H	1.422840	4.491027	-0.564975
H	2.646634	5.123097	0.518009
H	-5.091287	1.886097	-0.519200
H	-4.786868	1.865082	-2.254693
H	1.262321	4.563090	2.504943

Sum of electronic and zero-point Energies= -1201.599632

Sum of electronic and thermal Energies= -1201.570481

Sum of electronic and thermal Enthalpies= -1201.569537

Sum of electronic and thermal Free Energies= -1201.661026

daec[n=8]-3-E2 (benzene)

C	1.233120	-2.759761	-1.124783
H	0.867606	-2.879529	-2.143254
C	0.661012	-3.486313	-0.068380
C	1.184734	-3.301834	1.218309
H	0.768566	-3.860362	2.054718
C	2.234009	-2.406560	1.445907
H	2.640306	-2.259572	2.444046
C	2.781595	-1.683290	0.388559
O	3.863385	-0.850345	0.620214
C	2.283849	-1.864435	-0.915709
O	2.771235	-1.143299	-1.975615
C	4.084270	-1.510292	-2.413067
H	4.324384	-0.843073	-3.246911
H	4.100662	-2.552499	-2.765009
H	4.828066	-1.382306	-1.617370
C	3.486044	3.289363	0.928745
H	3.416765	4.371488	1.027372
C	2.316753	2.526167	0.805558
C	0.951868	3.183598	0.765628
H	0.921377	4.019886	1.479347
H	0.197695	2.460102	1.101398
C	0.572339	3.715620	-0.634829
H	1.272924	4.518789	-0.904850
C	-0.874005	4.236350	-0.730334
H	-0.976535	4.839519	-1.645119
H	-1.073266	4.922177	0.108766
C	-1.932017	3.122223	-0.752194
H	-1.794152	2.469058	0.120031
C	-3.379242	3.637956	-0.778667
H	-3.483258	4.370396	-1.594190
H	-3.586660	4.189819	0.152078
H	-1.758173	2.487579	-1.636278
H	0.723178	2.918282	-1.377811
C	2.423008	1.131650	0.691267
H	1.523483	0.528241	0.603361
C	3.677369	0.517309	0.695302
C	4.843268	1.281134	0.815889
H	5.807776	0.779539	0.825677
C	4.737517	2.666478	0.932625
H	5.641653	3.264424	1.032756
C	-5.626671	-0.669811	1.023611
C	-4.438792	2.537021	-0.970520
H	-4.247449	2.021459	-1.925464
H	-5.428228	3.008335	-1.075275
C	-3.736312	-2.231265	0.173232
H	-4.481644	-2.957947	-0.188437
H	-3.536263	-1.557248	-0.672895

C	-4.496963	1.494989	0.157422
H	-4.723588	1.999807	1.110824
H	-3.504916	1.041456	0.283231
C	-2.435265	-2.963430	0.534329
H	-2.621106	-3.653818	1.372779
H	-1.700722	-2.231054	0.900898
C	-1.834724	-3.744711	-0.642007
H	-1.697118	-3.067229	-1.498377
H	-2.550792	-4.512444	-0.971838
C	-4.328013	-1.434505	1.345658
H	-4.531720	-2.124929	2.178674
H	-3.568852	-0.732996	1.722428
C	-0.489830	-4.439807	-0.329338
H	-6.409177	-1.394966	0.750970
C	-5.530034	0.386666	-0.094222
H	-5.300504	-0.105852	-1.051140
H	-6.523393	0.842679	-0.226442
H	-0.617909	-5.101052	0.539152
H	-0.232053	-5.089897	-1.178019
H	-5.977252	-0.180175	1.945433

Sum of electronic and zero-point Energies= -1201.609260

Sum of electronic and thermal Energies= -1201.580072

Sum of electronic and thermal Enthalpies= -1201.579128

Sum of electronic and thermal Free Energies= -1201.670837

daec[n=8]-4-TS (benzene)

C	1.048307	-3.616058	0.086023
H	1.038573	-4.666730	0.372268
C	-0.151846	-2.897492	-0.041116
C	-0.051212	-1.551942	-0.408972
H	-0.939891	-0.943089	-0.532763
C	1.184650	-0.940653	-0.610259
H	1.210858	0.108864	-0.872435
C	2.371036	-1.650960	-0.444684
O	3.628495	-1.078517	-0.600463
C	2.299122	-3.018597	-0.107031
O	3.424971	-3.769344	0.122456
C	4.248205	-4.017269	-1.020280
H	3.683989	-4.547116	-1.802546
H	5.066044	-4.656970	-0.672151
H	4.661778	-3.088997	-1.431836
C	4.169421	2.664236	1.172262
H	4.273885	3.625112	1.673935
C	3.422921	2.578700	-0.010583
C	2.593035	3.739799	-0.523934
H	3.020473	4.697624	-0.197009
H	2.590957	3.747787	-1.623649
C	1.138839	3.606669	-0.008753
H	0.788526	2.593657	-0.247897
C	0.140802	4.635497	-0.559068
H	0.130065	4.590610	-1.659785
H	0.483756	5.648311	-0.298656
C	-1.292845	4.438620	-0.019776
H	-1.893261	5.327239	-0.266212
C	-2.019157	3.188904	-0.549750
H	-1.376375	2.304298	-0.430614
H	-2.183269	3.299872	-1.633534
H	-1.253998	4.396747	1.080439
H	1.150871	3.664306	1.090266
C	3.316966	1.331204	-0.644736
H	2.790667	1.251662	-1.592411
C	3.832866	0.182145	-0.043144
C	4.576625	0.270968	1.135804
H	4.982484	-0.635040	1.578339
C	4.762326	1.523617	1.724334
H	5.345574	1.605473	2.639586
C	-6.168477	0.120124	-0.199592
C	-3.359599	2.904758	0.148933
H	-3.173593	2.754547	1.224298
H	-4.013628	3.788006	0.075823

C	-5.082614	-1.987806	0.868964
H	-4.690768	-1.286074	1.620655
H	-6.001671	-2.409297	1.302743
C	-4.094262	1.675374	-0.413986
H	-4.402944	1.879149	-1.451916
H	-3.384170	0.837160	-0.469835
C	-4.040020	-3.110788	0.676872
H	-4.368420	-3.798356	-0.118544
H	-3.983833	-3.709393	1.598572
C	-2.653396	-2.542897	0.347325
H	-2.387872	-1.808488	1.123042
H	-2.725179	-1.979652	-0.591368
C	-5.447958	-1.225304	-0.420386
H	-4.547674	-1.047170	-1.022591
H	-6.090587	-1.870997	-1.037956
C	-1.504343	-3.554030	0.219030
H	-6.559110	0.465900	-1.169179
C	-5.320812	1.255003	0.414221
H	-4.988985	0.973033	1.424949
H	-5.974946	2.130010	0.551132
H	-1.730304	-4.267248	-0.589916
H	-1.436696	-4.159696	1.135322
H	-7.050535	-0.043088	0.439180

Sum of electronic and zero-point Energies= -1201.594648

Sum of electronic and thermal Energies= -1201.566275

Sum of electronic and thermal Enthalpies= -1201.565331

Sum of electronic and thermal Free Energies= -1201.653884

daec[n=8]-4-E1 (benzene)

C	0.377101	-3.264213	-0.559802
H	-0.066799	-3.848162	-1.363749
C	-0.351041	-2.976565	0.595277
C	0.273761	-2.215368	1.598472
H	-0.260245	-1.982361	2.518041
C	1.579783	-1.768301	1.432577
H	2.073522	-1.195544	2.214442
C	2.301233	-2.060537	0.268287
O	3.637524	-1.698115	0.172158
C	1.698115	-2.820721	-0.750598
O	2.284051	-3.227044	-1.911786
C	3.318269	-2.452664	-2.522031
H	3.071815	-1.382585	-2.529497
H	3.375204	-2.812181	-3.555152
H	4.284750	-2.601546	-2.030090
C	4.873426	2.260673	0.563041
H	5.222389	3.286572	0.667068
C	3.610389	2.013509	0.008394
C	2.729793	3.153727	-0.471265
H	3.256521	4.105080	-0.313451
H	2.583473	3.064501	-1.559319
C	1.344450	3.214880	0.201383
H	0.824041	2.263391	0.029088
C	0.480960	4.381661	-0.305931
H	0.491837	4.392518	-1.407703
H	0.943393	5.328935	0.009813
C	-0.981302	4.339186	0.179262
H	-1.450468	5.317402	-0.005167
C	-1.822092	3.246014	-0.497778
H	-1.321586	2.272923	-0.384864
H	-1.857096	3.441732	-1.581538
H	-0.998896	4.195247	1.271351
H	1.470476	3.298730	1.291227
C	3.177647	0.682785	-0.114132
H	2.203168	0.462576	-0.542365
C	3.992602	-0.368538	0.313828
C	5.256900	-0.117108	0.857483
H	5.873053	-0.953209	1.178378
C	5.689422	1.202677	0.976988
H	6.669569	1.408709	1.403142
C	-6.162951	0.510452	-0.669743

C	-3.253802	3.113024	0.041409
H	-3.214670	2.937464	1.128336
H	-3.797957	4.060906	-0.094579
C	-5.226299	-1.451770	0.744530
H	-4.844603	-0.681231	1.430644
H	-6.202513	-1.757329	1.150724
C	-4.022850	1.963830	-0.628044
H	-4.140006	2.177640	-1.702738
H	-3.400873	1.059266	-0.568582
C	-4.258917	-2.650708	0.784996
H	-4.559197	-3.400254	0.035666
H	-4.349575	-3.146122	1.763871
C	-2.789503	-2.256376	0.568237
H	-2.528210	-1.455040	1.276074
H	-2.651067	-1.830855	-0.435544
C	-5.441462	-0.851880	-0.656266
H	-4.477837	-0.753016	-1.173367
H	-6.025990	-1.565065	-1.257352
C	-1.792725	-3.420058	0.749996
H	-6.379466	0.777448	-1.715712
C	-5.399615	1.678201	-0.010801
H	-5.276593	1.484236	1.065265
H	-6.023215	2.582825	-0.079271
H	-2.017657	-4.213966	0.024564
H	-1.937492	-3.859232	1.748553
H	-7.141565	0.405997	-0.175805
Sum of electronic and zero-point Energies= -1201.606951			
Sum of electronic and thermal Energies= -1201.577719			
Sum of electronic and thermal Enthalpies= -1201.576774			
Sum of electronic and thermal Free Energies= -1201.668807			

daec[n=8]-4-E2 (benzene)

C	0.391618	-2.642033	0.751109
H	-0.048044	-2.703236	1.745282
C	-0.345226	-3.023130	-0.381519
C	0.278281	-2.937074	-1.633078
H	-0.265565	-3.234194	-2.528243
C	1.591345	-2.470371	-1.752564
H	2.078184	-2.404402	-2.722923
C	2.305927	-2.086059	-0.619560
O	3.630510	-1.705862	-0.745060
C	1.703911	-2.179404	0.650330
O	2.370313	-1.784529	1.783101
C	3.377669	-2.694045	2.236852
H	2.931060	-3.654725	2.534006
H	3.842703	-2.224853	3.109609
H	4.140215	-2.871620	1.468279
C	4.901541	2.201106	-0.059628
H	5.260777	3.213581	0.116192
C	3.568608	1.997668	-0.440923
C	2.630237	3.174910	-0.638644
H	3.174656	4.105069	-0.423638
H	2.340375	3.232234	-1.699931
C	1.346631	3.124991	0.212150
H	0.789692	2.211831	-0.036676
C	0.449093	4.357691	0.011416
H	0.334964	4.556320	-1.066464
H	0.959706	5.239036	0.427756
C	-0.949439	4.227002	0.645585
H	-1.415969	5.222133	0.701791
C	-1.882329	3.280159	-0.124421
H	-1.386522	2.307997	-0.263568
H	-2.042477	3.682959	-1.137454
H	-0.847069	3.880069	1.686106
H	1.614612	3.035789	1.275338
C	3.122352	0.684013	-0.661947
H	2.095748	0.498515	-0.967076
C	3.994824	-0.393187	-0.498003
C	5.329050	-0.184783	-0.132579
H	5.992008	-1.039837	-0.026903

C	5.773626	1.117582	0.085790
H	6.808821	1.289208	0.375399
C	-6.245465	0.590161	-0.322175
C	-3.241854	3.032423	0.544774
H	-3.077392	2.645724	1.563121
H	-3.783783	3.983899	0.663647
C	-5.172588	-1.603810	0.552367
H	-4.712589	-0.982351	1.334790
H	-6.098881	-2.002653	0.992886
C	-4.100640	2.031748	-0.243035
H	-4.341271	2.453781	-1.232207
H	-3.487820	1.140253	-0.438811
C	-4.213964	-2.768455	0.237088
H	-4.583938	-3.331115	-0.634806
H	-4.222139	-3.475517	1.080689
C	-2.765138	-2.318518	-0.008868
H	-2.422798	-1.731323	0.856707
H	-2.714252	-1.641862	-0.873619
C	-5.540286	-0.737066	-0.664984
H	-4.640776	-0.523629	-1.257752
H	-6.196321	-1.323167	-1.326560
C	-1.781910	-3.485586	-0.236907
H	-6.579854	1.057547	-1.261292
C	-5.398199	1.612848	0.462888
H	-5.151751	1.209991	1.456702
H	-6.015430	2.505059	0.649543
H	-2.081519	-4.046396	-1.133194
H	-1.859225	-4.185196	0.608680
H	-7.160776	0.375538	0.251164
Sum of electronic and zero-point Energies= -1201.607560			
Sum of electronic and thermal Energies= -1201.578239			
Sum of electronic and thermal Enthalpies= -1201.577294			
Sum of electronic and thermal Free Energies= -1201.669576			

daec[n=8]-5-TS (benzene)

C	-2.047365	3.405419	-0.014507
H	-2.297253	4.424713	0.275752
C	-0.709596	3.009394	-0.156453
C	-0.485310	1.683248	-0.539377
H	0.517629	1.306330	-0.699164
C	-1.537297	0.794270	-0.725220
H	-1.299568	-0.220868	-1.004885
C	-2.865025	1.180856	-0.552767
O	-3.933150	0.303258	-0.740331
C	-3.126028	2.527496	-0.211349
O	-4.373811	3.077409	-0.100133
C	-5.376454	2.392399	0.652819
H	-4.960834	1.970899	1.578843
H	-5.853411	1.599598	0.067830
H	-6.121848	3.152372	0.912859
C	-3.377209	-3.536859	0.822489
H	-3.186732	-4.502669	1.288059
C	-2.634262	-3.147470	-0.299710
C	-1.404614	-3.908017	-0.761045
H	-1.263915	-3.774561	-1.843218
H	-1.510622	-4.986235	-0.580007
C	-0.164723	-3.358706	-0.005825
H	-0.228554	-2.260925	-0.000854
C	1.212948	-3.750021	-0.561040
H	1.285441	-3.431078	-1.612951
H	1.332562	-4.844518	-0.562962
C	2.348921	-3.102600	0.254627
H	2.323044	-3.503425	1.280555
C	3.756453	-3.305534	-0.329266
H	3.818324	-2.818046	-1.314097
H	3.911249	-4.379179	-0.517729
H	2.142139	-2.025851	0.349299
H	-0.237205	-3.660265	1.050006
C	-2.916434	-1.905487	-0.889255
H	-2.405027	-1.622820	-1.804443

C	-3.786083	-1.002725	-0.272367
C	-4.527419	-1.397317	0.845035
H	-5.223230	-0.699873	1.303217
C	-4.340894	-2.680380	1.365152
H	-4.920948	-2.996658	2.230103
C	5.648372	1.033754	-0.137221
C	4.901793	-2.814081	0.582114
H	4.803774	-3.319407	1.555458
H	5.858168	-3.160086	0.160070
C	4.367283	3.281006	0.025535
H	5.224124	3.731751	0.548766
H	4.540472	3.458019	-1.047849
C	4.998912	-1.293256	0.829192
H	5.709528	-1.125738	1.653766
H	4.032111	-0.913101	1.188204
C	3.070002	4.015272	0.446488
H	3.102681	5.046243	0.063349
H	3.026996	4.095260	1.543908
C	1.819717	3.282144	-0.053249
H	1.790376	2.318374	0.465904
H	1.945482	3.047497	-1.121806
C	4.351241	1.758763	0.264858
H	4.116662	1.552825	1.320308
H	3.530212	1.318732	-0.317664
C	0.453227	3.954980	0.143772
H	6.038445	1.486103	-1.062153
C	5.466363	-0.477828	-0.388142
H	6.422002	-0.893979	-0.743647
H	4.753769	-0.607885	-1.217584
H	0.376921	4.855806	-0.484092
H	0.360472	4.309619	1.182392
H	6.423149	1.195366	0.628451

Sum of electronic and zero-point Energies= -1201.585222

Sum of electronic and thermal Energies= -1201.556910

Sum of electronic and thermal Enthalpies= -1201.555966

Sum of electronic and thermal Free Energies= -1201.644283

daec[n=8]-5-E1 (benzene)

C	1.763202	-3.018814	-0.444676
H	1.561206	-3.690941	-1.276782
C	0.945419	-3.022631	0.692685
C	1.262731	-2.143093	1.739128
H	0.655802	-2.138955	2.643097
C	2.336114	-1.260080	1.630870
H	2.572694	-0.567366	2.435410
C	3.112071	-1.233748	0.470473
O	4.170625	-0.345971	0.353718
C	2.841120	-2.134480	-0.573796
O	3.544875	-2.127188	-1.749587
C	4.923430	-2.501576	-1.658175
H	5.025395	-3.519451	-1.253201
H	5.494287	-1.800934	-1.038138
H	5.310060	-2.481354	-2.682251
C	3.449619	3.753750	0.122061
H	3.284181	4.828551	0.071289
C	2.439424	2.876859	-0.294037
C	1.108903	3.387047	-0.815981
H	0.933728	2.975675	-1.822010
H	1.156254	4.478415	-0.933904
C	-0.091840	3.015960	0.078979
H	-0.097548	1.927214	0.235518
C	-1.444933	3.443267	-0.508268
H	-1.524024	3.063224	-1.539374
H	-1.487314	4.541088	-0.586151
C	-2.644797	2.931587	0.303685
H	-2.596044	3.331519	1.329175
C	-4.003253	3.287299	-0.320104
H	-4.024160	2.932104	-1.361208
H	-4.093072	4.382881	-0.379814
H	-2.555590	1.839683	0.401249

H	0.043916	3.464317	1.074657
C	2.672822	1.494485	-0.220768
H	1.907693	0.797303	-0.551531
C	3.884487	1.005920	0.271700
C	4.895329	1.883978	0.677597
H	5.832513	1.480267	1.052508
C	4.668987	3.257203	0.595748
H	5.449032	3.947444	0.911939
C	-5.480623	-1.067259	-0.676989
C	-5.229028	2.741797	0.440109
H	-5.236966	3.171655	1.453808
H	-6.139413	3.115894	-0.053646
C	-4.052733	-3.186064	-0.333348
H	-4.976710	-3.704038	-0.033334
H	-3.951303	-3.351492	-1.417674
C	-5.320910	1.207387	0.560368
H	-6.193193	0.958659	1.184932
H	-4.446424	0.833871	1.110206
C	-2.862045	-3.840240	0.394602
H	-2.805248	-4.900278	0.102957
H	-3.052012	-3.833370	1.479773
C	-1.513118	-3.158341	0.125064
H	-1.540648	-2.130507	0.510444
H	-1.346208	-3.070410	-0.959645
C	-4.203763	-1.678485	-0.074360
H	-4.176245	-1.492443	1.009935
H	-3.333476	-1.152707	-0.494104
C	-0.303284	-3.877895	0.762501
H	-5.629889	-1.477210	-1.687925
C	-5.445809	0.468988	-0.781949
H	-6.355757	0.815846	-1.296220
H	-4.605807	0.746158	-1.436393
H	-0.140736	-4.841831	0.260057
H	-0.532083	-4.104733	1.813660
H	-6.356017	-1.385390	-0.089087

Sum of electronic and zero-point Energies= -1201.607442

Sum of electronic and thermal Energies= -1201.578155

Sum of electronic and thermal Enthalpies= -1201.577210

Sum of electronic and thermal Free Energies= -1201.669539

daec[n=8]-5-E2 (benzene)

C	1.212074	-2.552387	0.963818
H	0.703395	-2.591672	1.925493
C	0.711891	-3.262286	-0.137918
C	1.419220	-3.192907	-1.346080
H	1.064549	-3.747413	-2.213379
C	2.561254	-2.394929	-1.462802
H	3.099428	-2.317883	-2.404849
C	3.021254	-1.662328	-0.369715
O	4.153848	-0.875863	-0.500119
C	2.358070	-1.761484	0.867991
O	2.769070	-1.045358	1.962687
C	3.996946	-1.485118	2.552526
H	4.829071	-1.443143	1.839253
H	3.898228	-2.510954	2.937589
H	4.196140	-0.803098	3.385074
C	3.863302	3.283888	-0.435414
H	3.813606	4.371181	-0.413475
C	2.710367	2.542825	-0.724182
C	1.382942	3.220040	-1.013074
H	1.034360	2.919006	-2.013422
H	1.530039	4.308129	-1.054857
C	0.276136	2.887277	0.008579
H	0.172584	1.794840	0.081218
C	-1.087319	3.495177	-0.352096
H	-1.333960	3.230392	-1.392880
H	-1.024128	4.594499	-0.326716
C	-2.224099	3.016606	0.564097
H	-2.005283	3.300068	1.605966
C	-3.603982	3.562001	0.164537

H	-3.787837	3.332407	-0.895710
H	-3.586443	4.660787	0.230013
H	-2.240083	1.916958	0.548379
H	0.587736	3.227403	1.007334
C	2.796414	1.141710	-0.748527
H	1.915613	0.549343	-0.980700
C	4.005324	0.501389	-0.473170
C	5.158594	1.244114	-0.197538
H	6.093173	0.724884	-0.000084
C	5.077131	2.635528	-0.182002
H	5.969017	3.220713	0.035041
C	-5.581103	-0.557618	-0.464740
C	-4.778303	3.044098	1.019409
H	-4.614620	3.345732	2.065630
H	-5.697138	3.558291	0.697001
C	-4.357866	-2.824729	-0.560570
H	-5.292578	-3.288591	-0.209638
H	-4.398520	-2.857033	-1.660952
C	-5.019480	1.521615	0.982232
H	-5.827479	1.279521	1.690291
H	-4.127963	1.003613	1.360945
C	-3.170685	-3.676386	-0.069682
H	-3.260652	-4.689357	-0.491342
H	-3.237191	-3.795270	1.023506
C	-1.794213	-3.092486	-0.418821
H	-1.668231	-2.127534	0.089738
H	-1.739299	-2.876216	-1.497047
C	-4.314485	-1.355785	-0.109817
H	-4.138629	-1.314459	0.975669
H	-3.448688	-0.862286	-0.575555
C	-0.606613	-4.000586	-0.027539
H	-5.896512	-0.823599	-1.485622
C	-5.392417	0.969726	-0.403063
H	-6.316435	1.461223	-0.745744
H	-4.616112	1.245845	-1.132323
H	-0.600900	-4.896016	-0.664946
H	-0.746242	-4.349640	1.005531
H	-6.407500	-0.862680	0.196396

Sum of electronic and zero-point Energies= -1201.607522

Sum of electronic and thermal Energies= -1201.578331

Sum of electronic and thermal Enthalpies= -1201.577387

Sum of electronic and thermal Free Energies= -1201.668688

daec[n=8]-6-TS (benzene)

C	0.410909	-3.422505	-0.347846
H	0.765400	-4.308029	-0.872836
C	1.316683	-2.453829	0.110141
C	0.785527	-1.346582	0.783369
H	1.435469	-0.572594	1.178764
C	-0.587562	-1.197254	0.964460
H	-0.960847	-0.325562	1.488489
C	-1.481167	-2.140513	0.460191
O	-2.858345	-2.010282	0.594876
C	-0.973001	-3.280177	-0.191496
O	-1.796514	-4.227555	-0.746231
C	-2.551613	-5.010979	0.182540
H	-1.885144	-5.554239	0.869198
H	-3.115016	-5.733463	-0.417340
H	-3.249286	-4.393363	0.760281
C	-4.604066	1.496235	-0.856042
H	-5.053874	2.402623	-1.257148
C	-3.922441	1.538400	0.370896
C	-3.742049	2.828547	1.152667
H	-3.103156	2.623538	2.021747
H	-4.711292	3.152427	1.562521
C	-3.156773	4.011273	0.345217
H	-3.023038	4.854519	1.039735
C	-1.841767	3.758891	-0.414914
H	-1.631794	4.659058	-1.013256
H	-1.993164	2.947397	-1.141320

C	-0.594304	3.442568	0.429310
H	-0.471708	4.205779	1.214567
C	0.671128	3.394717	-0.444660
H	0.788543	4.372766	-0.938439
H	0.513971	2.668315	-1.257512
H	-0.722183	2.481386	0.949291
H	-3.908091	4.345214	-0.385197
C	-3.375844	0.346829	0.865761
H	-2.894366	0.342000	1.839611
C	-3.437299	-0.834185	0.121396
C	-4.108270	-0.868865	-1.100757
H	-4.145187	-1.798617	-1.662367
C	-4.705028	0.302567	-1.575173
H	-5.237518	0.286788	-2.524325
C	4.911778	1.413301	0.280832
C	1.985171	3.050091	0.277759
H	2.125762	3.723740	1.138176
H	1.921094	2.032277	0.691966
C	5.468175	-0.914403	-0.784594
H	5.226310	-1.500145	-1.683750
H	6.552274	-0.730308	-0.837458
C	3.193394	3.172791	-0.667982
H	3.209930	4.201744	-1.059467
H	3.029257	2.529435	-1.545179
C	5.199646	-1.772191	0.471146
H	5.727822	-1.329969	1.328691
H	5.658918	-2.760587	0.316068
C	3.725592	-1.935796	0.876751
H	3.670672	-2.525631	1.803478
H	3.346396	-0.941983	1.137090
C	4.729552	0.436257	-0.895461
H	5.082997	0.924059	-1.817463
H	3.657080	0.254706	-1.054217
C	2.807059	-2.575899	-0.179523
H	4.307834	1.085529	1.139105
C	4.582993	2.880746	-0.067660
H	5.336106	3.229402	-0.791471
H	4.723891	3.499477	0.832322
H	2.999382	-2.109030	-1.157720
H	3.069167	-3.636240	-0.305472
H	5.957707	1.380076	0.623703

Sum of electronic and zero-point Energies= -1201.590392

Sum of electronic and thermal Energies= -1201.562236

Sum of electronic and thermal Enthalpies= -1201.561292

Sum of electronic and thermal Free Energies= -1201.649120

daec[n=8]-6-E1 (benzene)

C	0.592049	1.909931	0.801443
H	1.243596	1.409565	1.515641
C	1.130596	2.676120	-0.242780
C	0.243273	3.314277	-1.120471
H	0.632531	3.926489	-1.932283
C	-1.138136	3.162734	-0.977324
H	-1.831278	3.646726	-1.661606
C	-1.657391	2.376924	0.050735
O	-3.030118	2.280682	0.197735
C	-0.785979	1.754049	0.963318
O	-1.253206	0.946895	1.969701
C	-1.914603	1.627777	3.041907
H	-1.223097	2.315323	3.551018
H	-2.236017	0.851317	3.743070
H	-2.790098	2.186709	2.689770
C	-5.122994	-1.222811	-0.644114
H	-5.697859	-2.121436	-0.862403
C	-3.775676	-1.149245	-1.029854
C	-3.108944	-2.323649	-1.720862
H	-2.207291	-1.980391	-2.244894
H	-3.785921	-2.712430	-2.495115
C	-2.750499	-3.492244	-0.770656
H	-2.461908	-4.358851	-1.385247



C	-1.634670	-3.207643	0.250326
H	-1.624721	-4.028362	0.983984
H	-1.873832	-2.296746	0.818352
C	-0.228241	-3.080378	-0.356482
H	-0.011199	-3.978907	-0.956747
C	0.872360	-2.900810	0.699841
H	0.841526	-3.749777	1.401503
H	0.654613	-2.003365	1.299894
H	-0.193615	-2.232695	-1.057434
H	-3.661207	-3.789995	-0.231014
C	-3.055418	0.021566	-0.753417
H	-2.015385	0.099986	-1.057523
C	-3.668850	1.087964	-0.089051
C	-5.011100	1.011658	0.293373
H	-5.469218	1.858699	0.798002
C	-5.731605	-0.148631	0.008896
H	-6.779048	-0.211518	0.298605
C	5.146955	-1.316881	-0.216804
C	2.284723	-2.785915	0.106334
H	2.490901	-3.668790	-0.520291
H	2.316019	-1.920511	-0.572632
C	5.473408	1.257878	-0.229541
H	5.414628	2.126601	0.442723
H	6.535918	1.166940	-0.503161
C	3.383030	-2.659620	1.173633
H	3.326950	-3.534712	1.839323
H	3.170649	-1.789325	1.812545
C	4.673187	1.549240	-1.515870
H	4.901646	0.779073	-2.266677
H	5.035732	2.497358	-1.942276
C	3.144483	1.616644	-1.356824
H	2.688776	1.738714	-2.350286
H	2.768355	0.657518	-0.974264
C	5.049709	0.005097	0.560436
H	5.683032	-0.065423	1.458627
H	4.024529	0.139633	0.932831
C	2.630667	2.749252	-0.440181
H	4.491102	-1.283342	-1.097997
C	4.819510	-2.567438	0.622652
H	5.521516	-2.614906	1.469785
H	5.021225	-3.462076	0.013219
H	3.127930	2.689351	0.536861
H	2.907981	3.720334	-0.874815
H	6.170053	-1.422470	-0.610550
Sum of electronic and zero-point Energies= -1201.606400			
Sum of electronic and thermal Energies= -1201.577474			
Sum of electronic and thermal Enthalpies= -1201.576530			
Sum of electronic and thermal Free Energies= -1201.667087			

daec[n=8]-6-E2 (benzene)

C	0.016733	3.290450	-0.260774
H	0.320777	4.074068	-0.952182
C	0.968193	2.589125	0.482190
C	0.518647	1.590576	1.362105
H	1.232922	1.036719	1.968694
C	-0.839489	1.309820	1.471301
H	-1.195879	0.547766	2.160898
C	-1.783759	2.005126	0.707991
O	-3.136319	1.756927	0.896630
C	-1.359488	3.019531	-0.171621
O	-2.156831	3.818156	-0.933876
C	-3.428998	3.361827	-1.398630
H	-3.372629	2.338106	-1.791184
H	-3.697400	4.041865	-2.214193
H	-4.192398	3.413064	-0.615640
C	-4.867030	-1.923921	-0.009906
H	-5.352526	-2.869828	-0.244404
C	-3.619225	-1.622586	-0.577411
C	-2.935688	-2.606973	-1.508675
H	-2.129911	-2.097591	-2.053243

H	-3.658820	-2.936680	-2.268782
C	-2.378214	-3.868104	-0.806479
H	-2.075808	-4.586975	-1.583257
C	-1.195406	-3.637534	0.150167
H	-1.027641	-4.567370	0.714964
H	-1.466761	-2.876189	0.896775
C	0.122128	-3.239482	-0.534652
H	0.356158	-3.974165	-1.321940
C	1.304897	-3.152649	0.441645
H	1.425264	-4.123331	0.948717
H	1.068065	-2.425180	1.234300
H	0.006694	-2.272460	-1.046872
H	-3.197245	-4.346920	-0.250520
C	-3.017935	-0.392936	-0.271762
H	-2.056839	-0.139123	-0.710147
C	-3.650266	0.511348	0.590237
C	-4.892858	0.206118	1.153147
H	-5.366372	0.925386	1.816619
C	-5.494322	-1.014645	0.845068
H	-6.463967	-1.255985	1.276817
C	5.307232	-0.943249	-0.420509
C	2.634012	-2.760556	-0.221592
H	2.858102	-3.466588	-1.037476
H	2.518545	-1.775301	-0.697710
C	5.418194	1.192768	0.118064
H	5.309750	2.289981	0.961975
H	6.472723	1.662776	-0.190445
C	3.813672	-2.737656	0.763125
H	3.903610	-3.733433	1.224046
H	3.583120	-2.049601	1.590279
C	4.544730	2.071413	-1.059504
H	4.807730	1.498715	-1.960652
H	4.807821	3.116718	-1.283792
C	3.023707	1.964550	-0.856932
H	2.520393	2.245011	-1.793656
H	2.746039	0.916991	-0.673620
C	5.140179	0.166416	0.629513
H	5.822408	-0.035642	1.470135
H	4.127483	0.123196	1.054466
C	2.449884	2.834003	0.284141
H	4.583073	-0.800509	-1.234921
C	5.176330	-2.371640	0.143526
H	5.955601	-2.518826	0.907530
H	5.402798	-3.089127	-0.660493
H	2.980165	2.614984	1.220488
H	2.633836	3.894149	0.058624
H	6.301162	-0.846178	-0.884875
Sum of electronic and zero-point Energies= -1201.604977			
Sum of electronic and thermal Energies= -1201.576147			
Sum of electronic and thermal Enthalpies= -1201.575203			
Sum of electronic and thermal Free Energies= -1201.665754			

daec[n=8]-7-TS (benzene)

C	0.389276	3.394828	-0.525521
H	0.805979	4.389781	-0.655686
C	1.262004	2.317319	-0.298089
C	0.703706	1.048129	-0.133645
H	1.343202	0.184101	0.027971
C	-0.677023	0.857566	-0.157656
H	-1.080556	-0.134648	0.005647
C	-1.541128	1.927653	-0.370489
O	-2.920101	1.804376	-0.405393
C	-1.001692	3.218205	-0.572478
O	-1.904834	4.214991	-0.784163
C	-1.413142	5.529008	-0.996071
H	-0.859360	5.903242	-0.122229
H	-0.767719	5.583933	-1.885163
H	-2.296269	6.155120	-1.155059
C	-4.445069	-1.386879	1.785012
H	-4.804069	-2.222942	2.384147

C	-3.934763	-1.635204	0.497302
C	-3.844079	-3.078734	0.021775
H	-4.861491	-3.499651	0.008504
H	-3.316687	-3.646806	0.802840
C	-3.201058	-3.399602	-1.341435
H	-3.330397	-4.482501	-1.485851
C	-1.710487	-3.060945	-1.571058
H	-1.590537	-1.991636	-1.789869
H	-1.405207	-3.577497	-2.494323
C	-0.713636	-3.422458	-0.455473
H	-0.875506	-4.455847	-0.110920
C	0.738670	-3.261827	-0.944844
H	0.811355	-2.339906	-1.543243
H	0.966582	-4.083253	-1.642517
H	-0.887170	-2.778173	0.419723
H	-3.787592	-2.925751	-2.142900
C	-3.494153	-0.540758	-0.256308
H	-3.120221	-0.669211	-1.266502
C	-3.468827	0.742077	0.304099
C	-3.976519	0.981261	1.578479
H	-3.952625	1.989057	1.984887
C	-4.488115	-0.095943	2.309197
H	-4.894443	0.072326	3.304813
C	4.632361	-1.503785	0.918986
C	1.822642	-3.209348	0.145597
H	1.687977	-2.295151	0.744225
H	1.700319	-4.050283	0.846275
C	5.487086	0.812055	0.024852
H	6.538131	0.620650	0.291000
H	5.522676	1.376092	-0.919119
C	3.236678	-3.254358	-0.462623
H	3.383295	-4.252861	-0.901973
C	3.285368	-2.554678	-1.310033
C	4.880987	1.707355	1.127334
H	5.388909	2.683398	1.087850
H	5.128412	1.284370	2.112340
C	3.357097	1.909031	1.088006
H	2.879088	0.942915	1.287690
H	3.061641	2.557624	1.925816
C	4.796814	-0.536520	-0.268820
H	3.814310	-0.349244	-0.724319
H	5.389225	-1.037989	-1.050398
C	2.770197	2.491715	-0.217727
H	5.537928	-1.470663	1.544531
C	4.411119	-2.973631	0.496757
H	4.299131	-3.592666	1.400460
H	5.334165	-3.321421	0.007522
H	3.034573	3.554666	-0.307634
H	3.232569	1.990513	-1.080689
H	3.810813	-1.167207	1.567674

Sum of electronic and zero-point Energies= -1201.588300

Sum of electronic and thermal Energies= -1201.560437

Sum of electronic and thermal Enthalpies= -1201.559493

Sum of electronic and thermal Free Energies= -1201.646296

daec[n=8]-7-E1 (benzene)

C	0.534973	2.066629	-0.894625
H	1.210776	1.651204	-1.637255
C	1.076052	2.748735	0.209191
C	0.205160	3.303124	1.152905
H	0.603349	3.847119	2.007432
C	-1.178518	3.151895	1.013270
H	-1.867505	3.573890	1.741418
C	-1.706000	2.456426	-0.068390
O	-3.076742	2.370506	-0.226963
C	-0.847470	1.917297	-1.050773
O	-1.454141	1.282271	-2.086892
C	-0.639502	0.751969	-3.122998
H	-0.049964	1.538484	-3.615771
H	0.036564	-0.030273	-2.748532

H	-1.330431	0.311657	-3.847560
C	-5.169036	-1.153503	0.518914
H	-5.746411	-2.055069	0.717840
C	-3.839546	-1.067498	0.959823
C	-3.199549	-2.226500	1.702187
H	-3.895398	-2.576518	2.478403
H	-2.303585	-1.875361	2.230810
C	-2.839761	-3.437042	0.807618
H	-2.586262	-4.285339	1.461865
C	-1.689486	-3.214761	-0.190023
H	-1.898432	-2.324395	-0.801813
H	-1.672516	-4.065410	-0.888627
C	-0.298927	-3.083292	0.452262
H	-0.120510	-3.949551	1.109557
C	0.836192	-2.991041	-0.578205
H	0.643974	-2.140379	-1.251865
H	0.820633	-3.889367	-1.215760
H	-0.265269	-2.197001	1.103507
H	-3.740138	-3.737822	0.252748
C	-3.118005	0.107995	0.706440
H	-2.093098	0.198611	1.056240
C	-3.713613	1.172071	0.020330
C	-5.038563	1.081809	-0.416255
H	-5.481230	1.923439	-0.942926
C	-5.758681	-0.085252	-0.161427
H	-6.792365	-0.158443	-0.495113
C	5.074893	-1.323879	0.340332
C	2.231860	-2.833377	0.043691
H	2.243040	-1.927029	0.667488
H	2.424445	-3.674453	0.728993
C	5.399994	1.245836	0.202363
H	6.465614	1.170423	0.468415
H	5.332355	2.076737	-0.515369
C	3.354875	-2.767617	-1.003244
H	3.320628	-3.683970	-1.612495
H	3.151941	-1.941428	-1.701391
C	4.613990	1.604114	1.480209
H	4.991437	2.565367	1.861907
H	4.839776	0.864717	2.262050
C	3.085226	1.685047	1.329107
H	2.695429	0.723467	0.966590
H	2.637323	1.830076	2.322820
C	4.970676	-0.049672	-0.512639
H	3.942673	0.063365	-0.885302
H	5.598584	-0.171422	-1.409196
C	2.578556	2.808508	0.397096
H	6.093965	-1.392004	0.752276
C	4.777301	-2.626653	-0.427550
H	4.973875	-3.480039	0.239871
H	5.498045	-2.718549	-1.255009
H	2.868865	3.781981	0.818165
H	3.071179	2.731335	-0.581144
H	4.407155	-1.248485	1.209925

Sum of electronic and zero-point Energies= -1201.608641

Sum of electronic and thermal Energies= -1201.579905

Sum of electronic and thermal Enthalpies= -1201.578961

Sum of electronic and thermal Free Energies= -1201.669073

daec[n=8]-7-E2 (benzene)

C	-0.036270	2.982064	0.324853
H	0.225273	3.578120	1.194949
C	0.990047	2.527944	-0.522385
C	0.650470	1.775709	-1.651363
H	1.430060	1.426293	-2.325658
C	-0.686156	1.460688	-1.917424
H	-0.963498	0.875273	-2.791147
C	-1.693232	1.893226	-1.064060
O	-3.015691	1.622155	-1.365220
C	-1.377454	2.674339	0.068822
O	-2.429563	3.063146	0.834290

C	-2.165698	3.840830	1.993828
H	-1.531789	3.298244	2.710052
H	-1.690490	4.799006	1.738592
H	-3.140784	4.033196	2.450492
C	-5.040391	-1.606257	0.317629
H	-5.595372	-2.440637	0.743755
C	-3.690195	-1.426776	0.652126
C	-2.990911	-2.402880	1.579484
H	-3.683338	-2.683907	2.385564
H	-2.140055	-1.906523	2.064773
C	-2.512079	-3.703680	0.888526
H	-2.217952	-4.419827	1.671223
C	-1.348704	-3.545847	-0.106552
H	-1.602236	-2.778022	-0.852442
H	-1.245240	-4.487855	-0.666589
C	0.005573	-3.210549	0.538689
H	0.241148	-3.973206	1.298497
C	1.158646	-3.132131	-0.473177
H	0.923841	-2.368174	-1.231184
H	1.229648	-4.087469	-1.017312
H	-0.059454	-2.254837	1.080481
H	-3.369710	-4.153898	0.367980
C	-2.994948	-0.339081	0.102310
H	-1.950421	-0.183033	0.356838
C	-3.638492	0.547139	-0.767860
C	-4.985606	0.364081	-1.097694
H	-5.465656	1.068697	-1.772100
C	-5.677898	-0.715065	-0.550009
H	-6.727878	-0.857986	-0.799656
C	5.239538	-1.080309	0.401689
C	2.518261	-2.809038	0.164958
H	2.441431	-1.848941	0.696978
H	2.749257	-3.563351	0.934459
C	5.387471	1.483861	0.036953
H	6.426828	1.519523	0.398190
H	5.326657	2.235303	-0.764044
C	3.669521	-2.757421	-0.851626
H	3.719490	-3.724936	-1.374599
H	3.435186	-2.013943	-1.628165
C	4.463122	1.897051	1.201046
H	4.723446	2.922852	1.504760
H	4.677739	1.264735	2.074583
C	2.953349	1.818126	0.916520
H	2.683919	0.792441	0.629069
H	2.404703	2.018258	1.848448
C	5.116756	0.097345	-0.578027
H	4.119333	0.093208	-1.039581
H	5.826306	-0.056292	-1.406082
C	2.441859	2.786719	-0.173466
H	6.234769	-1.046688	0.872106
C	5.057555	-2.466045	-0.248183
H	5.283363	-3.238449	0.503402
H	5.814085	-2.584954	-1.039498
H	2.574864	3.821919	0.174226
H	3.051103	2.681323	-1.080327
H	4.518657	-0.962120	1.222757

Sum of electronic and zero-point Energies= -1201.608289  
Sum of electronic and thermal Energies= -1201.579574  
Sum of electronic and thermal Enthalpies= -1201.578630  
Sum of electronic and thermal Free Energies= -1201.668930

#### jugcathanin-1-TS (benzene)

C	1.328887	2.723391	-0.134979
O	1.757658	3.986203	-0.017494
H	0.984804	4.565247	-0.283781
C	2.203069	1.627905	-0.269926
C	1.642001	0.410180	0.046650
H	2.258700	-0.453187	0.018039
C	0.339591	0.210178	0.404942
H	0.052771	-0.805161	0.558022

C	-0.548363	1.266376	0.536903
O	-1.879601	1.048030	0.924041
C	-0.030494	2.549873	0.274567
O	-0.773797	3.714421	0.307647
C	-1.395575	4.025239	1.563375
H	-1.840260	5.018501	1.443693
H	-2.178678	3.297813	1.802607
H	-0.653058	4.049742	2.373804
C	-2.475867	-2.852652	-0.333029
H	-2.490303	-3.831490	-0.811223
C	-1.599798	-2.610232	0.733225
C	-0.408389	-3.526960	1.020251
H	-0.733478	-4.574854	1.035747
H	0.017483	-3.310550	2.007336
C	0.737682	-3.391256	-0.056027
H	0.352128	-2.926779	-0.972234
H	1.060493	-4.398823	-0.364412
C	2.044149	-2.667870	0.355288
C	3.015855	-2.271336	-0.795744
H	2.421775	-2.006721	-1.679887
H	3.517377	-3.215353	-1.063770
C	4.115946	-1.176793	-0.508920
H	4.135101	-0.969602	0.568842
C	4.056317	0.166151	-1.350289
H	3.408265	0.003734	-2.223766
C	3.657065	1.547423	-0.710719
H	4.325033	1.760045	0.139682
H	3.877214	2.323070	-1.456742
H	5.063461	0.321685	-1.759090
H	5.085291	-1.640970	-0.726629
O	2.325309	-2.477084	1.520787
C	-1.670656	-1.338122	1.329947
H	-1.038957	-1.113363	2.185273
C	-2.298119	-0.269702	0.681014
C	-3.172007	-0.519534	-0.394831
O	-3.783062	0.557849	-0.949627
C	-4.618235	0.344553	-2.079450
H	-4.060351	-0.096653	-2.918047
H	-4.982498	1.334104	-2.370225
H	-5.476704	-0.297493	-1.833728
C	-3.305717	-1.845217	-0.841240
H	-3.981727	-2.077870	-1.658402

Sum of electronic and zero-point Energies= -1190.266199  
Sum of electronic and thermal Energies= -1190.242807  
Sum of electronic and thermal Enthalpies= -1190.241863  
Sum of electronic and thermal Free Energies= -1190.317758

#### jugcathanin-1-E1 (benzene)

C	-1.730207	-1.918417	-0.396189
O	-2.232953	-2.279493	-1.609615
H	-1.463876	-2.447241	-2.182011
C	-2.603956	-1.544804	0.638617
C	-2.036217	-1.229239	1.879760
H	-2.695169	-0.969475	2.705902
C	-0.652761	-1.175424	2.071590
H	-0.223960	-0.865778	3.020908
C	0.195412	-1.435267	0.996958
O	1.560567	-1.219186	1.110391
C	-0.335804	-1.864295	-0.226684
O	0.412347	-2.137561	-1.349483
C	1.411377	-3.165905	-1.219324
H	1.776034	-3.355950	-2.233741
H	2.237219	-2.833184	-0.583383
H	0.970070	-4.084830	-0.809310
C	2.997592	2.366289	-0.463288
H	3.399863	3.281581	-0.894471
C	1.659763	2.312437	-0.069180
C	0.729939	3.502621	-0.231871
H	1.273073	4.303950	-0.747757
H	0.440056	3.901149	0.750561

C	-0.570565	3.195566	-1.010427
H	-0.373852	2.542549	-1.869863
H	-0.970544	4.135839	-1.423739
C	-1.708224	2.624748	-0.154387
C	-2.600234	1.586730	-0.820836
H	-1.950351	0.715937	-0.997650
H	-2.861355	1.943492	-1.829633
C	-3.855579	1.180315	-0.032940
H	-3.605593	1.145306	1.034356
C	-4.464905	-0.169123	-0.490090
H	-4.178345	-0.373827	-1.529891
C	-4.088059	-1.395452	0.386985
H	-4.594310	-1.303136	1.357470
H	-4.489099	-2.297395	-0.095673
H	-5.561368	-0.098457	-0.485970
H	-4.603268	1.978427	-0.135063
O	-1.874089	2.990675	0.994487
C	1.188866	1.107029	0.478160
H	0.163630	1.036011	0.823928
C	2.008085	-0.010269	0.597826
C	3.363379	0.055089	0.207439
O	4.092148	-1.086667	0.365160
C	5.463844	-1.052522	-0.001365
H	5.593405	-0.840967	-1.073040
H	5.856256	-2.049805	0.218238
H	6.020980	-0.308264	0.585995
C	3.844425	1.257487	-0.317049
H	4.879328	1.336352	-0.635914

Sum of electronic and zero-point Energies= -1190.337603  
Sum of electronic and thermal Energies= -1190.313474  
Sum of electronic and thermal Enthalpies= -1190.312530  
Sum of electronic and thermal Free Energies= -1190.390784

#### jugcathanin-1-E2 (benzene)

C	-1.834455	-1.711998	0.547068
O	-2.404797	-1.781047	1.781057
H	-1.671338	-1.779367	2.420883
C	-2.639131	-1.586838	-0.597228
C	-1.994503	-1.563723	-1.842413
H	-2.599925	-1.505446	-2.745722
C	-0.601854	-1.543086	-1.954795
H	-0.110297	-1.457641	-2.920358
C	0.178255	-1.566744	-0.797753
O	1.550587	-1.398054	-0.880555
C	-0.431016	-1.717467	0.452832
O	0.249939	-1.741703	1.647789
C	1.215234	-2.795686	1.810505
H	1.565880	-2.721200	2.844364
H	0.748173	-3.777201	1.649362
H	2.057501	-2.669725	1.122799
C	3.107893	2.308721	0.225696
H	3.549179	3.261944	0.512967
C	1.725333	2.206220	0.047355
C	0.814646	3.399537	0.297802
H	1.335706	4.311979	-0.020873
H	0.643475	3.506870	1.378818
C	-0.566018	3.348962	-0.382191
H	-0.490186	3.017153	-1.425746
H	-0.976330	4.370899	-0.419897
C	-1.623065	2.524245	0.366094
C	-2.657596	1.817729	-0.500451
H	-2.102068	1.091952	-1.113337
H	-3.048664	2.547379	-1.228224
C	-3.802997	1.125282	0.254535
H	-3.403578	0.638699	1.151596
C	-4.578893	0.101577	-0.613026
H	-4.510568	0.393527	-1.671758
C	-4.133349	-1.380271	-0.463226
H	-4.460219	-1.748828	0.515296
H	-4.661807	-1.976999	-1.220234

H	-5.647779	0.141984	-0.361346
H	-4.494899	1.896417	0.619141
O	-1.630314	2.462748	1.580519
C	1.211636	0.958681	-0.332706
H	0.147919	0.836447	-0.491758
C	2.031294	-0.153390	-0.503150
C	3.423215	-0.046389	-0.307720
O	4.146485	-1.188834	-0.483104
C	5.551725	-1.117928	-0.293379
H	6.022473	-0.423332	-1.004486
H	5.929023	-2.128437	-0.476468
H	5.808966	-0.816843	0.732886
C	3.946728	1.200518	0.050324
H	5.015662	1.317173	0.201421

Sum of electronic and zero-point Energies= -1190.335968  
Sum of electronic and thermal Energies= -1190.311849  
Sum of electronic and thermal Enthalpies= -1190.310905  
Sum of electronic and thermal Free Energies= -1190.389287

#### jugcathanin-2-TS (benzene)

C	1.120079	2.829996	0.163391
O	1.434007	4.144143	-0.001435
H	0.635309	4.643868	0.244496
C	2.082811	1.830001	-0.072478
C	1.633408	0.545238	0.141598
H	2.323028	-0.254730	0.036033
C	0.361808	0.203173	0.502873
H	0.166964	-0.842133	0.580769
C	-0.603789	1.164731	0.755768
O	-1.893586	0.801445	1.173738
C	-0.209476	2.505061	0.578523
O	-1.028672	3.593358	0.811707
C	-2.208676	3.664069	-0.006582
H	-2.723737	4.584661	0.286526
H	-1.940632	3.715973	-1.071958
H	-2.859096	2.800661	0.165871
C	-2.217791	-3.006668	-0.420133
H	-2.171144	-3.937549	-0.984237
C	-1.326521	-2.786854	0.638493
C	-0.055985	-3.622675	0.808907
H	-0.294423	-4.691099	0.734134
H	0.382360	-3.462229	1.801150
C	1.040133	-3.294317	-0.277954
H	0.588610	-2.786512	-1.139468
H	1.435971	-4.239539	-0.683059
C	2.294350	-2.500238	0.165133
C	3.193256	-1.922868	-0.968498
H	2.551584	-1.629102	-1.809123
H	3.759221	-2.794447	-1.335326
C	4.211653	-0.772420	-0.608291
H	4.249327	-0.663525	0.483320
C	4.019537	0.632721	-1.318012
H	4.999049	0.908525	-1.730480
C	3.527369	1.911315	-0.543488
H	3.666566	2.768391	-1.216249
H	4.196464	2.097929	0.312019
H	3.362702	0.497759	-2.189680
H	5.207137	-1.133828	-0.892759
O	2.595195	-2.388855	1.335878
C	-1.478978	-1.583798	1.351378
H	-0.838708	-1.383051	2.206289
C	-2.213536	-0.518343	0.820668
C	-3.099477	-0.743945	-0.249920
O	-3.812005	0.327049	-0.691281
C	-4.677198	0.142463	-1.804126
H	-5.131575	1.119452	-1.992576
H	-5.470255	-0.586374	-1.583525
H	-4.123691	-0.178567	-2.698358
C	-3.143445	-2.030793	-0.811609
H	-3.827729	-2.246757	-1.626506

Sum of electronic and zero-point Energies= -1190.266892  
Sum of electronic and thermal Energies= -1190.243595  
Sum of electronic and thermal Enthalpies= -1190.242651  
Sum of electronic and thermal Free Energies= -1190.318089

jugcathanin-2-E1 (benzene)

C -2.049414 -1.973958 -0.206698  
O -2.798394 -2.459285 -1.236062  
H -2.171271 -2.833780 -1.878343  
C -2.683374 -1.336483 0.868298  
C -1.877333 -0.898647 1.928700  
H -2.348727 -0.438313 2.794452  
C -0.489265 -0.991293 1.875554  
H 0.132439 -0.595720 2.674323  
C 0.134392 -1.530355 0.747010  
O 1.517677 -1.477835 0.638334  
C -0.641786 -2.075395 -0.285520  
O -0.204804 -2.739099 -1.405260  
C 1.011465 -2.352739 -2.059142  
H 0.993664 -2.862517 -3.027687  
H 1.046990 -1.267608 -2.219515  
H 1.888059 -2.672944 -1.488926  
C 3.263987 2.194100 -0.302173  
H 3.755825 3.132591 -0.553118  
C 1.869748 2.124522 -0.265065  
C 1.004553 3.344633 -0.541539  
H 1.569971 4.036776 -1.178481  
H 0.806272 3.883445 0.396660  
C -0.360647 3.053321 -1.200469  
H -0.274205 2.284927 -1.979279  
H -0.707958 3.965768 -1.711140  
C -1.488226 2.699233 -0.219905  
C -2.511685 1.680418 -0.706535  
H -1.962347 0.733611 -0.823070  
H -2.811383 1.952407 -1.731189  
C -3.740464 1.485716 0.195117  
H -3.418958 1.517029 1.243384  
C -4.523236 0.179429 -0.089631  
H -5.599138 0.364877 0.035123  
C -4.162025 -1.023596 0.825336  
H -4.731339 -1.898155 0.483880  
H -4.500071 -0.800215 1.846451  
H -4.386739 -0.116832 -1.138655  
H -4.406195 2.349708 0.065204  
O -1.551641 3.220472 0.877115  
C 1.289901 0.888425 0.058891  
H 0.212919 0.797189 0.105017  
C 2.059076 -0.237013 0.342888  
C 3.468260 -0.158693 0.301764  
O 4.142687 -1.310372 0.571629  
C 5.561872 -1.264204 0.565634  
H 5.894105 -2.274917 0.820469  
H 5.947959 -0.557476 1.314852  
H 5.955910 -0.993972 -0.425318  
C 4.053418 1.069854 -0.020479  
H 5.134701 1.159421 -0.063362

Sum of electronic and zero-point Energies= -1190.333932  
Sum of electronic and thermal Energies= -1190.309890  
Sum of electronic and thermal Enthalpies= -1190.308946  
Sum of electronic and thermal Free Energies= -1190.387075

jugcathanin-2-E2 (benzene)

C -1.834332 -1.712090 0.547056  
O -2.404515 -1.781295 1.781120  
H -1.670967 -1.779417 2.420841  
C -2.639146 -1.586904 -0.597156  
C -1.994652 -1.563719 -1.842401  
H -2.600192 -1.505420 -2.745630  
C -0.602007 -1.543032 -1.954957  
H -0.110565 -1.457560 -2.920578

C 0.178217 -1.566662 -0.798002  
O 1.550545 -1.397966 -0.880833  
C -0.430929 -1.717456 0.452643  
O 0.250242 -1.741577 1.647511  
C 1.215277 -2.795846 1.810207  
H 1.566067 -2.721364 2.844017  
H 0.747938 -3.777253 1.649222  
H 2.057495 -2.670158 1.122390  
C 3.107783 2.308651 0.226009  
H 3.549037 3.261825 0.513491  
C 1.725266 2.206276 0.047173  
C 0.814660 3.399720 0.297344  
H 1.335712 4.312021 -0.021753  
H 0.643687 3.507444 1.378346  
C -0.566115 3.349034 -0.382438  
H -0.490414 3.017153 -1.425982  
H -0.976445 4.370960 -0.420175  
C -1.623040 2.524349 0.366062  
C -2.657631 1.817665 -0.500281  
H -2.102154 1.091904 -1.113221  
H -3.048885 2.547236 -1.228038  
C -3.802872 1.125164 0.254922  
H -3.403270 0.638528 1.151868  
C -4.578942 0.101507 -0.612547  
H -5.647777 0.141887 -0.360652  
C -4.133359 -1.380360 -0.462954  
H -4.661893 -1.976998 -1.219976  
H -4.460120 -1.749026 0.515559  
H -4.510833 0.393532 -1.671271  
H -4.494704 1.896268 0.619731  
O -1.630180 2.463029 1.580487  
C 1.211602 0.958802 -0.333123  
H 0.147937 0.836637 -0.492594  
C 2.031245 -0.153329 -0.503286  
C 3.423117 -0.046443 -0.307439  
O 4.146368 -1.188934 -0.482615  
C 5.551706 -1.117884 -0.293449  
H 5.929053 -2.128284 -0.476997  
H 5.809354 -0.817068 0.732797  
H 6.022070 -0.422995 -1.004520  
C 3.946603 1.200408 0.050854  
H 5.015491 1.316979 0.202347

Sum of electronic and zero-point Energies= -1190.335967  
Sum of electronic and thermal Energies= -1190.311849  
Sum of electronic and thermal Enthalpies= -1190.310905  
Sum of electronic and thermal Free Energies= -1190.389275

jugcathanin-3-TS (benzene)

C 0.387776 2.923647 -0.140771  
O 0.403980 4.260077 -0.398242  
H -0.520751 4.559000 -0.344353  
C 1.571159 2.164282 -0.230779  
C 1.413630 0.826034 0.057032  
H 2.272837 0.202941 0.045640  
C 0.230070 0.215119 0.361977  
H 0.274414 -0.838929 0.516393  
C -0.949484 0.935273 0.447712  
O -2.162074 0.308183 0.771706  
C -0.859118 2.317830 0.201950  
O -1.954882 3.165123 0.202715  
C -2.558224 3.367971 1.491116  
H -2.978263 2.432377 1.877976  
H -1.827203 3.766955 2.208535  
H -3.361294 4.096867 1.341038  
C -1.379471 -3.516411 -0.622884  
H -1.033071 -4.422929 -1.117996  
C -0.722338 -3.054546 0.532520  
C 0.675081 -3.553158 0.907235  
H 0.700343 -4.650232 0.900307  
H 0.940362 -3.234218 1.922253

C	1.788148	-3.036422	-0.084240
H	1.337166	-2.690210	-1.022744
H	2.431352	-3.882238	-0.376077
C	2.768363	-1.949446	0.421230
C	3.657930	-1.256326	-0.653455
H	3.099113	-1.207750	-1.596949
H	4.466909	-1.981108	-0.839491
C	4.303140	0.142233	-0.309992
H	4.170482	0.338025	0.761885
C	3.858123	1.389193	-1.182518
H	4.780324	1.865066	-1.540959
C	2.993877	2.563507	-0.592961
H	2.989433	3.368282	-1.340667
H	3.505238	2.984478	0.287824
H	3.349129	1.021789	-2.085367
H	5.385287	0.031731	-0.447804
O	2.883971	-1.694804	1.602593
C	-1.254537	-1.910197	1.142278
H	-0.796673	-1.525091	2.050084
C	-2.151688	-1.067663	0.461225
C	-2.806886	-1.537628	-0.688912
O	-3.709037	-0.850196	-1.436109
C	-4.485486	0.193675	-0.841020
H	-5.338989	0.338405	-1.511781
H	-3.918371	1.126136	-0.758019
H	-4.850504	-0.101743	0.151785
C	-2.448024	-2.811625	-1.171278
H	-2.965182	-3.176708	-2.055614

Sum of electronic and zero-point Energies= -1190.265876  
Sum of electronic and thermal Energies= -1190.242514  
Sum of electronic and thermal Enthalpies= -1190.241570  
Sum of electronic and thermal Free Energies= -1190.316998

#### jucathanan-3-E1 (benzene)

C	1.686749	1.904154	-0.449969
O	2.254743	2.217235	-1.647308
H	1.519116	2.350517	-2.270533
C	2.503940	1.595511	0.649968
C	1.870285	1.327830	1.870466
H	2.483931	1.118939	2.744457
C	0.479347	1.258723	1.984051
H	0.000309	0.986935	2.920886
C	-0.307847	1.453229	0.850895
O	-1.675846	1.215712	0.898483
C	0.284750	1.832387	-0.360684
O	-0.392642	2.036337	-1.539688
C	-1.462605	2.999891	-1.525344
H	-2.344796	2.603943	-1.013560
H	-1.136806	3.932307	-1.044490
H	-1.700798	3.193358	-2.575945
C	-2.962988	-2.448102	-0.640880
H	-3.316188	-3.383106	-1.072231
C	-1.654108	-2.355690	-0.152626
C	-0.698506	-3.535339	-0.217645
H	-1.197321	-4.363351	-0.735736
H	-0.463480	-3.892422	0.794742
C	0.641330	-3.232366	-0.927402
H	0.486958	-2.615275	-1.821310
H	1.080562	-4.179504	-1.280697
C	1.715078	-2.608965	-0.026479
C	2.639107	-1.592571	-0.682000
H	1.993437	-0.740540	-0.944802
H	2.971155	-1.993955	-1.652376
C	3.834124	-1.130762	0.166983
H	3.514397	-1.054773	1.213349
C	4.450783	0.208991	-0.308628
H	5.545792	0.157741	-0.234894
C	4.002615	1.463482	0.491778
H	4.416586	2.351982	-0.004665
H	4.451741	1.421262	1.493320

H	4.225541	0.365868	-1.371502
H	4.598945	-1.918815	0.148433
O	1.807953	-2.918724	1.146900
C	-1.235036	-1.130899	0.388077
H	-0.234810	-1.034748	0.795639
C	-2.078901	-0.020626	0.412681
C	-3.399121	-0.126141	-0.062436
O	-4.239531	0.962165	-0.099839
C	-4.728954	1.395254	1.173822
H	-5.398102	2.238392	0.972996
H	-3.913734	1.725106	1.829514
H	-5.295494	0.592306	1.668065
C	-3.826825	-1.349485	-0.579120
H	-4.843653	-1.415008	-0.960081

Sum of electronic and zero-point Energies= -1190.335842  
Sum of electronic and thermal Energies= -1190.311559  
Sum of electronic and thermal Enthalpies= -1190.310614  
Sum of electronic and thermal Free Energies= -1190.389136

#### jucathanan-3-E2 (benzene)

C	2.021782	1.882993	0.284056
O	2.840860	2.235651	1.311127
H	2.259561	2.574367	2.014702
C	2.562688	1.382214	-0.909558
C	1.667469	1.095894	-1.951105
H	2.063314	0.751578	-2.905356
C	0.287325	1.187841	-1.782924
H	-0.398908	0.913755	-2.579929
C	-0.234541	1.586137	-0.548297
O	-1.605583	1.542465	-0.329385
C	0.627038	1.988709	0.475130
O	0.231340	2.514208	1.687102
C	-0.456037	1.638790	2.597527
H	-1.463963	1.405690	2.240568
H	0.108515	0.710379	2.755568
H	-0.524728	2.188471	3.541737
C	-3.282827	-2.281009	-0.118862
H	-3.737152	-3.269927	-0.090899
C	-1.944718	-2.116230	0.260596
C	-1.096812	-3.288958	0.726048
H	-1.677489	-4.211637	0.606027
H	-0.876712	-3.193099	1.798592
C	0.250651	-3.447290	-0.013145
H	0.129263	-3.307463	-1.094706
H	0.611802	-4.479989	0.122017
C	1.384102	-2.556947	0.513106
C	2.389872	-2.074964	-0.521447
H	1.813529	-1.432137	-1.204381
H	2.692446	-2.934602	-1.140521
C	3.615489	-1.321913	0.021253
H	3.305197	-0.689690	0.861418
C	4.335201	-0.470889	-1.058973
H	5.422967	-0.591340	-0.963738
C	4.038293	1.054590	-1.013045
H	4.467823	1.517779	-1.913265
H	4.560092	1.492674	-0.155851
H	4.081300	-0.858308	-2.056542
H	4.315962	-2.053115	0.446103
O	1.455799	-2.256399	1.690956
C	-1.401811	-0.825748	0.198542
H	-0.371942	-0.661558	0.493527
C	-2.149201	0.266935	-0.244657
C	-3.500632	0.098997	-0.601699
O	-4.267120	1.125755	-1.088653
C	-4.560644	2.180042	-0.166907
H	-5.225842	2.869135	-0.697444
H	-3.654449	2.714781	0.141245
H	-5.079302	1.790163	0.721839
C	-4.048587	-1.184370	-0.526962
H	-5.088263	-1.308294	-0.821950

Sum of electronic and zero-point Energies= -1190.330714  
Sum of electronic and thermal Energies= -1190.306356  
Sum of electronic and thermal Enthalpies= -1190.305412  
Sum of electronic and thermal Free Energies= -1190.384548

jugcathanin-4-TS (benzene)

C	1.181998	2.771454	-0.196591
O	1.579790	4.045828	-0.461193
H	0.797552	4.607705	-0.318389
C	2.093634	1.703801	-0.322805
C	1.560036	0.468644	-0.025067
H	2.192067	-0.386994	-0.023393
C	0.252082	0.234234	0.285534
H	-0.012746	-0.790056	0.396143
C	-0.660699	1.262123	0.451444
O	-1.976853	0.995441	0.861502
C	-0.172265	2.562754	0.214545
O	-0.937873	3.711469	0.277153
C	-1.556575	3.982344	1.543834
H	-2.317284	3.229429	1.776500
H	-0.807622	4.012340	2.348133
H	-2.029268	4.964977	1.446195
C	-2.306210	-2.979405	-0.236195
H	-2.244899	-3.968577	-0.688691
C	-1.428638	-2.629057	0.798229
C	-0.133729	-3.403154	1.065323
H	-0.336192	-4.480404	1.115886
H	0.289156	-3.113142	2.034417
C	0.974136	-3.168093	-0.038996
H	0.582772	-2.580711	-0.881852
H	1.251744	-4.133633	-0.489022
C	2.310124	-2.525204	0.411318
C	3.434889	-2.317326	-0.654591
H	3.275222	-3.054987	-1.453291
H	4.354939	-2.604921	-0.128607
C	3.717731	-0.944186	-1.388377
H	4.492898	-1.196881	-2.124274
C	4.232622	0.285313	-0.545592
H	4.183393	0.046884	0.525210
C	3.549471	1.679723	-0.769136
H	4.140367	2.434558	-0.230901
H	3.619684	1.958292	-1.832838
H	5.299591	0.419467	-0.766009
H	2.840050	-0.666013	-1.983232
O	2.528623	-2.279814	1.581706
C	-1.600236	-1.350100	1.362421
H	-0.956682	-1.041007	2.182024
C	-2.322349	-0.357175	0.692072
C	-3.195700	-0.713862	-0.353453
O	-3.898924	0.291748	-0.933213
C	-4.731981	-0.025204	-2.040250
H	-5.534169	-0.722430	-1.757867
H	-4.154076	-0.451152	-2.873123
H	-5.176350	0.922503	-2.357805
C	-3.232076	-2.061915	-0.750549
H	-3.905837	-2.376899	-1.541543

Sum of electronic and zero-point Energies= -1190.259129  
Sum of electronic and thermal Energies= -1190.235980  
Sum of electronic and thermal Enthalpies= -1190.235036  
Sum of electronic and thermal Free Energies= -1190.310043

jugcathanin-4-E1 (benzene)

C	-1.494257	2.089449	0.425433
O	-1.977589	2.393778	1.663326
H	-1.199958	2.470543	2.243459
C	-2.375734	1.822663	-0.632979
C	-1.817420	1.579807	-1.896150
H	-2.484534	1.406546	-2.738885
C	-0.440266	1.452768	-2.083593
H	-0.021955	1.175453	-3.047526

C	0.408079	1.563679	-0.982034
O	1.740402	1.190911	-1.081322
C	-0.103497	1.958808	0.258565
O	0.646434	2.094515	1.405150
C	1.751473	3.013729	1.345358
H	2.552020	2.624970	0.708776
H	1.420550	3.993431	0.973989
H	2.110498	3.114799	2.374520
C	2.649317	-2.611675	0.376291
H	2.917999	-3.589597	0.772756
C	1.342403	-2.367807	-0.049576
C	0.271492	-3.443440	0.015905
H	0.721799	-4.353349	0.431083
H	-0.063127	-3.693488	-1.000416
C	-0.982974	-3.091601	0.847702
H	-0.743847	-2.405454	1.674061
H	-1.374042	-3.997149	1.339481
C	-2.162865	-2.512069	0.066614
C	-3.394171	-2.120914	0.884825
H	-3.320727	-2.552951	1.890879
H	-4.278382	-2.555691	0.398501
C	-3.556086	-0.580956	0.995675
H	-4.192598	-0.360197	1.863522
C	-4.153519	0.083400	-0.260165
H	-3.765165	-0.420492	-1.153772
C	-3.853226	1.602247	-0.386674
H	-4.436426	2.003394	-1.226853
H	-4.181122	2.131092	0.516048
H	-5.243259	-0.069846	-0.262560
H	-2.577638	-0.143694	1.227821
O	-2.135469	-2.376130	-1.143762
C	1.044481	-1.090511	-0.553701
H	0.043572	-0.883221	-0.916274
C	2.007868	-0.087038	-0.607400
C	3.330249	-0.344083	-0.184957
O	4.206006	0.697785	-0.277213
C	5.547248	0.472941	0.130628
H	6.025451	-0.316693	-0.467122
H	5.609784	0.209649	1.196978
H	6.072789	1.417722	-0.037280
C	3.636025	-1.617597	0.301583
H	4.642315	-1.843423	0.641288

Sum of electronic and zero-point Energies= -1190.335120  
Sum of electronic and thermal Energies= -1190.311087  
Sum of electronic and thermal Enthalpies= -1190.310143  
Sum of electronic and thermal Free Energies= -1190.387991

jugcathanin-4-E2 (benzene)

C	-1.812771	2.002008	-0.314112
O	-2.585011	2.268045	-1.401589
H	-1.972513	2.409187	-2.144443
C	-2.417031	1.614031	0.893296
C	-1.580702	1.397660	1.996920
H	-2.031396	1.142901	2.954578
C	-0.189342	1.412295	1.880110
H	0.453285	1.157847	2.718875
C	0.388127	1.657994	0.634697
O	1.745028	1.441191	0.444912
C	-0.412852	2.031157	-0.449268
O	0.061396	2.276115	-1.717432
C	1.021673	3.337505	-1.842465
H	0.616598	4.277685	-1.442577
H	1.953795	3.086406	-1.326063
H	1.210199	3.446194	-2.915023
C	2.894308	-2.494171	-0.329483
H	3.228646	-3.514928	-0.508362
C	1.547966	-2.163528	-0.491260
C	0.528280	-3.194238	-0.946596
H	1.022750	-4.172719	-0.983425
H	0.211591	-2.964950	-1.973906

C	-0.747597	-3.318735	-0.083969
H	-0.552852	-3.072946	0.970998
H	-1.089400	-4.366208	-0.068687
C	-1.952784	-2.502409	-0.053009
C	-3.221126	-2.607598	0.295717
H	-3.133566	-3.456056	0.986294
H	-4.063507	-2.812583	-0.379424
C	-3.499071	-1.312774	1.105087
H	-4.183899	-1.562642	1.927956
C	-4.091256	-0.155961	0.277365
H	-3.641831	-0.149309	-0.721935
C	-3.883494	1.246085	0.915422
H	-4.477227	1.978021	0.354221
H	-4.255799	1.249448	1.949608
H	-5.168065	-0.330186	0.134360
H	-2.561959	-0.993794	1.580118
O	-1.916227	-1.811667	-1.555505
C	1.165052	-0.834656	-0.243235
H	0.129510	-0.547989	-0.384362
C	2.087152	0.125856	0.163016
C	3.451525	-0.211167	0.306213
O	4.283265	0.796376	0.691659
C	5.660401	0.492542	0.849503
H	6.111894	0.147567	-0.092519
H	5.822944	-0.266871	1.628750
H	6.139437	1.427511	1.155418
C	3.837892	-1.530213	0.055254
H	4.877670	-1.822176	0.167976

Sum of electronic and zero-point Energies= -1190.334566  
Sum of electronic and thermal Energies= -1190.310489  
Sum of electronic and thermal Enthalpies= -1190.309544  
Sum of electronic and thermal Free Energies= -1190.387877

#### jugcathanin-5-TS (benzene)

C	1.476519	2.658954	-0.220028
O	1.988623	3.889019	-0.495591
H	1.255099	4.518587	-0.378415
C	2.288178	1.510634	-0.304019
C	1.639900	0.336132	0.000484
H	2.219682	-0.551304	0.061267
C	0.304971	0.212681	0.260358
H	-0.059016	-0.784283	0.361173
C	-0.508264	1.325611	0.404379
O	-1.845681	1.197875	0.806328
C	0.102209	2.574256	0.167933
O	-0.562319	3.785973	0.209211
C	-1.134966	4.138374	1.477608
H	-0.373477	4.122797	2.270519
H	-1.523908	5.155351	1.362938
H	-1.953304	3.458884	1.739384
C	-2.642779	-2.758572	-0.121361
H	-2.715204	-3.766731	-0.528053
C	-1.692240	-2.471008	0.867739
C	-0.497989	-3.393723	1.130447
H	-0.840067	-4.427111	1.267784
H	0.019097	-3.107928	2.054498
C	0.549887	-3.384029	-0.055386
H	0.099532	-2.959424	-0.960431
H	0.787756	-4.427543	-0.316975
C	1.938720	-2.729704	0.181736
C	2.688409	-2.243022	-1.085641
H	1.968998	-1.709791	-1.719389
H	2.919668	-3.163777	-1.649706
C	4.047227	-1.458017	-0.984861
H	4.768090	-2.147868	-0.524858
C	4.327993	-0.079740	-0.261044
H	4.145298	-0.200465	0.814612
C	3.743278	1.311733	-0.704543
H	3.852946	1.432139	-1.794506
H	4.383848	2.086764	-0.260607

H	5.418096	0.024633	-0.358102
H	4.373988	-1.348676	-2.029611
O	2.425867	-2.661423	1.292528
C	-1.693346	-1.159478	1.377734
H	-0.996753	-0.896498	2.169092
C	-2.324769	-0.117236	0.689927
C	-3.269969	-0.412109	-0.311128
O	-3.878048	0.643277	-0.909452
C	-4.785200	0.379275	-1.971345
H	-5.650759	-0.206570	-1.629278
H	-5.129596	1.358216	-2.317094
H	-4.293720	-0.145872	-2.803097
C	-3.473748	-1.761585	-0.647885
H	-4.207955	-2.027860	-1.401946

Sum of electronic and zero-point Energies= -1190.258218  
Sum of electronic and thermal Energies= -1190.234966  
Sum of electronic and thermal Enthalpies= -1190.234022  
Sum of electronic and thermal Free Energies= -1190.309636

#### jugcathanin-5-E1 (benzene)

C	-1.566628	1.849728	0.495800
O	-2.077711	1.989579	1.753494
H	-1.310469	2.068561	2.347397
C	-2.421091	1.644855	-0.596603
C	-1.833314	1.628750	-1.866945
H	-2.479777	1.431261	-2.734856
C	-0.449476	1.511027	-2.042351
H	-0.005440	1.344050	-3.020152
C	0.380001	1.575782	-0.923093
O	1.731735	1.282411	-1.035185
C	-0.168898	1.820748	0.340151
O	0.558089	1.890694	1.507134
C	1.615017	2.865782	1.549514
H	1.237306	3.858255	1.267634
H	1.959654	2.886257	2.588138
H	2.440097	2.581305	0.889376
C	2.780186	-2.540445	0.272142
H	3.079762	-3.518978	0.644145
C	1.454980	-2.310924	-0.100498
C	0.378861	-3.374706	0.026148
H	0.831328	-4.289069	0.429187
H	-0.025755	-3.630608	-0.962937
C	-0.809637	-2.964093	0.926144
H	-0.472729	-2.373853	1.788434
H	-1.274190	-3.869583	1.351541
C	-1.963100	-2.240008	0.217700
C	-2.858419	-1.395734	1.115902
H	-2.281101	-0.507082	1.407742
H	-2.991064	-1.952845	2.056947
C	-4.245259	-1.008400	0.568959
H	-4.767200	-1.934920	0.288538
C	-4.360121	-0.040854	-0.628563
H	-3.832372	-0.463980	-1.490642
C	-3.910435	1.432821	-0.418074
H	-4.231198	1.786561	0.568933
H	-4.441412	2.048586	-1.157898
H	-5.426105	-0.017509	-0.899445
H	-4.814625	-0.585647	1.410298
O	-2.162201	-2.377046	-0.975628
C	1.121002	-1.032014	-0.572875
H	0.106001	-0.834761	-0.897725
C	2.056646	-0.004421	-0.626408
C	3.397328	-0.243715	-0.255462
O	4.245251	0.821037	-0.341179
C	5.604385	0.614858	0.014376
H	6.080085	-0.142012	-0.626197
H	6.102114	1.577256	-0.137286
H	5.708676	0.316511	1.068119
C	3.744711	-1.524892	0.182464
H	4.766675	-1.738162	0.481078



Sum of electronic and zero-point Energies= -1190.334779  
Sum of electronic and thermal Energies= -1190.310815  
Sum of electronic and thermal Enthalpies= -1190.309871  
Sum of electronic and thermal Free Energies= -1190.387383

jugcathanin-5-E2 (benzene)

C	-1.720986	-1.937898	0.361799
O	-2.375786	-2.266204	1.507425
H	-1.689756	-2.444265	2.174191
C	-2.449931	-1.512923	-0.762027
C	-1.733594	-1.260734	-1.939673
H	-2.282662	-0.984185	-2.838355
C	-0.336566	-1.274156	-1.970356
H	0.214426	-0.989729	-2.863028
C	0.368634	-1.559204	-0.801319
O	1.736242	-1.333681	-0.739798
C	-0.315143	-1.964901	0.349561
O	0.285449	-2.255907	1.551723
C	1.286131	-3.287818	1.537485
H	2.168118	-2.972973	0.971003
H	1.557065	-3.454777	2.584511
H	0.880974	-4.215165	1.109204
C	2.914207	2.479537	0.484786
H	3.257626	3.469028	0.782503
C	1.548403	2.195441	0.449567
C	0.499402	3.225230	0.835634
H	0.971987	4.215056	0.856897
H	0.138555	3.031474	1.856317
C	-0.735698	3.273627	-0.090176
H	-0.459417	3.096440	-1.137676
H	-1.165840	4.288588	-0.065146
C	-1.901983	2.356648	0.307210
C	-2.830530	1.947736	-0.830076
H	-2.260834	1.248243	-1.458799
H	-2.976191	2.835950	-1.465203
C	-4.205811	1.371551	-0.443306
H	-4.692257	2.090662	0.231405
C	-4.290348	-0.016291	0.227798
H	-3.686530	-0.024376	1.140407
C	-3.936057	-1.257958	-0.638583
H	-4.375071	-1.151616	-1.640882
H	-4.416436	-2.130964	-0.176311
H	-5.334485	-0.139201	0.551207
H	-4.820167	1.355819	-1.356770
O	-2.082068	2.021915	1.462967
C	1.160169	0.907745	0.049019
H	0.107912	0.654615	0.025911
C	2.089859	-0.062936	-0.309630
C	3.471220	0.225101	-0.255416
O	4.310869	-0.788667	-0.607192
C	5.706717	-0.534258	-0.567901
H	6.044491	-0.275225	0.446501
H	6.189087	-1.465455	-0.879872
H	5.993024	0.269833	-1.261882
C	3.865011	1.505421	0.143559
H	4.920102	1.758810	0.185134

Sum of electronic and zero-point Energies= -1190.334091  
Sum of electronic and thermal Energies= -1190.310064  
Sum of electronic and thermal Enthalpies= -1190.309120  
Sum of electronic and thermal Free Energies= -1190.387033

jugcathanin-6-TS (benzene)

C	-0.983788	2.863266	-0.105042
O	-1.271672	4.183935	0.054829
H	-0.467642	4.668417	-0.203705
C	-1.976768	1.888405	0.120944
C	-1.549674	0.592611	-0.074203
H	-2.249389	-0.204916	0.004495
C	-0.273547	0.226186	-0.389981
H	-0.095341	-0.822024	-0.424891

C	0.707739	1.159863	-0.676825
O	1.978373	0.756343	-1.117581
C	0.337882	2.510443	-0.522249
O	1.172577	3.580883	-0.780297
C	2.373859	3.628953	0.007620
H	3.000445	2.750194	-0.177044
H	2.902581	4.535792	-0.303146
H	2.134197	3.691405	1.079117
C	2.051922	-3.113018	0.340446
H	1.934518	-4.049395	0.884784
C	1.165184	-2.791245	-0.695528
C	-0.192939	-3.482995	-0.850808
H	-0.074068	-4.572697	-0.802464
H	-0.625740	-3.253279	-1.831575
C	-1.241545	-3.058610	0.254959
H	-1.575379	-3.952318	0.804070
H	-0.778580	-2.425695	1.025600
C	-2.539632	-2.358093	-0.220584
C	-3.612188	-1.966848	0.847701
H	-3.483792	-2.638856	1.707695
H	-4.566826	-2.229200	0.372675
C	-3.768723	-0.514540	1.456364
H	-4.539306	-0.637877	2.229233
C	-4.212533	0.670346	0.514869
H	-4.212999	0.333252	-0.530201
C	-3.418293	2.020966	0.593901
H	-3.962143	2.767553	-0.002300
H	-3.440328	2.400889	1.627938
H	-5.259207	0.907670	0.745379
H	-2.855813	-0.252885	2.003752
O	-2.775406	-2.204149	-1.403080
C	1.410915	-1.586886	-1.382733
H	0.763700	-1.304289	-2.209011
C	2.229734	-0.596522	-0.830334
C	3.110061	-0.922469	0.218579
O	3.905331	0.077463	0.683650
C	4.763126	-0.205857	1.781384
H	4.194143	-0.510866	2.671532
H	5.292277	0.727572	1.993971
H	5.496399	-0.985945	1.531283
C	3.061836	-2.226931	0.739338
H	3.738914	-2.520448	1.535746

Sum of electronic and zero-point Energies= -1190.259703  
Sum of electronic and thermal Energies= -1190.236631  
Sum of electronic and thermal Enthalpies= -1190.235687  
Sum of electronic and thermal Free Energies= -1190.310335

jugcathanin-6-E1 (benzene)

C	-1.812533	2.001831	-0.314561
O	-2.584491	2.267500	-1.402323
H	-1.971814	2.408248	-2.145099
C	-2.417115	1.614361	0.892850
C	-1.581068	1.398406	1.996776
H	-2.032024	1.144087	2.954424
C	-0.189678	1.412947	1.880308
H	0.452746	1.158762	2.719306
C	0.388104	1.658055	0.634920
O	1.745047	1.441084	0.445584
C	-0.412585	2.030853	-0.449379
O	0.062016	2.275241	-1.717529
C	1.022441	3.336483	-1.842706
H	1.954282	3.085634	-1.325674
H	1.211535	3.444519	-2.915229
H	0.617228	4.276937	-1.443592
C	2.894250	-2.494125	-0.329697
H	3.228590	-3.514840	-0.508802
C	1.547847	-2.163520	-0.491026
C	0.528103	-3.194250	-0.946194
H	1.022527	-4.172762	-0.982850
H	0.211448	-2.965128	-1.973554

C	-0.747804	-3.318610	-0.083605
H	-1.089721	-4.366060	-0.068466
H	-0.553056	-3.072973	0.971392
C	-1.952924	-2.502196	-0.552651
C	-3.221275	-2.607315	0.296062
H	-3.133624	-3.455600	0.986844
H	-4.063590	-2.812604	-0.379073
C	-3.499607	-1.312394	1.105134
H	-4.184840	-1.562248	1.927666
C	-4.091439	-0.155646	0.277022
H	-3.641782	-0.149296	-0.722167
C	-3.883607	1.246513	0.914799
H	-4.477188	1.978377	0.353334
H	-4.256091	1.250159	1.948918
H	-5.168244	-0.329737	0.133829
H	-2.562740	-0.993373	1.580611
O	-1.916301	-1.811481	-1.555162
C	1.164933	-0.834692	-0.242726
H	0.129323	-0.548091	-0.383475
C	2.087115	0.125811	0.163334
C	3.451556	-0.211163	0.306050
O	4.283389	0.796408	0.691223
C	5.660366	0.492282	0.849907
H	5.822236	-0.267345	1.629082
H	6.139371	1.427096	1.156341
H	6.112433	0.147445	-0.091893
C	3.837913	-1.530154	0.054824
H	4.877752	-1.822065	0.167133

Sum of electronic and zero-point Energies= -1190.334564

Sum of electronic and thermal Energies= -1190.310488

Sum of electronic and thermal Enthalpies= -1190.309544

Sum of electronic and thermal Free Energies= -1190.387867

#### jugcathanin-6-E2 (benzene)

C	-1.771996	-2.154076	-0.264589
O	-2.418394	-2.582245	-1.386185
H	-1.724531	-2.843755	-2.015651
C	-2.505326	-1.645821	0.813760
C	-1.796454	-1.279879	1.967989
H	-2.347296	-0.920997	2.835345
C	-0.405790	-1.273175	1.991849
H	0.142558	-0.906239	2.855536
C	0.315034	-1.637637	0.850555
O	1.682810	-1.396356	0.806049
C	-0.357418	-2.155540	-0.263337
O	0.180824	-2.682742	-1.412068
C	1.416300	-2.195406	-1.951965
H	2.265568	-2.472189	-1.321269
H	1.509787	-2.675665	-2.931163
H	1.387255	-1.106461	-2.082332
C	2.911074	2.443182	-0.277272
H	3.269053	3.426750	-0.577375
C	1.550725	2.237586	-0.043533
C	0.544755	3.369959	-0.171283
H	1.047455	4.224711	-0.640192
H	0.238337	3.699950	0.831633
C	-0.741240	3.052210	-0.966246
H	-1.069109	3.945305	-1.522248
H	-0.566559	2.290177	-1.740753
C	-1.950650	2.625039	-0.131824
C	-3.223461	2.268501	-0.902132
H	-3.130857	2.606415	-1.942174
H	-4.058059	2.819468	-0.446579
C	-3.526562	0.745902	-0.881403
H	-4.214390	0.519892	-1.707813
C	-4.128524	0.235979	0.442488
H	-3.652092	0.761127	1.279205
C	-3.970572	-1.292638	0.669733
H	-4.516650	-1.565796	1.583288
H	-4.424570	-1.850599	-0.157077

H	-5.196945	0.497230	0.476246
H	-2.600701	0.202695	-1.108778
O	-1.911457	2.584339	1.084704
C	1.136946	0.950024	0.339112
H	0.089293	0.773561	0.550513
C	2.044264	-0.098886	0.474704
C	3.421039	0.119603	0.240424
O	4.232443	-0.966233	0.380998
C	5.625819	-0.782139	0.180068
H	5.850099	-0.458893	-0.847367
H	6.084431	-1.759666	0.356413
H	6.044768	-0.053564	0.889451
C	3.837810	1.400227	-0.130728
H	4.888703	1.594346	-0.323066

Sum of electronic and zero-point Energies= -1190.330054

Sum of electronic and thermal Energies= -1190.306433

Sum of electronic and thermal Enthalpies= -1190.305489

Sum of electronic and thermal Free Energies= -1190.381746

#### jugcathanin-7-TS (benzene)

C	-0.323670	-2.977038	-0.153386
O	-0.306870	-4.311386	0.115905
H	0.594127	-4.616240	-0.092559
C	-1.500217	-2.228090	0.048687
C	-1.381667	-0.892114	-0.271376
H	-2.213979	-0.240890	-0.142521
C	-0.239702	-0.298515	-0.715708
H	-0.297877	0.753787	-0.846094
C	0.941421	-0.994076	-0.897041
O	2.096178	-0.302405	-1.312091
C	0.890732	-2.373081	-0.616459
O	1.946762	-3.249681	-0.769715
C	3.127207	-2.940387	-0.008583
H	2.899218	-2.911536	1.066555
H	3.835682	-3.749778	-0.212315
H	3.553134	-1.980947	-0.316637
C	1.138760	3.300308	0.452378
H	0.733756	4.108458	1.058313
C	0.502860	2.947406	-0.742889
C	-0.890749	3.482323	-1.085447
H	-0.895457	3.887862	-2.107978
H	-1.107619	4.326434	-0.419213
C	-2.122972	2.501440	-1.031977
H	-1.996785	1.666430	-1.736703
H	-2.982874	3.059470	-1.434390
C	-2.579960	1.927463	0.329699
C	-3.971912	1.206437	0.432110
H	-4.653016	1.742342	-0.244892
H	-4.297019	1.428677	1.456505
C	-4.248443	-0.331548	0.179582
H	-5.343031	-0.405709	0.231515
C	-3.648829	-1.390446	1.185345
H	-3.002950	-0.879542	1.911650
C	-2.855424	-2.622131	0.619911
H	-3.464369	-3.139315	-0.139159
H	-2.730976	-3.345180	1.437557
H	-4.485131	-1.798192	1.767923
H	-4.001494	-0.589743	-0.857556
O	-1.942117	2.139908	1.341690
C	1.094083	1.906726	-1.487769
H	0.644953	1.589558	-2.427097
C	2.029505	1.045872	-0.900129
C	2.666594	1.416633	0.299239
O	3.591298	0.550785	0.793832
C	4.178302	0.849398	2.054105
H	3.420501	0.911055	2.848091
H	4.751720	1.786934	2.021705
H	4.860038	0.021156	2.268268
C	2.256126	2.602644	0.926387
H	2.725184	2.921806	1.851981

Sum of electronic and zero-point Energies= -1190.255579  
Sum of electronic and thermal Energies= -1190.232475  
Sum of electronic and thermal Enthalpies= -1190.231531  
Sum of electronic and thermal Free Energies= -1190.306376

jugcathanin-7-E1 (benzene)

C	-1.494928	-2.089347	-0.425152
O	-1.978673	-2.393711	-1.662890
H	-1.201211	-2.470912	-2.243174
C	-2.376043	-1.822114	0.633418
C	-1.817366	-1.578910	1.896368
H	-2.484260	-1.405231	2.739190
C	-0.440139	-1.452152	2.083420
H	-0.021483	-1.174485	3.047099
C	0.407883	-1.563673	0.981662
O	1.740338	-1.191276	1.080493
C	-0.104077	-1.959043	-0.258690
O	0.645530	-2.095388	-1.405394
C	1.750537	-3.014652	-1.345513
H	1.419815	-3.993932	-0.972873
H	2.108758	-3.116783	-2.374842
H	2.551586	-2.625323	-0.709914
C	2.649858	2.611454	-0.376364
H	2.918720	3.589425	-0.772584
C	1.342822	2.367631	0.049187
C	0.272056	3.443405	-0.016265
H	0.722426	4.353196	-0.431649
H	-0.062339	3.693640	1.000086
C	-0.982597	3.091768	-0.847840
H	-0.743630	2.405872	-1.674458
H	-1.373728	3.997470	-1.339332
C	-2.162373	2.512183	-0.066701
C	-3.393914	2.121292	-0.884694
H	-3.320665	2.553341	-1.890756
H	-4.277942	2.556196	-0.398149
C	-3.556078	0.581332	-0.995412
H	-4.192592	0.360538	-1.863241
C	-4.153587	-0.082675	0.260591
H	-3.765031	0.421295	1.154064
C	-3.853564	-1.601561	0.387394
H	-4.181695	-2.130566	-0.515141
H	-4.436658	-2.002397	1.227792
H	-5.243291	0.070839	0.263033
H	-2.577704	0.143858	-1.227456
O	-2.134744	2.375951	1.143641
C	1.044679	1.090273	0.552989
H	0.043689	0.882973	0.915315
C	2.008007	0.086731	0.606827
C	3.330490	0.343696	0.184685
O	4.206129	-0.698256	0.276846
C	5.547858	-0.472965	-0.129333
H	6.025029	0.316731	0.469138
H	5.611598	-0.209491	-1.195556
H	6.073400	-1.417639	0.039078
C	3.636438	1.617290	-0.301598
H	4.642809	1.843060	-0.641116

Sum of electronic and zero-point Energies= -1190.335119  
Sum of electronic and thermal Energies= -1190.311086  
Sum of electronic and thermal Enthalpies= -1190.310142  
Sum of electronic and thermal Free Energies= -1190.387988

jugcathanin-7-E2 (benzene)

C	-1.812917	-2.001733	0.314351
O	-2.585149	-2.267385	1.401914
H	-1.972647	-2.408056	2.144858
C	-2.417201	-1.614078	-0.893176
C	-1.580885	-1.398146	-1.996877
H	-2.031565	-1.143651	-2.954611
C	-0.189506	-1.412842	-1.880105
H	0.453096	-1.158707	-2.718985

C	0.387983	-1.658093	-0.634620
O	1.744910	-1.441342	-0.444997
C	-0.413022	-2.030855	0.449469
O	0.061369	-2.275281	1.717712
C	1.021102	-3.337122	1.843002
H	1.953183	-3.086828	1.326108
H	1.210026	-3.445322	2.915547
H	0.615389	-4.277331	1.443811
C	2.894522	2.493915	0.329580
H	3.228935	3.514646	0.508459
C	1.548190	2.163327	0.491510
C	0.528547	3.194056	0.946907
H	1.023106	4.172477	0.984071
H	0.211612	2.964543	1.974084
C	-0.747148	3.318820	0.084027
H	-0.552197	3.073239	-0.970945
H	-1.088890	4.366313	0.068913
C	-1.952461	2.502457	0.552659
C	-3.220600	2.607761	-0.296351
H	-3.132586	3.455942	-0.987216
H	-4.062997	2.813398	0.378587
C	-3.499001	1.312857	-1.105380
H	-4.183950	1.562795	-1.928130
C	-4.091285	0.156198	-0.277496
H	-3.641881	0.149653	0.721807
C	-3.883613	-1.245941	-0.915388
H	-4.255872	-1.249387	-1.949588
H	-4.477468	-1.977748	-0.354138
H	-5.168090	0.330482	-0.134566
H	-2.562047	0.993664	-1.580574
O	-1.916170	1.811604	1.555105
C	1.165159	0.834473	0.243490
H	0.129597	0.547932	0.384730
C	2.087142	-0.126068	-0.162931
C	3.451518	0.210903	-0.306240
O	4.283180	-0.796673	-0.691803
C	5.660215	-0.492821	-0.850107
H	6.112086	-0.147901	0.091765
H	5.822520	0.266632	-1.629377
H	6.139201	-1.427757	-1.156239
C	3.838013	1.529902	-0.055281
H	4.877805	1.821779	-0.168093

Sum of electronic and zero-point Energies= -1190.334565  
Sum of electronic and thermal Energies= -1190.310489  
Sum of electronic and thermal Enthalpies= -1190.309545  
Sum of electronic and thermal Free Energies= -1190.387872

jugcathanin-8-TS (benzene)

C	-0.814784	2.893504	0.176885
O	-0.997738	4.236247	0.049103
H	-0.143722	4.648521	0.269203
C	-1.893261	2.004785	0.001421
C	-1.567378	0.676666	0.168515
H	-2.341811	-0.045727	0.094142
C	-0.319560	0.195342	0.447700
H	-0.235072	-0.865275	0.507356
C	0.757597	1.045737	0.634815
O	2.031825	0.549106	0.955693
C	0.497546	2.421018	0.485625
O	1.468838	3.395412	0.634487
C	2.409464	3.451223	-0.451912
H	3.159966	4.197060	-0.170487
H	2.890074	2.478835	-0.606082
H	1.914259	3.760955	-1.383743
C	1.842573	-3.245342	-0.698602
H	1.649776	-4.149643	-1.274418
C	1.048707	-2.946898	0.421218
C	-0.291683	-3.645110	0.663127
H	-0.642296	-3.464991	1.686272
H	-0.176664	-4.730242	0.549996

C	-1.413559	-3.166864	-0.337661
H	-1.922723	-4.049638	-0.756422
H	-0.968708	-2.662641	-1.204898
C	-2.551586	-2.275943	0.219470
C	-3.483997	-1.595852	-0.826160
H	-4.176749	-2.397371	-1.129567
H	-2.899425	-1.370941	-1.727503
C	-4.329160	-0.341340	-0.376379
H	-5.380076	-0.582951	-0.575051
C	-4.036558	1.040097	-1.097634
H	-3.463910	0.841905	-2.015312
C	-3.351100	2.248503	-0.359460
H	-3.444651	3.123062	-1.017409
H	-3.929347	2.498184	0.544737
H	-5.006918	1.425840	-1.436807
H	-4.260926	-0.242750	0.714707
O	-2.744673	-2.162218	1.412567
C	1.374158	-1.787965	1.146097
H	0.807574	-1.539455	2.039467
C	2.192117	-0.796331	0.583328
C	2.997278	-1.110480	-0.522444
O	3.836108	-0.195835	-1.103582
C	4.884898	0.291529	-0.257697
H	4.488973	0.828465	0.612816
H	5.476896	0.977352	-0.872242
H	5.525414	-0.535735	0.081064
C	2.855181	-2.374941	-1.111755
H	3.483823	-2.612556	-1.966951

Sum of electronic and zero-point Energies= -1190.264450  
Sum of electronic and thermal Energies= -1190.240973  
Sum of electronic and thermal Enthalpies= -1190.240028  
Sum of electronic and thermal Free Energies= -1190.315993

#### jugcathanin-8-E1 (benzene)

C	1.920145	1.986654	0.300425
O	2.631124	2.455495	1.362850
H	1.978400	2.781584	2.006354
C	2.597088	1.419435	-0.788574
C	1.828856	1.003684	-1.884704
H	2.333319	0.599294	-2.759615
C	0.436616	1.045161	-1.857328
H	-0.154514	0.665724	-2.686662
C	-0.225171	1.507476	-0.717859
O	-1.609428	1.400732	-0.635214
C	0.509092	2.034684	0.354125
O	0.023304	2.641042	1.485641
C	-1.161609	2.150746	2.130904
H	-1.185208	2.646401	3.106427
H	-2.060682	2.408822	1.564391
H	-1.109984	1.064338	2.276105
C	-3.230142	-2.288499	0.479767
H	-3.678313	-3.227159	0.800865
C	-1.856968	-2.222753	0.216237
C	-0.959279	-3.440947	0.363349
H	-0.753041	-3.880206	-0.623411
H	-1.498134	-4.205369	0.936437
C	0.401911	-3.165573	1.041309
H	0.781335	-4.106428	1.471413
H	0.294678	-2.468449	1.881813
C	1.510540	-2.692521	0.090755
C	2.494474	-1.673688	0.652401
H	2.784456	-1.988207	1.667244
H	1.908296	-0.753941	0.805106
C	3.731234	-1.392489	-0.215152
H	4.424514	-2.238416	-0.113090
C	4.463546	-0.075560	0.145172
H	4.292679	0.170105	1.202130
C	4.084102	1.154000	-0.726078
H	4.616000	2.030880	-0.334134
H	4.451439	0.986344	-1.747650

H	5.547571	-0.220633	0.039362
H	3.429029	-1.385272	-1.269480
O	1.584906	-3.118436	-1.046347
C	-1.320174	-0.991263	-0.185860
H	-0.263183	-0.915823	-0.406839
C	-2.114063	0.149998	-0.309959
C	-3.496234	0.074306	-0.049583
O	-4.298692	1.188297	-0.076344
C	-4.546025	1.740074	-1.373967
H	-3.622326	2.095188	-1.846318
H	-5.223733	2.586110	-1.220012
H	-5.032407	1.000298	-2.026862
C	-4.035933	-1.154118	0.335205
H	-5.101939	-1.195070	0.548226

Sum of electronic and zero-point Energies= -1190.332414  
Sum of electronic and thermal Energies= -1190.308102  
Sum of electronic and thermal Enthalpies= -1190.307158  
Sum of electronic and thermal Free Energies= -1190.386516

#### jugcathanin-8-E2 (benzene)

C	1.948747	1.717987	-0.366296
O	2.771597	1.861454	-1.440678
H	2.193044	1.937725	-2.219611
C	2.483886	1.441130	0.901588
C	1.585594	1.332944	1.973679
H	1.980574	1.156743	2.973113
C	0.203193	1.381700	1.788181
H	-0.486752	1.237981	2.615545
C	-0.309039	1.559171	0.501167
O	-1.677430	1.455747	0.274943
C	0.557086	1.788029	-0.570115
O	0.145021	1.940489	-1.876239
C	-0.635883	3.113971	-2.152629
H	-0.805086	3.115891	-3.233850
H	-1.597377	3.076894	-1.629608
H	-0.091183	4.023355	-1.862592
C	-3.128394	-2.458695	0.053689
H	-3.515994	-3.475958	0.038785
C	-1.833321	-2.198432	-0.410838
C	-0.927648	-3.310450	-0.911124
H	-0.650651	-3.138811	-1.960148
H	-1.479713	-4.257533	-0.879177
C	0.380976	-3.465190	-0.100623
H	0.780960	-4.480602	-0.255555
H	0.192877	-3.371126	0.976181
C	1.511960	-2.522345	-0.530912
C	2.408592	-1.989653	0.577561
H	2.646678	-2.815587	1.266072
H	1.767141	-1.314804	1.166512
C	3.683248	-1.264772	0.115621
H	4.419355	-2.020434	-0.190422
C	4.301664	-0.347558	1.202203
H	3.993850	-0.699429	2.198071
C	3.963218	1.163255	1.068408
H	4.343007	1.683176	1.959499
H	4.504935	1.571724	0.208442
H	5.396692	-0.435385	1.181043
H	3.460201	-0.687106	-0.788371
O	1.666528	-2.221421	-1.700197
C	-1.372434	-0.874898	-0.369455
H	-0.383244	-0.640085	-0.746533
C	-2.152506	0.154158	0.158640
C	-3.460300	-0.110235	0.607771
O	-4.248840	0.851529	1.187131
C	-4.693677	1.899506	0.323421
H	-3.858287	2.515218	-0.031701
H	-5.370398	2.519153	0.921184
H	-5.242721	1.493101	-0.539098
C	-3.933781	-1.422538	0.535626
H	-4.940029	-1.619003	0.899174

Sum of electronic and zero-point Energies= -1190.333237  
Sum of electronic and thermal Energies= -1190.308736  
Sum of electronic and thermal Enthalpies= -1190.307792  
Sum of electronic and thermal Free Energies= -1190.387926

pterocarine-1-TS (benzene)

C	2.130674	1.898388	-0.068825
C	1.335368	3.053435	0.054433
H	1.742455	4.054569	-0.078538
C	-0.045844	2.963721	0.359184
O	-0.759337	4.123552	0.478245
H	-1.663238	3.899954	0.745867
C	-0.661461	1.704196	0.507956
O	-2.046673	1.589374	0.789263
C	0.141312	0.590011	0.374694
H	-0.241325	-0.403809	0.444056
C	1.480678	0.698297	0.132661
H	2.034233	-0.205725	0.108306
C	-2.833653	-2.201903	-0.684017
H	-2.888805	-3.156515	-1.205863
C	-3.535398	-1.111338	-1.200798
H	-4.159535	-1.212264	-2.085482
C	-3.325170	0.171382	-0.673649
O	-3.835109	1.254336	-1.316420
H	-3.524845	2.045089	-0.847232
C	-2.540714	0.300573	0.478582
C	-2.030907	-0.839249	1.114970
H	-1.445019	-0.705680	2.020677
C	-2.018478	-2.079104	0.456478
C	-0.924541	-3.102651	0.771128
H	-1.329381	-4.120415	0.707268
H	-0.553746	-2.970184	1.794582
C	0.302124	-3.007537	-0.218272
H	0.016966	-2.480372	-1.137465
H	0.573129	-4.023250	-0.548774
C	1.625482	-2.401576	0.313499
C	2.704048	-2.029887	-0.748610
H	2.196974	-1.682262	-1.657899
H	3.153160	-2.996951	-1.026931
C	3.859663	-1.037523	-0.333558
H	3.825178	-0.892276	0.753973
C	3.955226	0.351989	-1.093426
H	3.362897	0.288732	-2.017658
H	4.998073	0.454371	-1.421271
C	3.609389	1.720840	-0.395915
H	3.960602	2.520683	-1.063029
H	4.208923	1.817234	0.523567
H	4.804457	-1.561356	-0.521416
O	1.836375	-2.282506	1.503183

Sum of electronic and zero-point Energies= -1036.509094  
Sum of electronic and thermal Energies= -1036.489992  
Sum of electronic and thermal Enthalpies= -1036.489048  
Sum of electronic and thermal Free Energies= -1036.554945

pterocarine-1-E1 (benzene)

C	2.594449	-1.545804	-0.408892
C	2.004079	-1.995922	0.780869
H	2.598565	-2.146966	1.679923
C	0.621659	-2.188907	0.864411
O	0.065160	-2.561556	2.046113
H	-0.894194	-2.628450	1.911550
C	-0.171504	-1.941224	-0.266606
O	-1.558655	-1.975839	-0.095960
C	0.409416	-1.588868	-1.479519
H	-0.226935	-1.410972	-2.343210
C	1.790002	-1.396467	-1.549953
H	2.238774	-1.082720	-2.489631
C	-3.587962	1.667763	-0.023513
H	-4.151746	2.599260	-0.011306
C	-4.270746	0.465764	-0.226146

H	-5.348716	0.449467	-0.368711
C	-3.577775	-0.747160	-0.258784
O	-4.245961	-1.916067	-0.466092
H	-3.588083	-2.627243	-0.518927
C	-2.189845	-0.724403	-0.070113
C	-1.514079	0.474645	0.137265
H	-0.440781	0.442607	0.273032
C	-2.196117	1.696727	0.153769
C	-1.455386	3.016266	0.317056
H	-2.082354	3.701302	0.902815
H	-1.326599	3.487229	-0.668343
C	-0.064135	2.930401	0.972600
H	-0.075924	2.283659	1.859467
H	0.214733	3.933037	1.334410
C	1.072921	2.519842	0.025820
C	2.197782	1.698261	0.644308
H	1.743779	0.751501	0.973608
H	2.508555	2.191657	1.579250
C	3.407142	1.428614	-0.264477
H	3.049725	1.229451	-1.281997
C	4.304515	0.266092	0.230755
H	4.203260	0.161124	1.320894
H	5.359717	0.514330	0.051952
C	4.045436	-1.112437	-0.439144
H	4.680457	-1.860153	0.057054
H	4.378768	-1.061207	-1.484452
H	4.002484	2.348570	-0.335798
O	1.069130	2.851639	-1.144039

Sum of electronic and zero-point Energies= -1036.581242  
Sum of electronic and thermal Energies= -1036.561303  
Sum of electronic and thermal Enthalpies= -1036.560359  
Sum of electronic and thermal Free Energies= -1036.629315

pterocarine-1-E2 (benzene)

C	-2.572059	-1.571187	-0.326211
C	-2.038968	-1.770103	0.951976
H	-2.669567	-1.704751	1.835769
C	-0.668188	-1.985971	1.134761
O	-0.172122	-2.123607	2.390548
H	0.789898	-2.235434	2.317926
C	0.171946	-1.988268	0.015052
O	1.553282	-2.006907	0.248053
C	-0.353144	-1.886300	-1.271235
H	0.322318	-1.914782	-2.123551
C	-1.723713	-1.692567	-1.442328
H	-2.128507	-1.582488	-2.446615
C	3.508904	1.629362	-0.341515
H	4.039476	2.561298	-0.529778
C	4.145495	0.417896	-0.630048
H	5.154049	0.395625	-1.036034
C	3.479855	-0.793048	-0.429720
O	4.083314	-1.972053	-0.741782
H	3.442498	-2.681337	-0.571765
C	2.176079	-0.759162	0.086231
C	1.558314	0.444931	0.405290
H	0.558535	0.430253	0.827202
C	2.206960	1.667695	0.177022
C	1.493156	2.979805	0.453371
H	2.170278	3.808026	0.211618
H	1.250120	3.070765	1.520880
C	0.178246	3.161021	-0.342495
H	0.298944	2.837003	-1.383796
H	-0.071921	4.233778	-0.379612
C	-1.046486	2.487436	0.290497
C	-2.046971	1.856907	-0.667869
H	-1.513490	1.011296	-1.129993
H	-2.229032	2.557263	-1.498158
C	-3.367358	1.386289	-0.037029
H	-3.152824	0.956095	0.948414
C	-4.147097	0.371257	-0.912575

H	-3.838484	0.476320	-1.962845
H	-5.218845	0.611793	-0.892900
C	-4.008446	-1.117189	-0.488465
H	-4.524716	-1.737499	-1.235525
H	-4.539407	-1.263646	0.461543
H	-3.994688	2.266775	0.155597
O	-1.192448	2.461422	1.498601
Sum of electronic and zero-point Energies= -1036.581369			
Sum of electronic and thermal Energies= -1036.561518			
Sum of electronic and thermal Enthalpies= -1036.560574			
Sum of electronic and thermal Free Energies= -1036.629186			

pterocarine-2-TS (benzene)

C	-2.177849	1.825543	0.076217
C	-1.423244	3.013075	-0.013399
H	-1.868226	3.993327	0.150202
C	-0.041723	2.988032	-0.327041
O	0.619971	4.178998	-0.436798
H	1.537445	3.997487	-0.689705
C	0.624303	1.755641	-0.489742
O	2.013506	1.679817	-0.767030
C	-0.135063	0.612227	-0.373811
H	0.299990	-0.360364	-0.399147
C	-1.484399	0.658270	-0.168553
H	-1.992153	-0.274712	-0.164428
C	2.707025	-2.149883	0.621715
H	2.708228	-3.116124	1.122778
C	3.367896	-1.079775	1.226004
H	3.905977	-1.208947	2.161882
C	3.206296	0.216036	0.719060
O	3.659508	1.279309	1.432216
H	3.380387	2.083181	0.965763
C	2.513941	0.381592	-0.486704
C	2.051902	-0.735507	-1.196881
H	1.514391	-0.558717	-2.126266
C	1.996408	-1.998237	-0.581312
C	1.022153	-3.079570	-1.058844
H	1.126274	-3.949132	-0.398561
H	1.302013	-3.423635	-2.065743
C	-0.499911	-2.713939	-1.156637
H	-1.004763	-3.549695	-1.668095
H	-0.651073	-1.859845	-1.833331
C	-1.321139	-2.433752	0.122216
C	-2.851497	-2.187952	-0.072563
H	-3.297280	-3.178284	0.110497
H	-3.056347	-1.970103	-1.129151
C	-3.576191	-1.138068	0.863246
H	-4.413253	-1.662684	1.338491
C	-4.174887	0.157125	0.169513
H	-5.242921	0.191511	0.420496
H	-4.139029	0.022311	-0.921410
C	-3.626117	1.593542	0.493317
H	-4.301907	2.316057	0.012690
H	-3.720993	1.777960	1.575336
H	-2.897544	-0.872628	1.683241
O	-0.825065	-2.451044	1.229069

Sum of electronic and zero-point Energies= -1036.506444  
 Sum of electronic and thermal Energies= -1036.487484  
 Sum of electronic and thermal Enthalpies= -1036.486540  
 Sum of electronic and thermal Free Energies= -1036.551868

pterocarine-2-E1 (benzene)

C	-2.594644	1.545955	0.408466
C	-2.004043	1.995432	-0.781424
H	-2.598312	2.145944	-1.680710
C	-0.621604	2.188354	-0.864788
O	-0.064889	2.560160	-2.046682
H	0.894378	2.627700	-1.911878
C	0.171346	1.941339	0.266521
O	1.558534	1.975917	0.096291

C	-0.409831	1.589712	1.479528
H	0.226360	1.412383	2.343453
C	-1.790425	1.397320	1.549784
H	-2.239380	1.084096	2.489552
C	3.588071	-1.667550	0.023449
H	4.151954	-2.598986	0.011078
C	4.270775	-0.465487	0.226029
H	5.348766	-0.449081	0.368424
C	3.577686	0.747345	0.258840
O	4.245786	1.916339	0.466209
H	3.587858	2.627487	0.518732
C	2.189723	0.724498	0.070358
C	1.514041	-0.474603	-0.136958
H	0.440729	-0.442684	-0.272650
C	2.196215	-1.696636	-0.153651
C	1.455590	-3.016213	-0.316898
H	1.326771	-3.487189	0.668493
H	2.082590	-3.701232	-0.902640
C	0.064301	-2.930471	-0.972461
H	-0.214483	-3.933174	-1.334123
H	0.076045	-2.283787	-1.859363
C	-1.072722	-2.519900	-0.025606
C	-2.197523	-1.698180	-0.643910
H	-2.508410	-2.191518	-1.578866
H	-1.743553	-0.751421	-0.973233
C	-3.406887	-1.428534	0.264915
H	-4.002017	-2.348596	0.336564
C	-4.304516	-0.266356	-0.230660
H	-5.359664	-0.514661	-0.051619
H	-4.203416	-0.161806	-1.320850
C	-4.045599	1.112482	0.438694
H	-4.680616	1.859934	-0.057901
H	-4.379060	1.061665	1.483982
H	-3.049483	-1.228960	1.282359
O	-1.069030	-2.852061	1.144160
Sum of electronic and zero-point Energies= -1036.581241			
Sum of electronic and thermal Energies= -1036.561303			
Sum of electronic and thermal Enthalpies= -1036.560359			
Sum of electronic and thermal Free Energies= -1036.629305			

pterocarine-2-E2 (benzene)

C	-2.572002	1.571264	-0.326104
C	-2.038826	1.769938	0.952079
H	-2.669362	1.704457	1.835906
C	-0.668026	1.985731	1.134807
O	-0.171860	2.123129	2.390586
H	0.790127	2.235172	2.317899
C	0.172029	1.988245	0.015045
O	1.553372	2.006861	0.247979
C	-0.353135	1.886486	-1.271232
H	0.322275	1.915101	-2.123587
C	-1.723717	1.692796	-1.442259
H	-2.128581	1.582886	-2.446538
C	3.508932	-1.629459	-0.341475
H	4.039510	-2.561395	-0.529718
C	4.145580	-0.417992	-0.629922
H	5.154175	-0.395752	-1.035803
C	3.479978	0.792969	-0.429627
O	4.083510	1.971981	-0.741540
H	3.442673	2.681288	-0.571704
C	2.176135	0.759105	0.086183
C	1.558308	-0.444979	0.405128
H	0.558478	-0.430279	0.826916
C	2.206944	-1.667769	0.176912
C	1.493010	-2.979833	0.453153
H	1.249939	-3.070841	1.520647
H	2.170052	-3.808111	0.211361
C	0.178085	-3.160825	-0.342748
H	-0.072142	-4.233563	-0.380149
H	0.298814	-2.836580	-1.383977

C	-1.046636	-2.487347	0.290366
C	-2.047054	-1.856533	-0.667878
H	-2.229023	-2.556684	-1.498375
H	-1.513581	-1.010810	-1.129791
C	-3.367538	-1.386190	-0.037035
H	-3.994808	-2.266786	0.155290
C	-4.147319	-0.371036	-0.912386
H	-5.219096	-0.611430	-0.892476
H	-3.838941	-0.476156	-1.962722
C	-4.008426	1.117412	-0.488331
H	-4.524643	1.737745	-1.235409
H	-4.539367	1.263971	0.461673
H	-3.153161	-0.956238	0.948549
O	-1.192681	-2.461707	1.498467
Sum of electronic and zero-point Energies= -1036.581369			
Sum of electronic and thermal Energies= -1036.561519			
Sum of electronic and thermal Enthalpies= -1036.560574			
Sum of electronic and thermal Free Energies= -1036.629187			

pterocaraine-3-TS (benzene)

C	1.959633	2.016188	-0.112274
C	1.098677	3.125718	0.013535
H	1.454839	4.148391	-0.100646
C	-0.275751	2.964113	0.318183
O	-1.042547	4.085111	0.471177
H	-1.935691	3.812093	0.728829
C	-0.828653	1.672017	0.436027
O	-2.200079	1.470806	0.737503
C	0.031090	0.607682	0.272104
H	-0.301259	-0.403859	0.298840
C	1.370239	0.782299	0.073502
H	1.959024	-0.102657	0.073801
C	-2.646065	-2.416258	-0.609634
H	-2.605505	-3.381846	-1.112214
C	-3.468457	-1.418115	-1.136420
H	-4.092375	-1.605980	-2.006997
C	-3.379491	-0.105552	-0.648196
O	-3.998132	0.903211	-1.315862
H	-3.757248	1.734768	-0.877277
C	-2.596528	0.133517	0.487209
C	-1.966900	-0.932675	1.144176
H	-1.369073	-0.711158	2.024669
C	-1.828177	-2.179317	0.510714
C	-0.599555	-3.043964	0.812078
H	-0.863099	-4.108576	0.780829
H	-0.228748	-2.837452	1.822964
C	0.592386	-2.807914	-0.201508
H	0.289612	-2.155210	-1.032931
H	0.851967	-3.760491	-0.688316
C	1.925007	-2.262999	0.372800
C	3.129987	-2.052008	-0.602078
H	2.991686	-2.734836	-1.451812
H	3.996303	-2.415509	-0.033619
C	3.530133	-0.657120	-1.234986
H	4.341222	-0.911591	-1.930367
C	4.046902	0.498973	-0.293472
H	5.129729	0.595305	-0.445575
H	3.924995	0.204918	0.757435
C	3.440681	1.935460	-0.475076
H	4.036352	2.630396	0.134450
H	3.582912	2.261101	-1.517938
H	2.710733	-0.301284	-1.870079
O	2.074843	-2.098727	1.567915
Sum of electronic and zero-point Energies= -1036.501592			
Sum of electronic and thermal Energies= -1036.482689			
Sum of electronic and thermal Enthalpies= -1036.481745			
Sum of electronic and thermal Free Energies= -1036.546910			

pterocaraine-3-E1 (benzene)

C	-2.316032	1.927033	-0.243316
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C	-1.550754	2.158810	0.906214
H	-2.018794	2.222135	1.886287
C	-0.155252	2.210137	0.835912
O	0.564904	2.346765	1.980164
H	1.505459	2.355011	1.742567
C	0.468992	2.038760	-0.407304
O	1.851272	1.835154	-0.411988
C	-0.282161	1.945704	-1.574925
H	0.231160	1.833539	-2.527088
C	-1.673795	1.899534	-1.493282
H	-2.258723	1.756673	-2.399546
C	3.214182	-2.071185	0.124762
H	3.608144	-3.072747	0.289157
C	4.092841	-0.982700	0.161742
H	5.154373	-1.122736	0.351962
C	3.616661	0.312969	-0.033774
O	4.468680	1.376282	0.017510
H	3.961567	2.173576	-0.201584
C	2.243837	0.495761	-0.265545
C	1.375519	-0.589889	-0.328827
H	0.327131	-0.426591	-0.548367
C	1.847347	-1.896632	-0.126402
C	0.901036	-3.083967	-0.204286
H	1.444739	-3.978100	0.124342
H	0.618950	-3.258407	-1.252373
C	-0.402831	-2.970961	0.616214
H	-0.260513	-2.370824	1.527710
H	-0.702710	-3.966639	0.981157
C	-1.620089	-2.428506	-0.133622
C	-2.912264	-2.284802	0.672732
H	-2.817479	-2.827524	1.621655
H	-3.722735	-2.755187	0.098911
C	-3.265140	-0.801519	0.963784
H	-3.966211	-0.774002	1.809812
C	-3.876063	-0.045566	-0.231873
H	-4.936099	-0.322888	-0.329035
H	-3.382348	-0.369262	-1.156017
C	-3.765013	1.501932	-0.132436
H	-4.359144	1.946517	-0.942505
H	-4.200147	1.851124	0.814287
H	-2.357246	-0.290415	1.309386
O	-1.574294	-2.134791	-1.315104
Sum of electronic and zero-point Energies= -1036.579168			
Sum of electronic and thermal Energies= -1036.559411			
Sum of electronic and thermal Enthalpies= -1036.558467			
Sum of electronic and thermal Free Energies= -1036.626469			

pterocaraine-3-E2 (benzene)

C	-2.295427	1.885199	0.390665
C	-1.726394	2.161753	-0.859500
H	-2.342980	2.214259	-1.754486
C	-0.340448	2.255644	-1.008866
O	0.193285	2.445040	-2.242629
H	1.159980	2.423302	-2.152191
C	0.475479	2.063889	0.115148
O	1.846491	1.887249	-0.109390
C	-0.077292	1.921057	1.382823
H	0.581960	1.798116	2.239282
C	-1.464407	1.848444	1.522673
H	-1.897503	1.687153	2.507676
C	3.188799	-2.051603	0.192112
H	3.567480	-3.066970	0.297921
C	4.022475	-0.980301	0.528655
H	5.032783	-1.147055	0.894784
C	3.558662	0.332167	0.423268
O	4.356890	1.376768	0.776597
H	3.833473	2.188495	0.678350
C	2.252306	0.543122	-0.041950
C	1.431654	-0.522475	-0.399337
H	0.431246	-0.331694	-0.773799

C	1.882880	-1.845054	-0.274514
C	0.974097	-3.009366	-0.632033
H	1.537825	-3.940826	-0.499269
H	0.700775	-2.955087	-1.694656
C	-0.333782	-3.110088	0.185674
H	-0.192777	-2.764227	1.220713
H	-0.634834	-4.166362	0.281032
C	-1.549861	-2.394283	-0.402549
C	-2.835493	-2.438749	0.425595
H	-2.730829	-3.176495	1.231065
H	-3.650304	-2.775897	-0.230129
C	-3.187531	-1.055309	1.035723
H	-3.862774	-1.215623	1.888084
C	-3.838966	-0.070483	0.045646
H	-4.899484	-0.335028	-0.078392
H	-3.370246	-0.184156	-0.939176
C	-3.734977	1.422146	0.468303
H	-4.369447	2.019272	-0.200588
H	-4.128511	1.553285	1.486151
H	-2.271856	-0.617753	1.454189
O	-1.509745	-1.826677	-1.479800

Sum of electronic and zero-point Energies= -1036.579844  
Sum of electronic and thermal Energies= -1036.560124  
Sum of electronic and thermal Enthalpies= -1036.559180  
Sum of electronic and thermal Free Energies= -1036.627223

#### myricatomentogenin-1-TS (benzene)

C	2.918772	0.477128	-0.163225
O	4.228779	0.749365	-0.409349
H	4.314877	1.718703	-0.387484
C	2.444211	-0.848950	-0.204197
C	1.100456	-0.981915	0.066853
H	0.684974	-1.957711	0.094838
C	0.235194	0.047041	0.306358
H	-0.786460	-0.225774	0.441837
C	0.672821	1.359045	0.346860
O	-0.230328	2.410644	0.608421
C	2.044767	1.572346	0.119505
O	2.629213	2.825293	0.075788
C	2.636778	3.538402	1.323390
H	1.616024	3.774885	1.645775
H	3.143299	2.956381	2.106083
H	3.188042	4.466377	1.140347
C	-3.791110	0.749271	-0.697091
H	-4.609687	0.209094	-1.171382
C	-3.198583	0.228253	0.468370
C	-3.397104	-1.232285	0.879505
H	-4.463173	-1.490785	0.850437
H	-3.057026	-1.393570	1.909401
C	-2.632997	-2.243000	-0.060376
H	-2.426150	-1.782267	-1.034551
H	-3.298947	-3.091979	-0.284836
C	-1.331988	-2.895860	0.470115
C	-0.440741	-3.630773	-0.575553
H	-0.493691	-3.083763	-1.525885
H	-0.971293	-4.577708	-0.765669
C	1.056683	-3.955543	-0.196107
H	1.178840	-5.040310	-0.299105
C	2.199393	-3.284600	-1.068625
H	2.870335	-4.095709	-1.380452
C	3.148913	-2.164539	-0.501701
H	3.651805	-2.538274	0.404757
H	3.948616	-2.015551	-1.239844
H	1.751640	-2.902366	-1.997434
H	1.201723	-3.752192	0.872742
O	-1.054979	-2.890408	1.652192
C	-2.184904	0.995474	1.063927
H	-1.717918	0.650348	1.982853
C	-1.568047	2.031606	0.350794
C	-2.145364	2.522144	-0.826071

O	-1.560845	3.519302	-1.538522
H	-0.725313	3.741216	-1.094942
C	-3.319880	1.918091	-1.298188
H	-3.778858	2.309360	-2.202988

Sum of electronic and zero-point Energies= -1150.994995  
Sum of electronic and thermal Energies= -1150.973228  
Sum of electronic and thermal Enthalpies= -1150.972284  
Sum of electronic and thermal Free Energies= -1151.044173

#### myricatomentogenin-1-E1 (benzene)

C	1.734713	1.764995	-0.398424
O	2.305981	2.038304	-1.603367
H	1.581423	2.300552	-2.197552
C	2.530825	1.292013	0.657713
C	1.904646	1.074345	1.891816
H	2.507679	0.740289	2.733631
C	0.523840	1.210124	2.056394
H	0.039426	0.972709	2.999692
C	-0.260982	1.566210	0.961827
O	-1.648073	1.510423	1.054531
C	0.341040	1.898338	-0.258640
O	-0.333247	2.241791	-1.407535
C	-1.251382	3.343665	-1.335760
H	-2.204756	3.035902	-0.895037
H	-0.824188	4.173326	-0.757087
H	-1.418828	3.664329	-2.368728
C	-3.534750	-1.888667	-0.443217
H	-4.057380	-2.749370	-0.857142
C	-2.184015	-2.002647	-0.090903
C	-1.421091	-3.304332	-0.273063
H	-2.061611	-4.013159	-0.811923
H	-1.201645	-3.759867	0.702989
C	-0.081079	-3.163172	-1.031220
H	-0.178952	-2.483137	-1.886608
H	0.197871	-4.144424	-1.448467
C	1.109119	-2.752904	-0.154657
C	2.138930	-1.834199	-0.798036
H	1.607610	-0.890026	-0.993417
H	2.379656	-2.225082	-1.799261
C	3.414271	-1.585072	0.022419
H	4.053413	-2.475220	-0.050438
C	4.207507	-0.332402	-0.428820
H	5.284226	-0.549337	-0.404404
C	3.985149	0.939848	0.435841
H	4.455485	0.786538	1.416495
H	4.513943	1.775391	-0.043138
H	3.969491	-0.097504	-1.474318
H	3.141704	-1.504846	1.081814
O	1.210101	-3.147432	0.992265
C	-1.544092	-0.869065	0.434946
H	-0.506790	-0.922059	0.745425
C	-2.225939	0.334466	0.573045
C	-3.584344	0.436659	0.234685
O	-4.253825	1.617790	0.379830
H	-3.654865	2.239992	0.821700
C	-4.233542	-0.687786	-0.272046
H	-5.283336	-0.604503	-0.543419

Sum of electronic and zero-point Energies= -1151.064393  
Sum of electronic and thermal Energies= -1151.041798  
Sum of electronic and thermal Enthalpies= -1151.040854  
Sum of electronic and thermal Free Energies= -1151.115365

#### myricatomentogenin-1-E2 (benzene)

C	-2.141167	-1.637829	0.284857
O	-3.012820	-1.829916	1.310439
H	-2.504564	-2.262533	2.019153
C	-2.577249	-1.044884	-0.909401
C	-1.643939	-0.931128	-1.950512
H	-1.967393	-0.518208	-2.904671
C	-0.305065	-1.276514	-1.779687



H	0.421244	-1.127107	-2.574486
C	0.130823	-1.763920	-0.544270
O	1.492000	-1.946903	-0.311761
C	-0.790042	-2.000671	0.479229
O	-0.504865	-2.588835	1.691994
C	0.367524	-1.883125	2.592420
H	1.398418	-1.880503	2.225958
H	0.021905	-0.852944	2.749743
H	0.320595	-2.431495	3.538495
C	3.812068	1.511998	-0.136283
H	4.444212	2.398221	-0.114121
C	2.473784	1.605092	0.269952
C	1.868566	2.915290	0.747392
H	2.613908	3.711305	0.628790
H	1.637070	2.859472	1.820382
C	0.573771	3.333486	0.013414
H	0.670590	3.193664	-1.070635
H	0.408439	4.411997	0.170191
C	-0.704274	2.655475	0.525077
C	-1.766182	2.347102	-0.520261
H	-1.301499	1.613395	-1.196938
H	-1.912475	3.243771	-1.143502
C	-3.106791	1.816080	0.013065
H	-3.669723	2.655532	0.442146
C	-3.961292	1.110293	-1.074221
H	-5.006920	1.438100	-0.997034
C	-3.963716	-0.443053	-1.014972
H	-4.558520	-0.766002	-0.154271
H	-4.475033	-0.822772	-1.911539
H	-3.623614	1.432523	-2.070091
H	-2.914545	1.134250	0.849737
O	-0.842401	2.378716	1.702867
C	1.696260	0.438915	0.221123
H	0.660444	0.460899	0.539829
C	2.228400	-0.761826	-0.236964
C	3.571222	-0.850489	-0.635321
O	4.096555	-2.024282	-1.080813
H	3.384095	-2.683843	-1.076536
C	4.358761	0.300687	-0.574671
H	5.396847	0.236175	-0.892199

Sum of electronic and zero-point Energies= -1151.061237  
Sum of electronic and thermal Energies= -1151.038572  
Sum of electronic and thermal Enthalpies= -1151.037628  
Sum of electronic and thermal Free Energies= -1151.112822

#### myricatomentogenin-2-TS (benzene)

C	-1.124720	2.767095	0.112440
O	-1.566643	4.044528	-0.041471
H	-0.794027	4.620409	0.093388
C	-2.016199	1.686785	-0.017484
C	-1.444324	0.447736	0.171871
H	-2.071820	-0.408025	0.151148
C	-0.118318	0.221498	0.401115
H	0.174178	-0.802119	0.460797
C	0.782193	1.263391	0.551840
O	2.137788	0.992062	0.848889
C	0.262465	2.564719	0.408744
O	0.972841	3.738653	0.564022
C	2.221383	3.857378	-0.124560
H	2.459497	4.925884	-0.144617
H	3.015378	3.325164	0.412994
H	2.143708	3.484104	-1.155488
C	2.583809	-2.826086	-0.700863
H	2.559085	-3.772674	-1.239479
C	1.783237	-2.657074	0.444041
C	0.616532	-3.599809	0.744902
H	0.255380	-3.454802	1.770025
H	0.945578	-4.643709	0.666288
C	-0.598266	-3.404054	-0.241949
H	-0.976892	-4.395904	-0.537668

H	-0.264373	-2.937956	-1.177369
C	-1.847661	-2.651364	0.279729
C	-2.864357	-2.153398	-0.789635
H	-3.374810	-3.068914	-1.129936
H	-2.302741	-1.804194	-1.665914
C	-3.950480	-1.094394	-0.356468
H	-4.928815	-1.546250	-0.559308
C	-3.942275	0.314092	-1.085035
H	-3.354325	0.226592	-2.010227
C	-3.497701	1.638917	-0.360524
H	-3.767567	2.474050	-1.020787
H	-4.102667	1.776397	0.550125
H	-4.973929	0.500712	-1.411210
H	-3.912659	-0.975937	0.734173
O	-2.053116	-2.515102	1.468601
C	1.897537	-1.435505	1.126425
H	1.323288	-1.270083	2.034311
C	2.502629	-0.331383	0.510898
C	3.274678	-0.505348	-0.643747
O	3.876001	0.545523	-1.262165
H	3.656230	1.343616	-0.755879
C	3.374641	-1.789182	-1.198814
H	3.988513	-1.925742	-2.085926

Sum of electronic and zero-point Energies= -1150.993264  
Sum of electronic and thermal Energies= -1150.971602  
Sum of electronic and thermal Enthalpies= -1150.970657  
Sum of electronic and thermal Free Energies= -1151.042187

#### myricatomentogenin-2-E1 (benzene)

C	2.058905	-1.771739	-0.196298
O	2.865902	-2.151173	-1.224913
H	2.299277	-2.622315	-1.859901
C	2.597166	-1.037002	0.869511
C	1.740666	-0.711222	1.930439
H	2.143057	-0.176664	2.788158
C	0.380621	-1.006633	1.888024
H	-0.288264	-0.692928	2.684937
C	-0.158566	-1.645443	0.769418
O	-1.540767	-1.775347	0.656395
C	0.681057	-2.078148	-0.265688
O	0.332502	-2.806438	-1.376486
C	-0.891331	-2.531676	-2.072237
H	-0.783007	-3.005348	-3.053068
H	-1.750076	-2.965065	-1.550762
H	-1.041305	-1.452842	-2.202912
C	-3.791678	1.635334	-0.169492
H	-4.415509	2.501029	-0.386301
C	-2.396210	1.747533	-0.247220
C	-1.727689	3.070042	-0.592625
H	-1.617319	3.678054	0.317208
H	-2.391412	3.635567	-1.259387
C	-0.334943	2.961678	-1.245683
H	-0.117104	3.906530	-1.769078
H	-0.312375	2.179142	-2.015138
C	0.829664	2.778885	-0.261604
C	1.998500	1.929426	-0.749497
H	2.265253	2.260228	-1.765953
H	1.598841	0.913033	-0.888669
C	3.232714	1.904691	0.165622
H	3.772443	2.853671	0.045782
C	4.193364	0.721008	-0.112871
H	4.095148	0.397263	-1.157972
C	4.014225	-0.512400	0.815666
H	4.702800	-1.298608	0.479243
H	4.319902	-0.232359	1.832920
H	5.232387	1.059131	0.002615
H	2.897875	1.887280	1.209917
O	0.811565	3.299811	0.837015
C	-1.634103	0.605939	0.032983
H	-0.553759	0.648059	-0.010523

C	-2.238366	-0.596498	0.390802
C	-3.634832	-0.699943	0.472687
O	-4.234867	-1.875125	0.812633
H	-3.535409	-2.514335	1.021513
C	-4.404057	0.429704	0.187018
H	-5.486767	0.346435	0.246475
Sum of electronic and zero-point Energies= -1151.061651			
Sum of electronic and thermal Energies= -1151.039112			
Sum of electronic and thermal Enthalpies= -1151.038167			
Sum of electronic and thermal Free Energies= -1151.112739			

myricatomentogenin-2-E2 (benzene)

C	2.005608	-1.499199	0.386782
O	2.807938	-1.501691	1.485161
H	2.231480	-1.689748	2.246426
C	2.522661	-1.128940	-0.864752
C	1.654661	-1.177147	-1.965707
H	2.044300	-0.931517	-2.952361
C	0.296581	-1.465086	-1.823396
H	-0.381294	-1.435439	-2.672625
C	-0.215024	-1.730568	-0.552116
O	-1.590738	-1.838312	-0.359147
C	0.640914	-1.809870	0.548330
O	0.225148	-2.032557	1.841011
C	-0.428464	-3.287298	2.093277
H	-0.590093	-3.328945	3.174637
H	-1.391403	-3.339770	1.574837
H	0.207981	-4.127415	1.782508
C	-3.706707	1.740829	-0.069858
H	-4.283526	2.663527	-0.032273
C	-2.373928	1.739700	0.361761
C	-1.692149	3.002798	0.859203
H	-1.415158	2.901609	1.917689
H	-2.403329	3.835546	0.797366
C	-0.412028	3.378769	0.075691
H	-0.197915	4.448716	0.231676
H	-0.557200	3.248496	-1.004003
C	0.855515	2.648842	0.538227
C	1.845434	2.249845	-0.547580
H	1.960014	3.093159	-1.246669
H	1.332936	1.471349	-1.135110
C	3.211579	1.748465	-0.052184
H	3.801534	2.616474	0.271757
C	4.004190	0.951823	-1.120965
H	3.660979	1.242312	-2.125014
C	3.934431	-0.594889	-0.986849
H	4.427846	-1.040478	-1.862367
H	4.512274	-0.900222	-0.107885
H	5.066142	1.230270	-1.077504
H	3.066352	1.139226	0.847019
O	1.042834	2.403339	1.715605
C	-1.664158	0.530678	0.296605
H	-0.640460	0.482222	0.650477
C	-2.256065	-0.616802	-0.217721
C	-3.593151	-0.610967	-0.645914
O	-4.171946	-1.735490	-1.151074
H	-3.490797	-2.426687	-1.173005
C	-4.316082	0.578907	-0.556618
H	-5.349438	0.585670	-0.895307
Sum of electronic and zero-point Energies= -1151.063728			
Sum of electronic and thermal Energies= -1151.041022			
Sum of electronic and thermal Enthalpies= -1151.040078			
Sum of electronic and thermal Free Energies= -1151.115533			

myricatomentogenin-3-TS (benzene)

C	-0.066737	-2.958289	0.065526
O	-0.057769	-4.310550	-0.083281
H	0.858727	-4.598597	0.070997
C	-1.274062	-2.243865	-0.060612
C	-1.147694	-0.881983	0.109734

H	-2.018540	-0.270625	0.106012
C	0.033331	-0.226860	0.301875
H	-0.030859	0.835145	0.318577
C	1.226518	-0.902206	0.489698
O	2.401470	-0.184010	0.813636
C	1.171348	-2.304697	0.368523
O	2.229845	-3.172013	0.550540
C	3.456092	-2.867436	-0.121820
H	4.050862	-3.786407	-0.103295
H	3.273282	-2.573420	-1.164989
H	4.003710	-2.075244	0.402769
C	1.405940	3.563038	-0.635208
H	1.023252	4.436555	-1.161738
C	0.716595	3.070918	0.488601
C	-0.745180	3.438127	0.762165
H	-0.885513	4.524594	0.700186
H	-1.029242	3.137263	1.777476
C	-1.754282	2.758610	-0.248010
H	-1.221855	2.250424	-1.064927
H	-2.345413	3.537208	-0.754129
C	-2.792168	1.765991	0.332812
C	-3.823047	1.111590	-0.642916
H	-3.930302	1.779592	-1.508741
H	-4.771455	1.144897	-0.090269
C	-3.672101	-0.345622	-1.240142
H	-4.501467	-0.421743	-1.956042
C	-3.755693	-1.585568	-0.269533
H	-3.755225	-1.241411	0.773242
C	-2.677916	-2.715917	-0.414203
H	-2.690578	-3.107928	-1.443715
H	-2.983275	-3.558525	0.222358
H	-4.732822	-2.063102	-0.418074
H	-2.763194	-0.391942	-1.851087
O	-2.876661	1.570056	1.529675
C	1.289534	1.974908	1.155660
H	0.801789	1.570784	2.039069
C	2.271640	1.196675	0.527902
C	2.928965	1.678553	-0.609806
O	3.880776	0.944507	-1.245400
H	3.965382	0.104388	-0.767100
C	2.541506	2.920840	-1.133852
H	3.065902	3.303330	-2.006315
Sum of electronic and zero-point Energies= -1150.986391			
Sum of electronic and thermal Energies= -1150.964804			
Sum of electronic and thermal Enthalpies= -1150.963859			
Sum of electronic and thermal Free Energies= -1151.035136			

myricatomentogenin-3-E1 (benzene)

C	-1.713034	2.046630	0.271157
O	-2.381737	2.415574	1.398390
H	-1.709522	2.764698	2.009242
C	-2.407331	1.458325	-0.794378
C	-1.683486	1.164492	-1.958886
H	-2.208391	0.744517	-2.814782
C	-0.299228	1.302246	-2.010151
H	0.267824	0.987848	-2.882313
C	0.393945	1.743561	-0.881204
O	1.781161	1.624521	-0.846038
C	-0.307414	2.189318	0.245213
O	0.215442	2.775630	1.374725
C	1.358594	2.203108	2.026453
H	1.385973	2.656192	3.022518
H	1.257737	1.115225	2.122237
H	2.283455	2.445433	1.494200
C	3.404166	-2.054905	0.254132
H	3.866856	-2.990357	0.564400
C	2.027331	-2.011795	0.001820
C	1.159129	-3.253347	0.131103
H	1.759641	-4.045860	0.594070
H	0.884028	-3.614680	-0.870017

C	-0.146689	-3.085763	0.939537
H	-0.039916	-2.334163	1.736174
H	-0.381776	-4.022927	1.470025
C	-1.400535	-2.757105	0.126573
C	-2.688788	-2.523704	0.918377
H	-2.548852	-2.853828	1.955535
H	-3.475898	-3.148671	0.473967
C	-3.131295	-1.035278	0.906738
H	-3.814182	-0.870846	1.751488
C	-3.813483	-0.586941	-0.400237
H	-3.304423	-1.057807	-1.249942
C	-3.823547	0.950666	-0.623731
H	-4.317447	1.455367	0.214244
H	-4.413532	1.166400	-1.525144
H	-4.849155	-0.958297	-0.410832
H	-2.252576	-0.409283	1.107979
O	-1.383335	-2.697252	-1.089899
C	1.466032	-0.786661	-0.393559
H	0.407843	-0.731754	-0.618565
C	2.257099	0.352717	-0.517020
C	3.638709	0.299725	-0.268824
O	4.408247	1.420883	-0.372389
H	3.839538	2.138660	-0.693392
C	4.204998	-0.915298	0.113220
H	5.273513	-0.950671	0.312614

Sum of electronic and zero-point Energies= -1151.058699  
Sum of electronic and thermal Energies= -1151.036246  
Sum of electronic and thermal Enthalpies= -1151.035302  
Sum of electronic and thermal Free Energies= -1151.109319

#### myricatomentogenin-3-E2 (benzene)

C	-1.739786	1.889057	-0.282951
O	-2.542501	2.098123	-1.359807
H	-1.954624	2.315342	-2.104125
C	-2.292195	1.410157	0.916562
C	-1.431887	1.257400	2.012170
H	-1.847306	0.933331	2.964664
C	-0.050453	1.419798	1.891172
H	0.618715	1.209732	2.721532
C	0.488479	1.752304	0.649231
O	1.862162	1.654291	0.436528
C	-0.350759	2.064685	-0.424011
O	0.086559	2.379844	-1.689522
C	0.928114	3.537576	-1.804203
H	1.075648	3.696768	-2.876747
H	0.441283	4.419118	-1.364257
H	1.896168	3.368905	-1.321001
C	3.345499	-2.204193	-0.103271
H	3.763586	-3.203488	-0.214185
C	2.016183	-1.964206	-0.476108
C	1.135547	-3.070925	-1.032016
H	1.732566	-3.988943	-1.094803
H	0.830067	-2.823014	-2.057798
C	-0.144426	-3.374826	-0.220690
H	0.013121	-3.220954	0.857420
H	-0.405429	-4.441657	-0.317063
C	-1.401240	-2.611710	-0.639209
C	-2.659894	-2.860555	0.193740
H	-2.500430	-3.721571	0.854993
H	-3.477050	-3.117210	-0.494813
C	-3.056200	-1.622844	1.042802
H	-3.702959	-1.962096	1.864427
C	-3.771052	-0.509740	0.252957
H	-3.329113	-0.425505	-0.745980
C	-3.710658	0.886706	0.933234
H	-4.073799	0.819484	1.968401
H	-4.383075	1.567180	0.396631
H	-4.824174	-0.792143	0.106580
H	-2.149781	-1.224494	1.517761
O	-1.412175	-1.853504	-1.592777

C	1.512356	-0.663515	-0.319961
H	0.494248	-0.444527	-0.622446
C	2.306585	0.345681	0.215096
C	3.638668	0.100523	0.584484
O	4.412103	1.090174	1.112202
H	3.853440	1.879618	1.194829
C	4.153223	-1.184602	0.412346
H	5.183092	-1.375931	0.704753

Sum of electronic and zero-point Energies= -1151.062797  
Sum of electronic and thermal Energies= -1151.040179  
Sum of electronic and thermal Enthalpies= -1151.039235  
Sum of electronic and thermal Free Energies= -1151.114306

#### myricatomentogenin-4-TS (benzene)

C	0.808721	2.823104	-0.210381
O	1.152065	4.118480	-0.443115
H	0.326406	4.632293	-0.398649
C	1.791254	1.811836	-0.241694
C	1.308198	0.545972	0.008259
H	1.988947	-0.268471	0.074423
C	-0.007318	0.228462	0.187616
H	-0.221047	-0.810851	0.268948
C	-0.986733	1.201519	0.262311
O	-2.324431	0.850511	0.543925
C	-0.562102	2.529815	0.070522
O	-1.414576	3.618813	0.064377
C	-2.041311	3.907950	1.324875
H	-2.713414	3.095162	1.623851
H	-1.289156	4.069673	2.109775
H	-2.619012	4.825563	1.174524
C	-2.296241	-3.126077	-0.594340
H	-2.136702	-4.107010	-1.040568
C	-1.548321	-2.745947	0.535648
C	-0.249685	-3.461013	0.922019
H	-0.401187	-4.547658	0.934890
H	0.057788	-3.169662	1.933353
C	0.950250	-3.150426	-0.060494
H	0.608665	-2.601638	-0.949984
H	1.346069	-4.095618	-0.462669
C	2.179104	-2.404439	0.516935
C	3.391954	-2.124618	-0.429644
H	3.359928	-2.868065	-1.238099
H	4.269811	-2.357240	0.187878
C	3.664555	-0.734765	-1.136568
H	4.521711	-0.940517	-1.791534
C	4.022412	0.522483	-0.253492
H	5.095310	0.721093	-0.372894
C	3.282307	1.874783	-0.546003
H	3.772562	2.662082	0.044113
H	3.436412	2.159986	-1.598889
H	3.887010	0.279794	0.808920
H	2.835409	-0.507672	-1.816701
O	2.252840	-2.130113	1.699025
C	-1.838804	-1.490382	1.095524
H	-1.298091	-1.160283	1.978883
C	-2.553731	-0.534918	0.361102
C	-3.266149	-0.912918	-0.782694
O	-3.958753	-0.006190	-1.519164
H	-3.810793	0.866842	-1.119562
C	-3.199454	-2.250539	-1.201335
H	-3.767212	-2.549093	-2.079387

Sum of electronic and zero-point Energies= -1150.987744  
Sum of electronic and thermal Energies= -1150.966153  
Sum of electronic and thermal Enthalpies= -1150.965209  
Sum of electronic and thermal Free Energies= -1151.036501

#### myricatomentogenin-4-E1 (benzene)

C	1.398322	2.026985	-0.423971
O	1.939563	2.281447	-1.648011
H	1.190684	2.412780	-2.255085

C	2.227385	1.707009	0.661063
C	1.619079	1.519217	1.910608
H	2.247663	1.305961	2.773334
C	0.232176	1.496643	2.059073
H	-0.232757	1.258417	3.011981
C	-0.574064	1.659453	0.932784
O	-1.931012	1.359428	1.003196
C	-0.003945	1.998221	-0.298448
O	-0.695963	2.169092	-1.474752
C	-1.798926	3.087205	-1.477085
H	-2.701786	2.621843	-1.069497
H	-1.556543	3.993217	-0.906248
H	-1.971318	3.349438	-2.525749
C	-3.084879	-2.395291	-0.388328
H	-3.422117	-3.356654	-0.772371
C	-1.750739	-2.236901	0.008414
C	-0.761667	-3.388458	-0.068792
H	-1.270847	-4.249578	-0.518600
H	-0.469959	-3.692200	0.946343
C	0.533853	-3.114458	-0.865137
H	0.361231	-2.410322	-1.693107
H	0.876993	-4.041419	-1.352788
C	1.728700	-2.617413	-0.051015
C	3.005687	-2.308443	-0.833692
H	2.931419	-2.733016	-1.842798
H	3.844785	-2.802361	-0.324509
C	3.273733	-0.782695	-0.935275
H	3.948093	-0.604396	-1.784036
C	3.879286	-0.161313	0.338582
H	4.954066	-0.394443	0.374321
C	3.690464	1.376381	0.456504
H	4.277213	1.734303	1.313399
H	4.082482	1.877369	-0.436365
H	3.427856	-0.633236	1.219918
H	2.334051	-0.280471	-1.194523
O	1.676971	-2.480328	1.158620
C	-1.351157	-0.982305	0.496152
H	-0.331186	-0.837265	0.834455
C	-2.255102	0.073831	0.559932
C	-3.595064	-0.097170	0.178676
O	-4.479834	0.940729	0.252980
H	-4.021393	1.682661	0.677950
C	-4.002743	-1.342639	-0.295427
H	-5.038836	-1.470725	-0.600027

Sum of electronic and zero-point Energies= -1151.062233  
Sum of electronic and thermal Energies= -1151.039700  
Sum of electronic and thermal Enthalpies= -1151.038756  
Sum of electronic and thermal Free Energies= -1151.112944

#### myricatomentogenin-4-E2 (benzene)

C	1.739826	1.889063	0.282921
O	2.542571	2.098190	1.359743
H	1.954693	2.315438	2.104050
C	2.292207	1.410124	-0.916578
C	1.431898	1.257354	-2.012190
H	1.847323	0.933275	-2.964684
C	0.050475	1.419771	-1.891170
H	-0.618718	1.209705	-2.721508
C	-0.488444	1.752317	-0.649223
O	-1.862138	1.654312	-0.436498
C	0.350798	2.064711	0.424005
O	-0.086448	2.379905	1.689524
C	-0.928198	3.537487	1.804282
H	-0.441767	4.419011	1.363878
H	-1.896433	3.368451	1.321572
H	-1.075287	3.696930	2.876850
C	-3.345513	-2.204159	0.103261
H	-3.763610	-3.203450	0.214180
C	-2.016203	-1.964177	0.476123
C	-1.135591	-3.070904	1.032038

H	-1.732631	-3.988911	1.094782
H	-0.830120	-2.823017	2.057827
C	0.144390	-3.734817	0.220727
H	-0.013157	-3.221056	-0.857395
H	0.405420	-4.441635	0.317217
C	1.401213	-2.611695	0.639238
C	2.659844	-2.860578	-0.193722
H	2.500342	-3.721620	-0.854933
H	3.477024	-3.117202	0.494809
C	3.056143	-1.622886	-1.042827
H	3.702924	-1.962156	-1.864425
C	3.771002	-0.509794	-0.252979
H	4.824118	-0.792228	-0.106593
C	3.710659	0.886662	-0.933237
H	4.383091	1.567107	-0.396620
H	4.073798	0.819448	-1.968404
H	3.329055	-0.425573	0.745954
H	2.149737	-1.224538	-1.517809
O	1.412163	-1.853509	1.592818
C	-1.512359	-0.663497	0.319973
H	-0.494244	-0.444525	0.622453
C	-2.306572	0.345697	-0.215101
C	-3.638649	0.100548	-0.584520
O	-4.412063	1.090209	-1.112252
H	-3.853396	1.879652	-1.194875
C	-4.153219	-1.184570	-0.412385
H	-5.183081	-1.375897	-0.704816

Sum of electronic and zero-point Energies= -1151.062797  
Sum of electronic and thermal Energies= -1151.040179  
Sum of electronic and thermal Enthalpies= -1151.039235  
Sum of electronic and thermal Free Energies= -1151.114307

#### myricatomentogenin-5-TS (benzene)

C	2.792722	1.238030	0.154171
O	4.035352	1.760883	-0.024952
H	4.656076	1.011893	-0.002368
C	1.663568	2.078021	0.176298
C	0.471091	1.417131	0.374758
H	-0.419597	1.987549	0.486140
C	0.328202	0.063441	0.411655
H	-0.672595	-0.297591	0.403327
C	1.417515	-0.788861	0.467814
O	1.196586	-2.170534	0.683652
C	2.682076	-0.183461	0.338828
O	3.899788	-0.828927	0.392941
C	4.038295	-2.046107	-0.348371
H	3.650024	-1.932028	-1.370395
H	5.111934	-2.255397	-0.389773
H	3.528429	-2.873653	0.158074
C	-2.777326	-2.342818	-0.447672
H	-3.768997	-2.204708	-0.874053
C	-2.461961	-1.728728	0.777513
C	-3.354839	-0.634682	1.368201
H	-3.454476	-0.774911	2.453377
H	-4.360373	-0.714881	0.940997
C	-2.867369	0.852541	1.165983
H	-1.855077	0.989636	1.553795
H	-3.506687	1.477560	1.811425
C	-3.046908	1.462359	-0.244850
C	-2.069041	2.481359	-0.927093
H	-2.670080	2.886082	-1.749233
H	-1.336409	1.821698	-1.414900
C	-1.299239	3.675022	-0.236329
H	-1.898215	4.575519	-0.422389
C	0.156437	3.966137	-0.805840
H	0.211429	3.538135	-1.817010
C	1.486011	3.574327	-0.048085
H	2.317479	3.982594	-0.636962
H	1.518656	4.104664	0.917277
H	0.223266	5.053479	-0.944363

H	-1.279016	3.582607	0.857622
O	-4.002781	1.102115	-0.906302
C	-1.174627	-1.963837	1.296660
H	-0.873517	-1.489058	2.228352
C	-0.169013	-2.507052	0.484384
C	-0.495898	-3.098826	-0.742104
O	0.461346	-3.617802	-1.554993
H	1.316880	-3.482771	-1.117033
C	-1.832301	-3.081515	-1.162989
H	-2.085839	-3.547199	-2.112258
Sum of electronic and zero-point Energies= -1150.975043			
Sum of electronic and thermal Energies= -1150.953560			
Sum of electronic and thermal Enthalpies= -1150.952616			
Sum of electronic and thermal Free Energies= -1151.023971			

myricatomentogenin-5-E1 (benzene)

C	-2.084927	-1.721350	0.159353
O	-2.964885	-1.922569	1.176251
H	-2.455611	-2.311370	1.908790
C	-2.522384	-1.101533	-1.020041
C	-1.597844	-0.978922	-2.066864
H	-1.926311	-0.551662	-3.012293
C	-0.259987	-1.330774	-1.904767
H	0.465722	-1.161329	-2.695757
C	0.189255	-1.804786	-0.669763
O	1.558284	-1.902941	-0.432465
C	-0.727465	-2.062305	0.357858
O	-0.467481	-2.625366	1.582301
C	0.683454	-2.210900	2.335490
H	0.796745	-1.119938	2.319296
H	0.496428	-2.542038	3.361755
H	1.594197	-2.685710	1.958465
C	3.693429	1.671478	-0.134380
H	4.286929	2.582378	-0.071841
C	2.292905	1.753335	-0.185576
C	1.580939	3.101590	-0.185394
H	2.051959	3.739145	-0.946372
H	1.739632	3.612124	0.774576
C	0.057170	3.070271	-0.447413
H	-0.198479	2.390572	-1.268076
H	-0.250493	4.074761	-0.775262
C	-0.777242	2.785117	0.809441
C	-1.915749	1.768281	0.765979
H	-2.396546	1.804653	1.751200
H	-1.441981	0.779835	0.684105
C	-2.986490	1.896629	-0.340651
H	-3.462004	2.883123	-0.251543
C	-4.081367	0.800140	-0.233708
H	-4.179169	0.494220	0.815576
C	-3.893891	-0.470483	-1.111472
H	-4.672955	-1.190379	-0.825558
H	-4.078857	-0.205557	-2.161271
H	-5.050596	1.234981	-0.514146
H	-2.519932	1.869267	-1.335294
O	-0.506576	3.357519	1.849594
C	1.578452	0.554496	-0.267620
H	0.500061	0.572669	-0.316969
C	2.225203	-0.678476	-0.330754
C	3.622857	-0.753402	-0.279225
O	4.270412	-1.951431	-0.333121
H	3.602798	-2.643848	-0.459861
C	4.348162	0.437363	-0.174055
H	5.433543	0.377784	-0.138643
Sum of electronic and zero-point Energies= -1151.053828			
Sum of electronic and thermal Energies= -1151.031187			
Sum of electronic and thermal Enthalpies= -1151.030242			
Sum of electronic and thermal Free Energies= -1151.105379			

myricatomentogenin-5-E2 (benzene)

C	2.026023	-1.549778	0.378960
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O	2.836274	-1.533402	1.473511
H	2.301920	-1.868971	2.214150
C	2.484303	-1.050440	-0.849288
C	1.615381	-1.133031	-1.947648
H	1.964045	-0.791889	-2.920859
C	0.290857	-1.547957	-1.809628
H	-0.400974	-1.514601	-2.647481
C	-0.183184	-1.909586	-0.547253
O	-1.558322	-2.050361	-0.327383
C	0.699075	-1.997728	0.531554
O	0.329796	-2.321806	1.819252
C	-0.310179	-3.596341	2.001930
H	0.312123	-4.403740	1.592605
H	-0.416502	-3.725787	3.083216
H	-1.296745	-3.610501	1.528148
C	-3.320173	1.718286	-0.000290
H	-3.763615	2.712286	0.020117
C	-2.192975	1.446682	0.789809
C	-1.553287	2.503117	1.677676
H	-1.825641	2.323048	2.728672
H	-1.953570	3.490475	1.417555
C	-0.005195	2.574912	1.599598
H	0.445014	1.604132	1.836081
H	0.338444	3.285398	2.364234
C	0.493260	3.098645	0.248016
C	1.344395	2.189792	-0.631621
H	1.374655	2.653056	-1.625605
H	0.834950	1.222627	-0.724071
C	2.795993	1.974701	-0.130833
H	3.243633	2.963437	0.040242
C	3.689362	1.201223	-1.138269
H	3.333668	1.407010	-2.157939
C	3.814799	-0.334298	-0.940054
H	4.402460	-0.734229	-1.779107
H	4.392677	-0.531663	-0.030978
H	4.708868	1.608978	-1.090663
H	2.797423	1.463980	0.842291
O	0.191208	4.222307	-0.110795
C	-1.652987	0.156412	0.729393
H	-0.801127	-0.110191	1.344773
C	-2.171102	-0.798761	-0.138161
C	-3.301615	-0.526596	-0.919739
O	-3.808155	-1.457399	-1.773179
H	-3.241004	-2.243235	-1.709675
C	-3.883524	0.741487	-0.826585
H	-4.752475	0.961203	-1.442356
Sum of electronic and zero-point Energies= -1151.055251			
Sum of electronic and thermal Energies= -1151.032544			
Sum of electronic and thermal Enthalpies= -1151.031600			
Sum of electronic and thermal Free Energies= -1151.107280			

myricatomentogenin-6-TS (benzene)

C	1.120240	2.767136	-0.039484
O	1.576674	4.038370	0.121216
H	0.812735	4.624472	-0.019222
C	2.005783	1.676964	0.052426
C	1.415259	0.447554	-0.129233
H	2.043669	-0.407211	-0.181341
C	0.075893	0.233107	-0.281379
H	-0.234050	-0.786968	-0.293867
C	-0.809609	1.284300	-0.452681
O	-2.161301	1.027776	-0.778091
C	-0.270580	2.580653	-0.328751
O	-0.965807	3.761681	-0.496205
C	-2.217203	3.897240	0.184702
H	-2.446685	4.967788	0.192158
H	-3.012159	3.364629	-0.350565
H	-2.147611	3.533340	1.219398
C	-2.621672	-2.883240	0.509215
H	-2.605559	-3.858480	0.994368

C	-1.756397	-2.629936	-0.571920
C	-0.533770	-3.512577	-0.838590
H	-0.092199	-3.281506	-1.815586
H	-0.827335	-4.569413	-0.866960
C	0.584714	-3.352861	0.268388
H	0.925968	-4.358549	0.562227
H	0.160914	-2.917340	1.181178
C	1.896667	-2.606544	-0.097832
C	2.674349	-1.972238	1.083673
H	2.988022	-2.826481	1.709088
H	1.953311	-1.430272	1.708378
C	3.974974	-1.121285	0.846654
H	4.347298	-0.908418	1.859707
C	4.133578	0.206844	0.002549
H	5.218846	0.380184	0.027465
C	3.491453	1.594254	0.371719
H	4.054350	2.366345	-0.171401
H	3.657099	1.809487	1.439725
H	3.901658	-0.009946	-1.048214
H	4.712635	-1.804022	0.402949
O	2.311210	-2.578371	-1.239589
C	-1.864240	-1.374191	-1.190796
H	-1.236385	-1.142461	-2.046941
C	-2.525407	-0.319015	-0.546543
C	-3.357293	-0.575337	0.549201
O	-4.009981	0.426367	1.196199
H	-3.765989	1.258711	0.760759
C	-3.464693	-1.893398	1.017451
H	-4.127153	-2.095065	1.855845

Sum of electronic and zero-point Energies= -1150.985326  
Sum of electronic and thermal Energies= -1150.963847  
Sum of electronic and thermal Enthalpies= -1150.962903  
Sum of electronic and thermal Free Energies= -1151.033579

#### myricatomentogenin-6-E2 (benzene)

C	1.424746	1.797999	0.502494
O	1.961047	1.889201	1.753151
H	1.211578	2.009340	2.362242
C	2.250827	1.554070	-0.603087
C	1.644207	1.513447	-1.867633
H	2.271544	1.366730	-2.744919
C	0.259234	1.565200	-2.025532
H	-0.206392	1.437095	-2.999076
C	-0.550076	1.668811	-0.894819
O	-1.918767	1.435733	-0.999016
C	0.024810	1.857442	0.366117
O	-0.672329	1.949488	1.548291
C	-1.717903	2.929858	1.630966
H	-1.917259	3.068036	2.698217
H	-1.396536	3.882495	1.189554
H	-2.629420	2.580572	1.135686
C	-3.186318	-2.328191	0.267809
H	-3.546857	-3.288470	0.632877
C	-1.840409	-2.182209	-0.090668
C	-0.838696	-3.316301	0.042450
H	-0.461268	-3.612319	-0.946247
H	-1.349714	-4.192107	0.460717
C	0.382397	-2.978723	0.928486
H	0.798610	-3.911369	1.545099
H	0.090458	-2.373260	1.796641
C	1.566763	-2.319018	0.208397
C	2.518446	-1.527707	1.096939
H	2.632011	-2.092899	2.035527
H	1.994230	-0.609469	1.397631
C	3.917868	-1.217131	0.533036
H	4.521108	-0.829727	1.367692
C	4.073638	-0.255440	-0.664813
H	5.134046	-0.299658	-0.953844
C	3.725067	1.244389	-0.444830
H	4.284561	1.826151	-1.190934

H	4.081658	1.573181	0.538391
H	3.505425	-0.641196	-1.518666
H	4.382534	-2.171131	0.244274
O	1.743809	-2.462256	-0.987797
C	-1.415255	-0.928652	-0.554253
H	-0.386290	-0.790948	-0.865475
C	-2.294390	0.146786	-0.611476
C	-3.644806	-0.007498	-0.263353
O	-4.507674	1.049403	-0.323413
H	-4.027474	1.796916	-0.712868
C	-4.084437	-1.258137	0.168995
H	-5.129522	-1.374483	0.446405

Sum of electronic and zero-point Energies= -1151.061800  
Sum of electronic and thermal Energies= -1151.039265  
Sum of electronic and thermal Enthalpies= -1151.038321  
Sum of electronic and thermal Free Energies= -1151.112743

#### myricatomentogenin-6-E1 (benzene)

C	1.684216	1.845792	-0.278125
O	2.440978	2.154055	-1.363932
H	1.823605	2.444521	-2.057730
C	2.288856	1.272424	0.853451
C	1.478376	1.041808	1.972893
H	1.935863	0.651615	2.880479
C	0.093836	1.220892	1.929910
H	-0.537764	0.952638	2.772815
C	-0.499683	1.655804	0.745401
O	-1.881972	1.578571	0.587936
C	0.291856	2.038944	-0.340989
O	-0.198354	2.460397	-1.554624
C	-1.036694	3.626437	-1.536773
H	-1.221999	3.878726	-2.585248
H	-1.987541	3.419382	-1.034874
H	-0.528625	4.464430	-1.039765
C	-3.394475	-2.205866	-0.297238
H	-3.820068	-3.189141	-0.490903
C	-2.033855	-1.978274	-0.537504
C	-1.104241	-3.072055	-1.034740
H	-0.724695	-2.828433	-2.036910
H	-1.674859	-4.003758	-1.131724
C	0.116571	-3.323985	-0.119743
H	0.467586	-4.360377	-0.258837
H	-0.157455	-3.243696	0.940131
C	1.353509	-2.461246	-0.408394
C	2.284617	-2.229573	0.775191
H	2.312666	-3.162286	1.359685
H	1.770424	-1.508192	1.427527
C	3.727464	-1.785971	0.465030
H	4.303758	-1.885599	1.397801
C	3.991591	-0.384199	-0.125746
H	5.056012	-0.363131	-0.401920
C	3.738773	0.845358	0.792638
H	4.344821	1.676223	0.407069
H	4.103364	0.635177	1.808221
H	3.432325	-0.264035	-1.058393
H	4.159685	-2.519155	-0.231342
O	1.577869	-2.025293	-1.522553
C	-1.524809	-0.698533	-0.272247
H	-0.481405	-0.484781	-0.472163
C	-2.338156	0.301774	0.247933
C	-3.702541	0.069669	0.485103
O	-4.501650	1.047327	0.997804
H	-3.940653	1.818011	1.178689
C	-4.223710	-1.191886	0.197565
H	-5.279011	-1.372460	0.388643

Sum of electronic and zero-point Energies= -1151.061606  
Sum of electronic and thermal Energies= -1151.039035  
Sum of electronic and thermal Enthalpies= -1151.038090  
Sum of electronic and thermal Free Energies= -1151.112781

## galeon-1-TS (benzene)

C	-0.110924	3.095523	-0.009765
H	-0.170653	4.168222	-0.174468
C	1.130857	2.431465	-0.119114
C	1.103930	1.074115	0.098970
H	2.005991	0.517401	0.067273
C	-0.038112	0.373767	0.371553
H	0.082116	-0.681543	0.472994
C	-1.265487	0.986855	0.496920
O	-2.419337	0.232091	0.800192
C	-1.304201	2.390704	0.301192
O	-2.534691	2.968389	0.409145
C	-2.639674	4.373700	0.235443
H	-3.697341	4.613241	0.380299
H	-2.335288	4.682681	-0.775434
H	-2.040801	4.919820	0.978685
C	-1.359435	-3.475244	-0.703167
H	-0.967984	-4.342824	-1.233268
C	-0.697865	-3.007695	0.447595
C	0.742193	-3.418340	0.764928
H	0.852608	-4.506992	0.682687
H	1.003094	-3.147651	1.795064
C	1.793618	-2.752401	-0.205425
H	1.303796	-2.408160	-1.125129
H	2.510015	-3.520381	-0.539445
C	-1.279267	-1.918731	1.116903
H	-0.823225	-1.541789	2.029020
C	-2.250254	-1.131749	0.483933
C	-2.881403	-1.590317	-0.678522
O	-3.818865	-0.838140	-1.310482
H	-3.894335	-0.002906	-0.818302
C	-2.479307	-2.819766	-1.220545
H	-2.980087	-3.184252	-2.114386
C	2.675474	-1.604083	0.345282
C	3.494324	-0.786572	-0.699541
H	2.922938	-0.735440	-1.635374
H	4.357101	-1.432514	-0.929202
C	4.028655	0.640958	-0.288818
H	3.888171	0.771665	0.791887
C	3.481635	1.893321	-1.094225
H	4.361944	2.461485	-1.422462
C	2.524239	2.959321	-0.442648
H	2.995736	3.354510	0.471712
H	2.469578	3.809831	-1.137383
H	3.003247	1.535552	-2.017361
H	5.115134	0.623826	-0.435729
O	2.775927	-1.392684	1.536473

Sum of electronic and zero-point Energies= -1075.784143

Sum of electronic and thermal Energies= -1075.763522

Sum of electronic and thermal Enthalpies= -1075.762578

Sum of electronic and thermal Free Energies= -1075.832663

## galeon-1-E1 (benzene)

C	1.606334	-1.980999	0.481887
H	1.954726	-2.250175	1.475539
C	2.534297	-1.504916	-0.464597
C	2.091280	-1.212682	-1.757427
H	2.800579	-0.876940	-2.510677
C	0.728060	-1.272659	-2.072439
H	0.362919	-0.978801	-3.053665
C	-0.190774	-1.632708	-1.099178
O	-1.555550	-1.513402	-1.340208
C	0.244241	-2.052807	0.176882
O	-0.735377	-2.456610	1.028361
C	-0.368445	-2.816415	2.354544
H	-1.299881	-3.095236	2.855055
H	0.090825	-1.972019	2.888045
H	0.319665	-3.673653	2.363699
C	-3.336875	1.765420	0.516318
H	-3.820032	2.597201	1.026828

C	-2.084060	1.955321	-0.082150
C	-1.338831	3.274048	0.020444
H	-2.005146	4.028812	0.456072
H	-1.050255	3.639620	-0.974099
C	-0.054336	3.190024	0.882435
H	-0.238408	2.621464	1.802461
H	0.234151	4.206631	1.195547
C	-1.497653	0.861312	-0.737803
H	-0.537768	0.973664	-1.232495
C	-2.120847	-0.381228	-0.745439
C	-3.365649	-0.571283	-0.125509
O	-3.951676	-1.797297	-0.110998
H	-3.299167	-2.422485	-0.468751
C	-3.979464	0.522502	0.487049
H	-4.944402	0.377542	0.967319
C	1.170586	2.636348	0.143522
C	2.058475	1.671602	0.918026
H	1.454423	0.757297	1.034134
H	2.187618	2.053465	1.942655
C	3.414243	1.348183	0.270359
H	3.272468	1.257957	-0.812914
C	4.087197	0.070766	0.836889
H	5.160482	0.252191	0.985608
C	3.958589	-1.198128	-0.051386
H	4.568205	-1.058368	-0.954158
H	4.396045	-2.046858	0.494408
H	3.681920	-0.147726	1.835734
H	4.080523	2.209812	0.411159
O	1.404140	2.956859	-1.007414

Sum of electronic and zero-point Energies= -1075.855156

Sum of electronic and thermal Energies= -1075.833793

Sum of electronic and thermal Enthalpies= -1075.832849

Sum of electronic and thermal Free Energies= -1075.905209

## galeon-1-E2 (benzene)

C	-1.808652	-1.622339	0.758379
H	-2.283251	-1.512372	1.728861
C	-2.599393	-1.527405	-0.398832
C	-1.993529	-1.710130	-1.648458
H	-2.593067	-1.675030	-2.556232
C	-0.606059	-1.865331	-1.742720
H	-0.111596	-1.936924	-2.708878
C	0.177117	-1.868524	-0.594638
O	1.561472	-1.865617	-0.700541
C	-0.422726	-1.802389	0.679714
O	0.419507	-1.864170	1.739403
C	-0.109241	-1.613257	3.037542
H	0.745477	-1.659699	3.718119
H	-0.844245	-2.377125	3.328566
H	-0.567131	-0.616279	3.095736
C	3.587161	1.711888	-0.021840
H	4.153060	2.626190	0.150502
C	2.188062	1.762882	-0.092713
C	1.434659	3.068422	0.116696
H	2.055022	3.896384	-0.250504
H	1.294255	3.245625	1.193123
C	0.047144	3.152836	-0.549587
H	0.072486	2.769501	-1.577759
H	-0.241453	4.213437	-0.629473
C	1.503526	0.563474	-0.326166
H	0.423658	0.556085	-0.395448
C	2.181964	-0.643261	-0.461115
C	3.581508	-0.689143	-0.376639
O	4.253700	-1.867433	-0.506164
H	3.592199	-2.571115	-0.600901
C	4.276055	0.502409	-0.161709
H	5.361489	0.465090	-0.103372
C	-1.094004	2.492070	0.235168
C	-2.207826	1.868856	-0.599297
H	-1.747614	1.032026	-1.146543

H	-2.492320	2.586269	-1.385353
C	-3.441441	1.390851	0.182455
H	-3.112441	0.957398	1.134526
C	-4.316803	0.378620	-0.598088
H	-5.377550	0.569017	-0.383935
C	-4.053662	-1.119785	-0.279676
H	-4.402319	-1.325417	0.741570
H	-4.676121	-1.727561	-0.951658
H	-4.195757	0.543706	-1.678736
H	-4.045462	2.267785	0.451193
O	-1.103489	2.483289	1.451770

Sum of electronic and zero-point Energies= -1075.854672

Sum of electronic and thermal Energies= -1075.833358

Sum of electronic and thermal Enthalpies= -1075.832414

Sum of electronic and thermal Free Energies= -1075.904056

#### galeon-2-TS (benzene)

C	-0.164455	3.077293	-0.056700
H	-0.218680	4.153106	-0.201837
C	1.080439	2.413783	-0.158635
C	1.044394	1.053467	0.041454
H	1.941068	0.482349	0.051447
C	-0.111817	0.353713	0.245992
H	0.000912	-0.704472	0.289979
C	-1.334446	0.966639	0.401262
O	-2.482516	0.207667	0.718126
C	-1.361986	2.376767	0.246902
O	-2.583842	2.964422	0.388926
C	-2.674677	4.375863	0.264939
H	-2.383144	4.716081	-0.739685
H	-2.057066	4.889139	1.016236
H	-3.726931	4.622360	0.435283
C	-1.278399	-3.522370	-0.598931
H	-0.843884	-4.389429	-1.095239
C	-0.633515	-2.966434	0.521604
C	0.840131	-3.250595	0.830251
H	1.038021	-4.329344	0.795810
H	1.087641	-2.913477	1.843807
C	1.834849	-2.542236	-0.175163
H	1.294295	-2.078315	-1.012816
H	2.473157	-3.300835	-0.653551
C	-1.271246	-1.881681	1.147370
H	-0.817765	-1.429068	2.025826
C	-2.278904	-1.169986	0.482496
C	-2.892528	-1.714862	-0.651584
O	-3.863648	-1.039684	-1.319194
H	-3.974888	-0.182658	-0.874028
C	-2.435645	-2.950756	-1.133892
H	-2.923739	-3.382046	-2.004740
C	2.811422	-1.487207	0.402510
C	3.836753	-0.809798	-0.565364
H	4.005822	-1.499604	-1.403918
H	4.767306	-0.775452	0.016691
C	3.633178	0.616962	-1.219120
H	4.487518	0.713867	-1.902506
C	3.608715	1.893129	-0.292208
H	3.596538	1.586178	0.761904
C	2.467202	2.948304	-0.508493
H	2.713538	3.835813	0.092735
H	2.480543	3.288819	-1.556449
H	4.558554	2.425745	-0.430572
H	2.750017	0.593315	-1.867917
O	2.859302	-1.257658	1.595317

Sum of electronic and zero-point Energies= -1075.776490

Sum of electronic and thermal Energies= -1075.756137

Sum of electronic and thermal Enthalpies= -1075.755193

Sum of electronic and thermal Free Energies= -1075.823966

#### galeon-2-E1 (benzene)

C	-1.280743	2.166700	0.571158
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H	-1.639036	2.340530	1.581935
C	-2.213316	1.908667	-0.448649
C	-1.754446	1.747688	-1.760969
H	-2.464635	1.582700	-2.568792
C	-0.383343	1.676108	-2.024551
H	-0.011987	1.451399	-3.021679
C	0.527722	1.782825	-0.982732
O	1.863891	1.451855	-1.183215
C	0.094157	2.111152	0.317231
O	1.073818	2.276327	1.245074
C	0.691137	2.530172	2.590481
H	0.105736	1.698324	3.007752
H	0.115676	3.462862	2.677209
H	1.624969	2.629185	3.151032
C	2.964137	-2.257845	0.367858
H	3.280485	-3.209413	0.792759
C	1.685562	-2.141378	-0.193985
C	0.709032	-3.305431	-0.196004
H	1.237524	-4.204329	0.144773
H	0.366372	-3.508540	-1.219408
C	-0.541531	-3.110534	0.691736
H	-0.305085	-2.536319	1.599791
H	-0.896905	-4.087354	1.060859
C	1.316187	-0.901585	-0.739608
H	0.338278	-0.786680	-1.195950
C	2.185767	0.183272	-0.689355
C	3.458965	0.065339	-0.110170
O	4.289821	1.139812	-0.041217
H	3.778676	1.908248	-0.345439
C	3.847176	-1.172522	0.403622
H	4.833256	-1.264536	0.853121
C	-1.756129	-2.475119	0.015510
C	-2.954453	-2.170243	0.917463
H	-2.812547	-2.650993	1.893526
H	-3.849027	-2.612316	0.457024
C	-3.163314	-0.644799	1.117118
H	-3.744401	-0.492238	2.037707
C	-3.872077	0.057326	-0.057104
H	-3.517233	-0.372744	-1.001306
C	-3.655667	1.596000	-0.108796
H	-4.328553	2.016067	-0.868847
H	-3.937094	2.048509	0.852770
H	-4.950778	-0.151765	-0.001288
H	-2.184436	-0.181337	1.296719
O	-1.786054	-2.237245	-1.178865

Sum of electronic and zero-point Energies= -1075.853224

Sum of electronic and thermal Energies= -1075.831981

Sum of electronic and thermal Enthalpies= -1075.831036

Sum of electronic and thermal Free Energies= -1075.902761

#### galeon-2-E2 (benzene)

C	-1.673393	2.006508	-0.530639
H	-2.256044	2.061792	-1.445858
C	-2.330986	1.712224	0.676683
C	-1.587102	1.670025	1.860511
H	-2.084673	1.484460	2.810262
C	-0.191391	1.759577	1.815348
H	0.409193	1.627661	2.712626
C	0.456612	1.919680	0.598708
O	1.834801	1.759374	0.523436
C	-0.280106	2.118711	-0.587262
O	0.444887	2.325361	-1.714047
C	-0.243836	2.358616	-2.959052
H	-0.956345	3.194706	-3.004363
H	-0.770869	1.413387	-3.150099
H	0.528286	2.502980	-3.720011
C	3.288574	-2.104270	-0.044001
H	3.706092	-3.102538	-0.165782
C	1.924082	-1.889792	-0.273576
C	1.008538	-3.018956	-0.718814



H	1.571297	-3.959071	-0.666734
H	0.735782	-2.877359	-1.774356
C	-0.301504	-3.185530	0.082815
H	-0.175229	-2.888015	1.134770
H	-0.582016	-4.250664	0.125729
C	1.422150	-0.590151	-0.101058
H	0.373077	-0.394763	-0.289273
C	2.255566	0.451048	0.296919
C	3.626454	0.230522	0.513860
O	4.442994	1.250092	0.901797
H	3.895626	2.048265	0.973965
C	4.134086	-1.055845	0.338516
H	5.193469	-1.224784	0.517620
C	-1.529649	-2.467375	-0.476479
C	-2.820781	-2.591330	0.335740
H	-2.707024	-3.379565	1.090596
H	-3.623079	-2.899687	-0.349025
C	-3.208940	-1.261703	1.036303
H	-3.904940	-1.493963	1.854715
C	-3.846694	-0.213959	0.103617
H	-3.350680	-0.252253	-0.873632
C	-3.770704	1.244023	0.636483
H	-4.371023	1.887386	-0.021808
H	-4.220120	1.303183	1.637596
H	-4.900343	-0.478649	-0.069163
H	-2.312304	-0.844708	1.513090
O	-1.495680	-1.838570	-1.519758
Sum of electronic and zero-point Energies= -1075.852924			
Sum of electronic and thermal Energies= -1075.831591			
Sum of electronic and thermal Enthalpies= -1075.830647			
Sum of electronic and thermal Free Energies= -1075.902970			

#### galeon-3-TS (benzene)

C	-0.767101	3.012545	0.084928
H	-1.025919	4.056911	0.238330
C	-1.766063	2.015013	0.152167
C	-1.336312	0.727619	-0.056193
H	-2.050826	-0.053962	-0.120378
C	-0.023295	0.382941	-0.219593
H	0.179279	-0.664156	-0.256347
C	0.968601	1.328750	-0.360262
O	2.288540	0.946046	-0.680198
C	0.585136	2.686184	-0.203065
O	1.589034	3.600734	-0.326920
C	1.269550	4.977891	-0.196908
H	2.208779	5.517198	-0.352052
H	0.880740	5.212808	0.804956
H	0.539658	5.298104	-0.954646
C	2.311777	-3.029055	0.472859
H	2.186207	-4.011662	0.926358
C	1.488054	-2.649752	-0.604076
C	0.177148	-3.382663	-0.905647
H	0.350674	-4.464577	-0.962999
H	-0.224914	-3.075781	-1.878889
C	-0.929519	-3.129790	0.196551
H	-0.471513	-2.754000	1.119254
H	-1.372110	-4.100459	0.472463
C	1.735941	-1.393278	-1.180018
H	1.141131	-1.066779	-2.029189
C	2.501317	-0.436583	-0.498922
C	3.290154	-0.815086	0.593497
O	4.032379	0.095776	1.274345
H	3.861844	0.963693	0.870812
C	3.251412	-2.151723	1.018732
H	3.878369	-2.450248	1.855612
C	-2.156958	-2.248727	-0.164002
C	-2.894736	-1.583439	1.027861
H	-2.138759	-1.162444	1.702288
H	-3.330158	-2.423877	1.596476
C	-4.078451	-0.572750	0.800125

H	-4.876787	-1.140682	0.303031
C	-4.055529	0.804199	0.020504
H	-3.826277	0.610299	-1.035169
C	-3.257394	2.085483	0.467082
H	-3.728094	2.946688	-0.029341
H	-3.402224	2.252991	1.546760
H	-5.112698	1.105535	0.035715
H	-4.454893	-0.365848	1.812892
O	-2.546691	-2.142109	-1.309685
Sum of electronic and zero-point Energies= -1075.775605			
Sum of electronic and thermal Energies= -1075.755231			
Sum of electronic and thermal Enthalpies= -1075.754287			
Sum of electronic and thermal Free Energies= -1075.823191			

#### galeon-3-E1 (benzene)

C	-1.593551	1.925734	-0.534836
H	-2.107296	2.024096	-1.486818
C	-2.337418	1.584112	0.609042
C	-1.681813	1.502901	1.841547
H	-2.246650	1.282828	2.745401
C	-0.286555	1.609138	1.905053
H	0.247364	1.448482	2.839053
C	0.448037	1.826720	0.748176
O	1.829701	1.678675	0.764856
C	-0.202882	2.054896	-0.482665
O	0.600499	2.309325	-1.544193
C	0.005668	2.379074	-2.835475
H	0.830917	2.551483	-3.532063
H	-0.707432	3.212709	-2.907016
H	-0.499222	1.438186	-3.094949
C	3.332941	-2.077798	-0.242939
H	3.764310	-3.048035	-0.484201
C	1.943500	-1.907236	-0.269588
C	0.997730	-3.036277	-0.647377
H	1.542813	-3.986449	-0.586299
H	0.678701	-2.929261	-1.694551
C	-0.276777	-3.131662	0.219467
H	-0.059841	-2.912229	1.272870
H	-0.646472	-4.170503	0.202835
C	1.432351	-0.643605	0.057287
H	0.362884	-0.476796	0.037467
C	2.272681	0.410375	0.399959
C	3.666240	0.236063	0.413079
O	4.496255	1.264585	0.745304
H	3.943467	2.044833	0.910027
C	4.185534	-1.017354	0.089247
H	5.264755	-1.150872	0.109159
C	-1.475163	-2.296722	-0.253877
C	-2.457850	-1.883849	0.836269
H	-1.955143	-1.104764	1.428226
H	-2.556533	-2.736295	1.526400
C	-3.861306	-1.434965	0.386426
H	-4.274328	-2.221747	-0.260939
C	-4.032760	-0.092694	-0.357103
H	-3.400435	-0.089908	-1.252267
C	-3.798948	1.213830	0.451366
H	-4.323216	2.026029	-0.073319
H	-4.272992	1.129049	1.439408
H	-5.072347	-0.068066	-0.715187
H	-4.500689	-1.418179	1.282175
O	-1.637776	-2.023670	-1.428936

Sum of electronic and zero-point Energies= -1075.852131  
Sum of electronic and thermal Energies= -1075.830778  
Sum of electronic and thermal Enthalpies= -1075.829834  
Sum of electronic and thermal Free Energies= -1075.902144

#### galeon-3-E2 (benzene)

C	-1.414514	1.960688	0.598592
H	-1.818132	2.079509	1.600451
C	-2.292007	1.669444	-0.459641

C	-1.778825	1.585081	-1.759496
H	-2.448316	1.402801	-2.597585
C	-0.399461	1.631379	-1.978486
H	0.019754	1.470087	-2.968957
C	0.468044	1.782321	-0.905396
O	1.831773	1.565519	-1.076273
C	-0.030876	2.022901	0.390747
O	0.900644	2.231769	1.357150
C	0.454944	2.423797	2.693395
H	1.358957	2.586590	3.286957
H	-0.072781	1.538002	3.075372
H	-0.198127	3.303976	2.778744
C	3.163644	-2.157622	0.246960
H	3.538019	-3.108931	0.622013
C	1.841475	-2.060921	-0.204185
C	0.873076	-3.228679	-0.135173
H	1.414032	-4.121215	0.202536
H	0.470249	-3.459323	-1.130858
C	-0.324344	-2.983298	0.813426
H	-0.005517	-2.455336	1.721366
H	-0.722823	-3.953375	1.155823
C	1.399111	-0.818505	-0.682796
H	0.387794	-0.718684	-1.061576
C	2.233708	0.293516	-0.664302
C	3.555538	0.193996	-0.201287
O	4.364066	1.288180	-0.169099
H	3.819228	2.052041	-0.420308
C	4.017215	-1.047170	0.238028
H	5.040210	-1.122801	0.599478
C	-1.535106	-2.273900	0.190925
C	-2.385396	-1.455629	1.155331
H	-1.812905	-0.537407	1.354602
H	-2.401466	-1.990693	2.117218
C	-3.833040	-1.138516	0.732979
H	-4.323104	-2.088622	0.475725
C	-4.100443	-0.156831	-0.428240
H	-3.599447	-0.517563	-1.333433
C	-3.750016	1.341799	-0.203735
H	-4.374881	1.933622	-0.887883
H	-4.037003	1.643594	0.813761
H	-5.180152	-0.209496	-0.630765
H	-4.356506	-0.766054	1.626853
O	-1.805662	-2.393448	-0.989955

Sum of electronic and zero-point Energies= -1075.851657  
Sum of electronic and thermal Energies= -1075.830434  
Sum of electronic and thermal Enthalpies= -1075.829490  
Sum of electronic and thermal Free Energies= -1075.900966

#### galeon-4-TS (benzene)

C	-0.197866	3.145470	-0.244558
H	-0.198082	4.212852	-0.460653
C	-1.378705	2.378212	-0.275291
C	-1.216383	1.041063	0.019022
H	-2.065320	0.405530	0.052460
C	-0.010202	0.456227	0.278065
H	-0.034688	-0.599232	0.433279
C	1.165687	1.181778	0.312046
O	2.393445	0.538795	0.587086
C	1.063629	2.567387	0.049134
O	2.173654	3.375833	-0.006853
C	2.855909	3.562399	1.237104
H	3.687392	4.243946	1.029508
H	3.249983	2.616820	1.630782
H	2.190553	4.019120	1.984676
C	1.583741	-3.326958	-0.655552
H	1.243262	-4.254570	-1.114303
C	0.942910	-2.849225	0.502982
C	-0.436345	-3.363102	0.921875
H	-0.672002	-3.048297	1.945495
H	-0.450143	-4.460330	0.913316

C	-1.588623	-2.859702	-0.030776
H	-2.255186	-3.705667	-0.264359
H	-1.178470	-2.550093	-1.000395
C	1.460463	-1.677890	1.078157
H	1.019324	-1.286989	1.991779
C	2.328174	-0.852345	0.351170
C	2.935122	-1.322475	-0.819303
O	3.770540	-0.537593	-1.546514
H	3.795119	0.334539	-1.118273
C	2.613760	-2.611607	-1.269563
H	3.097884	-2.984140	-2.169159
C	-2.532764	-1.746186	0.486532
C	-3.461263	-1.070387	-0.567165
H	-4.270804	-1.802169	-0.720226
H	-2.932492	-1.029315	-1.528323
C	-4.104274	0.328457	-0.219401
H	-5.189815	0.208859	-0.316595
C	-3.701509	1.569292	-1.121846
H	-3.222980	1.197065	-2.039205
C	-2.825412	2.756110	-0.573568
H	-2.871772	3.563017	-1.318577
H	-3.299692	3.163555	0.333823
H	-4.640272	2.033966	-1.450610
H	-3.934108	0.539036	0.844340
O	-2.593137	-1.459112	1.664634

Sum of electronic and zero-point Energies= -1075.782130  
Sum of electronic and thermal Energies= -1075.761436  
Sum of electronic and thermal Enthalpies= -1075.760492  
Sum of electronic and thermal Free Energies= -1075.830289

#### galeon-4-E1 (benzene)

C	-1.666206	2.017811	-0.634777
H	-2.075136	2.245980	-1.617403
C	-2.506510	1.649342	0.424590
C	-1.929021	1.423283	1.682337
H	-2.560534	1.173625	2.532279
C	-0.542536	1.450706	1.841773
H	-0.082334	1.204841	2.796098
C	0.285153	1.706235	0.750822
O	1.659800	1.524100	0.883252
C	-0.273146	2.051175	-0.495576
O	0.452133	2.329139	-1.615920
C	1.588068	3.193701	-1.509995
H	1.722452	3.631882	-2.504692
H	2.495814	2.645707	-1.236263
H	1.409059	3.997636	-0.783702
C	3.266543	-2.145075	-0.264716
H	3.721894	-3.080948	-0.584251
C	1.892287	-2.098582	0.000191
C	1.014863	-3.331405	-0.142884
H	0.725888	-3.712747	0.846950
H	1.601760	-4.124031	-0.622905
C	-0.283700	-3.109477	-0.951405
H	-0.637418	-4.081601	-1.331522
H	-0.100294	-2.483640	-1.833645
C	1.341548	-0.871724	0.404438
H	0.286773	-0.799501	0.642720
C	2.134578	0.264994	0.514798
C	3.514626	0.206384	0.261730
O	4.292737	1.322507	0.373889
H	3.729485	2.036813	0.711388
C	4.073618	-1.009819	-0.125976
H	5.140754	-1.049971	-0.331524
C	-1.456814	-2.553024	-0.135207
C	-2.373166	-1.571402	-0.852377
H	-2.617305	-1.982040	-1.844851
H	-1.750564	-0.688694	-1.065281
C	-3.644947	-1.169486	-0.089393
H	-4.364028	-1.997319	-0.148743
C	-4.300778	0.130757	-0.619868

H	-4.009358	0.290439	-1.668179
C	-3.985718	1.413230	0.197547
H	-4.435433	2.271772	-0.321994
H	-4.486862	1.340271	1.172233
H	-5.393458	0.017125	-0.628968
H	-3.400990	-1.067523	0.974962
O	-1.631245	-2.884973	1.022653
Sum of electronic and zero-point Energies= -1075.851697			
Sum of electronic and thermal Energies= -1075.830144			
Sum of electronic and thermal Enthalpies= -1075.829199			
Sum of electronic and thermal Free Energies= -1075.901733			

galeon-4-E2 (benzene)

C	-1.808433	1.622197	0.758616
H	-2.282868	1.512163	1.729172
C	-2.599411	1.527498	-0.398471
C	-1.993794	1.710429	-1.648172
H	-2.593513	1.675539	-2.555835
C	-0.606325	1.865593	-1.742694
H	-0.112069	1.937353	-2.708945
C	0.177081	1.868529	-0.594780
O	1.561404	1.865571	-0.700952
C	-0.422534	1.802210	0.679692
O	0.419907	1.863808	1.739218
C	-0.108547	1.612516	3.037374
H	0.746314	1.658654	3.717795
H	-0.566520	0.615564	3.095383
H	-0.843442	2.376351	3.328793
C	3.587054	-1.711861	-0.021758
H	4.152930	-2.626150	0.150746
C	2.187974	-1.762912	-0.093057
C	1.434559	-3.068477	0.116161
H	1.294242	-3.245868	1.192568
H	2.054869	-3.896384	-0.251249
C	0.046985	-3.152700	-0.550000
H	-0.241689	-4.213267	-0.630068
H	0.072223	-2.769182	-1.578106
C	1.503482	-0.563528	-0.326717
H	0.423639	-0.556131	-0.396364
C	2.181925	0.643237	-0.461379
C	3.581427	0.689189	-0.376452
O	4.253612	1.867518	-0.505666
H	3.592116	2.571185	-0.600580
C	4.275951	-0.502360	-0.161379
H	5.361364	-0.465002	-0.102692
C	-1.094033	-2.491990	0.235006
C	-2.207973	-1.868697	-0.599269
H	-2.492563	-2.585999	-1.385378
H	-1.747818	-1.031783	-1.146446
C	-3.441476	-1.390748	0.182691
H	-4.045488	-2.267682	0.451449
C	-4.316914	-0.378420	-0.597647
H	-4.195995	-0.543392	-1.678327
C	-4.053685	1.119939	-0.279122
H	-4.676225	1.727805	-0.950946
H	-4.402177	1.325475	0.742200
H	-5.377642	-0.568809	-0.383389
H	-3.112305	-0.957379	1.134741
O	-1.103333	-2.483263	1.451602
Sum of electronic and zero-point Energies= -1075.854671			
Sum of electronic and thermal Energies= -1075.833358			
Sum of electronic and thermal Enthalpies= -1075.832413			
Sum of electronic and thermal Free Energies= -1075.904051			

galeon-5-TS (benzene)

C	-3.088690	0.606933	-0.010035
H	-4.141978	0.811132	0.163940
C	-2.152534	1.668364	-0.010440
C	-0.846784	1.305061	-0.235167
H	-0.086800	2.043415	-0.300169

C	-0.433688	0.005395	-0.326984
H	0.621633	-0.138177	-0.314965
C	-1.315349	-1.048535	-0.393735
O	-0.837863	-2.360227	-0.619542
C	-2.691153	-0.737866	-0.237388
O	-3.549106	-1.796967	-0.290303
C	-4.935334	-1.553922	-0.107001
H	-5.334964	-0.878892	-0.878050
H	-5.146924	-1.134586	0.887724
H	-5.423120	-2.529311	-0.196081
C	3.157449	-1.833864	0.337341
H	4.131457	-1.547563	0.731170
C	2.653540	-1.204961	-0.815476
C	3.246698	0.075751	-1.404773
H	2.660629	0.349665	-2.291401
H	4.272339	-0.094350	-1.763903
C	3.374943	1.353825	-0.474946
H	3.773704	2.149094	-1.119509
H	4.146837	1.137000	0.275336
C	1.410018	-1.652282	-1.290555
H	0.978099	-1.188251	-2.174070
C	0.567601	-2.428767	-0.484864
C	1.070237	-3.024733	0.676887
O	0.275056	-3.766450	1.489221
H	-0.623172	-3.734192	1.118932
C	2.406934	-2.783500	1.032769
H	2.796307	-3.254058	1.932358
C	2.194568	1.923311	0.363449
C	1.567248	3.290202	-0.039765
H	1.371803	3.281296	-1.122826
H	2.390219	4.014244	0.076229
C	0.315921	3.785342	0.784988
H	0.167542	3.087214	1.617159
C	-1.047123	4.025396	0.009466
H	-1.353770	5.061387	0.203759
C	-2.318129	3.150106	0.315194
H	-3.160252	3.595571	-0.235718
H	-2.575561	3.256885	1.381166
H	-0.857482	3.979581	-1.073096
O	0.596975	4.739872	1.246233
O	1.859193	1.356830	1.383372
Sum of electronic and zero-point Energies= -1075.771435			
Sum of electronic and thermal Energies= -1075.751132			
Sum of electronic and thermal Enthalpies= -1075.750188			
Sum of electronic and thermal Free Energies= -1075.818546			

galeon-5-E1 (benzene)

C	2.118071	1.843169	-0.253725
H	2.789319	2.100469	-1.068681
C	2.596117	1.036219	0.794565
C	1.743634	0.744613	1.864737
H	2.104955	0.156654	2.705207
C	0.401983	1.131407	1.820288
H	-0.291682	0.828714	2.601385
C	-0.089654	1.830043	0.725521
O	-1.465874	1.996078	0.570784
C	0.778686	2.253504	-0.301238
O	0.217206	2.974802	-1.305278
C	1.049732	3.387832	-2.381063
H	1.464942	2.527723	-2.926344
H	1.871123	4.030357	-2.033152
H	0.403802	3.960759	-3.052445
C	-3.446675	-1.524713	-0.475565
H	-3.979588	-2.447106	-0.701372
C	-2.128071	-1.352222	-0.919493
C	-1.360093	-2.425148	-1.668973
H	-0.673332	-1.953790	-2.385171
H	-2.055435	-3.030328	-2.265910
C	-0.567990	-3.408876	-0.764942
H	-0.119262	-4.175548	-1.418287

H	-1.253127	-3.923924	-0.081780
C	-1.488006	-0.146849	-0.611938
H	-0.478116	0.026580	-0.964537
C	-2.107418	0.828662	0.161210
C	-3.428622	0.654185	0.599035
O	-4.049049	1.605003	1.349998
H	-3.405743	2.314665	1.508966
C	-4.094607	-0.527544	0.261490
H	-5.117173	-0.660880	0.606918
C	0.573028	-2.858709	0.098478
C	1.677623	-2.033237	-0.567228
H	1.287641	-1.010180	-0.654428
H	1.828346	-2.379457	-1.600324
C	3.005955	-2.014681	0.212416
H	2.777342	-1.948783	1.282173
C	3.981760	-0.883396	-0.199503
H	5.010571	-1.268971	-0.178597
C	3.959652	0.385449	0.699004
H	4.697932	1.097639	0.303438
H	4.299177	0.105709	1.705631
H	3.793965	-0.588835	-1.242762
H	3.499085	-2.986737	0.074317
O	0.609544	-3.112507	1.287909

Sum of electronic and zero-point Energies= -1075.848275

Sum of electronic and thermal Energies= -1075.826808

Sum of electronic and thermal Enthalpies= -1075.825864

Sum of electronic and thermal Free Energies= -1075.898569

#### galeon-5-E2 (benzene)

C	-1.691348	-1.570653	0.777496
H	-2.076020	-1.351882	1.768916
C	-2.569208	-1.532488	-0.319105
C	-2.081241	-1.866704	-1.588407
H	-2.753716	-1.880811	-2.444263
C	-0.713714	-2.098593	-1.780696
H	-0.305955	-2.275519	-2.773502
C	0.162664	-2.012273	-0.706567
O	1.540057	-1.992546	-0.921358
C	-0.325255	-1.810661	0.601280
O	0.604693	-1.802949	1.588357
C	0.212494	-1.338262	2.878848
H	-0.520747	-2.013293	3.342722
H	-0.196017	-0.320582	2.823916
H	1.126153	-1.334357	3.479791
C	3.174724	1.779483	-0.201987
H	3.610689	2.750033	0.030372
C	1.918269	1.708240	-0.820728
C	1.071558	2.932415	-1.112491
H	0.425402	2.735083	-1.978437
H	1.712997	3.778689	-1.393049
C	0.200817	3.403622	0.086142
H	-0.341999	4.310609	-0.226346
H	0.845064	3.677863	0.929347
C	1.404973	0.439429	-1.113252
H	0.449010	0.347085	-1.617882
C	2.078250	-0.716530	-0.735687
C	3.325072	-0.642055	-0.099982
O	3.976184	-1.769494	0.290163
H	3.363703	-2.511377	0.154226
C	3.877978	0.619619	0.139714
H	4.846260	0.675930	0.631683
C	-0.842450	2.426488	0.634783
C	-1.905280	1.868726	-0.314633
H	-1.451474	0.990665	-0.794389
H	-2.094539	2.584824	-1.127001
C	-3.218812	1.458391	0.379619
H	-2.972468	1.001951	1.345002
C	-4.121197	0.509134	-0.448237
H	-5.173905	0.770852	-0.271928
C	-3.976962	-1.006876	-0.134045

H	-4.674702	-1.556903	-0.781038
H	-4.302902	-1.181089	0.900805
H	-3.947355	0.671279	-1.522193
H	-3.780066	2.372485	0.618022
O	-0.830362	2.121958	1.814441

Sum of electronic and zero-point Energies= -1075.851019

Sum of electronic and thermal Energies= -1075.829761

Sum of electronic and thermal Enthalpies= -1075.828817

Sum of electronic and thermal Free Energies= -1075.900375

#### galeon-6-TS (benzene)

C	-0.219298	3.188611	0.070913
H	-0.210915	4.269043	-0.063335
C	-1.399665	2.435104	-0.035806
C	-1.246851	1.076845	0.151177
H	-2.100695	0.447050	0.146407
C	-0.041665	0.474823	0.361339
H	-0.065410	-0.590530	0.419693
C	1.135914	1.187716	0.507542
O	2.334527	0.495475	0.819052
C	1.040448	2.593430	0.361004
O	2.078993	3.472801	0.511463
C	3.356974	3.120968	-0.014136
H	3.876331	2.398903	0.627627
H	3.934442	4.050978	-0.044703
H	3.271745	2.725165	-1.037154
C	1.569422	-3.290169	-0.685216
H	1.253968	-4.190144	-1.211813
C	0.859530	-2.867049	0.453997
C	-0.537413	-3.406177	0.766599
H	-0.832304	-3.148175	1.790715
H	-0.541271	-4.501441	0.699157
C	-1.642037	-2.862582	-0.218942
H	-2.315922	-3.693191	-0.484653
H	-1.191952	-2.547477	-1.168541
C	1.344491	-1.731022	1.120927
H	0.847384	-1.383592	2.023147
C	2.264926	-0.877337	0.496850
C	2.947052	-1.298085	-0.650880
O	3.847841	-0.493957	-1.274766
H	3.888026	0.337161	-0.775051
C	2.643145	-2.555869	-1.191588
H	3.185861	-2.887942	-2.073457
C	-2.587868	-1.747137	0.292003
C	-3.395567	-0.961631	-0.783302
H	-4.158385	-1.676153	-1.132502
H	-2.745897	-0.798985	-1.653167
C	-4.106526	0.378567	-0.352123
H	-5.176358	0.247007	-0.553736
C	-3.669806	1.717488	-1.080747
H	-3.142417	1.456708	-2.009753
C	-2.835447	2.836714	-0.352566
H	-2.858581	3.727979	-0.995311
H	-3.355723	3.125898	0.574735
H	-4.596110	2.213293	-1.399662
H	-4.032811	0.481377	0.738277
O	-2.737807	-1.542089	1.479353

Sum of electronic and zero-point Energies= -1075.780955

Sum of electronic and thermal Energies= -1075.760266

Sum of electronic and thermal Enthalpies= -1075.759322

Sum of electronic and thermal Free Energies= -1075.829166

#### galeon-6-E1 (benzene)

C	1.666498	2.017811	0.634774
H	2.075525	2.246064	1.617349
C	2.506682	1.649195	-0.424601
C	1.929083	1.423147	-1.682332
H	2.560539	1.173470	-2.532316
C	0.542610	1.450667	-1.841646
H	0.082282	1.204864	-2.795921

C	-0.285003	1.706275	-0.750607
O	-1.659648	1.524212	-0.882920
C	0.273416	2.051302	0.495690
O	-0.451694	2.329486	1.616084
C	-1.587828	3.193757	1.509983
H	-1.409057	3.997481	0.783383
H	-1.722167	3.632277	2.504539
H	-2.495511	2.645491	1.236584
C	-3.266854	-2.144942	0.264471
H	-3.722362	-3.080818	0.583771
C	-1.892493	-2.098477	0.000047
C	-1.015171	-3.331344	0.143343
H	-0.726411	-3.713028	-0.846428
H	-1.602091	-4.123752	0.623702
C	0.283548	-3.109407	0.951589
H	0.637208	-4.081549	1.331719
H	0.100347	-2.483493	1.833817
C	-1.341605	-0.871629	-0.403943
H	-0.286776	-0.799397	-0.641969
C	-2.134546	0.265135	-0.514545
C	-3.514666	0.206581	-0.261929
O	-4.292759	1.322692	-0.374263
H	-3.729526	2.037002	-0.711773
C	-4.073822	-1.009653	0.125492
H	-5.141041	-1.049771	0.330631
C	1.456599	-2.553138	0.135191
C	2.373100	-1.571553	0.852175
H	2.617324	-1.982170	1.844652
H	1.750629	-0.688764	1.065169
C	3.644791	-1.169736	0.089046
H	4.363777	-1.997660	0.148190
C	4.300870	0.130384	0.619547
H	4.009572	0.290064	1.667893
C	3.985891	1.412988	-0.197711
H	4.435736	2.271424	0.321893
H	4.486934	1.340080	-1.172450
H	5.393532	0.016596	0.628547
H	3.400666	-1.067640	-0.975261
O	1.630885	-2.885258	-1.022644

Sum of electronic and zero-point Energies= -1075.851696  
Sum of electronic and thermal Energies= -1075.830143  
Sum of electronic and thermal Enthalpies= -1075.829199  
Sum of electronic and thermal Free Energies= -1075.901730

#### galeon-6-E2 (benzene)

C	1.922485	1.820491	-0.665584
H	2.503963	1.878986	-1.583107
C	2.542193	1.537571	0.553261
C	1.750943	1.520998	1.716307
H	2.210941	1.350508	2.687997
C	0.368778	1.655699	1.622425
H	-0.264152	1.572771	2.503529
C	-0.247571	1.833549	0.380177
O	-1.639314	1.759412	0.304088
C	0.531306	1.985657	-0.778385
O	0.055269	2.190672	-2.034683
C	-1.148626	2.937893	-2.233476
H	-2.040812	2.314160	-2.114289
H	-1.097290	3.302106	-3.264955
H	-1.204201	3.794484	-1.549425
C	-3.353592	-2.036998	0.236601
H	-3.829229	-3.016146	0.254574
C	-2.035485	-1.916757	-0.221281
C	-1.237254	-3.126992	-0.674994
H	-1.011016	-3.062190	-1.748443
H	-1.852218	-4.024687	-0.537147
C	0.103881	-3.318698	0.072746
H	0.413284	-4.372921	-0.013551
H	-0.009148	-3.117168	1.145220
C	-1.455582	-0.637772	-0.227467

H	-0.445565	-0.500024	-0.597823
C	-2.160090	0.466156	0.240448
C	-3.484089	0.339075	0.693596
O	-4.172615	1.421262	1.151363
H	-3.570146	2.181755	1.119918
C	-4.076452	-0.923137	0.678872
H	-5.098196	-1.022132	1.037840
C	1.274413	-2.513981	-0.506077
C	2.249928	-1.913125	0.496411
H	2.487581	-2.674631	1.255778
H	1.675650	-1.147689	1.041744
C	3.529308	-1.310022	-0.104134
H	4.200089	-2.131379	-0.389609
C	4.269852	-0.341971	0.852942
H	4.012845	-0.583026	1.894791
C	4.010445	1.168316	0.599450
H	4.523481	1.742123	1.384947
H	4.480418	1.450016	-0.352248
H	5.354130	-0.498711	0.770428
H	3.273204	-0.799939	-1.040475
O	1.401366	-2.370345	-1.707857

Sum of electronic and zero-point Energies= -1075.851445  
Sum of electronic and thermal Energies= -1075.829858  
Sum of electronic and thermal Enthalpies= -1075.828913  
Sum of electronic and thermal Free Energies= -1075.901913

#### daec[n=1]-1-TS (dmf)

C	-3.011441	-0.021379	0.075931
H	-4.090635	0.004342	0.202947
C	-2.260537	1.175198	0.160984
C	-0.904335	1.036521	-0.018104
H	-0.270432	1.886473	-0.005865
C	-0.286460	-0.171662	-0.188006
H	0.777846	-0.136889	-0.220480
C	-0.978856	-1.356893	-0.302054
O	-0.289008	-2.560281	-0.529975
C	-2.392553	-1.276855	-0.176688
O	-3.070038	-2.453580	-0.297389
C	-4.488633	-2.433120	-0.174211
H	-4.952060	-1.800832	-0.944728
H	-4.803838	-2.084772	0.819528
H	-4.813770	-3.468461	-0.312919
C	3.458537	-1.498124	0.882649
H	4.334297	-1.070203	1.368104
C	3.015464	-0.964205	-0.339393
C	3.589785	0.346328	-0.886137
H	3.998169	0.170127	-1.892630
H	4.441121	0.640435	-0.257221
C	2.609963	1.568358	-1.036693
H	1.762397	1.256515	-1.663184
H	3.153663	2.310840	-1.639859
C	1.902766	-1.576443	-0.948223
H	1.532491	-1.194969	-1.897500
C	1.078011	-2.435460	-0.202038
C	1.527040	-2.966780	1.006366
H	0.891323	-3.644360	1.571679
C	2.761913	-2.538235	1.509064
H	3.130374	-2.947901	2.447646
C	2.054193	2.301510	0.221402
H	2.894637	2.715517	0.796901
H	1.568652	1.583567	0.893833
C	1.057631	3.467727	-0.153046
H	0.680740	3.282356	-1.169059
C	-0.189942	3.769771	0.787177
H	1.645105	4.391382	-0.237982
H	-0.158401	3.123656	1.675194
C	-1.629634	3.707799	0.116859
H	-1.500319	3.686047	-0.975213
C	-2.684366	2.602463	0.495784
H	-2.901559	2.670195	1.574351

H -3.625477 2.867420 -0.008229  
H -2.129178 4.661595 0.332086  
H -0.064059 4.789693 1.171767  
Sum of electronic and zero-point Energies= -926.530658  
Sum of electronic and thermal Energies= -926.512162  
Sum of electronic and thermal Enthalpies= -926.511218  
Sum of electronic and thermal Free Energies= -926.575602

daec[n=1]-1-E1 (dmf)

C -2.143013 -1.415809 -0.355709  
H -2.782817 -1.483800 -1.231280  
C -2.623269 -0.755062 0.789741  
C -1.810235 -0.700137 1.927908  
H -2.179036 -0.228785 2.836503  
C -0.504348 -1.198470 1.888336  
H 0.154799 -1.108706 2.749324  
C -0.003775 -1.760436 0.720435  
O 1.335090 -2.123061 0.644652  
C -0.835547 -1.918967 -0.408684  
O -0.273352 -2.517930 -1.489671  
C -1.065765 -2.651958 -2.668233  
H -1.366828 -1.672112 -3.063990  
H -1.960421 -3.262403 -2.484115  
H -0.427115 -3.156837 -3.398602  
C 4.104510 0.952424 0.104625  
H 4.844354 1.742284 -0.017676  
C 2.749717 1.220057 -0.157075  
C 2.318198 2.614033 -0.602873  
H 3.027618 2.954247 -1.370969  
H 2.451812 3.310844 0.240470  
C 0.883736 2.749442 -1.151635  
H 0.693457 1.918478 -1.846874  
H 0.834828 3.660796 -1.763467  
C 1.825741 0.180484 0.004574  
H 0.777837 0.353501 -0.201365  
C 2.230887 -1.087461 0.441755  
C 3.580107 -1.351599 0.690451  
H 3.884452 -2.341141 1.023107  
C 4.509106 -0.321443 0.513783  
H 5.562661 -0.517614 0.705991  
C -0.240956 2.803617 -0.088765  
H -0.376074 3.843040 0.247468  
H 0.053410 2.236723 0.805906  
C -1.567621 2.232877 -0.614317  
H -1.391716 1.189060 -0.908096  
C -2.749335 2.283995 0.375160  
H -1.855265 2.757126 -1.539904  
H -2.393087 2.041031 1.387028  
C -3.909154 1.329010 -0.009305  
H -3.863786 1.123381 -1.088781  
C -3.948154 -0.020662 0.762698  
H -4.259710 0.178195 1.797103  
H -4.728248 -0.650996 0.312250  
H -4.876427 1.821651 0.162056  
H -3.123599 3.316353 0.430848  
Sum of electronic and zero-point Energies= -926.604635  
Sum of electronic and thermal Energies= -926.585007  
Sum of electronic and thermal Enthalpies= -926.584063  
Sum of electronic and thermal Free Energies= -926.652406

daec[n=1]-1-E2 (dmf)

C -1.845873 -1.465139 0.624274  
H -2.256376 -1.477329 1.629550  
C -2.659705 -1.030027 -0.436165  
C -2.146861 -1.067214 -1.739209  
H -2.770241 -0.768543 -2.580088  
C -0.808590 -1.414452 -1.961017  
H -0.379518 -1.380565 -2.960301  
C 0.016028 -1.749240 -0.892592  
O 1.372779 -1.964469 -1.094178

C -0.512647 -1.835537 0.412997  
O 0.348247 -2.234582 1.383906  
C -0.126513 -2.274764 2.728570  
H -0.962480 -2.979067 2.838621  
H -0.437895 -1.279534 3.074545  
H 0.718992 -2.619708 3.330480  
C 3.959753 1.039010 0.214423  
H 4.651110 1.804973 0.563188  
C 2.606784 1.362019 0.010560  
C 2.109088 2.778890 0.280973  
H 2.818144 3.478069 -0.185682  
H 2.180536 2.976738 1.362755  
C 0.684610 3.113794 -0.204270  
H 0.564524 2.737050 -1.230708  
H 0.596250 4.206320 -0.280922  
C 1.747804 0.354655 -0.444217  
H 0.704186 0.574912 -0.626800  
C 2.211184 -0.948973 -0.662249  
C 3.558143 -1.262673 -0.470709  
H 3.908245 -2.276369 -0.650432  
C 4.425035 -0.255288 -0.034467  
H 5.477068 -0.489680 0.119626  
C -0.468213 2.582214 0.682206  
H -0.679012 3.309373 1.481291  
H -0.159134 1.659037 1.192981  
C -1.743216 2.289797 -0.124864  
H -1.499786 1.527646 -0.877765  
C -2.952679 1.813104 0.704862  
H -2.034406 3.186885 -0.694633  
H -2.610960 1.127507 1.494158  
C -4.047272 1.119359 -0.146388  
H -3.972631 1.471050 -1.185824  
C -4.020461 -0.435720 -0.135256  
H -4.350428 -0.782896 0.853327  
H -4.762336 -0.796022 -0.862017  
H -5.044140 1.422716 0.203047  
H -3.386308 2.676973 1.229006  
Sum of electronic and zero-point Energies= -926.605173  
Sum of electronic and thermal Energies= -926.585622  
Sum of electronic and thermal Enthalpies= -926.584677  
Sum of electronic and thermal Free Energies= -926.652329

daec[n=1]-2-TS (dmf)

C -2.894349 0.752418 0.024488  
H -3.918273 1.073231 0.198288  
C -1.845065 1.701193 0.046304  
C -0.585765 1.195819 -0.181452  
H 0.269331 1.828101 -0.186665  
C -0.337808 -0.133549 -0.362191  
H 0.690766 -0.383215 -0.455263  
C -1.321238 -1.096174 -0.380489  
O -0.971965 -2.450958 -0.551553  
C -2.651581 -0.634115 -0.193786  
O -3.626309 -1.586436 -0.216914  
C -4.976712 -1.179293 -0.019602  
H -5.305384 -0.477394 -0.799015  
H -5.120400 -0.719003 0.968189  
H -5.574393 -2.093531 -0.081706  
C 2.892933 -2.221054 0.904271  
H 3.831323 -1.964993 1.393829  
C 2.608234 -1.692464 -0.366199  
C 3.444496 -0.554531 -0.959777  
H 4.393355 -0.496480 -0.409060  
H 3.701915 -0.796232 -2.001310  
C 2.807958 0.893873 -1.004193  
H 1.898561 0.865179 -1.618389  
H 3.524263 1.499754 -1.579399  
C 1.401662 -2.089887 -0.977010  
H 1.151077 -1.708775 -1.965199  
C 0.380326 -2.662598 -0.198715

C	0.670591	-3.191544	1.058547
H	-0.117711	-3.651583	1.649979
C	1.963422	-3.027671	1.572323
H	2.209079	-3.441880	2.548379
C	2.544726	1.632252	0.339031
H	3.488882	1.607083	0.905011
H	1.831180	1.073898	0.957390
C	2.165099	3.165044	0.285058
H	2.918049	3.642119	-0.360818
C	0.783716	3.802720	-0.147470
H	2.368824	3.549819	1.295822
H	1.020450	4.869363	-0.266608
C	-0.449411	3.719143	0.842362
H	-0.173144	3.112963	1.716784
C	-1.843057	3.201793	0.327501
H	-2.597726	3.455626	1.085483
H	-2.129604	3.762804	-0.576797
H	-0.624125	4.731320	1.230514
H	0.500837	3.472724	-1.155711

Sum of electronic and zero-point Energies= -926.524957  
Sum of electronic and thermal Energies= -926.506560  
Sum of electronic and thermal Enthalpies= -926.505615  
Sum of electronic and thermal Free Energies= -926.569614

daec[n=1]-2-E1 (dmf)

C	-1.778118	-1.712222	-0.527502
H	-2.308594	-1.716017	-1.475202
C	-2.448836	-1.271280	0.625022
C	-1.779813	-1.306853	1.856057
H	-2.296411	-1.006022	2.765632
C	-0.421901	-1.630280	1.906764
H	0.133610	-1.575208	2.840686
C	0.266199	-1.941976	0.739499
O	1.651298	-2.038906	0.762815
C	-0.418917	-2.054829	-0.486725
O	0.325612	-2.417885	-1.562120
C	-0.316171	-2.470459	-2.835417
H	-0.696525	-1.483987	-3.134644
H	-1.139921	-3.197268	-2.840552
H	0.454502	-2.791421	-3.541981
C	3.795070	1.468609	0.036330
H	4.378507	2.368248	-0.154582
C	2.393308	1.515197	-0.054811
C	1.706371	2.826358	-0.422288
H	1.794879	3.520517	0.429188
H	2.302268	3.286473	-1.223202
C	0.227646	2.782713	-0.775914
H	0.047178	1.878819	-1.475598
H	0.071850	3.628489	-1.561386
C	1.671193	0.341599	0.189697
H	0.591029	0.359711	0.125479
C	2.326838	-0.856598	0.510938
C	3.721086	-0.897650	0.597199
H	4.217884	-1.832480	0.845864
C	4.444797	0.274116	0.359220
H	5.531467	0.249792	0.422526
C	-0.824876	2.907102	0.244627
H	-0.607968	3.826989	0.808592
H	-0.727413	2.081648	0.965792
C	-2.276074	2.972296	-0.286380
H	-2.285147	3.603085	-1.188045
C	-2.909814	1.598655	-0.606292
H	-2.909773	3.492848	0.447477
H	-3.639468	1.703209	-1.422643
C	-3.616265	0.955450	0.604665
H	-3.053324	1.179979	1.522266
C	-3.794240	-0.585139	0.520849
H	-4.450713	-0.906058	1.341615
H	-4.294524	-0.854970	-0.419383
H	-4.604210	1.422363	0.731591

H	-2.129365	0.926717	-0.988264
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Sum of electronic and zero-point Energies= -926.603984  
Sum of electronic and thermal Energies= -926.584405  
Sum of electronic and thermal Enthalpies= -926.583461  
Sum of electronic and thermal Free Energies= -926.651792

daec[n=1]-2-E2 (dmf)

C	1.688805	1.777386	0.511825
H	2.154324	1.847940	1.490934
C	2.449813	1.299159	-0.571603
C	1.866914	1.254506	-1.841801
H	2.450358	0.920710	-2.697541
C	0.503682	1.539213	-2.000755
H	0.014895	1.415917	-2.964959
C	-0.268915	1.880679	-0.899672
O	-1.652199	1.935839	-1.002808
C	0.330996	2.072882	0.364582
O	-0.494797	2.472944	1.364884
C	0.054464	2.601583	2.675207
H	0.859918	3.348295	2.701936
H	0.434105	1.640069	3.047406
H	-0.770480	2.936126	3.310593
C	-3.723665	-1.471072	0.235062
H	-4.286516	-2.347098	0.554731
C	-2.341363	-1.578981	0.000397
C	-1.656681	-2.932106	0.166073
H	-1.800019	-3.272256	1.203988
H	-2.219849	-3.652406	-0.445957
C	-0.161459	-3.060600	-0.198397
H	0.042733	-2.532091	-1.140939
H	0.026425	-4.123333	-0.410887
C	-1.646737	-0.437072	-0.411748
H	-0.583401	-0.500189	-0.603909
C	-2.308729	0.788267	-0.585270
C	-3.683487	0.887407	-0.362056
H	-4.185080	1.841848	-0.503002
C	-4.381324	-0.252624	0.049261
H	-5.452973	-0.183927	0.229049
C	0.840799	-2.629010	0.890772
H	0.604818	-3.190505	1.807443
H	0.707100	-1.566540	1.143791
C	2.313838	-2.895432	0.499607
H	2.361725	-3.861566	-0.024910
C	2.960224	-1.795517	-0.374659
H	2.916597	-3.022110	1.411540
H	3.716910	-2.239486	-1.037967
C	3.625818	-0.675296	0.451059
H	3.033371	-0.485680	1.357727
C	3.801087	0.674882	-0.294488
H	4.414361	1.341178	0.328721
H	4.347086	0.517905	-1.234820
H	4.610084	-1.022415	0.798564
H	2.195004	-1.370175	-1.038504

Sum of electronic and zero-point Energies= -926.604352  
Sum of electronic and thermal Energies= -926.584780  
Sum of electronic and thermal Enthalpies= -926.583836  
Sum of electronic and thermal Free Energies= -926.652141

daec[n=1]-3-TS (dmf)

C	3.035521	0.392877	0.078753
H	4.096801	0.572882	0.229661
C	2.126904	1.479001	0.057876
C	0.811813	1.136787	-0.141931
H	0.066125	1.884799	-0.224397
C	0.368625	-0.152603	-0.220382
H	-0.689716	-0.257304	-0.260754
C	1.215690	-1.237597	-0.248038
O	0.701572	-2.536286	-0.420102
C	2.601389	-0.951155	-0.102343
O	3.438423	-2.027003	-0.130853

C	4.836488	-1.802318	0.020017
H	5.231010	-1.158160	-0.778549
H	5.304704	-2.788844	-0.047178
H	5.071783	-1.355633	0.996508
C	-3.260395	-1.865661	0.608960
H	-4.214237	-1.524782	1.008311
C	-2.743542	-1.289641	-0.565595
C	-3.298281	0.005925	-1.173662
H	-4.293920	-0.178606	-1.605062
H	-2.654119	0.293960	-2.015044
C	-3.496844	1.231959	-0.203562
H	-4.205405	0.902752	0.569184
H	-4.042522	1.987267	-0.789288
C	-1.533926	-1.813410	-1.058735
H	-1.114164	-1.400666	-1.972913
C	-0.696645	-2.572595	-0.222595
C	-1.207241	-3.132697	0.946227
H	-0.567692	-3.729941	1.592121
C	-2.528617	-2.830780	1.310748
H	-2.946769	-3.273275	2.212981
C	-2.322289	1.948317	0.550313
H	-1.608588	1.202631	0.916751
H	-2.767773	2.375889	1.461014
C	-1.562431	3.118021	-0.156556
H	-2.281527	3.932873	-0.320683
C	-0.322034	3.705317	0.653738
H	-1.247025	2.814847	-1.165311
H	-0.179618	3.113377	1.568473
C	1.072677	3.860044	-0.092393
H	0.907659	3.751129	-1.174464
C	2.317548	2.975207	0.300272
H	2.552576	3.142751	1.363911
H	3.182978	3.366273	-0.255091
H	1.404340	4.897092	0.048712
H	-0.611325	4.705001	1.002082

Sum of electronic and zero-point Energies= -926.521100  
Sum of electronic and thermal Energies= -926.502615  
Sum of electronic and thermal Enthalpies= -926.501670  
Sum of electronic and thermal Free Energies= -926.565870

#### daec[n=1]-3-E1 (dmf)

C	2.202521	-1.375132	-0.388603
H	2.781854	-1.436484	-1.305865
C	2.684789	-0.584093	0.670153
C	1.959105	-0.540633	1.866652
H	2.341020	0.023698	2.714646
C	0.703682	-1.150988	1.950235
H	0.090146	-1.048604	2.842961
C	0.180935	-1.829621	0.856838
O	-1.151484	-2.230815	0.874414
C	0.956201	-2.011244	-0.308269
O	0.385404	-2.738567	-1.302294
C	1.110601	-2.892368	-2.521278
H	1.287338	-1.923795	-3.009032
H	0.479804	-3.512489	-3.164481
H	2.071096	-3.399223	-2.355667
C	-3.892897	0.766487	-0.127458
H	-4.620784	1.539850	-0.367902
C	-2.557783	0.909768	-0.535094
C	-2.066930	2.115329	-1.315905
H	-2.911812	2.552258	-1.865625
H	-1.345381	1.777870	-2.072842
C	-1.423170	3.249808	-0.476782
H	-2.174677	3.624732	0.234252
H	-1.215944	4.081654	-1.167398
C	-1.650944	-0.107725	-0.214107
H	-0.623435	-0.009236	-0.540997
C	-2.045979	-1.234386	0.513970
C	-3.381224	-1.383009	0.903710
H	-3.686162	-2.265141	1.461873

C	-4.294347	-0.376450	0.575363
H	-5.334276	-0.485234	0.878829
C	-0.134984	2.930759	0.308584
H	-0.346260	2.173839	1.078422
H	0.141740	3.844649	0.857663
C	1.079346	2.467155	-0.516698
H	1.203691	3.114817	-1.399333
C	2.392788	2.466492	0.298185
H	0.899126	1.458214	-0.909888
H	2.178310	2.109632	1.315168
C	3.537164	1.614392	-0.315216
H	3.281403	1.344018	-1.349913
C	3.885424	0.315000	0.466583
H	4.301244	0.591937	1.444989
H	4.677543	-0.215438	-0.080468
H	4.458514	2.209801	-0.378793
H	2.728744	3.506479	0.417258

Sum of electronic and zero-point Energies= -926.604152  
Sum of electronic and thermal Energies= -926.584558  
Sum of electronic and thermal Enthalpies= -926.583614  
Sum of electronic and thermal Free Energies= -926.651731

#### daec[n=1]-3-E2 (dmf)

C	1.966002	-1.338975	0.611712
H	2.404623	-1.222266	1.598102
C	2.683489	-0.887575	-0.509923
C	2.146977	-1.101807	-1.786210
H	2.704855	-0.798615	-2.670382
C	0.855885	-1.624347	-1.928889
H	0.394634	-1.716665	-2.910039
C	0.102475	-1.943082	-0.804829
O	-1.252830	-2.234928	-0.918995
C	0.676090	-1.866651	0.481819
O	-0.110813	-2.262158	1.515108
C	0.411472	-2.150009	2.837905
H	1.318384	-2.756966	2.964940
H	-0.373078	-2.529316	3.498879
H	0.630995	-1.105121	3.096685
C	-3.760210	0.983004	0.013655
H	-4.424240	1.806920	0.270766
C	-2.463458	1.247626	-0.453575
C	-1.925190	2.656779	-0.619751
H	-2.761494	3.338118	-0.828566
H	-1.272842	2.685104	-1.503389
C	-1.152454	3.230684	0.596225
H	-1.838971	3.272169	1.455252
H	-0.903458	4.275474	0.354782
C	-1.641376	0.163340	-0.783134
H	-0.648830	0.359097	-1.170465
C	-2.076405	-1.156048	-0.624126
C	-3.374743	-1.417439	-0.176906
H	-3.711685	-2.445378	-0.065659
C	-4.207864	-0.338434	0.135521
H	-5.219531	-0.534409	0.487029
C	0.134056	2.509184	1.045480
H	-0.112606	1.496639	1.398001
H	0.511680	3.047928	1.928917
C	1.269929	2.407721	0.010530
H	1.398628	3.374247	-0.502519
C	2.617946	1.991108	0.641385
H	0.998452	1.687438	-0.771846
H	2.431519	1.224531	1.406467
C	3.675052	1.465909	-0.367176
H	3.375066	1.736783	-1.389890
C	3.940185	-0.066336	-0.315343
H	4.394240	-0.312686	0.654284
H	4.680843	-0.313417	-1.088734
H	4.638894	1.964536	-0.193845
H	3.025907	2.854631	1.186097

Sum of electronic and zero-point Energies= -926.604170



Sum of electronic and thermal Energies= -926.584645  
Sum of electronic and thermal Enthalpies= -926.583701  
Sum of electronic and thermal Free Energies= -926.651289

daec[n=1]-4-TS (dmf)

C	-2.505417	1.963852	-0.002251
H	-3.377572	2.606175	0.110543
C	-1.189646	2.466790	0.037160
C	-0.214969	1.511234	-0.117617
H	0.800414	1.807310	-0.137813
C	-0.463189	0.179600	-0.229675
H	0.397096	-0.444452	-0.259287
C	-1.728587	-0.356273	-0.318103
O	-1.839340	-1.752717	-0.529413
C	-2.794117	0.578159	-0.202816
O	-4.125690	0.282120	-0.298209
C	-4.576919	-0.997665	0.144409
H	-4.218772	-1.217222	1.160387
H	-4.260690	-1.800053	-0.530940
H	-5.670193	-0.936454	0.154856
C	1.870956	-3.128100	0.777207
H	2.843266	-3.334352	1.222454
C	1.797201	-2.434336	-0.444648
C	3.030743	-1.766302	-1.066459
H	2.789553	-1.488663	-2.101945
H	3.850321	-2.496896	-1.127432
C	3.626059	-0.486131	-0.352146
H	4.472740	-0.161967	-0.975773
H	4.053834	-0.777593	0.618192
C	0.517202	-2.240308	-0.998952
H	0.419806	-1.719130	-1.948970
C	-0.642263	-2.439233	-0.221177
C	-0.553255	-3.124591	0.986812
H	-1.447216	-3.286860	1.584037
C	0.710256	-3.522136	1.447814
H	0.788092	-4.069366	2.385325
C	2.611940	0.667178	-0.154449
H	1.934686	0.337214	0.639138
H	2.024627	0.719241	-1.078192
C	3.085297	2.113569	0.213279
H	3.552259	2.580865	-0.667026
C	2.043786	3.141493	0.848829
H	3.885323	2.028988	0.963900
H	1.537888	2.641528	1.686665
C	0.973765	3.930384	-0.033000
H	1.225005	4.996696	0.040825
C	-0.575386	3.848149	0.290228
H	-1.071617	4.625990	-0.308370
H	-0.736649	4.138138	1.340805
H	1.110176	3.676261	-1.093885
H	2.677124	3.907376	1.316814

Sum of electronic and zero-point Energies= -926.516805  
Sum of electronic and thermal Energies= -926.498173  
Sum of electronic and thermal Enthalpies= -926.497229  
Sum of electronic and thermal Free Energies= -926.562330

daec[n=1]-4-E1 (dmf)

C	1.756336	1.857083	-0.601455
H	2.268460	2.022298	-1.547999
C	2.436950	1.293066	0.484949
C	1.744962	1.153680	1.699460
H	2.260391	0.777742	2.580677
C	0.377057	1.420490	1.762140
H	-0.186902	1.227707	2.672624
C	-0.318052	1.852579	0.630616
O	-1.714016	1.858324	0.665205
C	0.386466	2.157112	-0.548711
O	-0.179130	2.615780	-1.700892
C	-1.274756	3.538079	-1.623741
H	-1.123181	4.265886	-0.816304

H	-2.230246	3.024096	-1.477774
H	-1.286032	4.062644	-2.584978
C	-3.374702	-1.956545	0.238671
H	-3.801125	-2.955937	0.167946
C	-2.210797	-1.642878	-0.479986
C	-1.491239	-2.662350	-1.345524
H	-1.240247	-2.196944	-2.310287
H	-2.174101	-3.493649	-1.566304
C	-0.187671	-3.250561	-0.739695
H	0.193646	-3.997191	-1.452994
H	-0.432460	-3.801402	0.181354
C	-1.694901	-0.343795	-0.372307
H	-0.812956	-0.078054	-0.943215
C	-2.276919	0.597375	0.480623
C	-3.447141	0.289489	1.179944
H	-3.900404	1.033342	1.830836
C	-3.993279	-0.990357	1.041558
H	-4.902205	-1.241975	1.585319
C	0.913300	-2.220600	-0.437337
H	0.569737	-1.559761	0.369117
H	1.056200	-1.576586	-1.317705
C	2.264568	-2.828956	-0.019753
H	2.742266	-3.313925	-0.885820
C	3.225469	-1.802069	0.617460
H	2.084495	-3.628323	0.715975
H	2.694601	-1.334688	1.458114
C	3.768499	-0.702375	-0.330658
H	4.779395	-0.974304	-0.665478
C	3.826621	0.721101	0.294287
H	4.412229	1.370717	-0.370492
H	4.357725	0.679443	1.255351
C	3.155532	-0.644351	-1.240308
H	4.075737	-2.337031	1.064584

Sum of electronic and zero-point Energies= -926.600294  
Sum of electronic and thermal Energies= -926.580573  
Sum of electronic and thermal Enthalpies= -926.579628  
Sum of electronic and thermal Free Energies= -926.647958

daec[n=1]-4-E2 (dmf)

C	-1.623381	-1.700875	0.644521
H	-2.026430	-1.736404	1.654428
C	-2.441799	-1.353972	-0.440490
C	-1.884373	-1.400923	-1.728787
H	-2.506507	-1.181496	-2.594985
C	-0.519078	-1.638960	-1.909934
H	-0.071089	-1.594816	-2.900452
C	0.308523	-1.831680	-0.803973
O	1.694134	-1.814230	-0.950492
C	-0.254044	-1.935064	0.481417
O	0.512343	-2.131560	1.599802
C	1.229409	-3.373185	1.652665
H	1.939026	-3.468810	0.823246
H	0.532011	-4.222981	1.639300
H	1.774815	-3.367895	2.601576
C	3.396638	1.813842	0.252050
H	3.840035	2.746175	0.598223
C	2.149481	1.831342	-0.391111
C	1.370821	3.115885	-0.617539
H	1.028939	3.144106	-1.663016
H	2.045918	3.972124	-0.486288
C	0.134705	3.326594	0.298489
H	-0.290122	4.310482	0.047034
H	0.466231	3.393113	1.345999
C	1.614426	0.611993	-0.830268
H	0.666623	0.607317	-1.355604
C	2.267453	-0.597381	-0.580736
C	3.520130	-0.610768	0.037905
H	4.031750	-1.554539	0.210603
C	4.078626	0.605578	0.442913
H	5.051821	0.606976	0.930771

C	-0.958091	2.251100	0.180467
H	-0.564362	1.301690	0.565690
H	-1.181824	2.078483	-0.882739
C	-2.260967	2.575429	0.934358
H	-2.803127	3.382895	0.417199
C	-3.178673	1.348517	1.125201
H	-2.008508	2.968166	1.931697
H	-2.587059	0.574869	1.633072
C	-3.807101	0.761800	-0.164946
H	-4.838244	1.127923	-0.268006
C	-3.832354	-0.793390	-0.226125
H	-4.488832	-1.099944	-1.051845
H	-4.270256	-1.190306	0.700157
H	-3.269249	1.123261	-1.051845
H	-3.985463	1.610626	1.824852
Sum of electronic and zero-point Energies= -926.600152			
Sum of electronic and thermal Energies= -926.580456			
Sum of electronic and thermal Enthalpies= -926.579511			
Sum of electronic and thermal Free Energies= -926.647464			

daec[n=2]-1-TS (dmf)

C	-3.048924	-0.542773	-0.019245
H	-4.127862	-0.651820	0.055097
C	-2.471069	0.743426	0.073212
C	-1.094480	0.804632	-0.038991
H	-0.578016	1.740174	-0.013773
C	-0.312159	-0.320405	-0.171012
H	0.746344	-0.162756	-0.182034
C	-0.849301	-1.588981	-0.279010
O	-0.034294	-2.714997	-0.445644
C	-2.262118	-1.703360	-0.211469
O	-2.764929	-2.964175	-0.329296
C	-4.176762	-3.136167	-0.254489
H	-4.351922	-4.209520	-0.373724
H	-4.572914	-2.809847	0.717535
H	-4.693421	-2.592909	-1.058333
C	3.650474	-1.404717	0.944501
H	4.520608	-0.938566	1.404174
C	3.173511	-0.918312	-0.284211
C	3.726315	0.363637	-0.902277
H	4.198679	0.127268	-1.868031
H	4.528009	0.746580	-0.255992
C	2.696491	1.504661	-1.188051
H	1.898250	1.100600	-1.827296
H	3.221605	2.243185	-1.812446
C	2.068193	-1.569481	-0.857830
H	1.675460	-1.229037	-1.813074
C	1.302377	-2.462899	-0.096023
C	1.783330	-2.949529	1.119143
H	1.188601	-3.654311	1.695455
C	2.998339	-2.452030	1.605071
H	3.390879	-2.823760	2.549684
C	2.042094	2.270369	-0.006369
H	2.826052	2.750116	0.599709
H	1.528468	1.574770	0.669599
C	1.065027	3.364313	-0.527943
C	0.189096	4.165985	0.487455
C	-1.139427	3.596246	1.081474
H	-1.491190	4.350780	1.799975
H	-0.931763	2.708266	1.690179
H	-0.071917	5.110204	-0.014676
H	0.826009	4.454862	1.337741
H	0.423361	2.931719	-1.309154
H	1.679690	4.109770	-1.054978
C	-2.300848	3.319002	0.066885
H	-2.963728	4.194651	0.057361
H	-1.897177	3.248306	-0.953153
C	-3.193298	2.064590	0.315978
H	-3.578424	2.089429	1.348453
H	-4.081052	2.135986	-0.329584

Sum of electronic and zero-point Energies= -965.843558  
Sum of electronic and thermal Energies= -965.823961  
Sum of electronic and thermal Enthalpies= -965.823017  
Sum of electronic and thermal Free Energies= -965.889747

daec[n=2]-1-E1 (dmf)

C	-1.574859	-1.903255	-0.624235
H	-2.094996	-1.930448	-1.577686
C	-2.312008	-1.647407	0.546828
C	-1.647094	-1.642431	1.777786
H	-2.204506	-1.471167	2.696430
C	-0.256521	-1.796808	1.829267
H	0.278835	-1.741527	2.774801
C	0.472327	-1.972645	0.660261
O	1.857534	-2.032684	0.711673
C	-0.185887	-2.070161	-0.584764
O	0.606927	-2.281098	-1.666245
C	-0.011126	-2.322425	-2.951549
H	0.800228	-2.492870	-3.664850
H	-0.736386	-3.144594	-3.022545
H	-0.510466	-1.372585	-3.187391
C	4.041017	1.482398	0.202363
H	4.635264	2.386104	0.075327
C	2.646293	1.540204	0.043179
C	1.984284	2.873046	-0.287830
H	2.672568	3.423473	-0.944017
H	1.925616	3.475691	0.633350
C	0.588191	2.838906	-0.949681
H	0.542128	2.005373	-1.666573
H	0.479729	3.754536	-1.549332
C	1.907899	0.359854	0.203208
H	0.832408	0.375150	0.078989
C	2.543019	-0.847392	0.522372
C	3.931679	-0.899392	0.677203
H	4.410003	-1.844666	0.922492
C	4.671095	0.274188	0.514421
H	5.753172	0.242383	0.630472
C	-0.611104	2.763688	0.013544
H	-0.580626	3.634859	0.687361
H	-0.526445	1.880818	0.661154
C	-1.959743	2.744746	-0.727230
C	-3.200155	2.648951	0.185240
C	-3.413836	1.276958	0.856090
H	-4.123111	1.387832	1.690194
H	-2.469497	0.948389	1.310022
H	-4.096236	2.902866	-0.402277
H	-3.122208	3.421703	0.965506
H	-1.963722	1.911625	-1.446833
H	-2.037736	3.661632	-1.331749
C	-3.939920	0.186824	-0.095260
H	-5.005583	0.368023	-0.299835
H	-3.426933	0.254133	-1.065102
C	-3.772640	-1.259570	0.437527
H	-4.256850	-1.350501	1.419703
H	-4.295815	-1.945642	-0.243480

Sum of electronic and zero-point Energies= -965.895194  
Sum of electronic and thermal Energies= -965.874293  
Sum of electronic and thermal Enthalpies= -965.873349  
Sum of electronic and thermal Free Energies= -965.944824

daec[n=2]-1-E2 (dmf)

C	1.531227	1.965842	0.500972
H	2.011997	2.080096	1.468062
C	2.317259	1.627652	-0.614106
C	1.702790	1.521314	-1.868365
H	2.299084	1.286736	-2.748271
C	0.315372	1.654019	-1.989058
H	-0.179562	1.524369	-2.949273
C	-0.464421	1.902144	-0.865359
O	-1.847498	1.936178	-0.967499

C	0.141731	2.104984	0.392612
O	-0.695692	2.386588	1.423530
C	-0.129208	2.550953	2.722523
H	-0.970669	2.766047	3.387232
H	0.376504	1.635599	3.059362
H	0.578522	3.390895	2.748793
C	-3.981248	-1.423052	0.277363
H	-4.559734	-2.286631	0.602765
C	-2.615932	-1.575292	-0.022623
C	-1.976585	-2.953863	0.107723
H	-2.640071	-3.668857	-0.400358
H	-2.000095	-3.250290	1.168722
C	-0.545894	-3.148736	-0.433469
H	-0.455865	-2.670608	-1.420539
H	-0.404930	-4.224994	-0.611694
C	-1.898573	-0.449228	-0.444612
H	-0.849371	-0.538008	-0.699152
C	-2.522190	0.802135	-0.548748
C	-3.880851	0.945728	-0.259901
H	-4.350328	1.922229	-0.351331
C	-4.602627	-0.178361	0.151821
H	-5.662149	-0.076779	0.380997
C	0.593592	-2.668226	0.483867
H	0.519559	-3.195094	1.448704
H	0.472752	-1.600926	0.712215
C	1.983338	-2.923511	-0.126468
C	3.172247	-2.478639	0.750222
C	3.362171	-0.953271	0.871926
H	4.019048	-0.736843	1.728004
H	2.396034	-0.491794	1.113771
H	4.096672	-2.923767	0.350243
H	3.043547	-2.904892	1.757122
H	2.041322	-2.430229	-1.108961
H	2.081567	-4.001558	-0.327720
C	3.957364	-0.288973	-0.383036
H	5.031742	-0.519537	-0.438126
H	3.505085	-0.718311	-1.288326
C	3.774217	1.250555	-0.440600
H	4.178320	1.704806	0.474858
H	4.363864	1.641176	-1.281453

Sum of electronic and zero-point Energies= -965.895239  
Sum of electronic and thermal Energies= -965.874367  
Sum of electronic and thermal Enthalpies= -965.873423  
Sum of electronic and thermal Free Energies= -965.944659

daec[n=2]-2-TS (dmf)

C	-2.893437	-1.135959	0.004652
H	-3.923490	-1.471181	0.094077
C	-2.598436	0.244095	0.059327
C	-1.270190	0.592327	-0.072060
H	-0.990919	1.620685	-0.086028
C	-0.261804	-0.337029	-0.194820
H	0.739021	0.042492	-0.235332
C	-0.520540	-1.693053	-0.265737
O	0.509480	-2.626366	-0.426358
C	-1.875984	-2.104582	-0.171056
O	-2.097096	-3.446966	-0.251055
C	-3.438020	-3.915783	-0.150284
H	-3.379594	-5.004447	-0.241225
H	-4.067577	-3.517703	-0.958683
H	-3.885449	-3.656614	0.819763
C	3.921788	-0.628254	0.855813
H	4.709853	-0.010513	1.283655
C	3.327567	-0.247138	-0.358739
C	3.626213	1.104734	-1.001286
H	4.053824	0.950286	-2.003528
H	4.401599	1.610610	-0.409944
C	2.401064	2.058062	-1.180697
H	1.652636	1.544777	-1.801927
H	2.746645	2.912330	-1.781921

C	2.335752	-1.087776	-0.892345
H	1.864427	-0.833643	-1.838925
C	1.772829	-2.104353	-0.107983
C	2.371655	-2.484143	1.093142
H	1.936444	-3.285079	1.686103
C	3.488180	-1.768677	1.541200
H	3.969996	-2.055230	2.474140
C	1.699507	2.594300	0.091944
H	2.400823	3.218696	0.665944
H	1.448300	1.752830	0.751612
C	0.399074	3.402145	-0.210965
C	-0.615003	3.466535	0.974344
C	-2.124031	3.719392	0.650451
H	-2.183778	4.708795	0.170952
H	-2.630056	3.838518	1.621135
H	-0.312607	4.290583	1.637837
H	-0.518768	2.562045	1.588852
H	-0.081878	2.962157	-1.095485
H	0.663301	4.426029	-0.513256
C	-3.029482	2.792449	-0.235106
H	-3.927657	3.400309	-0.414030
H	-2.574240	2.657380	-1.226652
C	-3.562056	1.405469	0.263776
H	-4.507623	1.202806	-0.259572
H	-3.830178	1.483167	1.330320

Sum of electronic and zero-point Energies= -965.842858  
Sum of electronic and thermal Energies= -965.823222  
Sum of electronic and thermal Enthalpies= -965.822278  
Sum of electronic and thermal Free Energies= -965.889161

daec[n=2]-2-E1 (dmf)

C	-1.739571	-1.697799	-0.532313
H	-2.282233	-1.788481	-1.469021
C	-2.428658	-1.260487	0.614574
C	-1.735699	-1.183183	1.827493
H	-2.256440	-0.875707	2.732151
C	-0.364260	-1.459814	1.878129
H	0.192138	-1.362000	2.807970
C	0.320866	-1.831501	0.727864
O	1.692945	-2.040998	0.776687
C	-0.370130	-1.988002	-0.492906
O	0.374781	-2.384648	-1.556396
C	-0.274405	-2.508963	-2.820805
H	0.501176	-2.831749	-3.521119
H	-0.690464	-1.548419	-3.154765
H	-1.073163	-3.262607	-2.789990
C	4.210863	1.225208	0.152604
H	4.886063	2.068163	0.011934
C	2.847883	1.364659	-0.160891
C	2.323707	2.694024	-0.696181
H	2.961041	2.989436	-1.542731
H	2.487542	3.468514	0.070138
C	0.851440	2.729669	-1.147870
H	0.658736	1.869407	-1.806199
H	0.706760	3.620280	-1.775861
C	2.007710	0.260486	0.027933
H	0.955705	0.333120	-0.213599
C	2.502335	-0.945708	0.538499
C	3.860098	-1.083350	0.838593
H	4.233435	-2.026661	1.230068
C	4.706122	0.011367	0.637083
H	5.765260	-0.085643	0.870031
C	-0.185488	2.751385	-0.005989
H	-0.210596	3.757128	0.441422
H	0.130389	2.075847	0.800817
C	-1.597765	2.343248	-0.458771
C	-2.588463	2.202543	0.706878
C	-4.011371	1.759341	0.314332
H	-4.435060	2.515374	-0.365790
H	-4.641536	1.784162	1.217295

H	-2.668717	3.171628	1.224373
H	-2.172671	1.502310	1.444137
H	-1.526839	1.386202	-0.995802
H	-1.982588	3.073939	-1.188617
C	-4.190633	0.381924	-0.358273
H	-5.243210	0.315431	-0.669916
H	-3.603343	0.329714	-1.285798
C	-3.891935	-0.870993	0.507423
H	-4.443791	-1.714576	0.067159
H	-4.305263	-0.723969	1.514966
Sum of electronic and zero-point Energies= -965.893568			
Sum of electronic and thermal Energies= -965.872722			
Sum of electronic and thermal Enthalpies= -965.871778			
Sum of electronic and thermal Free Energies= -965.942718			

daec[n=2]-2-E2 (dmf)

C	-1.656363	-1.690084	0.538807
H	-2.136107	-1.761414	1.510525
C	-2.427211	-1.312031	-0.573257
C	-1.814070	-1.264192	-1.832746
H	-2.398980	-1.006508	-2.713743
C	-0.443300	-1.510982	-1.964202
H	0.049043	-1.438978	-2.931769
C	0.325597	-1.815210	-0.846400
O	1.697757	-1.990016	-0.966155
C	-0.282527	-1.940333	0.420920
O	0.538486	-2.274395	1.449583
C	-0.024967	-2.365385	2.757041
H	0.803481	-2.635797	3.417902
H	-0.799088	-3.143337	2.808102
H	-0.449418	-1.404707	3.079658
C	4.149449	1.174053	0.209823
H	4.804856	1.983419	0.528804
C	2.806038	1.447628	-0.100929
C	2.277115	2.875234	0.000322
H	2.904981	3.513883	-0.639126
H	2.449239	3.238538	1.025813
C	0.800749	3.097311	-0.377438
H	0.608702	2.641701	-1.360249
H	0.641526	4.176096	-0.516842
C	1.991564	0.384916	-0.509690
H	0.956744	0.562883	-0.772634
C	2.489352	-0.921800	-0.580062
C	3.828034	-1.187440	-0.284682
H	4.204010	-2.205670	-0.349579
C	4.651011	-0.126294	0.106224
H	5.695443	-0.322724	0.342895
C	-0.221355	2.568743	0.648944
H	-0.246742	3.246554	1.516383
H	0.111156	1.597183	1.039949
C	-1.637784	2.401953	0.073338
C	-2.617962	1.762839	1.068799
C	-4.042499	1.518558	0.534629
H	-4.476579	2.488813	0.244994
H	-4.663014	1.151269	1.367172
H	-2.697863	2.413401	1.954080
H	-2.191566	0.817223	1.430145
H	-1.575000	1.780409	-0.831936
H	-2.026219	3.379700	-0.255032
C	-4.225196	0.556930	-0.658565
H	-5.284835	0.610683	-0.947876
H	-3.661024	0.916301	-1.530544
C	-3.891146	-0.940587	-0.417843
H	-4.473945	-1.528690	-1.141508
H	-4.245913	-1.237894	0.578787
Sum of electronic and zero-point Energies= -965.893623			
Sum of electronic and thermal Energies= -965.872821			
Sum of electronic and thermal Enthalpies= -965.871876			
Sum of electronic and thermal Free Energies= -965.942431			

daec[n=2]-3-TS (dmf)			
C	-3.206698	0.763583	0.046493
H	-4.247675	1.062603	0.138060
C	-2.167400	1.721293	0.121506
C	-0.903707	1.211679	-0.010225
H	-0.108319	1.894732	-0.003903
C	-0.582806	-0.112752	-0.129292
H	0.463482	-0.352366	-0.137227
C	-1.567781	-1.070984	-0.237322
O	-1.229376	-2.416457	-0.424005
C	-2.916107	-0.616471	-0.153790
O	-3.868917	-1.587112	-0.264056
C	-5.237466	-1.206898	-0.170771
H	-5.811176	-2.131318	-0.286465
H	-5.518010	-0.504283	-0.968345
H	-5.467773	-0.757814	0.805906
C	2.750756	-2.682119	0.799725
H	3.760089	-2.636845	1.205618
C	2.463709	-2.030903	-0.412250
C	3.499161	-1.140737	-1.101642
H	3.560579	-1.433889	-2.159607
H	4.488311	-1.341561	-0.667510
C	3.224540	0.404504	-1.082700
H	2.169143	0.558616	-1.335369
H	3.795489	0.840161	-1.916205
C	1.154687	-2.145370	-0.919400
H	0.898511	-1.659652	-1.858823
C	0.123645	-2.677623	-0.126516
C	0.422792	-3.327983	1.070212
H	-0.379407	-3.749086	1.671644
C	1.753640	-3.367048	1.502615
H	2.000020	-3.877121	2.432002
C	3.592189	1.184513	0.208463
H	4.685188	1.154138	0.332098
H	3.173961	0.660733	1.082098
C	3.120677	2.679594	0.285942
C	1.580343	2.711378	0.219045
C	0.654293	3.935447	0.541261
H	1.138437	4.847001	0.161561
H	0.581019	4.065603	1.631135
H	1.294395	1.896002	0.890309
H	1.340073	2.389007	-0.800890
H	3.572790	3.268831	-0.526277
H	3.494268	3.100741	1.231106
C	-0.812015	3.989826	-0.101779
H	-0.701312	3.786929	-1.177947
H	-1.088263	5.051249	-0.033016
C	-2.126201	3.233052	0.388364
H	-2.261777	3.413818	1.466974
H	-2.967199	3.746426	-0.100070
Sum of electronic and zero-point Energies= -965.814187			
Sum of electronic and thermal Energies= -965.794260			
Sum of electronic and thermal Enthalpies= -965.793316			
Sum of electronic and thermal Free Energies= -965.860922			

daec[n=2]-3-E1 (dmf)

C	-1.992149	-1.663827	-0.477977
H	-2.544903	-1.754258	-1.408807
C	-2.640930	-1.133738	0.652248
C	-1.937828	-1.050354	1.858763
H	-2.430585	-0.665300	2.749352
C	-0.583714	-1.400032	1.912902
H	-0.015018	-1.298673	2.834923
C	0.070928	-1.848845	0.772384
O	1.424824	-2.147018	0.825730
C	-0.639494	-2.022820	-0.435462
O	0.074157	-2.504962	-1.484914
C	-0.593546	-2.653852	-2.736901
H	0.157255	-3.048041	-3.427651
H	-0.963256	-1.689755	-3.112313

H	-1.429171	-3.363408	-2.664739
C	4.236427	0.827051	0.034253
H	4.990386	1.590702	-0.151683
C	2.890264	1.092714	-0.269298
C	2.521269	2.431795	-0.901749
H	2.962866	2.453635	-1.910347
H	3.035976	3.230695	-0.346375
C	1.026186	2.777231	-1.022613
H	0.503543	1.952338	-1.524886
H	0.933073	3.640021	-1.698734
C	1.939019	0.094799	-0.014480
H	0.893264	0.272880	-0.234855
C	2.321704	-1.137034	0.532982
C	3.664572	-1.401006	0.818061
H	3.944321	-2.362697	1.241569
C	4.614965	-0.409206	0.563750
H	5.662017	-0.603945	0.789859
C	0.337290	3.119958	0.310148
H	0.769568	4.056155	0.695821
H	0.572399	2.347982	1.057647
C	-1.195615	3.262152	0.228485
C	-1.908402	1.953845	-0.157517
C	-3.421674	1.948609	0.120790
H	-3.872268	2.819492	-0.380739
H	-3.597427	2.098773	1.198228
H	-1.434657	1.132831	0.391826
H	-1.746347	1.741888	-1.224673
H	-1.464484	4.061963	-0.480013
H	-1.561279	3.592438	1.213290
C	-4.177124	0.686960	-0.350930
H	-3.869787	0.444957	-1.379589
H	-5.249781	0.924316	-0.404718
C	-4.047757	-0.582700	0.530725
H	-4.432838	-0.359239	1.535242
H	-4.711058	-1.350117	0.104442

Sum of electronic and zero-point Energies= -965.894453  
Sum of electronic and thermal Energies= -965.873522  
Sum of electronic and thermal Enthalpies= -965.872578  
Sum of electronic and thermal Free Energies= -965.943999

#### daec[n=2]-3-E2 (dmf)

C	-1.890395	-1.585493	0.634108
H	-2.365309	-1.540000	1.609852
C	-2.645591	-1.256461	-0.504271
C	-2.043003	-1.346986	-1.765295
H	-2.618053	-1.124547	-2.662257
C	-0.686055	-1.668293	-1.877823
H	-0.196476	-1.702632	-2.848875
C	0.075115	-1.912158	-0.739743
O	1.431722	-2.180052	-0.849672
C	-0.531208	-1.909641	0.534984
O	0.278687	-2.200930	1.584973
C	-0.281431	-2.159215	2.896616
H	0.536031	-2.417528	3.575688
H	-1.093357	-2.890571	3.010279
H	-0.655622	-1.155764	3.142067
C	4.169796	0.845861	0.007218
H	4.902282	1.617733	0.239215
C	2.850759	1.213690	-0.307896
C	2.479974	2.692007	-0.376293
H	2.925574	3.106500	-1.294516
H	2.985224	3.214000	0.450129
C	0.982150	3.048269	-0.365349
H	0.474260	2.511228	-1.177395
H	0.887374	4.115798	-0.613847
C	1.927122	0.199175	-0.596174
H	0.903571	0.450989	-0.848741
C	2.308063	-1.148212	-0.561828
C	3.625433	-1.507496	-0.265273
H	3.904547	-2.558226	-0.246407

C	4.550285	-0.498866	0.016681
H	5.577127	-0.769153	0.257349
C	0.275070	2.786166	0.975150
H	0.694913	3.467032	1.731714
H	0.508835	1.768352	1.321034
C	-1.257844	2.943833	0.942910
C	-1.959697	1.930391	0.019694
C	-3.463583	1.762235	0.299665
H	-3.945027	2.749718	0.222426
H	-3.607431	1.440268	1.343718
H	-1.458403	0.962594	0.130238
H	-1.826634	2.225439	-1.031677
H	-1.527445	3.971218	0.650481
H	-1.634265	2.811914	1.969331
C	-4.211986	0.792374	-0.640835
H	-3.916859	0.994385	-1.681611
H	-5.287751	1.014407	-0.583285
C	-4.057063	-0.724771	-0.354166
H	-4.418890	-0.932526	0.662307
H	-4.726962	-1.261219	-1.042107

Sum of electronic and zero-point Energies= -965.894697  
Sum of electronic and thermal Energies= -965.873767  
Sum of electronic and thermal Enthalpies= -965.872823  
Sum of electronic and thermal Free Energies= -965.944148

#### daec[n=2]-4-TS (dmf)

C	-3.109422	0.327137	0.057076
H	-4.171945	0.517070	0.185595
C	-2.196983	1.404171	0.122943
C	-0.864195	1.085262	-0.059450
H	-0.104788	1.835289	-0.052856
C	-0.430326	-0.207604	-0.239295
H	0.628859	-0.339985	-0.312127
C	-1.297623	-1.280576	-0.311108
O	-0.828135	-2.585554	-0.507649
C	-2.681956	-1.003399	-0.170848
O	-3.517639	-2.075914	-0.257750
C	-4.916618	-1.854151	-0.109346
H	-5.386005	-2.836562	-0.216574
H	-5.304048	-1.180416	-0.886619
H	-5.158347	-1.443217	0.881113
C	3.094986	-2.352762	0.830191
H	4.066586	-2.148941	1.277532
C	2.751140	-1.739959	-0.386342
C	3.607136	-0.634889	-0.994943
H	3.831650	-0.879752	-2.043709
H	4.570788	-0.604377	-0.468154
C	2.991839	0.808014	-0.997193
H	2.071269	0.802308	-1.597404
H	3.704595	1.434803	-1.554701
C	1.503305	-2.058812	-0.948601
H	1.211099	-1.615638	-1.898113
C	0.531476	-2.714745	-0.180046
C	0.878229	-3.328635	1.023437
H	0.121113	-3.851097	1.603452
C	2.189761	-3.189569	1.493016
H	2.478614	-3.668176	2.426905
C	2.732530	1.479420	0.374548
H	3.617094	1.306188	1.007289
H	1.900811	0.985429	0.894502
C	2.512926	3.024676	0.346876
C	1.210265	3.628764	-0.260978
C	-0.005539	3.835894	0.705982
H	0.152343	4.785984	1.234670
H	-0.002828	3.072022	1.494049
H	0.907547	3.036013	-1.134924
H	1.463608	4.615807	-0.673537
H	3.366048	3.457323	-0.197573
H	2.612130	3.390114	1.380556
C	-1.410048	3.880019	-0.005092

H	-1.840648	4.879650	0.139421
H	-1.262150	3.778798	-1.090223
C	-2.515584	2.863381	0.423959
H	-3.453879	3.158029	-0.068426
H	-2.705097	2.975260	1.504339

Sum of electronic and zero-point Energies= -965.840755  
Sum of electronic and thermal Energies= -965.821031  
Sum of electronic and thermal Enthalpies= -965.820087  
Sum of electronic and thermal Free Energies= -965.887180

daec[n=2]-4-E1 (dmf)

C	-1.759317	-1.987109	-0.496791
H	-2.301924	-2.083148	-1.433133
C	-2.445191	-1.535835	0.645333
C	-1.754443	-1.443256	1.858483
H	-2.275735	-1.119648	2.757180
C	-0.375791	-1.675404	1.902761
H	0.186399	-1.539902	2.824350
C	0.313144	-2.019891	0.746758
O	1.696577	-2.121643	0.776357
C	-0.381772	-2.236978	-0.462167
O	0.369110	-2.625289	-1.524364
C	-0.286885	-2.804342	-2.778721
H	0.492463	-3.120808	-3.477725
H	-0.736893	-1.867265	-3.134582
H	-1.060511	-3.582152	-2.719548
C	3.969947	1.300885	0.066372
H	4.585774	2.183020	-0.102916
C	2.607880	1.329631	-0.278738
C	2.045505	2.572483	-0.960313
H	2.416130	2.568340	-1.997993
H	2.505918	3.457361	-0.496252
C	0.518687	2.774944	-1.011379
H	0.039962	1.899371	-1.471723
H	0.334449	3.609752	-1.704735
C	1.834117	0.184792	-0.043546
H	0.779975	0.186289	-0.296522
C	2.410319	-0.965598	0.515257
C	3.769917	-0.993265	0.839255
H	4.198980	-1.893532	1.272616
C	4.541444	0.148368	0.611260
H	5.598904	0.138003	0.870075
C	-0.149510	3.108028	0.333954
H	0.450263	3.881835	0.838053
H	-0.122759	2.231557	0.996370
C	-1.593314	3.642783	0.208716
C	-2.635727	2.682140	-0.399331
C	-2.924620	1.447306	0.466885
H	-3.377105	1.762471	1.420815
H	-1.970291	0.976445	0.729932
H	-2.296428	2.352843	-1.393230
H	-3.569319	3.240001	-0.570781
H	-1.567553	4.560039	-0.400154
H	-1.938168	3.952995	1.207598
C	-3.822166	0.398332	-0.211361
H	-4.852492	0.775427	-0.292718
H	-3.469594	0.239367	-1.241502
C	-3.846933	-0.978298	0.508001
H	-4.487610	-1.662270	-0.066345
H	-4.300091	-0.869222	1.502784

Sum of electronic and zero-point Energies= -965.893875  
Sum of electronic and thermal Energies= -965.872977  
Sum of electronic and thermal Enthalpies= -965.872033  
Sum of electronic and thermal Free Energies= -965.943527

daec[n=2]-4-E2 (dmf)

C	-1.646440	-1.930252	0.606086
H	-2.119568	-1.913992	1.583623
C	-2.426350	-1.655904	-0.530362
C	-1.825410	-1.710957	-1.793953

H	-2.418737	-1.530949	-2.688634
C	-0.444976	-1.910837	-1.909284
H	0.045385	-1.891466	-2.880347
C	0.336704	-2.066758	-0.770350
O	1.719201	-2.125696	-0.868462
C	-0.265725	-2.135661	0.503915
O	0.569789	-2.349237	1.552669
C	0.008603	-2.363013	2.864202
H	0.845883	-2.549627	3.542655
H	-0.734610	-3.164571	2.974627
H	-0.454188	-1.398193	3.113329
C	3.868863	1.316743	0.095030
H	4.449634	2.200705	0.354422
C	2.542336	1.463609	-0.344792
C	1.971464	2.863550	-0.540422
H	2.324155	3.227155	-1.519236
H	2.436497	3.531298	0.199434
C	0.442499	3.056534	-0.495365
H	-0.039339	2.410888	-1.242600
H	0.243401	4.087757	-0.824930
C	1.814168	0.308742	-0.663697
H	0.790273	0.393360	-1.011719
C	2.398118	-0.960437	-0.547482
C	3.724675	-1.098341	-0.131077
H	4.160755	-2.090961	-0.048400
C	4.452428	0.050222	0.188792
H	5.483071	-0.047423	0.525808
C	-0.204374	2.854080	0.885200
H	0.389722	3.403840	1.631871
H	-0.144327	1.796099	1.176915
C	-1.661655	3.356672	0.983576
C	-2.699929	2.651580	0.086604
C	-2.932585	1.176817	0.445967
H	-3.339684	1.105336	1.467490
H	-1.961170	0.670113	0.474708
H	-2.385085	2.719890	-0.965797
H	-3.650834	3.202773	0.151970
H	-1.670330	4.432406	0.748046
H	-1.988091	3.274769	2.032232
C	-3.852839	0.425861	-0.531217
H	-4.888777	0.780872	-0.424301
H	-3.549673	0.662375	-1.562257
C	-3.833392	-1.119345	-0.366476
H	-4.507149	-1.559345	-1.114813
H	-4.226229	-1.391080	0.622877

Sum of electronic and zero-point Energies= -965.893919  
Sum of electronic and thermal Energies= -965.873129  
Sum of electronic and thermal Enthalpies= -965.872185  
Sum of electronic and thermal Free Energies= -965.942952

daec[n=2]-5-TS (dmf)

C	-2.953793	-1.088638	0.053072
H	-3.972936	-1.428247	0.218652
C	-2.671939	0.295311	0.069228
C	-1.356760	0.659654	-0.156476
H	-1.074222	1.689501	-0.201022
C	-0.349506	-0.269698	-0.324880
H	0.648586	0.111429	-0.421779
C	-0.600871	-1.628875	-0.350405
O	0.414013	-2.569390	-0.542134
C	-1.944159	-2.050943	-0.171446
O	-2.157534	-3.395452	-0.216976
C	-3.484929	-3.873121	-0.020621
H	-3.423304	-4.962457	-0.100437
H	-4.170214	-3.491192	-0.790477
H	-3.868824	-3.603555	0.973501
C	3.995901	-0.882485	0.753810
H	4.853044	-0.367774	1.185745
C	3.363176	-0.343866	-0.381361
C	3.690314	1.065035	-0.859681

H	3.435011	1.178391	-1.921962
H	4.771800	1.232478	-0.772856
C	2.950104	2.166734	-0.013064
H	3.645618	3.001701	0.149511
H	2.750868	1.750308	0.984460
C	2.290197	-1.058285	-0.934007
H	1.822678	-0.700362	-1.847284
C	1.696673	-2.111235	-0.219195
C	2.326288	-2.640720	0.906300
H	1.870351	-3.471510	1.439467
C	3.513533	-2.048100	1.355370
H	4.022360	-2.460483	2.224704
C	1.630045	2.733858	-0.601963
H	1.111088	1.953556	-1.173790
H	1.868976	3.520711	-1.333697
C	0.655479	3.289305	0.468948
C	-0.705546	3.820630	-0.090649
C	-1.990166	3.485458	0.757500
H	-2.345074	4.413268	1.224269
H	-1.712842	2.832170	1.595705
H	-0.842466	3.433953	-1.110510
H	-0.636498	4.909699	-0.214237
H	1.156650	4.084436	1.040672
H	0.462542	2.485124	1.193344
C	-3.195184	2.844656	-0.026202
H	-4.071797	3.494249	0.097187
H	-2.972194	2.854448	-1.103049
C	-3.666935	1.410102	0.362197
H	-3.916348	1.396131	1.436069
H	-4.616215	1.214109	-0.158158

Sum of electronic and zero-point Energies= -965.844758  
Sum of electronic and thermal Energies= -965.824863  
Sum of electronic and thermal Enthalpies= -965.823919  
Sum of electronic and thermal Free Energies= -965.891589

daec[n=2]-5-E1 (dmf)

C	-1.954628	-1.635801	-0.425311
H	-2.448715	-1.825918	-1.374110
C	-2.693845	-1.059555	0.625518
C	-2.060406	-0.845306	1.854279
H	-2.619763	-0.423851	2.687022
C	-0.702615	-1.151761	2.019613
H	-0.200401	-0.974431	2.968239
C	0.033037	-1.669619	0.962112
O	1.375569	-1.979133	1.124935
C	-0.596166	-1.937115	-0.276419
O	0.194365	-2.471111	-1.242211
C	-0.387331	-2.727211	-2.519360
H	0.416990	-3.142528	-3.133194
H	-0.760094	-1.803631	-2.983154
H	-1.205276	-3.457256	-2.448964
C	4.276503	0.625951	-0.350588
H	5.049517	1.287023	-0.740233
C	3.017906	1.154264	-0.013848
C	2.767487	2.649967	-0.190292
H	2.950464	2.909400	-1.245077
H	3.542351	3.188525	0.375695
C	1.386479	3.181089	0.231678
H	1.441837	4.277277	0.292243
H	1.169476	2.838259	1.254157
C	2.043820	0.279376	0.487550
H	1.068061	0.650932	0.777272
C	2.310597	-1.088509	0.625799
C	3.566851	-1.605283	0.302491
H	3.758185	-2.668951	0.421905
C	4.546569	-0.734278	-0.182949
H	5.528447	-1.127003	-0.441897
C	0.231453	2.774782	-0.705554
H	0.396651	1.747161	-1.056843
H	0.252740	3.403036	-1.608973

C	-1.158139	2.836124	-0.044899
C	-2.206871	2.001050	-0.793393
C	-3.560648	1.858795	-0.067421
H	-4.167604	2.756897	-0.251399
H	-3.393171	1.830157	1.020107
H	-1.782453	1.001333	-0.949915
H	-2.375805	2.414406	-1.800314
H	-1.490459	3.880875	0.060607
H	-1.076569	2.439004	0.979027
C	-4.352969	0.599144	-0.489789
H	-5.431158	0.812690	-0.480604
H	-4.105164	0.344041	-1.530822
C	-4.138118	-0.644854	0.413355
H	-4.588418	-0.440774	1.394390
H	-4.702954	-1.482210	-0.022371

Sum of electronic and zero-point Energies= -965.892063  
Sum of electronic and thermal Energies= -965.871087  
Sum of electronic and thermal Enthalpies= -965.870143  
Sum of electronic and thermal Free Energies= -965.941469

daec[n=2]-5-E2 (dmf)

C	-1.958859	-1.399076	0.745775
H	-2.474469	-1.266704	1.692455
C	-2.677363	-1.221627	-0.449001
C	-2.017705	-1.426784	-1.668640
H	-2.559101	-1.317701	-2.606599
C	-0.655824	-1.742212	-1.690460
H	-0.128958	-1.883652	-2.631865
C	0.058614	-1.875173	-0.502932
O	1.404386	-2.211107	-0.547288
C	-0.595754	-1.731018	0.737332
O	0.169059	-1.912145	1.844477
C	-0.445672	-1.741397	3.120769
H	0.343083	-1.924851	3.855769
H	-1.260469	-2.462262	3.273786
H	-0.831389	-0.720464	3.247379
C	4.345311	0.737458	-0.391892
H	5.132707	1.489517	-0.366603
C	3.024022	1.106235	-0.086660
C	2.720845	2.559940	0.268401
H	2.869503	3.177946	-0.631931
H	3.491759	2.895991	0.976707
C	1.331735	2.857496	0.862645
H	1.374506	3.828087	1.376870
H	1.115441	2.114988	1.644990
C	2.032145	0.115104	-0.119786
H	1.005885	0.360319	0.121721
C	2.346587	-1.204082	-0.467884
C	3.664252	-1.565848	-0.762812
H	3.892064	-2.595758	-1.026955
C	4.657656	-0.584714	-0.718546
H	5.686709	-0.857498	-0.946556
C	0.180046	2.875682	-0.163814
H	0.349538	2.093120	-0.915546
H	0.199718	3.825064	-0.720035
C	-1.209663	2.651071	0.461966
C	-2.247383	2.141499	-0.548560
C	-3.598643	1.733406	0.073850
H	-4.212823	2.632531	0.226558
H	-3.429319	1.315465	1.078097
H	-1.813932	1.273851	-1.062045
H	-2.420194	2.896047	-1.332132
H	-1.563452	3.569613	0.955908
H	-1.117411	1.896396	1.258623
C	-4.385787	0.705938	-0.771586
H	-5.465546	0.876408	-0.655541
H	-4.167254	0.863995	-1.838177
C	-4.128565	-0.780182	-0.405730
H	-4.523683	-0.959967	0.603501
H	-4.720443	-1.404752	-1.090492

Sum of electronic and zero-point Energies= -965.891718  
Sum of electronic and thermal Energies= -965.870712  
Sum of electronic and thermal Enthalpies= -965.869768  
Sum of electronic and thermal Free Energies= -965.941543

daec[n=2]-6-TS (dmf)

C	-3.146817	-0.286186	0.060628
H	-4.229894	-0.310570	0.149578
C	-2.466616	0.946283	0.189037
C	-1.091299	0.900407	0.055223
H	-0.499805	1.789063	0.108474
C	-0.410174	-0.279957	-0.133905
H	0.656052	-0.217261	-0.170707
C	-1.044549	-1.496951	-0.271801
O	-0.309482	-2.668948	-0.489306
C	-2.460247	-1.501600	-0.183028
O	-3.067158	-2.711943	-0.333542
C	-4.487609	-2.769420	-0.246713
H	-4.752275	-3.819926	-0.399173
H	-4.964979	-2.158370	-1.025729
H	-4.846073	-2.444948	0.740399
C	3.554428	-1.775541	0.797200
H	4.500347	-1.443045	1.222409
C	3.076956	-1.182125	-0.385828
C	3.752633	0.042226	-0.994603
H	3.425035	0.147326	-2.038209
H	4.840125	-0.116733	-1.020107
C	3.511733	1.411960	-0.267567
H	4.116628	2.153715	-0.811188
H	3.932215	1.359794	0.747581
C	1.875467	-1.672660	-0.922558
H	1.490939	-1.250731	-1.848356
C	1.052612	-2.529200	-0.171489
C	1.532652	-3.113550	0.998385
H	0.896956	-3.786114	1.569538
C	2.814690	-2.766659	1.448119
H	3.204853	-3.225471	2.354724
C	2.042813	1.893652	-0.205964
H	1.527463	1.303292	0.557117
H	1.565486	1.655007	-1.168037
C	1.791912	3.398450	0.084127
C	0.365608	3.920174	-0.297647
C	-0.822067	3.825883	0.729048
H	-0.881436	4.785201	1.260235
H	-0.608329	3.089309	1.513017
H	0.073952	3.416027	-1.230244
H	0.467342	4.979679	-0.570965
H	2.513120	3.983642	-0.506286
H	2.013195	3.625027	1.138322
C	-2.226166	3.540744	0.065773
H	-2.865134	4.418828	0.228516
H	-2.093144	3.474882	-1.023623
C	-3.074234	2.305995	0.513118
H	-4.066692	2.399587	0.048848
H	-3.253168	2.368367	1.599315

Sum of electronic and zero-point Energies= -965.839990  
Sum of electronic and thermal Energies= -965.820132  
Sum of electronic and thermal Enthalpies= -965.819188  
Sum of electronic and thermal Free Energies= -965.886664

daec[n=2]-6-E1 (dmf)

C	-2.082388	-1.735023	-0.390152
H	-2.759670	-1.764247	-1.239205
C	-2.542135	-1.208268	0.830142
C	-1.673939	-1.193476	1.927727
H	-2.017169	-0.810535	2.886817
C	-0.345095	-1.602928	1.781603
H	0.350720	-1.546782	2.616252
C	0.126112	-2.040277	0.548349
O	1.471579	-2.353612	0.390997

C	-0.754604	-2.155833	-0.547765
O	-0.220606	-2.631648	-1.702752
C	-1.074728	-2.740013	-2.840077
H	-0.451104	-3.148351	-3.640504
H	-1.464059	-1.759350	-3.146742
H	-1.913978	-3.422783	-2.648515
C	4.088174	0.896186	0.340491
H	4.777567	1.738907	0.349439
C	2.880230	0.998518	-0.369639
C	2.534437	2.270501	-1.125524
H	2.207539	2.012933	-2.144205
H	3.452175	2.863137	-1.235241
C	1.449090	3.172305	-0.480080
H	1.505633	4.156709	-0.968978
H	1.695929	3.340015	0.579323
C	2.014446	-0.106457	-0.369967
H	1.089078	-0.070007	-0.936549
C	2.330141	-1.264001	0.350595
C	3.541425	-1.366032	1.039558
H	3.774944	-2.277667	1.584332
C	4.418646	-0.278482	1.023442
H	5.363276	-0.345387	1.560321
C	0.015893	2.636127	-0.608246
H	-0.054090	1.669535	-0.094495
H	-0.190666	2.432484	-1.671582
C	-1.073855	3.579984	-0.069512
C	-2.499531	3.011509	-0.239167
C	-2.799800	1.818235	0.690596
H	-3.086007	2.186926	1.687834
H	-1.872935	1.253691	0.840101
H	-2.621275	2.696241	-1.287567
H	-3.238320	3.810030	-0.076393
H	-1.004621	4.544278	-0.595965
H	-0.885820	3.797124	0.994266
C	-3.870420	0.845583	0.166451
H	-4.870112	1.300499	0.230160
H	-3.685432	0.656138	-0.901447
C	-3.892781	-0.522579	0.900439
H	-4.671543	-1.150523	0.444853
H	-4.173744	-0.374415	1.952137

Sum of electronic and zero-point Energies= -965.893408  
Sum of electronic and thermal Energies= -965.872439  
Sum of electronic and thermal Enthalpies= -965.871495  
Sum of electronic and thermal Free Energies= -965.943099

daec[n=2]-6-E2 (dmf)

C	-1.655156	-1.876531	0.620362
H	-2.069765	-1.902659	1.623918
C	-2.502785	-1.565658	-0.456880
C	-1.972910	-1.566502	-1.753225
H	-2.616056	-1.354486	-2.605475
C	-0.602482	-1.769622	-1.957547
H	-0.172099	-1.723614	-2.955737
C	0.245010	-1.982270	-0.875701
O	1.616179	-2.092125	-1.063373
C	-0.285085	-2.089067	0.428885
O	0.605110	-2.359549	1.417957
C	0.121708	-2.416866	2.758802
H	0.994449	-2.641562	3.378476
H	-0.626340	-3.211965	2.882431
H	-0.309903	-1.456245	3.072011
C	3.924615	1.134366	0.233550
H	4.538087	1.962279	0.585327
C	2.690925	1.400049	-0.382189
C	2.214438	2.831149	-0.570171
H	1.918105	2.982008	-1.619349
H	3.066806	3.499744	-0.391363
C	1.040492	3.290367	0.335019
H	1.003007	4.389473	0.291124
H	1.261961	3.031602	1.381624



C	1.925712	0.311313	-0.832699
H	0.984121	0.484710	-1.344098
C	2.365654	-1.002087	-0.638721
C	3.603293	-1.258827	-0.043366
H	3.932367	-2.286545	0.089232
C	4.379362	-0.180276	0.385805
H	5.343361	-0.368290	0.855492
C	-0.332104	2.731328	-0.067267
H	-0.314153	1.638330	0.019619
H	-0.503329	2.950812	-1.133696
C	-1.517811	3.284973	0.742670
C	-2.877250	2.716687	0.279989
C	-3.071216	1.226488	0.628303
H	-3.419083	1.130009	1.668520
H	-2.093465	0.733893	0.597518
H	-2.950640	2.848497	-0.811100
H	-3.694140	3.313336	0.711913
H	-1.534811	4.381749	0.649882
H	-1.370830	3.069842	1.813320
C	-4.018129	0.461156	-0.312075
H	-5.061740	0.763378	-0.138564
H	-3.785437	0.736961	-1.351467
C	-3.916241	-1.084007	-0.191853
H	-4.616844	-1.535897	-0.907956
H	-4.234200	-1.398955	0.811582

Sum of electronic and zero-point Energies= -965.893848  
Sum of electronic and thermal Energies= -965.872898  
Sum of electronic and thermal Enthalpies= -965.871954  
Sum of electronic and thermal Free Energies= -965.943342

#### daec[n=2]-7-TS (dmf)

C	0.508573	3.118011	-0.187585
H	0.714023	4.182305	-0.296488
C	1.547346	2.166811	-0.215180
C	1.154845	0.847772	-0.049470
H	1.876413	0.059164	-0.020478
C	-0.160827	0.468281	0.067783
H	-0.346547	-0.584375	0.122734
C	-1.198380	1.387478	0.098562
O	-2.528630	0.972151	0.230692
C	-0.846897	2.752819	-0.021602
O	-1.789982	3.751554	-0.054195
C	-2.549997	3.919567	1.149253
H	-3.215221	4.771270	0.973550
H	-1.890187	4.144652	1.999960
H	-3.150187	3.030677	1.377785
C	-2.406102	-3.006584	0.946274
H	-2.224549	-4.002831	-1.346526
C	-1.838235	-2.643240	0.286332
C	-0.823610	-3.539530	0.991468
H	-0.690995	-4.453653	0.396860
H	-1.234848	-3.861596	1.960392
C	0.572717	-2.907456	1.297688
H	1.081011	-3.601058	1.984356
H	0.417082	-1.986769	1.878421
C	-2.123809	-1.359754	0.782184
H	-1.710925	-1.043627	1.737299
C	-2.701012	-0.394827	-0.053768
C	-3.270023	-0.759314	-1.273077
H	-3.727983	-0.003773	-1.907037
C	-3.166570	-2.093267	-1.685196
H	-3.608734	-2.397968	-2.631833
C	1.552456	-2.596973	0.133888
H	1.081192	-1.933555	-0.602824
H	1.784926	-3.526276	-0.408657
C	2.876092	-1.981371	0.674235
C	3.955543	-1.465026	-0.330280
C	3.863376	-0.061349	-1.010946
H	2.982007	-0.012911	-1.661523
H	4.719559	-0.007672	-1.698881

H	4.060415	-2.208831	-1.135128
H	4.912663	-1.487153	0.213017
H	3.365996	-2.764837	1.272051
H	2.636098	-1.189517	1.398471
C	3.928736	1.184542	-0.062969
H	4.969146	1.534507	-0.028996
H	3.688865	0.884180	0.967026
C	3.037792	2.412804	-0.422760
H	3.366940	3.271006	0.181004
H	3.220645	2.702626	-1.470247

Sum of electronic and zero-point Energies= -965.841033  
Sum of electronic and thermal Energies= -965.821256  
Sum of electronic and thermal Enthalpies= -965.820311  
Sum of electronic and thermal Free Energies= -965.887622

#### daec[n=2]-7-E1 (dmf)

C	-1.347441	2.051226	0.633995
H	-1.753435	2.188564	1.634284
C	-2.200759	1.833193	-0.457496
C	-1.628022	1.707437	-1.732894
H	-2.269266	1.568835	-2.601774
C	-0.240579	1.697243	-1.896736
H	0.207384	1.546833	-2.876720
C	0.594013	1.819222	-0.786550
O	1.967904	1.686634	-0.933265
C	0.042571	2.044942	0.487291
O	0.828331	2.157095	1.605389
C	1.644056	3.335971	1.666147
H	2.196463	3.275467	2.609102
H	1.018630	4.240193	1.668311
H	2.351908	3.382893	0.830308
C	3.712156	-1.902951	0.276547
H	4.189159	-2.829129	0.594303
C	2.345266	-1.905334	-0.054897
C	1.568143	-3.215216	0.022693
H	1.591552	-3.572059	1.064678
H	2.138315	-3.964814	-0.545849
C	0.111163	-3.232563	-0.478928
H	-0.154313	-4.281291	-0.678250
H	0.047982	-2.721455	-1.451492
C	1.758738	-0.701623	-0.464076
H	0.711371	-0.672848	-0.740513
C	2.513910	0.477830	-0.524459
C	3.873122	0.473189	-0.208069
H	4.445874	1.395282	-0.270332
C	4.463972	-0.729483	0.191627
H	5.522868	-0.745107	0.443975
C	-0.939777	-2.651608	0.484146
H	-0.697004	-1.608225	0.725658
H	-0.892732	-3.202628	1.437096
C	-2.367537	-2.744065	-0.083194
C	-3.471990	-2.188873	0.839541
C	-3.484904	-0.655103	0.995868
H	-2.466721	-0.311527	1.220547
H	-4.091609	-0.385114	1.873430
H	-3.361666	-2.648830	1.833689
H	-4.452237	-2.518799	0.461412
H	-2.588936	-3.801331	-0.296458
H	-2.402966	-2.229950	-1.056085
C	-4.031868	0.099415	-0.229385
H	-5.125718	-0.012952	-0.263855
H	-3.647895	-0.353345	-1.154648
C	-3.684927	1.611131	-0.255756
H	-4.247943	2.085802	-1.071147
H	-4.014783	2.081817	0.680837

Sum of electronic and zero-point Energies= -965.892013  
Sum of electronic and thermal Energies= -965.870899  
Sum of electronic and thermal Enthalpies= -965.869955  
Sum of electronic and thermal Free Energies= -965.941958

## daec[n=2]-7-E2 (dmf)

C	-1.574629	1.903396	-0.624172
H	-2.094646	1.930650	-1.577691
C	-2.311897	1.647539	0.546804
C	-1.647081	1.642502	1.777820
H	-2.204565	1.471235	2.696427
C	-0.256514	1.796817	1.829441
H	0.278733	1.741454	2.775034
C	0.472434	1.972634	0.660503
O	1.857661	2.032557	0.711956
C	-0.185656	2.070260	-0.584580
O	0.607246	2.281292	-1.665976
C	-0.010696	2.322663	-2.951350
H	0.800746	2.493055	-3.664565
H	-0.735860	3.144912	-3.022382
H	-0.510088	1.372871	-3.187254
C	4.040967	-1.482525	0.201816
H	4.635209	-2.386191	0.074471
C	2.646177	-1.540469	0.043516
C	1.984029	-2.873358	-0.286948
H	1.924889	-3.475461	0.634551
H	2.672358	-3.424275	-0.942659
C	0.588083	-2.839284	-0.949265
H	0.479759	-3.755002	-1.548802
H	0.542237	-2.005839	-1.666263
C	1.907769	-0.360135	0.203970
H	0.832196	-0.375546	0.080510
C	2.543031	0.847202	0.522499
C	3.931786	0.899267	0.676565
H	4.410227	1.844584	0.921474
C	4.671164	-0.274260	0.513464
H	5.753299	-0.242401	0.628933
C	-0.611440	-2.763821	0.013650
H	-0.526799	-1.880871	0.661168
H	-0.581238	-3.634914	0.687575
C	-1.959903	-2.744770	-0.727441
C	-3.200500	-2.648763	0.184732
C	-3.414166	-1.276766	0.855578
H	-2.469896	-0.948369	1.309806
H	-4.123673	-1.387622	1.689486
H	-3.122836	-3.421511	0.965029
H	-4.096490	-2.902545	-0.402984
H	-2.037862	-3.661680	-1.331929
H	-1.963575	-1.911683	-1.447079
C	-3.939884	-0.186450	-0.095758
H	-5.005529	-0.367455	-0.300583
H	-3.426723	-0.253646	-1.065513
C	-3.772529	1.259799	0.437372
H	-4.295651	1.946092	-0.243449
H	-4.256751	1.350501	1.419564

Sum of electronic and zero-point Energies= -965.895196  
 Sum of electronic and thermal Energies= -965.874294  
 Sum of electronic and thermal Enthalpies= -965.873350  
 Sum of electronic and thermal Free Energies= -965.944833

## daec[n=3]-1-TS (dmf)

C	2.978976	1.318008	0.036313
H	3.976619	1.675079	-0.205369
C	2.759833	-0.067374	0.174208
C	1.466028	-0.470924	0.476954
H	1.223971	-1.509702	0.606944
C	0.422851	0.431225	0.594710
H	-0.552875	0.020878	0.786657
C	0.616334	1.795577	0.434032
O	-0.422041	2.725405	0.502053
C	1.931323	2.252996	0.169372
O	2.078280	3.599756	0.032229
C	3.378475	4.109101	-0.248671
H	3.265185	5.195692	-0.306829
H	4.091129	3.861097	0.550536

H	3.762459	3.733090	-1.207623
C	-3.990261	0.931829	-0.700742
H	-4.852059	0.393631	-1.091962
C	-3.373994	0.501433	0.487159
C	-3.718285	-0.818142	1.160553
H	-4.765914	-0.822616	1.496950
H	-3.101982	-0.922710	2.063127
C	-3.535872	-2.059816	0.237599
H	-4.317450	-2.000617	-0.533064
H	-3.776259	-2.953711	0.832758
C	-2.293756	1.248933	0.972860
H	-1.847424	0.980380	1.925835
C	-1.685542	2.228463	0.178325
C	-2.294827	2.651447	-1.002706
H	-1.827462	3.425539	-1.606606
C	-3.481143	2.025640	-1.408077
H	-3.972768	2.354420	-2.321884
C	-2.188115	-2.278257	-0.501394
H	-1.813153	-1.314759	-0.875397
H	-2.422330	-2.866107	-1.402126
C	-1.038608	-3.020883	0.223164
C	0.081691	-3.387729	-0.784548
C	1.319651	-4.183616	-0.282645
H	0.983308	-4.939707	0.443665
H	1.702458	-4.754491	-1.142638
C	2.532121	-3.432295	0.332174
H	2.236612	-2.925697	1.258270
H	3.248074	-4.201039	0.657983
H	-0.393766	-4.001896	-1.564433
H	0.410727	-2.475351	-1.302034
H	-1.429307	-3.946800	0.674149
H	-0.648348	-2.417647	1.055473
C	3.271448	-2.457557	-0.636545
H	2.611737	-2.191436	-1.473689
H	4.113727	-3.000658	-1.086773
C	3.825929	-1.135067	-0.032962
H	4.335553	-1.354471	0.919569
H	4.604073	-0.739642	-0.700548

Sum of electronic and zero-point Energies= -1005.142064  
 Sum of electronic and thermal Energies= -1005.120940  
 Sum of electronic and thermal Enthalpies= -1005.119995  
 Sum of electronic and thermal Free Energies= -1005.190500

## daec[n=3]-1-E1 (dmf)

C	1.727233	-1.784197	0.689627
H	2.228566	-1.627720	1.640507
C	2.477931	-1.709153	-0.499017
C	1.836750	-1.943844	-1.719130
H	2.403989	-1.906476	-2.647036
C	0.456326	-2.183328	-1.760165
H	-0.058847	-2.332333	-2.706761
C	-0.286923	-2.191951	-0.587734
O	-1.659907	-2.381558	-0.628670
C	0.349943	-2.021330	0.662329
O	-0.453818	-2.082141	1.754741
C	0.139198	-1.876848	3.035884
H	-0.677550	-1.965746	3.757817
H	0.900736	-2.638426	3.252754
H	0.588270	-0.877200	3.114736
C	-4.172982	0.924223	-0.220953
H	-4.851645	1.769998	-0.121739
C	-2.842525	1.142156	-0.611972
C	-2.332581	2.542191	-0.896109
H	-3.153883	3.134722	-1.322210
H	-1.549553	2.496757	-1.664675
C	-1.795518	3.303734	0.340663
H	-2.576815	3.306428	1.115259
H	-1.651028	4.354768	0.047313
C	-1.988922	0.036489	-0.743009
H	-0.962316	0.189744	-1.062687

C	-2.453317	-1.258201	-0.483954
C	-3.782644	-1.472010	-0.105002
H	-4.128582	-2.485426	0.084301
C	-4.634652	-0.373256	0.024020
H	-5.670664	-0.533583	0.317762
C	-0.483912	2.783534	0.955826
H	-0.612040	1.742984	1.290831
H	-0.288745	3.370957	1.866630
C	0.747768	2.875005	0.038190
C	2.073615	2.656522	0.788447
C	3.315347	2.592218	-0.126084
H	3.240677	3.391638	-0.879069
H	4.216460	2.818200	0.464662
C	3.511698	1.235374	-0.832588
H	2.545803	0.893389	-1.230324
H	4.167935	1.363270	-1.706467
H	2.199482	3.474410	1.514059
H	2.006989	1.734027	1.385974
H	0.773104	3.866946	-0.441424
H	0.657393	2.145062	-0.779056
C	4.110597	0.152970	0.083536
H	3.656755	0.219201	1.082383
H	5.183402	0.351578	0.224565
C	3.935136	-1.294388	-0.434235
H	4.387851	-1.391216	-1.430689
H	4.488669	-1.971824	0.232602

Sum of electronic and zero-point Energies= -1005.182739  
Sum of electronic and thermal Energies= -1005.160621  
Sum of electronic and thermal Enthalpies= -1005.159677  
Sum of electronic and thermal Free Energies= -1005.233598

#### daec[n=3]-1-E2 (dmf)

C	1.739931	-2.095573	-0.501924
H	2.254240	-2.281464	-1.440360
C	2.473264	-1.594159	0.585852
C	1.814954	-1.374575	1.803607
H	2.370300	-1.010094	2.665646
C	0.437623	-1.582278	1.907507
H	-0.091749	-1.382941	2.836929
C	-0.291218	-2.025642	0.808752
O	-1.664896	-2.186912	0.918223
C	0.358802	-2.322295	-0.405873
O	-0.428310	-2.778795	-1.413480
C	0.186776	-3.061389	-2.669561
H	-0.617156	-3.419792	-3.318724
H	0.635167	-2.160013	-3.109514
H	0.953398	-3.842535	-2.574431
C	-4.203999	0.963788	-0.096010
H	-4.889215	1.769965	-0.353262
C	-2.847429	1.068386	-0.439070
C	-2.319213	2.292964	-1.161884
H	-3.129899	2.715519	-1.770926
H	-1.528562	1.991797	-1.862136
C	-1.786744	3.418203	-0.240179
H	-2.570704	3.672367	0.488703
H	-1.643019	4.315602	-0.861157
C	-1.982743	0.014470	-0.104697
H	-0.933155	0.083178	-0.373436
C	-2.464169	-1.120130	0.558103
C	-3.820417	-1.224078	0.889438
H	-4.178517	-2.115337	1.399359
C	-4.681295	-0.176382	0.559564
H	-5.736830	-0.253312	0.814951
C	-0.475291	3.132287	0.513849
H	-0.600271	2.257801	1.170039
H	-0.283780	3.985665	1.183046
C	0.756715	2.924204	-0.383627
C	2.082706	2.937131	0.397175
C	3.319891	2.592432	-0.458871
H	3.245022	3.127479	-1.417888

H	4.225400	2.980387	0.032558
C	3.504081	1.083800	-0.722299
H	2.529931	0.641802	-0.974482
H	4.139511	0.935334	-1.608168
H	2.214567	3.935617	0.840956
H	2.014318	2.238256	1.245327
H	0.789289	3.717945	-1.147569
H	0.659317	1.977508	-0.934352
C	4.127498	0.329511	0.466091
H	3.705573	0.705327	1.409047
H	5.204955	0.548085	0.506497
C	3.930179	-1.205318	0.426819
H	4.323481	-1.607143	-0.517129
H	4.524621	-1.653495	1.235960

Sum of electronic and zero-point Energies= -1005.182321  
Sum of electronic and thermal Energies= -1005.160157  
Sum of electronic and thermal Enthalpies= -1005.159213  
Sum of electronic and thermal Free Energies= -1005.233478

#### daec[n=3]-2-TS (dmf)

C	2.377502	2.145146	-0.084380
H	3.230523	2.798051	0.081224
C	2.567938	0.748179	-0.069687
C	1.446134	-0.042547	-0.280869
H	1.519392	-1.114095	-0.281426
C	0.187284	0.504527	-0.468304
H	-0.636023	-0.175642	-0.602982
C	-0.021642	1.874681	-0.443706
O	-1.293822	2.436962	-0.560419
C	1.102607	2.718939	-0.268545
O	0.850712	4.056975	-0.267281
C	1.948862	4.946537	-0.089482
H	2.694170	4.833160	-0.889372
H	2.436028	4.798679	0.884706
H	1.524787	5.954127	-0.131467
C	-4.020740	-0.260274	1.064142
H	-4.634514	-1.015420	1.552742
C	-3.474399	-0.527278	-0.200911
C	-3.591363	-1.900574	-0.847049
H	-4.155455	-1.823755	-1.788999
H	-4.178258	-2.553570	-0.186815
C	-2.228800	-2.575779	-1.174893
H	-1.691349	-1.942807	-1.896377
H	-2.442043	-3.515996	-1.704985
C	-2.704198	0.476654	-0.810017
H	-2.292011	0.318542	-1.803443
C	-2.320009	1.611594	-0.088890
C	-2.873794	1.878789	1.164557
H	-2.578883	2.774603	1.705797
C	-3.761684	0.950455	1.717030
H	-4.203719	1.144770	2.692514
C	-1.297672	-2.864279	0.021604
H	-1.761597	-3.616413	0.678837
H	-1.196927	-1.954813	0.630848
C	0.115654	-3.336602	-0.396443
C	1.117156	-3.412014	0.779203
C	2.601589	-3.677698	0.410844
H	2.639470	-4.524576	-0.291830
H	3.114885	-4.024779	1.321089
C	3.439553	-2.516860	-0.189013
H	4.388114	-2.946401	-0.543160
H	2.952532	-2.134670	-1.094642
H	0.791988	-4.219797	1.452381
H	1.045173	-2.491300	1.376419
H	0.495394	-2.656437	-1.172672
H	0.048911	-4.324969	-0.877557
C	3.771077	-1.360460	0.800695
H	4.716533	-1.606112	1.303706
H	3.015199	-1.320514	1.597338
C	3.904635	0.066082	0.196940

H 4.495879 0.015397 -0.732149  
H 4.492544 0.689941 0.884909  
Sum of electronic and zero-point Energies= -1005.151700  
Sum of electronic and thermal Energies= -1005.130725  
Sum of electronic and thermal Enthalpies= -1005.129781  
Sum of electronic and thermal Free Energies= -1005.199696

daec[n=3]-2-E1 (dmf)

C 1.630472 2.031773 -0.531857  
H 2.238502 2.183398 -1.418914  
C 2.265076 1.703095 0.677210  
C 1.479843 1.522548 1.824738  
H 1.952914 1.284003 2.775509  
C 0.090306 1.643073 1.756816  
H -0.527260 1.503904 2.641767  
C -0.533288 1.945799 0.549275  
O -1.910464 2.106174 0.499873  
C 0.233971 2.154776 -0.614038  
O -0.455644 2.454488 -1.744888  
C 0.284211 2.656054 -2.947827  
H 0.844504 1.754335 -3.231230  
H 0.977390 3.503637 -2.856688  
H -0.459190 2.877750 -3.718807  
C -4.422285 -1.212369 0.358036  
H -5.098928 -2.065414 0.331147  
C -3.083334 -1.378276 -0.037421  
C -2.622763 -2.751374 -0.515909  
H -3.322163 -3.076794 -1.300197  
H -2.760507 -3.472080 0.305820  
C -1.187766 -2.870117 -1.056879  
H -0.994137 -2.045518 -1.759328  
H -1.125428 -3.789797 -1.656378  
C -2.232245 -0.265221 0.003949  
H -1.195836 -0.354500 -0.301423  
C -2.706054 0.979462 0.439509  
C -4.040775 1.140882 0.820380  
H -4.389936 2.115853 1.151821  
C -4.892943 0.034636 0.774207  
H -5.933840 0.149719 1.071872  
C -0.081776 -2.909681 0.012771  
H -0.152359 -3.857335 0.569676  
H -0.240130 -2.112128 0.752882  
C 1.322311 -2.753656 -0.588624  
C 2.457722 -2.779623 0.447618  
C 3.823720 -2.343479 -0.121306  
H 4.008060 -2.891302 -1.058203  
H 4.623869 -2.648593 0.570634  
C 3.937015 -0.827880 -0.383212  
H 4.764487 -0.633911 -1.081711  
H 3.028426 -0.482562 -0.895551  
H 2.542445 -3.795306 0.862677  
H 2.189818 -2.129474 1.294702  
H 1.351553 -1.804252 -1.143740  
H 1.495749 -3.544527 -1.336023  
C 4.160249 0.007394 0.890700  
H 5.218990 -0.054759 1.182306  
H 3.589166 -0.418631 1.727678  
C 3.766963 1.497172 0.745405  
H 4.244354 1.919966 -0.149528  
H 4.166553 2.049107 1.608103  
Sum of electronic and zero-point Energies= -1005.181123  
Sum of electronic and thermal Energies= -1005.158870  
Sum of electronic and thermal Enthalpies= -1005.157926  
Sum of electronic and thermal Free Energies= -1005.232961

daec[n=3]-2-E2 (dmf)

C 1.445519 1.964334 0.597265  
H 1.900339 2.039590 1.580919  
C 2.278071 1.811078 -0.528043  
C 1.690535 1.742589 -1.795064

H 2.315845 1.638287 -2.679494  
C 0.296179 1.790379 -1.935257  
H -0.170117 1.724826 -2.915953  
C -0.519150 1.912403 -0.817582  
O -1.893830 2.001953 -0.968454  
C 0.054412 2.020494 0.470884  
O -0.816535 2.172688 1.501199  
C -0.285875 2.250860 2.823144  
H 0.370196 3.124116 2.941298  
H 0.267000 1.339078 3.087837  
H -1.151060 2.355681 3.483869  
C -4.347313 -1.150403 0.211592  
H -5.008753 -1.959649 0.518115  
C -3.009530 -1.435820 -0.114037  
C -2.528599 -2.882012 -0.052686  
H -3.211670 -3.482162 -0.672178  
H -2.672870 -3.254721 0.973814  
C -1.083957 -3.168149 -0.496411  
H -0.891324 -2.665383 -1.456062  
H -0.999016 -4.244467 -0.704753  
C -2.179693 -0.377484 -0.508360  
H -1.145942 -0.559829 -0.780617  
C -2.671497 0.932894 -0.562517  
C -4.004540 1.209055 -0.252099  
H -4.367890 2.232394 -0.306569  
C -4.836960 0.155051 0.134254  
H -5.877238 0.359298 0.382120  
C 0.004829 -2.779939 0.519830  
H -0.056292 -3.454032 1.388769  
H -0.182296 -1.768611 0.908634  
C 1.416348 -2.822977 -0.083028  
C 2.532597 -2.445341 0.904551  
C 3.901493 -2.212147 0.232352  
H 4.110909 -3.054135 -0.445182  
H 4.693853 -2.233868 0.996436  
C 3.996688 -0.887421 -0.551660  
H 4.834094 -0.938090 -1.263288  
H 3.092692 -0.765255 -1.164335  
H 2.627361 -3.239906 1.660023  
H 2.236454 -1.539662 1.456083  
H 1.440139 -2.140626 -0.945811  
H 1.616311 -3.827786 -0.488604  
C 4.183146 0.351038 0.343634  
H 5.235636 0.416474 0.656343  
H 3.598968 0.240198 1.268111  
C 3.777028 1.683154 -0.330373  
H 4.285856 1.777416 -1.299763  
H 4.133341 2.513883 0.295943  
Sum of electronic and zero-point Energies= -1005.181973  
Sum of electronic and thermal Energies= -1005.159792  
Sum of electronic and thermal Enthalpies= -1005.158848  
Sum of electronic and thermal Free Energies= -1005.233041

daec[n=3]-3-TS (dmf)

C -3.159345 -1.085497 -0.017471  
H -4.194039 -1.400268 0.090327  
C -2.855705 0.292538 -0.047348  
C -1.520985 0.636602 -0.192664  
H -1.227725 1.664625 -0.270159  
C -0.511032 -0.313715 -0.244112  
H 0.503844 0.045016 -0.291590  
C -0.796041 -1.669884 -0.229596  
O 0.176150 -2.661521 -0.306912  
C -2.155378 -2.065829 -0.126484  
O -2.383422 -3.408549 -0.125846  
C -3.729411 -3.860132 -0.012442  
H -4.184992 -3.540383 0.935475  
H -3.679162 -4.952682 -0.038084  
H -4.346701 -3.505562 -0.850018  
C 4.020893 -1.272139 0.541250

H	4.984733	-0.859396	0.834743
C	3.322994	-0.716957	-0.545878
C	3.781266	0.554860	-1.241513
H	3.103521	0.763129	-2.079733
H	4.780753	0.411610	-1.678700
C	3.869484	1.795811	-0.306992
H	4.208485	2.645934	-0.918384
H	4.676827	1.608170	0.415523
C	2.104022	-1.300764	-0.913073
H	1.575823	-0.923668	-1.784014
C	1.495629	-2.265314	-0.099121
C	2.188972	-2.811546	0.980605
H	1.716599	-3.572482	1.597143
C	3.474245	-2.333950	1.267495
H	4.028331	-2.761319	2.101226
C	2.617530	2.213809	0.500634
H	2.960846	2.898387	1.291802
H	2.216499	1.334871	1.027366
C	1.467845	2.908768	-0.257658
C	0.314442	3.322905	0.687948
C	-0.965428	3.856438	-0.021157
H	-0.980009	3.480403	-1.054074
H	-0.890713	4.947716	-0.123212
C	-2.324912	3.491834	0.673424
H	-2.751808	4.404782	1.108260
H	-2.126640	2.832631	1.529446
H	0.684344	4.073776	1.402152
H	0.049482	2.447369	1.297155
H	1.068900	2.237632	-1.033119
H	1.854931	3.793148	-0.788166
C	-3.411929	2.830445	-0.244448
H	-3.060043	2.828874	-1.286291
H	-4.309008	3.463720	-0.239178
C	-3.890149	1.397008	0.116215
H	-4.774402	1.167378	-0.497036
H	-4.252553	1.395408	1.157513

Sum of electronic and zero-point Energies= -1005.144863  
Sum of electronic and thermal Energies= -1005.123712  
Sum of electronic and thermal Enthalpies= -1005.122768  
Sum of electronic and thermal Free Energies= -1005.193259

daec[n=3]-3-E1 (dmf)

C	-2.314868	-1.610707	-0.443579
H	-2.920648	-1.793710	-1.326716
C	-2.880261	-0.907786	0.636273
C	-2.102467	-0.692904	1.780680
H	-2.528668	-0.175339	2.637411
C	-0.778647	-1.142471	1.834272
H	-0.169273	-0.981694	2.721233
C	-0.219531	-1.815225	0.753956
O	1.068706	-2.321792	0.846741
C	-0.989956	-2.067260	-0.402308
O	-0.368177	-2.746860	-1.399846
C	-1.109003	-3.018744	-2.588417
H	-1.989558	-3.641624	-2.379210
H	-0.425789	-3.565955	-3.244145
H	-1.426531	-2.091681	-3.085309
C	4.412170	0.036174	0.047263
H	5.303203	0.628183	-0.155853
C	3.169464	0.462006	-0.446081
C	3.056786	1.738916	-1.258476
H	2.270750	1.619459	-2.015225
H	3.995724	1.888785	-1.808730
C	2.786359	3.023581	-0.434478
H	2.830910	3.876946	-1.128358
H	3.612629	3.163376	0.278360
C	2.033275	-0.321325	-0.181345
H	1.065517	-0.014025	-0.566793
C	2.140542	-1.500629	0.562882
C	3.384640	-1.924937	1.045147

H	3.448339	-2.847917	1.616576
C	4.514616	-1.149908	0.781713
H	5.484442	-1.476408	1.153269
C	1.454690	3.065669	0.334993
H	1.417292	4.001740	0.913493
H	1.437409	2.252360	1.075891
C	0.199184	2.957564	-0.543163
C	-1.116265	2.921539	0.257386
C	-2.251339	2.230001	-0.510372
H	-1.905723	1.222898	-0.779411
H	-2.430531	2.747581	-1.466235
C	-3.581190	2.117677	0.261136
H	-4.129131	3.067045	0.175422
H	-3.375906	1.988847	1.334638
H	-1.411418	3.939913	0.554751
H	-0.951234	2.366800	1.194215
H	0.260053	2.038765	-1.142827
H	0.177040	3.786409	-1.268112
C	-4.475360	0.954699	-0.225731
H	-4.295845	0.778076	-1.296768
H	-5.535095	1.233171	-0.138182
C	-4.298273	-0.374372	0.555049
H	-4.948932	-1.130761	0.093262
H	-4.670655	-0.221396	1.577397

Sum of electronic and zero-point Energies= -1005.179710  
Sum of electronic and thermal Energies= -1005.157454  
Sum of electronic and thermal Enthalpies= -1005.156510  
Sum of electronic and thermal Free Energies= -1005.231126

daec[n=3]-3-E2 (dmf)

C	-2.105652	-1.327552	0.732270
H	-2.549992	-1.121912	1.701606
C	-2.897404	-1.188654	-0.421907
C	-2.331615	-1.495004	-1.666204
H	-2.930456	-1.414618	-2.571643
C	-0.992484	-1.893561	-1.757765
H	-0.543616	-2.131957	-2.719752
C	-0.207197	-1.997529	-0.614057
O	1.096479	-2.460337	-0.704984
C	-0.765570	-1.726833	0.654443
O	0.062140	-1.885890	1.719003
C	-0.463027	-1.638268	3.022178
H	-0.796939	-0.597346	3.130821
H	0.361976	-1.828206	3.714568
H	-1.296383	-2.315668	3.253878
C	4.333849	0.111171	-0.159300
H	5.198459	0.759798	-0.026940
C	3.127666	0.650632	-0.633594
C	3.015211	2.127365	-0.965246
H	2.278208	2.263079	-1.767166
H	3.977551	2.473406	-1.367085
C	2.650012	3.043347	0.230178
H	2.684525	4.084028	-0.126852
H	3.437056	2.954049	0.993717
C	2.029183	-0.206901	-0.807145
H	1.092403	0.185848	-1.192619
C	2.134481	-1.568580	-0.506552
C	3.341688	-2.103478	-0.045763
H	3.405928	-3.166462	0.173964
C	4.436614	-1.254280	0.125500
H	5.379437	-1.664166	0.483709
C	1.286870	2.777979	0.891691
H	1.179977	3.458074	1.751004
H	1.279095	1.759944	1.309548
C	0.073299	2.935749	-0.036806
C	-1.268236	2.607049	0.645144
C	-2.349948	2.167313	-0.351171
H	-1.955007	1.314799	-0.919597
H	-2.527238	2.962873	-1.092280
C	-3.691617	1.768173	0.294263

H	-4.267745	2.677873	0.517005
H	-3.504810	1.289803	1.267785
H	-1.614960	3.466440	1.240007
H	-1.112605	1.785712	1.362050
H	0.193719	2.266955	-0.900195
H	0.047198	3.956523	-0.449517
C	-4.540699	0.818089	-0.580248
H	-4.347921	1.027038	-1.643152
H	-5.609587	1.019193	-0.420627
C	-4.326846	-0.693693	-0.304073
H	-4.964902	-1.259154	-0.998016
H	-4.693786	-0.911335	0.708607

Sum of electronic and zero-point Energies= -1005.180149  
Sum of electronic and thermal Energies= -1005.157972  
Sum of electronic and thermal Enthalpies= -1005.157028  
Sum of electronic and thermal Free Energies= -1005.230974

#### daec[n=3]-4-TS (dmf)

C	3.281825	-0.383999	-0.093889
H	4.365787	-0.423647	-0.023497
C	2.629752	0.862916	0.018627
C	1.245136	0.854045	-0.074239
H	0.678677	1.763186	-0.016290
C	0.527997	-0.320334	-0.224777
H	-0.544036	-0.247726	-0.247257
C	1.150969	-1.551742	-0.326710
O	0.432178	-2.738137	-0.462999
C	2.566803	-1.586320	-0.274241
O	3.139190	-2.817240	-0.383975
C	4.559607	-2.904467	-0.326588
H	4.796921	-3.966292	-0.440885
H	5.032704	-2.337474	-1.140761
H	4.948036	-2.548161	0.637957
C	-3.464228	-2.176560	0.923624
H	-4.444606	-1.961022	1.346087
C	-3.078564	-1.564407	-0.282158
C	-3.942168	-0.500863	-0.940439
H	-4.995118	-0.813858	-0.901880
H	-3.673742	-0.423338	-2.003276
C	-3.858293	0.921516	-0.305049
H	-4.170521	0.865040	0.748521
H	-4.616033	1.535753	-0.815183
C	-1.823749	-1.892697	-0.815605
H	-1.510984	-1.458881	-1.762500
C	-0.908586	-2.653040	-0.074106
C	-1.297371	-3.260230	1.119022
H	-0.583226	-3.860478	1.677738
C	-2.597904	-3.045210	1.592563
H	-2.916197	-3.522179	2.517719
C	-2.490976	1.630382	-0.407688
H	-2.087266	1.475473	-1.420596
H	-1.785596	1.155623	0.284406
C	-2.520582	3.150892	-0.130976
C	-1.184938	3.879375	-0.441141
C	-0.086775	3.812897	0.652181
H	-0.180246	2.868328	1.203129
H	-0.271987	4.594548	1.403499
C	1.363554	3.962369	0.098730
H	1.583375	5.033187	-0.012309
H	1.396282	3.559586	-0.923002
H	-1.399449	4.935169	-0.662180
H	-0.784464	3.459371	-1.376730
H	-2.820810	3.339233	0.911883
H	-3.307412	3.598002	-0.757476
C	2.497698	3.292110	0.945536
H	2.071493	2.871745	1.868072
H	3.201934	4.068951	1.271541
C	3.345223	2.188511	0.246202
H	4.245605	2.009448	0.851376
H	3.713349	2.582560	-0.715587

Sum of electronic and zero-point Energies= -1005.147562  
Sum of electronic and thermal Energies= -1005.126276  
Sum of electronic and thermal Enthalpies= -1005.125332  
Sum of electronic and thermal Free Energies= -1005.196485

#### daec[n=3]-4-E1 (dmf)

C	1.914570	-1.766986	-0.723754
H	2.484510	-1.758442	-1.648348
C	2.563808	-1.428185	0.474764
C	1.830058	-1.454181	1.669026
H	2.314023	-1.216352	2.614121
C	0.469061	-1.767256	1.653062
H	-0.112739	-1.776148	2.572546
C	-0.175708	-2.070881	0.456274
O	-1.526535	-2.399756	0.465066
C	0.550149	-2.094936	-0.750837
O	-0.149446	-2.417785	-1.870429
C	0.548885	-2.442341	-3.114483
H	-0.194088	-2.727008	-3.864925
H	0.959666	-1.454704	-3.365438
H	1.359505	-3.183796	-3.105374
C	-4.287197	0.722962	0.628972
H	-5.015017	1.530550	0.689977
C	-3.178856	0.853311	-0.223533
C	-2.980059	2.109582	-1.051195
H	-3.943897	2.629053	-1.134765
H	-2.683502	1.832371	-2.073719
C	-1.934568	3.107147	-0.491689
H	-2.177252	3.336381	0.557310
H	-2.043443	4.051187	-1.046867
C	-2.259091	-0.204858	-0.290743
H	-1.413196	-0.145371	-0.968412
C	-2.426617	-1.346686	0.498773
C	-3.540128	-1.478431	1.333529
H	-3.658964	-2.379269	1.930846
C	-4.470245	-0.437398	1.387690
H	-5.339357	-0.529348	2.036756
C	-0.479437	2.630279	-0.598051
H	-0.259972	2.387942	-1.650979
H	-0.362971	1.694371	-0.038188
C	0.550473	3.652799	-0.094212
C	2.015371	3.226673	-0.310778
C	2.418627	1.938610	0.423974
H	1.791800	1.109156	0.078103
H	2.206426	2.055882	1.499245
C	3.901107	1.572614	0.243905
H	4.509257	2.438209	0.549939
H	4.115540	1.419123	-0.826136
H	2.674412	4.047256	0.013597
H	2.196850	3.099799	-1.390444
H	0.381019	3.842085	0.977976
H	0.383754	4.614691	-0.603745
C	4.388103	0.345499	1.041434
H	4.029600	0.418393	2.079108
H	5.485564	0.388291	1.100357
C	4.033567	-1.046635	0.466587
H	4.593390	-1.794289	1.049582
H	4.415702	-1.113892	-0.561502

Sum of electronic and zero-point Energies= -1005.181177  
Sum of electronic and thermal Energies= -1005.158858  
Sum of electronic and thermal Enthalpies= -1005.157914  
Sum of electronic and thermal Free Energies= -1005.232735

#### daec[n=3]-4-E2 (dmf)

C	1.811400	-1.806308	0.437724
H	2.321236	-1.877557	1.393866
C	2.543935	-1.427105	-0.703016
C	1.885251	-1.368569	-1.935459
H	2.436206	-1.091846	-2.832300
C	0.513894	-1.645074	-2.025247

H	-0.006250	-1.592611	-2.979288
C	-0.211621	-1.973600	-0.887513
O	-1.567435	-2.257477	-0.970593
C	0.440757	-2.073081	0.363757
O	-0.341229	-2.425272	1.416641
C	0.263403	-2.499275	2.706380
H	-0.539631	-2.778724	3.394276
H	1.051465	-3.264329	2.737691
H	0.682611	-1.529977	3.009611
C	-4.269711	0.631715	0.353781
H	-4.986846	1.371183	0.706650
C	-3.143017	1.051057	-0.370976
C	-2.914621	2.522016	-0.668477
H	-3.863829	3.056200	-0.528941
H	-2.641145	2.642801	-1.727394
C	-1.832819	3.217117	0.196296
H	-2.049958	3.041440	1.261093
H	-1.927547	4.302035	0.037147
C	-2.238240	0.075406	-0.820878
H	-1.374247	0.366878	-1.410619
C	-2.441741	-1.275660	-0.527389
C	-3.574108	-1.689799	0.179197
H	-3.718271	-2.746928	0.388041
C	-4.486332	-0.726070	0.613567
H	-5.370222	-1.036942	1.167923
C	-0.392400	2.791078	-0.119981
H	-0.204873	2.940209	-1.196144
H	-0.284287	1.715294	0.063386
C	0.675174	3.549292	0.683515
C	2.122703	3.205626	0.281278
C	2.502651	1.730460	0.482237
H	1.847558	1.098520	-0.127536
H	2.310192	1.449503	1.530669
C	3.970503	1.422680	0.144120
H	4.609471	2.104413	0.727014
H	4.163422	1.661895	-0.914189
H	2.811611	3.837962	0.863058
H	2.277156	3.479201	-0.775084
H	0.537205	3.343632	1.757233
H	0.521159	4.632410	0.558008
C	4.431378	-0.020795	0.432504
H	4.095282	-0.316778	1.437606
H	5.530488	-0.028420	0.472048
C	4.023877	-1.104544	-0.593526
H	4.565567	-2.025966	-0.327830
H	4.393913	-0.810908	-1.585747

Sum of electronic and zero-point Energies= -1005.181703  
Sum of electronic and thermal Energies= -1005.159410  
Sum of electronic and thermal Enthalpies= -1005.158466  
Sum of electronic and thermal Free Energies= -1005.233039

daec[n=3]-5-TS (dmf)

C	2.303126	2.406448	-0.255718
H	3.058915	3.182998	-0.144133
C	2.650295	1.045528	-0.244934
C	1.603573	0.145540	-0.398756
H	1.812191	-0.904593	-0.423811
C	0.283547	0.534331	-0.498008
H	-0.453932	-0.246988	-0.555606
C	-0.072322	1.880403	-0.501238
O	-1.394888	2.309957	-0.599458
C	0.966347	2.831543	-0.399075
O	0.706941	4.181516	-0.462075
C	0.135551	4.740846	-0.726404
H	0.805264	4.600655	1.587631
H	-0.843385	4.298655	0.949909
H	0.013312	5.812115	0.534880
C	-3.990056	-0.685198	0.711739
H	-4.584523	-1.495645	1.130251
C	-3.223204	-0.904901	-0.446148

C	-3.039096	-2.288327	-1.051383
H	-2.421874	-2.199247	-1.954931
H	-4.008550	-2.694282	-1.377132
C	-2.417490	-3.336338	-0.081362
H	-2.359814	-4.291186	-0.625777
H	-3.141237	-3.501026	0.729812
C	-2.505555	0.177156	-0.972382
H	-1.952515	0.049905	-1.898680
C	-2.362563	1.364397	-0.242855
C	-3.121101	1.579237	0.906814
H	-3.021614	2.510343	1.459497
C	-3.971899	0.558045	1.350502
H	-4.577999	0.718019	2.240282
C	-1.046672	-3.046256	0.580145
H	-0.953688	-3.739661	1.430465
H	-1.060937	-2.039303	1.023142
C	0.222258	-3.193514	-0.286720
C	1.526719	-3.017036	0.534299
C	2.815564	-2.883807	-0.320935
H	2.592039	-2.357997	-1.259976
H	3.125226	-3.891011	-0.638314
C	4.053879	-2.235832	0.359774
H	4.888784	-2.309947	-0.354357
H	4.335225	-2.883624	1.204828
H	1.639339	-3.868084	1.222890
H	1.411806	-2.135607	1.179803
H	0.205340	-2.454928	-1.101808
H	0.225292	-4.181371	-0.773806
C	4.049493	-0.785483	0.933788
H	3.240712	-0.675699	1.669381
H	4.979834	-0.719307	1.515300
C	4.035007	0.458430	-0.019953
H	4.689295	1.231639	0.404012
H	4.488656	0.182102	-0.985468

Sum of electronic and zero-point Energies= -1005.139888  
Sum of electronic and thermal Energies= -1005.118563  
Sum of electronic and thermal Enthalpies= -1005.117619  
Sum of electronic and thermal Free Energies= -1005.188789

daec[n=3]-5-E1 (dmf)

C	1.921802	1.811724	-0.619483
H	2.465793	1.984646	-1.546339
C	2.576401	1.277596	0.498550
C	1.830667	1.096353	1.675970
H	2.315891	0.714287	2.572125
C	0.467405	1.388874	1.712085
H	-0.113966	1.230492	2.618092
C	-0.178240	1.879354	0.575344
O	-1.539133	2.154394	0.623171
C	0.553942	2.114898	-0.599159
O	-0.044125	2.557736	-1.751519
C	-0.523248	3.909643	-1.715298
H	0.301702	4.609415	-1.518459
H	-1.304947	4.041532	-0.957964
H	-0.939441	4.111461	-2.707450
C	-4.282267	-0.955498	0.166195
H	-5.016736	-1.751669	0.055331
C	-2.993361	-1.121533	-0.363265
C	-2.599513	-2.397677	-1.082177
H	-1.938309	-2.151119	-1.923452
H	-3.500360	-2.851154	-1.517389
C	-1.916722	-3.466382	-0.191266
H	-1.788579	-4.372772	-0.802559
H	-2.608163	-3.738297	0.620194
C	-2.065827	-0.078149	-0.215430
H	-1.070549	-0.181669	-0.636206
C	-2.416269	1.096026	0.456711
C	-3.705050	1.262642	0.974612
H	-3.961453	2.185953	1.488613
C	-4.632142	0.229997	0.821729

H	-5.637368	0.352159	1.221356
C	-0.559639	-3.080315	0.423895
H	-0.233613	-3.906745	1.074475
H	-0.689919	-2.210773	1.085133
C	0.553171	-2.772973	-0.589917
C	1.898499	-2.422955	0.068168
C	2.915058	-1.845212	-0.928152
H	2.496975	-0.929924	-1.371269
H	3.035568	-2.553896	-1.762955
C	4.313410	-1.553907	-0.353636
H	4.962075	-1.216345	-1.177259
H	4.748677	-2.501658	0.001058
H	2.318614	-3.319565	0.551796
H	1.721282	-1.696179	0.873609
H	0.247450	-1.931725	-1.228530
H	0.685558	-3.632283	-1.266853
C	4.424002	-0.532710	0.795840
H	3.836928	-0.868280	1.661942
H	5.471870	-0.536893	1.129213
C	4.055384	0.934541	0.459924
H	4.570702	1.579397	1.187729
H	4.465611	1.198535	-0.524641

Sum of electronic and zero-point Energies= -1005.177652

Sum of electronic and thermal Energies= -1005.155263

Sum of electronic and thermal Enthalpies= -1005.154319

Sum of electronic and thermal Free Energies= -1005.229268

daec[n=3]-5-E2 (dmf)

C	1.819429	1.593115	0.641192
H	2.282846	1.531099	1.621440
C	2.602958	1.348780	-0.502756
C	2.008246	1.471403	-1.762874
H	2.599925	1.305698	-2.661115
C	0.646695	1.783845	-1.880068
H	0.172586	1.862267	-2.856130
C	-0.128943	1.978134	-0.744531
O	-1.475251	2.291924	-0.857987
C	0.459457	1.902026	0.538365
O	-0.368592	2.134232	1.589142
C	0.175200	2.046451	2.905166
H	0.971799	2.786942	3.060579
H	0.565164	1.040519	3.112624
H	-0.655549	2.260601	3.583485
C	-4.330468	-0.648872	-0.079405
H	-5.094496	-1.399029	0.118674
C	-3.047386	-1.052850	-0.479097
C	-2.700088	-2.521033	-0.637696
H	-2.033342	-2.644047	-1.501538
H	-3.617389	-3.078206	-0.871714
C	-2.051648	-3.181829	0.605111
H	-1.956688	-4.258087	0.394518
H	-2.749365	-3.094879	1.451382
C	-2.082806	-0.066367	-0.737959
H	-1.090868	-0.358626	-1.068778
C	-2.389106	1.289239	-0.588217
C	-3.673037	1.688551	-0.202325
H	-3.896698	2.747796	-0.100269
C	-4.637259	0.710509	0.048952
H	-5.638722	1.013641	0.349793
C	-0.680016	-2.632607	1.037004
H	-0.378375	-3.156477	1.957405
H	-0.779934	-1.572418	1.313697
C	0.438819	-2.771084	-0.007212
C	1.796951	-2.238139	0.481190
C	2.820805	-2.083700	-0.653833
H	2.422172	-1.378632	-1.397073
H	2.918665	-3.048173	-1.177263
C	4.230354	-1.641090	-0.218820
H	4.881217	-1.636710	-1.107366
H	4.644439	-2.411210	0.451264

H	2.199393	-2.907404	1.258615
H	1.641265	-1.264582	0.967056
H	0.157515	-2.228590	-0.921350
H	0.540932	-3.827385	-0.303754
C	4.376357	-0.281018	0.492967
H	3.774025	-0.266258	1.411913
H	5.422111	-0.202960	0.824269
C	4.069266	0.984177	-0.347082
H	4.582154	1.830813	0.134335
H	4.523275	0.879204	-1.342372

Sum of electronic and zero-point Energies= -1005.181644

Sum of electronic and thermal Energies= -1005.159591

Sum of electronic and thermal Enthalpies= -1005.158647

Sum of electronic and thermal Free Energies= -1005.232033

daec[n=4]-1-TS (dmf)

C	-0.075691	3.336305	-0.113224
H	-0.018450	4.386494	-0.387171
C	1.087971	2.545180	-0.192936
C	0.976439	1.204556	0.162731
H	1.831425	0.546289	0.128762
C	-0.240531	0.655356	0.554255
H	-0.258659	-0.393428	0.804055
C	-1.401402	1.416460	0.589006
O	-2.651791	0.890509	0.913594
C	-1.315161	2.794079	0.269140
O	-2.477844	3.497479	0.335464
C	-2.441784	4.884727	0.013119
H	-3.466473	5.245617	0.141828
H	-2.127214	5.050333	-1.026922
H	-1.774477	5.439188	0.687828
C	-3.239206	-2.847879	-0.853990
H	-3.325644	-3.789648	-1.393969
C	-2.304770	-2.721638	0.185150
C	-1.209643	-3.741277	0.434262
H	-1.582919	-4.770895	0.348493
H	-0.823142	-3.619636	1.455433
C	-0.056783	-3.525295	-0.591791
H	0.055473	-2.448232	-0.776852
H	-0.374112	-3.958776	-1.550481
C	-2.241186	-1.503132	0.875849
H	-1.583974	-1.416082	1.735171
C	-2.923015	-0.378530	0.404108
C	-3.853667	-0.504096	-0.630348
H	-4.397386	0.372046	-0.975459
C	-4.035477	-1.757610	-1.225336
H	-4.764581	-1.868367	-2.026002
C	1.312089	-4.110051	-0.176879
H	1.149044	-5.029118	0.406047
H	1.858284	-4.422601	-1.079591
C	3.891946	-1.208180	0.650672
C	2.218114	-3.152691	0.630660
H	2.994921	-3.750148	1.132491
H	1.633773	-2.683787	1.438691
C	4.694057	-0.089459	-0.083215
H	4.739140	-0.313156	-1.159857
C	2.920680	-2.055783	-0.198116
H	2.173797	-1.412878	-0.685365
H	3.486688	-2.533963	-1.013454
H	5.733039	-0.148937	0.267174
C	4.206323	1.375775	0.125627
H	5.075083	2.010801	0.349883
H	3.584958	1.418148	1.029828
H	4.610767	-1.904818	1.107611
H	3.342377	-0.763996	1.494691
C	3.453841	2.019313	-1.069151
H	2.948400	1.244176	-1.661736
H	4.193914	2.470084	-1.744734
C	2.417982	3.101957	-0.685793
H	2.224807	3.743009	-1.558120



H 2.851464 3.769844 0.076459  
Sum of electronic and zero-point Energies= -1044.433532  
Sum of electronic and thermal Energies= -1044.410708  
Sum of electronic and thermal Enthalpies= -1044.409764  
Sum of electronic and thermal Free Energies= -1044.485138

daec[n=4]-1-E1 (dmf)

C -1.355966 2.374371 0.689253  
H -1.897853 2.345732 1.630218  
C -2.081616 2.378884 -0.517007  
C -1.381072 2.438733 -1.725996  
H -1.925240 2.455068 -2.668208  
C 0.019495 2.443375 -1.735523  
H 0.573478 2.464857 -2.671634  
C 0.727843 2.386344 -0.542669  
O 2.114833 2.369929 -0.554672  
C 0.043302 2.371607 0.693244  
O 0.820875 2.336277 1.805433  
C 0.173087 2.287007 3.075650  
H 0.976943 2.259820 3.816755  
H -0.445977 1.384987 3.176231  
H -0.447329 3.177755 3.244852  
C 4.170390 -1.256115 -0.332519  
H 4.731673 -2.187734 -0.282605  
C 2.779295 -1.288855 -0.498782  
C 2.011324 -2.593553 -0.579697  
H 2.676925 -3.398055 -0.922452  
H 1.220608 -2.493078 -1.335414  
C 1.379970 -3.000183 0.770150  
H 0.824968 -2.144249 1.178520  
H 2.189102 -3.204111 1.486944  
C 2.075135 -0.075638 -0.567019  
H 0.998159 -0.092869 -0.708616  
C 2.747216 1.145624 -0.467265  
C 4.138377 1.175230 -0.303680  
H 4.647443 2.133590 -0.233445  
C 4.839216 -0.029189 -0.238333  
H 5.920588 -0.009935 -0.113602  
C 0.458365 -4.231932 0.696063  
H 1.026410 -5.080228 0.283411  
H 0.188584 -4.519103 1.724227  
C -3.120724 -2.881450 -0.339574  
C -0.839085 -4.059725 -0.119511  
H -1.380460 -5.018614 -0.105641  
H -0.598368 -3.868671 -1.176332  
C -3.975258 -1.662521 0.063460  
H -3.975630 -1.577192 1.162111  
C -1.770089 -2.950580 0.393338  
H -1.260824 -1.980728 0.309233  
H -1.957697 -3.101226 1.468951  
H -5.022899 -1.832439 -0.226975  
C -3.489114 -0.339485 -0.553075  
H -3.719967 -0.335182 -1.630290  
H -2.394655 -0.285390 -0.479768  
H -3.682034 -3.806179 -0.136762  
H -2.950561 -2.861681 -1.428180  
C -4.084841 0.910195 0.110019  
H -3.842419 0.892370 1.183210  
H -5.183094 0.884363 0.044466  
C -3.593166 2.246795 -0.496047  
H -4.036198 3.072426 0.080576  
H -3.971843 2.342416 -1.522752  
Sum of electronic and zero-point Energies= -1044.469489  
Sum of electronic and thermal Energies= -1044.445891  
Sum of electronic and thermal Enthalpies= -1044.444947  
Sum of electronic and thermal Free Energies= -1044.522808

daec[n=4]-1-E2 (dmf)

C -1.180736 2.574955 -0.641459  
H -1.646208 2.718250 -1.612312

C -2.002311 2.433262 0.489535  
C -1.402154 2.267689 1.744772  
H -2.018431 2.177252 2.637241  
C -0.011041 2.178287 1.855198  
H 0.465724 2.018008 2.819971  
C 0.792768 2.271276 0.723859  
O 2.170250 2.165523 0.848206  
C 0.215453 2.505000 -0.541466  
O 1.078590 2.616916 -1.583297  
C 0.535499 2.824262 -2.886395  
H 1.395767 2.887456 -3.558786  
H -0.036532 3.760710 -2.938165  
H -0.105329 1.986160 -3.192884  
C 4.106455 -1.413955 -0.079502  
H 4.636636 -2.335015 -0.316100  
C 2.710156 -1.366981 -0.185730  
C 1.894032 -2.576567 -0.598886  
H 2.538018 -3.301087 -1.116428  
H 1.131611 -2.258037 -1.322951  
C 1.204379 -3.272693 0.594933  
H 0.667895 -2.519508 1.188308  
H 1.981343 -3.680828 1.258165  
C 2.046008 -0.167924 0.120769  
H 0.963506 -0.124710 0.040232  
C 2.762956 0.962466 0.520982  
C 4.159669 0.913069 0.624063  
H 4.703546 1.802133 0.934579  
C 4.820273 -0.277942 0.323204  
H 5.905442 -0.319353 0.400615  
C 0.240701 -4.407721 0.201104  
H 0.792986 -5.161050 -0.382055  
H -0.082804 -4.915447 1.123009  
C -3.233490 -2.682690 -0.610020  
C -1.013479 -3.988898 -0.592416  
H -1.595123 -4.897233 -0.814606  
H -0.721139 -3.576156 -1.569931  
C -4.054905 -1.541447 0.023418  
H -4.109023 -1.702809 1.112132  
C -1.917454 -2.978178 0.129702  
H -1.365737 -2.040074 0.279942  
H -2.153609 -3.355021 1.138161  
H -5.092021 -1.586862 -0.341691  
C -3.481858 -0.142628 -0.259610  
H -3.623612 0.096770 -1.325710  
H -2.396182 -0.156127 -0.095436  
H -3.840084 -3.600740 -0.634297  
H -3.018099 -2.433106 -1.661595  
C -4.093372 0.968252 0.605201  
H -3.942007 0.718568 1.666173  
H -5.182339 1.008570 0.450901  
C -3.510360 2.377100 0.333992  
H -3.985857 3.088201 1.024974  
H -3.782190 2.693619 -0.682218  
Sum of electronic and zero-point Energies= -1044.469578  
Sum of electronic and thermal Energies= -1044.445973  
Sum of electronic and thermal Enthalpies= -1044.445029  
Sum of electronic and thermal Free Energies= -1044.522792

daec[n=4]-2-TS (dmf)

C -2.902134 -1.816032 0.035612  
H -3.847958 -2.311193 0.238866  
C -2.878486 -0.411765 -0.094702  
C -1.648799 0.179784 -0.362193  
H -1.558856 1.244170 -0.507321  
C -0.478802 -0.569209 -0.449053  
H 0.442824 -0.032975 -0.610322  
C -0.493666 -1.950781 -0.319652  
O 0.634366 -2.757589 -0.403796  
C -1.737670 -2.591337 -0.086410  
O -1.698026 -3.947989 0.017928

C	-2.918125	-4.635486	0.278115
H	-3.651410	-4.476778	-0.525096
H	-3.358022	-4.329162	1.237722
H	-2.656882	-5.696895	0.237596
C	4.255913	-0.887727	0.502526
H	5.162662	-0.365920	0.803949
C	3.499300	-0.408464	-0.580283
C	3.802093	0.916854	-1.257731
H	3.095361	1.061894	-2.085350
H	4.807465	0.901088	-1.704405
C	3.748575	2.128978	-0.287464
H	3.963371	3.037615	-0.870058
H	4.587352	2.021258	0.414989
C	2.357697	-1.125923	-0.958719
H	1.804732	-0.814518	-1.839400
C	1.873178	-2.172913	-0.165549
C	2.624402	-2.643769	0.912317
H	2.248615	-3.470148	1.510729
C	3.838096	-2.015524	1.215154
H	4.436507	-2.382532	2.047044
C	2.468615	2.349341	0.553977
H	2.136344	1.390514	0.978451
H	2.762747	2.964406	1.418260
C	-0.959864	4.346411	0.459552
C	1.269556	3.057703	-0.113691
H	0.842474	2.433161	-0.912634
H	1.623918	3.981075	-0.599433
C	-2.101127	3.691988	-0.347087
H	-1.671131	3.102670	-1.170616
C	0.189543	3.423353	0.930925
H	0.700649	3.934240	1.761449
H	-0.223019	2.499803	1.364354
H	-2.687582	4.484153	-0.836985
C	-3.065637	2.813728	0.484129
H	-3.676646	3.471282	1.119252
H	-2.489021	2.193294	1.181693
H	-0.526201	5.163018	-0.138188
H	-1.398703	4.828896	1.346861
C	-3.997102	1.909782	-0.378854
H	-5.005545	2.344143	-0.400531
H	-3.650638	1.916098	-1.422719
C	-4.130338	0.438356	0.078392
H	-4.434041	0.416088	1.137992
H	-4.961384	-0.028222	-0.471072

Sum of electronic and zero-point Energies= -1044.440421  
Sum of electronic and thermal Energies= -1044.417835  
Sum of electronic and thermal Enthalpies= -1044.416891  
Sum of electronic and thermal Free Energies= -1044.491076

daec[n=4]-2-E1 (dmf)

C	-1.175177	-2.629662	-0.501645
H	-1.574979	-2.950629	-1.459549
C	-2.069492	-2.272016	0.523843
C	-1.554620	-1.884982	1.766093
H	-2.230879	-1.625363	2.577967
C	-0.171935	-1.782792	1.957318
H	0.240005	-1.447114	2.906611
C	0.703101	-2.082792	0.921179
O	2.069003	-1.955157	1.121601
C	0.210122	-2.548211	-0.317462
O	1.142862	-2.858163	-1.253816
C	0.688853	-3.293231	-2.534660
H	0.089908	-2.518674	-3.032968
H	0.101138	-4.218293	-2.459067
H	1.592862	-3.485144	-3.119487
C	4.111211	1.426063	-0.216844
H	4.671679	2.293683	-0.561530
C	2.744956	1.315496	-0.519488
C	2.042020	2.396632	-1.319344
H	1.180841	1.963416	-1.844917

H	2.730793	2.758570	-2.095341
C	1.582231	3.619292	-0.487806
H	1.330160	4.430501	-1.187694
H	2.438222	3.979247	0.101838
C	2.042557	0.184949	-0.074299
H	0.986325	0.088179	-0.307506
C	2.695739	-0.818786	0.651473
C	4.059226	-0.705728	0.946399
H	4.550362	-1.496773	1.508197
C	4.757342	0.421404	0.510224
H	5.818694	0.511274	0.735489
C	0.384453	3.389991	0.450997
H	0.591624	2.541768	1.121472
H	0.290493	4.272844	1.102172
C	-3.533074	2.957372	0.054948
C	-0.960518	3.165057	-0.261619
H	-0.922610	2.233846	-0.844627
H	-1.121832	3.975638	-0.991051
C	-3.778703	1.633517	-0.695045
H	-3.076015	1.546544	-1.537725
C	-2.148760	3.123948	0.712878
H	-2.157610	4.061361	1.290655
H	-1.986480	2.323228	1.449807
H	-4.783434	1.670841	-1.144365
C	-3.658875	0.381114	0.184823
H	-4.347708	0.463156	1.041202
H	-2.648928	0.341699	0.612220
H	-3.694585	3.792432	-0.644712
H	-4.301697	3.065006	0.836345
C	-3.933282	-0.930932	-0.565311
H	-4.997685	-0.988410	-0.837768
H	-3.371585	-0.934310	-1.511891
C	-3.555288	-2.204348	0.233577
H	-4.118145	-2.224346	1.177091
H	-3.866380	-3.085772	-0.344526

Sum of electronic and zero-point Energies= -1044.468736  
Sum of electronic and thermal Energies= -1044.445275  
Sum of electronic and thermal Enthalpies= -1044.444331  
Sum of electronic and thermal Free Energies= -1044.521544

daec[n=4]-2-E2 (dmf)

C	-1.500822	-2.097915	0.758257
H	-2.074867	-1.889620	1.656378
C	-2.182163	-2.269764	-0.459688
C	-1.444291	-2.571536	-1.611045
H	-1.955614	-2.729019	-2.558986
C	-0.047494	-2.635153	-1.559832
H	0.538130	-2.844543	-2.452533
C	0.621162	-2.400730	-0.363818
O	2.006317	-2.439397	-0.318106
C	-0.102992	-2.154044	0.821818
O	0.635261	-1.966506	1.945784
C	-0.053273	-1.674461	3.160523
H	-0.725570	-2.494170	3.448613
H	-0.627063	-0.740566	3.082848
H	0.724240	-1.559843	3.921125
C	4.198913	1.108488	-0.378099
H	4.799515	2.016412	-0.403783
C	2.855110	1.150863	-0.783887
C	2.234215	2.449923	-1.264471
H	1.339170	2.229391	-1.860722
H	2.944415	2.945561	-1.941552
C	1.878569	3.451055	-0.139100
H	1.677001	4.428126	-0.603957
H	2.766972	3.591712	0.493961
C	2.103143	-0.033180	-0.753572
H	1.067271	-0.017366	-1.080417
C	2.683422	-1.235019	-0.328121
C	4.023761	-1.273050	0.069363
H	4.458493	-2.216141	0.391865

C	4.772964	-0.094944	0.041974
H	5.817335	-0.120130	0.348468
C	0.681804	3.072935	0.751370
H	0.835641	2.069692	1.178110
H	0.665172	3.765294	1.607329
C	-3.264453	3.037862	0.411116
C	-0.688694	3.129221	0.054010
H	-0.739950	2.362373	-0.731987
H	-0.793714	4.099573	-0.458280
C	-3.631735	1.933863	-0.599769
H	-2.972592	1.996855	-1.478975
C	-1.857954	2.953016	1.036356
H	-1.781887	3.733368	1.809573
H	-1.743737	1.996784	1.568761
H	-4.649371	2.130097	-0.972166
C	-3.561405	0.511785	-0.025725
H	-4.179786	0.449035	0.884483
H	-2.531352	0.310390	0.293672
H	-3.375312	4.016907	-0.080930
H	-4.004445	3.024164	1.226683
C	-4.000176	-0.580150	-1.012582
H	-5.083133	-0.504302	-1.191515
H	-3.513390	-0.412650	-1.985499
C	-3.674873	-2.022160	-0.544190
H	-4.142507	-2.201332	0.434159
H	-4.128105	-2.730248	-1.251473

Sum of electronic and zero-point Energies= -1044.468766  
Sum of electronic and thermal Energies= -1044.445261  
Sum of electronic and thermal Enthalpies= -1044.444317  
Sum of electronic and thermal Free Energies= -1044.521735

#### daec[n=4]-3-TS (dmf)

C	2.728093	2.037113	-0.081928
H	3.638553	2.619579	0.033142
C	2.817170	0.631108	-0.152477
C	1.629490	-0.073863	-0.303776
H	1.632316	-1.147551	-0.396147
C	0.393210	0.566130	-0.333647
H	-0.489894	-0.050460	-0.397638
C	0.298163	1.948700	-0.271127
O	-0.897172	2.653240	-0.308226
C	1.494399	2.703273	-0.155358
O	1.340776	4.055052	-0.106883
C	2.509998	4.856912	0.029368
H	3.195149	4.720657	-0.819281
H	3.043143	4.638743	0.965448
H	2.159068	5.892934	0.047195
C	-4.357248	0.501700	0.607597
H	-5.226619	-0.083370	0.903155
C	-3.574960	0.088524	-0.484490
C	-3.813101	-1.234490	-1.190753
H	-3.138201	-1.303970	-2.053808
H	-4.837079	-1.273500	-1.590962
C	-3.630300	-2.472901	-0.270973
H	-3.825446	-3.371244	-0.876233
H	-4.424957	-2.444619	0.488555
C	-2.482948	0.883206	-0.855815
H	-1.904289	0.613583	-1.734235
C	-2.077422	1.961902	-0.060115
C	-2.855174	2.367351	1.025326
H	-2.540638	3.217909	1.625207
C	-4.016194	1.647759	1.331198
H	-4.634672	1.962926	2.169627
C	-2.283643	-2.637097	0.467772
H	-2.045717	-1.705720	1.003187
H	-2.433866	-3.396911	1.250346
C	1.443069	-3.721784	-0.306676
C	-1.065462	-3.062419	-0.374073
H	-0.850772	-2.304054	-1.142413
H	-1.304851	-3.989871	-0.918817

C	2.761031	-3.777262	0.505062
H	3.502113	-4.346185	-0.077961
C	0.196062	-3.283267	0.488094
H	-0.020717	-4.044586	1.254291
H	0.408908	-2.356789	1.040537
H	2.580595	-4.367946	1.416600
C	3.396559	-2.426936	0.915241
H	4.166179	-2.626781	1.675338
H	2.644946	-1.807937	1.421069
H	1.254977	-4.724882	-0.719145
H	1.573360	-3.069682	-1.183364
C	4.056059	-1.639231	-0.246788
H	3.528826	-1.840234	-1.190076
H	5.074683	-2.024767	-0.393748
C	4.145992	-0.108224	-0.050452
H	4.844726	0.303233	-0.794506
H	4.604287	0.107928	0.928248

Sum of electronic and zero-point Energies= -1044.446838  
Sum of electronic and thermal Energies= -1044.424506  
Sum of electronic and thermal Enthalpies= -1044.423561  
Sum of electronic and thermal Free Energies= -1044.496664

#### daec[n=4]-3-E1 (dmf)

C	1.530559	2.213987	-0.666912
H	1.960335	2.394291	-1.648390
C	2.388558	1.899167	0.403114
C	1.834988	1.691035	1.671911
H	2.481329	1.471042	2.518815
C	0.448830	1.753298	1.857886
H	0.006935	1.582745	2.837250
C	-0.393542	2.039646	0.790089
O	-1.755441	2.160048	1.016945
C	0.144259	2.298428	-0.489768
O	-0.750060	2.608134	-1.463217
C	-0.253146	2.853544	-2.778073
H	0.259974	1.971390	-3.184789
H	0.429326	3.714313	-2.794706
H	-1.132124	3.076238	-3.389503
C	-4.471422	-0.838412	0.014286
H	-5.204363	-1.603188	-0.237652
C	-3.134715	-1.002407	-0.379258
C	-2.703818	-2.240771	-1.142250
H	-1.919733	-1.973019	-1.862761
H	-3.556851	-2.603221	-1.731770
C	-2.210506	-3.409552	-0.252698
H	-2.118010	-4.302558	-0.889583
H	-2.993112	-3.638464	0.485686
C	-2.203895	-0.001638	-0.052689
H	-1.167508	-0.113825	-0.357375
C	-2.606529	1.138596	0.650607
C	-3.943557	1.299865	1.034948
H	-4.236586	2.195557	1.577547
C	-4.867930	0.305859	0.714241
H	-5.908413	0.428637	1.010163
C	-0.877977	-3.177316	0.480622
H	-0.946641	-2.261229	1.086130
H	-0.727393	-4.000338	1.196015
C	2.874787	-2.638539	-0.600821
C	0.351142	-3.088784	-0.437854
H	0.190441	-2.316394	-1.204825
H	0.466505	-4.039042	-0.983732
C	4.170338	-2.212132	0.117985
H	5.017421	-2.317982	-0.577792
C	1.648006	-2.762702	0.317029
H	1.839078	-3.536940	1.077625
H	1.499045	-1.823775	0.869992
H	4.364267	-2.917772	0.940688
C	4.160295	-0.778987	0.684506
H	5.008088	-0.659259	1.376075
H	3.257822	-0.638237	1.293745

H	3.048788	-3.607024	-1.094646
H	2.647878	-1.927442	-1.409790
C	4.241454	0.326578	-0.381513
H	3.580403	0.092531	-1.227981
H	5.262654	0.357523	-0.789616
C	3.873966	1.736287	0.146144
H	4.197331	2.482290	-0.592756
H	4.436250	1.937401	1.068931

Sum of electronic and zero-point Energies= -1044.468736  
Sum of electronic and thermal Energies= -1044.445296  
Sum of electronic and thermal Enthalpies= -1044.444352  
Sum of electronic and thermal Free Energies= -1044.521491

#### daec[n=4]-3-E2 (dmf)

C	1.716967	1.900509	0.619738
H	2.275888	1.798504	1.544919
C	2.412256	1.879467	-0.602827
C	1.690773	2.051197	-1.791182
H	2.212282	2.052873	-2.746573
C	0.301724	2.215559	-1.762238
H	-0.265358	2.355427	-2.680117
C	-0.381657	2.204761	-0.551411
O	-1.748303	2.433773	-0.518114
C	0.324359	2.052588	0.661589
O	-0.423335	2.072089	1.794694
C	0.245885	1.909243	3.044076
H	0.967645	2.718265	3.221769
H	0.760524	0.940251	3.100708
H	-0.537244	1.949142	3.806527
C	-4.487888	-0.687743	-0.162441
H	-5.228791	-1.481547	-0.080533
C	-3.196541	-0.988834	-0.622692
C	-2.825956	-2.410717	-0.999291
H	-2.048409	-2.393276	-1.774089
H	-3.703302	-2.895413	-1.449341
C	-2.356648	-3.287517	0.187860
H	-2.287134	-4.327662	-0.165557
H	-3.140969	-3.276664	0.959064
C	-2.257551	0.050034	-0.731163
H	-1.258663	-0.163227	-1.102572
C	-2.606813	1.360464	-0.385818
C	-3.897832	1.656343	0.065581
H	-4.150318	2.682494	0.321913
C	-4.831619	0.625017	0.175164
H	-5.837975	0.850352	0.524052
C	-1.017541	-2.882989	0.827405
H	-1.065377	-1.829715	1.143105
H	-0.882843	-3.468375	1.749945
C	2.751085	-2.759555	-0.321145
C	0.212408	-3.086957	-0.071189
H	0.078437	-2.543248	-1.018265
H	0.294519	-4.152242	-0.340785
C	4.057724	-2.219546	0.294080
H	4.905365	-2.518537	-0.342232
C	1.517918	-2.614775	0.584734
H	1.685223	-3.174655	1.519102
H	1.393835	-1.562451	0.879141
H	4.218497	-2.713809	1.264745
C	4.095990	-0.692782	0.500013
H	4.928320	-0.439441	1.173995
H	3.184135	-0.378267	1.023625
H	2.890602	-3.823939	-0.565607
H	2.555005	-2.255328	-1.279876
C	4.256914	0.119121	-0.796731
H	3.630750	-0.303403	-1.595218
H	5.296768	0.031886	-1.145022
C	3.906226	1.621857	-0.648120
H	4.333442	2.167183	-1.500410
H	4.387147	2.019440	0.257004

Sum of electronic and zero-point Energies= -1044.468757

Sum of electronic and thermal Energies= -1044.445217  
Sum of electronic and thermal Enthalpies= -1044.444272  
Sum of electronic and thermal Free Energies= -1044.521895

#### daec[n=4]-4-TS (dmf)

C	-1.273835	-3.183586	0.012900
H	-1.542496	-4.234036	-0.062425
C	0.087377	-2.818186	-0.051099
C	0.382758	-1.464784	0.062815
H	1.402818	-1.115918	0.068184
C	-0.615550	-0.504623	0.181879
H	-0.313338	0.528673	0.211058
C	-1.955906	-0.853094	0.255193
O	-2.990087	0.065759	0.401642
C	-2.293151	-2.228711	0.179505
O	-3.619753	-2.521798	0.267704
C	-4.011438	-3.888884	0.187914
H	-5.101216	-3.891449	0.284081
H	-3.573919	-4.482885	1.002693
C	-3.731742	-4.334219	-0.777345
C	-1.977452	3.961864	-0.712892
H	-1.656935	4.933771	-1.085108
C	-1.281150	3.357182	0.343827
C	0.062704	3.868522	0.837008
H	0.171709	3.659331	1.910713
H	0.146461	4.955507	0.704500
C	1.195747	3.141771	0.057570
H	1.192636	3.496890	-0.984246
H	0.937079	2.078442	0.010311
C	-1.734589	2.114074	0.813935
H	-1.239347	1.656180	1.665697
C	-2.710054	1.399317	0.111813
C	-3.404657	2.005307	-0.938845
H	-4.180550	1.451372	-1.461791
C	-3.058076	3.306714	-1.316132
H	-3.599028	3.789674	-2.127833
C	2.613031	3.261561	0.639990
H	2.949100	4.308190	0.586375
H	2.588617	3.001601	1.710254
C	4.556159	-0.043642	-0.463029
C	3.656520	2.362451	-0.068692
H	4.656081	2.636344	0.302579
H	3.660295	2.589151	-1.146877
C	4.464772	-1.539783	-0.071898
H	4.322453	-1.592067	1.018324
C	3.450952	0.847960	0.139976
H	2.481985	0.554814	-0.281669
H	3.390139	0.648332	1.222202
H	5.441466	-2.007355	-0.261562
C	3.355811	-2.376322	-0.774867
H	3.799962	-2.960595	-1.593676
H	2.645095	-1.702148	-1.264737
H	5.532189	0.336276	-0.122917
H	4.558309	0.056499	-1.560103
C	2.612409	-3.345658	0.184619
H	3.248271	-4.228108	0.344468
H	2.514346	-2.870286	1.171285
C	1.207473	-3.833780	-0.250852
H	0.962387	-4.747912	0.308643
H	1.236746	-4.139765	-1.309676

Sum of electronic and zero-point Energies= -1044.439903  
Sum of electronic and thermal Energies= -1044.417155  
Sum of electronic and thermal Enthalpies= -1044.416211  
Sum of electronic and thermal Free Energies= -1044.491128

#### daec[n=4]-4-E1 (dmf)

C	-0.932308	-2.384350	0.768082
H	-1.415988	-2.368554	1.740417
C	-1.719076	-2.592176	-0.378560
C	-1.088475	-2.636591	-1.628393

H	-1.674525	-2.813511	-2.528453
C	0.293624	-2.439286	-1.733090
H	0.790982	-2.461750	-2.700460
C	1.060092	-2.204200	-0.596678
O	2.433842	-2.047706	-0.706371
C	0.452071	-2.193233	0.677870
O	1.279476	-1.987653	1.734586
C	0.704930	-1.946775	3.039771
H	1.538975	-1.770858	3.724998
H	0.219378	-2.898818	3.294339
H	-0.022241	-1.128559	3.133245
C	4.166402	1.698354	-0.098346
H	4.639866	2.664549	0.067798
C	2.813575	1.640643	-0.459082
C	1.977737	2.895929	-0.640268
H	1.640615	2.949666	-1.687283
H	2.603217	3.782929	-0.470710
C	0.732998	2.940002	0.269203
H	1.048858	3.012025	1.320905
H	0.209182	1.980418	0.178563
C	2.224658	0.381903	-0.67625
H	1.181171	0.314711	-0.963090
C	2.966234	-0.788839	-0.499985
C	4.321507	-0.727553	-0.152759
H	4.885592	-1.649423	-0.032789
C	4.911993	0.520906	0.043535
H	5.963721	0.576463	0.319274
C	-0.245128	4.082810	-0.057001
H	0.167876	5.034657	0.308366
H	-0.332286	4.188043	-1.150160
C	-3.767255	2.352953	0.453206
C	-1.653427	3.860606	0.532751
H	-2.220318	4.803275	0.498526
H	-1.562955	3.596544	1.598618
C	-4.376563	1.083261	-0.177153
H	-4.365214	1.189493	-1.273855
C	-2.439939	2.764214	-0.204466
H	-1.803873	1.874390	-0.299556
H	-2.639957	3.098743	-1.234910
H	-5.435623	0.996926	0.108525
C	-3.637726	-0.206735	0.221633
H	-3.850115	-0.430625	1.279290
H	-2.554332	-0.039138	0.162278
H	-4.484461	3.184425	0.380063
H	-3.608525	2.180242	1.529807
C	-3.990002	-1.424894	-0.641975
H	-5.069277	-1.630597	-0.576642
H	-3.783787	-1.190452	-1.697449
C	-3.226737	-2.716324	-0.257805
H	-3.579827	-3.531404	-0.905223
H	-3.487786	-2.994686	0.772668

Sum of electronic and zero-point Energies= -1044.468600  
Sum of electronic and thermal Energies= -1044.445002  
Sum of electronic and thermal Enthalpies= -1044.444058  
Sum of electronic and thermal Free Energies= -1044.521606

#### daec[n=4]-4-E2 (dmf)

C	-0.893579	-2.709347	-0.512067
H	-1.409982	-3.027653	-1.413333
C	-1.638724	-2.509396	0.664576
C	-0.968375	-2.115266	1.828400
H	-1.524771	-1.968010	2.751893
C	0.413464	-1.896136	1.810850
H	0.941043	-1.581671	2.708983
C	1.138492	-2.070600	0.637895
O	2.513683	-1.882272	0.637771
C	0.490745	-2.493426	-0.542980
O	1.280821	-2.650367	-1.636009
C	0.664972	-3.066833	-2.853640
H	1.472762	-3.126463	-3.588610

H	-0.084533	-2.339505	-3.194738
H	0.195196	-4.054418	-2.748654
C	4.127899	1.930692	0.139099
H	4.571367	2.918651	0.027443
C	2.779270	1.734210	-0.185608
C	1.913180	2.865556	-0.713136
H	1.619395	2.633052	-1.748898
H	2.506312	3.789000	-0.761342
C	0.630068	3.100315	0.108737
H	0.897993	3.443904	1.119212
H	0.126816	2.135126	0.244193
C	2.227082	0.450815	-0.030885
H	1.185108	0.277772	-0.283545
C	3.003689	-0.606094	0.448697
C	4.355597	-0.408251	0.760785
H	4.946530	-1.243299	1.129652
C	4.907423	0.862244	0.600796
H	5.955550	1.023485	0.847135
C	-0.353116	4.096313	-0.533198
H	0.013380	5.122410	-0.382540
H	-0.374706	3.937668	-1.623153
C	-3.856508	2.396627	0.165623
C	-1.789893	3.964522	0.013600
H	-2.375271	4.852819	-0.268104
H	-1.759898	3.954257	1.114954
C	-4.392060	0.995454	-0.195689
H	-4.306185	0.852497	-1.284903
C	-2.502091	2.700429	-0.494891
H	-1.838601	1.837561	-0.350418
H	-2.646857	2.785409	-1.583723
H	-5.466373	0.935572	0.034051
C	-3.654822	-0.143578	0.531633
H	-3.952653	-0.146226	1.592270
H	-2.575143	0.056555	0.524418
H	-4.588454	3.162388	-0.132593
H	-3.760589	2.475329	1.260428
C	-3.895941	-1.532442	-0.074062
H	-4.971766	-1.764364	-0.063698
H	-3.593718	-1.520538	-1.132374
C	-3.146846	-2.677178	0.650038
H	-3.408103	-3.625909	0.159537
H	-3.509436	-2.746047	1.684929

Sum of electronic and zero-point Energies= -1044.468239  
Sum of electronic and thermal Energies= -1044.444525  
Sum of electronic and thermal Enthalpies= -1044.443580  
Sum of electronic and thermal Free Energies= -1044.522049

#### daec[n=5]-1-TS (dmf)

C	2.883731	2.009879	-0.245555
H	3.808447	2.559330	-0.093070
C	2.950767	0.632230	-0.524697
C	1.747425	-0.048352	-0.717770
H	1.745056	-1.102972	-0.967799
C	0.517456	0.603376	-0.601834
H	-0.386569	0.022785	-0.724046
C	0.452960	1.967916	-0.333833
O	-0.710010	2.710045	-0.225990
C	1.659829	2.688503	-0.160453
O	1.529562	4.018626	0.096004
C	2.716291	4.782858	0.287802
H	3.356924	4.766694	-0.605217
H	2.381982	5.807897	0.473263
H	3.291389	4.427166	1.154324
C	-4.402860	0.976468	0.659286
H	-5.356406	0.524103	0.926401
C	-3.700521	0.512322	-0.464971
C	-4.180667	-0.683062	-1.266843
H	-3.504219	-0.834227	-2.117803
H	-5.175186	-0.480964	-1.691573
C	-4.280779	-1.986329	-0.432654

H	-5.114310	-1.876477	0.276063
C	-3.030519	-2.394305	0.369871
H	-3.320476	-3.213748	1.045490
H	-2.735732	-1.560869	1.024706
C	-1.805607	-2.855300	-0.438548
H	-1.504123	-2.076790	-1.155818
H	-2.077679	-3.737626	-1.040031
H	-4.567524	-2.803065	-1.112347
C	-2.487557	1.130568	-0.799421
H	-1.970956	0.827232	-1.704703
C	-1.930720	2.108377	0.033701
C	-2.631178	2.561844	1.154412
H	-2.192699	3.333950	1.781807
C	-3.879760	2.005426	1.446967
H	-4.434693	2.361541	2.313031
C	1.777120	-4.134514	0.705691
C	-0.614562	-3.198390	0.474858
H	-0.297261	-2.284114	0.999109
H	-0.957923	-3.891261	1.260155
C	2.640010	-2.914202	1.096692
H	3.132451	-3.113030	2.060663
C	0.590241	-3.836191	-0.237642
H	0.921268	-3.192399	-1.067003
H	0.261028	-4.778060	-0.702884
H	1.996176	-2.040204	1.267021
C	3.733259	-2.568404	0.067116
H	3.299860	-2.525367	-0.941778
H	4.441022	-3.409954	0.039230
H	2.429264	-4.889794	0.240434
H	1.379018	-4.605908	1.617323
C	4.516698	-1.257176	0.360553
H	4.302130	-0.916317	1.384232
H	5.593128	-1.476860	0.339865
C	4.289574	-0.079105	-0.621456
H	4.430008	-0.456171	-1.646818
H	5.086408	0.659490	-0.459971

Sum of electronic and zero-point Energies= -1083.735336  
Sum of electronic and thermal Energies= -1083.711345  
Sum of electronic and thermal Enthalpies= -1083.710400  
Sum of electronic and thermal Free Energies= -1083.788320

daec[n=5]-1-E1 (dmf)

C	1.121463	2.473850	-0.758375
H	1.575737	2.610576	-1.735578
C	1.952054	2.420017	0.373498
C	1.363082	2.253695	1.634615
H	1.983637	2.223139	2.527872
C	-0.022756	2.128383	1.756408
H	-0.490895	2.003907	2.730565
C	-0.839079	2.177353	0.630288
O	-2.214340	2.158647	0.798883
C	-0.273164	2.365332	-0.647498
O	-1.145157	2.425935	-1.686700
C	-0.615732	2.600938	-3.000123
H	0.044011	1.768870	-3.281789
H	-1.481623	2.618885	-3.667993
H	-0.067979	3.549018	-3.088926
C	-4.585310	-1.198977	0.128828
H	-5.232790	-2.057333	-0.043035
C	-3.237228	-1.260941	-0.256256
C	-2.692577	-2.519876	-0.904371
H	-1.937253	-2.252168	-1.654823
H	-3.511768	-3.007156	-1.450088
C	-2.098605	-3.555357	0.083983
H	-2.819642	-3.713193	0.899431
C	-0.723102	-3.204141	0.677987
H	-0.493118	-3.932422	1.470966
H	-0.768884	-2.222166	1.172964
C	0.419279	-3.209845	-0.349176
H	0.215159	-2.467372	-1.135211

H	0.443232	-4.187822	-0.856537
H	-2.016721	-4.517799	-0.443637
C	-2.415550	-0.141753	-0.036436
H	-1.371984	-0.171521	-0.336762
C	-2.941398	1.014734	0.550105
C	-4.289267	1.071972	0.926471
H	-4.675743	1.982977	1.377199
C	-5.103486	-0.039767	0.714250
H	-6.152117	0.001941	1.003757
C	4.317204	-2.536510	-0.296118
C	1.802042	-2.915628	0.250824
H	1.751875	-1.973814	0.817239
H	2.064039	-3.698325	0.980923
C	4.477376	-1.257477	0.547129
H	5.542357	-1.140563	0.802004
C	2.897598	-2.819305	-0.821893
H	2.614476	-2.040512	-1.545977
H	2.921882	-3.760786	-1.392588
H	3.952659	-1.380385	1.506668
C	3.971555	0.027234	-0.124663
H	2.893514	-0.064507	-0.315534
H	4.446719	0.148183	-1.111423
H	4.998606	-2.482996	-1.159575
H	4.657070	-3.394259	0.305087
C	4.224804	1.283276	0.721738
H	3.944930	1.080927	1.766331
H	5.301315	1.509538	0.733775
C	3.460608	2.534477	0.235891
H	3.717310	2.739203	-0.812583
H	3.809128	3.401174	0.817180

Sum of electronic and zero-point Energies= -1083.753372  
Sum of electronic and thermal Energies= -1083.728522  
Sum of electronic and thermal Enthalpies= -1083.727578  
Sum of electronic and thermal Free Energies= -1083.808406

daec[n=5]-1-E2 (dmf)

C	1.225533	2.308242	0.634302
H	1.725073	2.318068	1.598513
C	1.998843	2.392813	-0.539717
C	1.344499	2.400594	-1.775608
H	1.922729	2.466274	-2.695197
C	-0.053642	2.327815	-1.842272
H	-0.570171	2.346994	-2.799522
C	-0.808725	2.238035	-0.679990
O	-2.191483	2.277084	-0.746601
C	-0.169404	2.225547	0.581348
O	-0.987268	2.145536	1.662148
C	-0.388471	2.107231	2.956392
H	0.176928	3.025988	3.164386
H	-1.218187	2.024668	3.664124
H	0.273219	1.237223	3.066871
C	-4.572992	-1.069417	-0.054789
H	-5.224722	-1.926657	0.106773
C	-3.268987	-1.272406	-0.534651
C	-2.779734	-2.677517	-0.830430
H	-2.031256	-2.645989	-1.632751
H	-3.624922	-3.263227	-1.217322
C	-2.201441	-3.431859	0.392364
H	-2.927719	-3.370041	1.216120
C	-0.827262	-2.949981	0.888149
H	-0.604358	-3.462678	1.836647
H	-0.871909	-1.876329	1.127245
C	0.323121	-3.207317	-0.097206
H	0.144353	-2.652637	-1.030548
H	0.330470	-4.273660	-0.375136
H	-2.126709	-4.497737	0.128287
C	-2.445175	-0.154827	-0.747453
H	-1.438676	-0.288139	-1.136989
C	-2.924064	1.134647	-0.489106
C	-4.226901	1.331396	-0.020332

H	-4.578428	2.343433	0.165457
C	-5.045072	0.221849	0.196513
H	-6.060734	0.368323	0.560091
C	4.237369	-2.625009	-0.097021
C	1.703674	-2.815690	0.449832
H	1.662020	-1.776470	0.808527
H	1.940187	-3.433931	1.330884
C	4.415283	-1.228676	0.528030
H	5.473755	-1.101894	0.804157
C	2.818724	-2.957618	-0.597292
H	2.574986	-2.320778	-1.460946
H	2.821073	-3.990053	-0.980355
H	3.852437	-1.176452	1.472269
C	3.979816	-0.059230	-0.366216
H	2.919941	-0.178327	-0.629234
H	4.535190	-0.086360	-1.317518
H	4.935646	-2.733032	-0.941661
H	4.542189	-3.378257	0.646191
C	4.174952	1.307856	0.304439
H	3.774322	1.268248	1.328368
H	5.249413	1.520177	0.408344
C	3.512914	2.481379	-0.448694
H	3.927679	2.547473	-1.464054
H	3.789038	3.417675	0.060047

Sum of electronic and zero-point Energies= -1083.753882  
Sum of electronic and thermal Energies= -1083.729080  
Sum of electronic and thermal Enthalpies= -1083.728136  
Sum of electronic and thermal Free Energies= -1083.808644

daec[n=5]-2-TS (dmf)

C	-2.964864	-1.925667	-0.187401
H	-3.918369	-2.400747	0.025561
C	-2.942910	-0.547837	-0.473018
C	-1.703717	0.038737	-0.741887
H	-1.629866	1.090863	-0.992776
C	-0.525728	-0.709780	-0.701112
H	0.413628	-0.208348	-0.893416
C	-0.549609	-2.071349	-0.413584
O	0.571944	-2.885403	-0.372122
C	-1.793317	-2.696615	-0.161601
O	-1.750595	-4.029800	0.107347
C	-2.979795	-4.697192	0.378278
H	-3.476090	-4.285884	1.268625
H	-2.715100	-5.742451	0.563339
H	-3.666602	-4.643426	-0.478172
C	4.225393	-1.244971	0.805102
H	5.162681	-0.804713	1.142096
C	3.666483	-0.836775	-0.416738
C	4.268672	0.300893	-1.216899
H	3.860046	0.286395	-2.236625
H	5.355986	0.166313	-1.305977
C	4.004536	1.688312	-0.576548
H	4.514644	1.726904	0.397941
C	2.522717	2.048547	-0.373177
H	2.044481	1.273787	0.243125
H	2.002878	2.035011	-1.343405
C	2.331639	3.410478	0.317139
H	2.655013	4.218399	-0.358657
H	3.011053	3.452590	1.182806
H	4.486895	2.451668	-1.205701
C	2.471955	-1.436414	-0.839788
H	2.053178	-1.171917	-1.807003
C	1.794542	-2.335204	-0.009366
C	2.352084	-2.736140	1.206735
H	1.819116	-3.449707	1.830297
C	3.583605	-2.201201	1.597057
H	4.031004	-2.515784	2.538151
C	-1.522259	4.395227	0.333060
C	0.906284	3.704656	0.825137
H	0.578487	2.872221	1.467343

H	0.954673	4.588572	1.480501
C	-2.371646	3.234366	0.909861
H	-2.842377	3.545496	1.854147
C	-0.154910	3.980463	-0.254376
H	-0.281221	3.101343	-0.904664
H	0.213325	4.789826	-0.904108
H	-1.719233	2.387972	1.169055
C	-3.480643	2.749774	-0.043387
H	-3.053240	2.562564	-1.037841
H	-4.188382	3.578738	-0.190688
H	-2.106956	4.909012	-0.444823
H	-1.342231	5.149612	1.113587
C	-4.255891	1.495613	0.453403
H	-5.310080	1.765633	0.604146
H	-3.882237	1.194233	1.442823
C	-4.230686	0.260201	-0.482398
H	-5.056532	-0.406491	-0.200044
H	-4.450979	0.595226	-1.508398

Sum of electronic and zero-point Energies= -1083.734601  
Sum of electronic and thermal Energies= -1083.710463  
Sum of electronic and thermal Enthalpies= -1083.709518  
Sum of electronic and thermal Free Energies= -1083.788414

daec[n=5]-2-E1 (dmf)

C	-0.730132	-2.709329	-0.698731
H	-1.145371	-2.991541	-1.662006
C	-1.593381	-2.596139	0.403728
C	-1.054947	-2.239202	1.647924
H	-1.698860	-2.159881	2.521201
C	0.311672	-1.981323	1.777616
H	0.740249	-1.703318	2.738232
C	1.159099	-2.086141	0.678546
O	2.522364	-1.900638	0.854818
C	0.646903	-2.468110	-0.577648
O	1.546964	-2.563176	-1.590264
C	1.068665	-2.935284	-2.881997
H	0.608658	-3.932810	-2.867670
H	1.949661	-2.952020	-3.529869
H	0.345856	-2.204249	-3.269517
C	4.358521	1.786701	0.228861
H	4.864902	2.738116	0.074526
C	3.098393	1.571602	-0.349374
C	2.448718	2.654563	-1.190502
H	1.985065	2.201069	-2.079001
H	3.237969	3.323948	-1.557925
C	1.383417	3.513931	-0.467607
H	1.799127	3.892910	0.478550
C	0.048881	2.800913	-0.208028
H	0.200897	1.951511	0.474346
H	-0.306163	2.372710	-1.157114
C	-1.028060	3.727840	0.377585
H	-1.163570	4.594104	-0.290070
H	-0.664451	4.134867	1.333881
H	1.191385	4.397780	-1.094756
C	2.462582	0.334822	-0.146298
H	1.493396	0.147639	-0.598444
C	3.078425	-0.660160	0.619597
C	4.340986	-0.443245	1.185445
H	4.803606	-1.233173	1.772391
C	4.973102	0.783666	0.985721
H	5.954229	0.957647	1.424272
C	-4.530110	2.059358	-0.469653
C	-2.392598	3.052338	0.610350
H	-2.250857	2.176714	1.261757
H	-3.039731	3.745951	1.170150
C	-4.616382	0.776677	0.378671
H	-5.675395	0.484213	0.454756
C	-3.117330	2.635872	-0.680072
H	-2.507165	1.908461	-1.232768
H	-3.199824	3.517112	-1.335815

H	-4.290796	0.989455	1.408151
C	-3.806342	-0.410409	-0.162807
H	-2.740269	-0.145688	-0.191218
H	-4.099121	-0.614636	-1.205502
H	-4.973921	1.860222	-1.457740
H	-5.163687	2.829606	-0.002355
C	-3.984595	-1.683769	0.675588
H	-5.032535	-2.014843	0.621564
H	-3.794627	-1.450726	1.733842
C	-3.081346	-2.859903	0.246526
H	-3.355146	-3.741117	0.846503
H	-3.292986	-3.121140	-0.799438
Sum of electronic and zero-point Energies= -1083.753316			
Sum of electronic and thermal Energies= -1083.728390			
Sum of electronic and thermal Enthalpies= -1083.727446			
Sum of electronic and thermal Free Energies= -1083.808800			

daec[n=5]-2-E2 (dmf)

C	-1.013905	-2.379080	0.607997
H	-1.569457	-2.362807	1.540790
C	-1.708604	-2.566686	-0.602325
C	-0.980071	-2.607209	-1.795429
H	-1.497041	-2.753863	-2.741792
C	0.413578	-2.459101	-1.785597
H	0.987255	-2.495828	-2.709193
C	1.089514	-2.258479	-0.589116
O	2.473166	-2.185700	-0.571313
C	0.375214	-2.219793	0.630675
O	1.119934	-2.033839	1.750749
C	0.442549	-1.961074	3.003913
H	-0.268831	-1.124042	3.027788
H	1.222394	-1.796221	3.752775
H	-0.086381	-2.897253	3.229587
C	4.430861	1.443148	0.034044
H	4.969625	2.377264	0.185132
C	3.194361	1.457289	-0.630308
C	2.614225	2.762028	-1.142573
H	2.110932	2.587243	-2.104616
H	3.442843	3.454432	-1.343656
C	1.619096	3.463596	-0.187589
H	2.080757	3.570937	0.805919
C	0.254974	2.771603	-0.059637
H	0.381322	1.767492	0.372379
H	-0.156741	2.622038	-1.068764
C	-0.743943	3.565977	0.796425
H	-0.866505	4.574091	0.368428
H	-0.313604	3.711962	1.799428
H	1.461289	4.485244	-0.565389
C	2.518920	0.240871	-0.822995
H	1.570206	0.225678	-1.353357
C	3.070647	-0.956784	-0.356992
C	4.308948	-0.967133	0.292708
H	4.721527	-1.911641	0.638779
C	4.982186	0.239929	0.485836
H	5.945873	0.240529	0.992246
C	-4.369837	2.299599	-0.208375
C	-2.128694	2.908140	0.941902
H	-2.001903	1.900879	1.366926
H	-2.713812	3.478266	1.680811
C	-4.505399	0.874533	0.359668
H	-5.577193	0.635890	0.443659
C	-2.931576	2.828307	-0.366921
H	-2.393650	2.208184	-1.097035
H	-2.983182	3.835708	-0.809535
H	-4.112318	0.847110	1.387259
C	-3.811973	-0.218498	-0.466609
H	-2.737963	0.001161	-0.540019
H	-4.198416	-0.204819	-1.498613
H	-4.865006	2.338549	-1.191340
H	-4.932060	2.988198	0.441851

C	-3.996151	-1.620309	0.130833
H	-5.064071	-1.885293	0.124598
H	-3.696782	-1.603492	1.189323
C	-3.218780	-2.734493	-0.601037
H	-3.473561	-3.696567	-0.129887
H	-3.567189	-2.801000	-1.640968
Sum of electronic and zero-point Energies= -1083.753833			
Sum of electronic and thermal Energies= -1083.728999			
Sum of electronic and thermal Enthalpies= -1083.728055			
Sum of electronic and thermal Free Energies= -1083.809014			

daec[n=5]-3-TS (dmf)

C	1.670452	2.835615	0.228581
H	2.238031	3.660088	0.651032
C	2.278676	1.569096	0.139173
C	1.527790	0.528200	-0.413732
H	1.937078	-0.466412	-0.504000
C	0.216340	0.731406	-0.836546
H	-0.328217	-0.102148	-1.260461
C	-0.403747	1.966527	-0.690401
O	-1.734688	2.174976	-1.042420
C	0.338802	3.049281	-0.168163
O	-0.314854	4.238044	-0.071019
C	0.393236	5.349910	0.470441
H	0.707417	5.163140	1.506960
H	-0.310788	6.187030	0.451924
H	1.273453	5.603129	-0.136800
C	-4.397606	-0.502994	0.751692
H	-5.066516	-1.199855	1.254280
C	-3.623907	-0.940787	-0.336433
C	-3.612519	-2.392250	-0.778625
H	-3.038047	-2.477148	-1.710182
H	-4.635842	-2.721667	-1.011715
C	-3.040530	-3.364332	0.285258
H	-3.720511	-3.361103	1.149656
C	-1.614932	-3.087836	0.803246
H	-1.449625	-3.743529	1.672233
H	-1.560147	-2.059743	1.191652
C	-0.461166	-3.312810	-0.190382
H	-0.545756	-2.612080	-1.035057
H	-0.542144	-4.323438	-0.622143
H	-3.085353	-4.382433	-0.130615
C	-2.792980	-0.011752	-0.976453
H	-2.235968	-0.315465	-1.857680
C	-2.649256	1.286844	-0.476196
C	-3.418620	1.716984	0.605700
H	-3.303233	2.732683	0.975838
C	-4.310221	0.817628	1.201201
H	-4.920772	1.145270	2.040753
C	3.501664	-3.256370	0.191535
C	0.920171	-3.150713	0.474003
H	0.975158	-2.153891	0.935145
H	1.002328	-3.872920	1.302366
C	3.951518	-1.850337	0.648281
H	4.788654	-1.959175	1.354857
C	2.111832	-3.352201	-0.479203
H	2.023925	-4.348197	-0.940505
H	2.044459	-2.633733	-1.310477
H	3.140976	-1.380615	1.221874
C	4.398159	-0.928203	-0.501953
H	3.658491	-0.951942	-1.311704
H	5.316498	-1.345638	-0.943318
H	4.256139	-3.657540	-0.503135
H	3.508499	-3.929316	1.062928
C	4.699760	0.539926	-0.116911
H	4.909660	1.099022	-1.040986
H	5.633992	0.557708	0.464739
C	3.662545	1.329607	0.722097
H	3.539998	0.820129	1.690530
H	4.111733	2.302994	0.962260



Sum of electronic and zero-point Energies= -1083.733893  
Sum of electronic and thermal Energies= -1083.710201  
Sum of electronic and thermal Enthalpies= -1083.709257  
Sum of electronic and thermal Free Energies= -1083.785783

daec[n=5]-3-E1 (dmf)

C	1.685661	2.540519	-0.111975
H	2.376666	3.054616	-0.773682
C	2.200102	1.705308	0.896672
C	1.302130	1.054943	1.750694
H	1.677020	0.416835	2.548483
C	-0.078345	1.234998	1.605059
H	-0.775320	0.742683	2.279741
C	-0.578575	2.052326	0.596580
O	-1.931908	2.314521	0.475829
C	0.306629	2.718964	-0.279519
O	-0.266421	3.501546	-1.230583
C	0.593051	4.192406	-2.134594
H	1.249374	4.898746	-1.607321
H	-0.068377	4.746480	-2.806890
H	1.205560	3.494107	-2.721676
C	-4.749993	-0.716461	0.004078
H	-5.507864	-1.488184	-0.121468
C	-3.456093	-0.928121	-0.500057
C	-3.108883	-2.230743	-1.194029
H	-2.317789	-2.055735	-1.934777
H	-3.988920	-2.577993	-1.752527
C	-2.678015	-3.363834	-0.229065
H	-3.456236	-3.478744	0.539675
C	-1.313020	-3.172009	0.455139
H	-1.215506	-3.923164	1.253906
H	-1.284911	-2.192891	0.956698
C	-0.109097	-3.299577	-0.490627
H	-0.209009	-2.587049	-1.323304
H	-0.116638	-4.302395	-0.947508
H	-2.664023	-4.307351	-0.795683
C	-2.494753	0.081219	-0.337992
H	-1.493062	-0.054958	-0.738073
C	-2.821067	1.269831	0.326575
C	-4.112030	1.477273	0.822643
H	-4.345663	2.411214	1.328113
C	-5.072626	0.478004	0.653431
H	-6.080379	0.634879	1.034062
C	3.818028	-2.982780	-0.127832
C	1.243397	-3.062386	0.197307
H	1.245501	-2.053640	0.636496
H	1.357348	-3.763578	1.039963
C	4.077867	-1.566587	0.421406
H	5.097267	-1.542274	0.838227
C	2.434064	-3.219751	-0.760240
H	2.416832	-4.237593	-1.180184
H	2.298791	-2.541895	-1.616482
H	3.403527	-1.367865	1.266086
C	3.940528	-0.450953	-0.626347
H	2.893342	-0.372947	-0.951300
H	4.514808	-0.731946	-1.523261
H	4.586568	-3.211523	-0.882868
H	3.967438	-3.708927	0.686663
C	4.428163	0.932435	-0.163394
H	4.343647	1.634596	-1.005753
H	5.500290	0.876942	0.079718
C	3.698847	1.529792	1.061342
H	3.885181	0.904467	1.943747
H	4.155371	2.507662	1.277667

Sum of electronic and zero-point Energies= -1083.752819  
Sum of electronic and thermal Energies= -1083.728080  
Sum of electronic and thermal Enthalpies= -1083.727136  
Sum of electronic and thermal Free Energies= -1083.807945

daec[n=5]-3-E2 (dmf)

C	1.341615	1.801188	0.972563
H	1.798984	1.476547	1.902637
C	2.172487	2.176522	-0.097562
C	1.577617	2.616709	-1.287248
H	2.196496	2.924511	-2.127639
C	0.184697	2.669075	-1.405365
H	-0.286681	3.014763	-2.322925
C	-0.631115	2.295153	-0.342001
O	-2.001319	2.464265	-0.448508
C	-0.054682	1.862816	0.872236
O	-0.920349	1.543009	1.868377
C	-0.382936	1.107761	3.116473
H	0.205452	0.187374	3.002949
H	-1.247102	0.908557	3.756444
H	0.240005	1.886345	3.577684
C	-4.661522	-0.741215	-0.442399
H	-5.378947	-1.560366	-0.444523
C	-3.321791	-0.993170	-0.778494
C	-2.871188	-2.400720	-1.117372
H	-2.053347	-2.361583	-1.848851
H	-3.702143	-2.927270	-1.606238
C	-2.431643	-3.237351	0.110928
H	-3.230909	-3.191896	0.865080
C	-1.097646	-2.820886	0.755921
H	-1.000608	-3.338555	1.722531
H	-1.119716	-1.745904	0.990269
C	0.137949	-3.138712	-0.100128
H	0.029411	-2.686217	-1.097363
H	0.187595	-4.227016	-0.266023
H	-2.362555	-4.290748	-0.200666
C	-2.412404	0.076747	-0.780961
H	-1.374897	-0.093716	-1.057637
C	-2.835222	1.364729	-0.436125
C	-4.172938	1.612622	-0.110477
H	-4.480821	2.624019	0.143986
C	-5.080321	0.552400	-0.117432
H	-6.123157	0.739313	0.133156
C	4.035085	-2.526006	0.195977
C	1.460207	-2.655067	0.513088
H	1.408010	-1.564916	0.652214
H	1.582590	-3.087155	1.519583
C	4.205484	-0.998912	0.315123
H	5.218817	-0.796230	0.696631
C	2.680068	-3.014678	-0.348336
H	2.725761	-4.109656	-0.455618
H	2.529133	-2.622093	-1.365177
H	3.514991	-0.607599	1.075336
C	4.006598	-0.239010	-1.005705
H	2.955522	-0.309185	-1.319704
H	4.591313	-0.736523	-1.795482
H	4.830102	-2.916503	-0.458572
H	4.207694	-2.977759	1.185488
C	4.422689	1.241331	-0.967825
H	4.286529	1.670361	-1.971231
H	5.499804	1.309921	-0.751637
C	3.682091	2.124926	0.060677
H	3.921332	1.788008	1.077262
H	4.085613	3.145472	-0.024267

Sum of electronic and zero-point Energies= -1083.753552  
Sum of electronic and thermal Energies= -1083.728809  
Sum of electronic and thermal Enthalpies= -1083.727864  
Sum of electronic and thermal Free Energies= -1083.808063

daec[n=5]-4-TS (dmf)

C	1.966014	2.897906	0.024216
H	2.632141	3.691598	-0.302726
C	2.483883	1.598862	0.184668
C	1.602050	0.598442	0.594960
H	1.942214	-0.418147	0.738429
C	0.253885	0.869614	0.821333

H	-0.387001	0.057008	1.132293
C	-0.265933	2.145134	0.632888
O	-1.606770	2.462643	0.824252
C	0.608164	3.186362	0.240382
O	0.045288	4.414026	0.077615
C	0.889251	5.489921	-0.323072
H	0.240543	6.368740	-0.383130
H	1.341191	5.304967	-1.307842
H	1.684353	5.675565	0.412664
C	-4.401258	-0.126949	-0.900663
H	-5.098017	-0.803392	-1.393339
C	-3.638133	-0.580612	0.186710
C	-3.602354	-2.038019	0.603427
H	-4.616063	-2.446119	0.719124
H	-3.116348	-2.112249	1.585280
C	-2.820187	-2.899094	-0.430896
H	-3.515739	-3.208756	-1.222857
C	-2.120289	-4.139313	0.166139
H	-2.023636	-4.908425	-0.615125
H	-2.763623	-4.578890	0.943369
C	-0.717225	-3.867954	0.753780
H	-0.413479	-4.737199	1.357052
H	-0.764937	-3.017237	1.452329
H	-2.069772	-2.268617	-0.925663
C	-2.769311	0.322876	0.814638
H	-2.234666	0.006511	1.704358
C	-2.557651	1.600181	0.286554
C	-3.316244	2.047148	-0.798102
H	-3.153985	3.048904	-1.188377
C	-4.257565	1.183667	-1.368414
H	-4.858890	1.527532	-2.208148
C	2.795672	-3.042165	-0.865632
C	0.361894	-3.600802	-0.311419
H	0.396346	-4.457347	-1.003987
H	0.070655	-2.732254	-0.921059
C	4.218734	-2.665573	-0.397869
H	4.896273	-2.730593	-1.263769
C	1.774839	-3.349748	0.246389
H	2.110635	-4.230304	0.817141
H	1.735742	-2.520081	0.967121
H	4.570431	-3.426509	0.316068
C	4.381482	-1.271376	0.244674
H	5.387996	-1.204087	0.684871
H	3.692182	-1.178432	1.092670
H	2.394273	-2.242094	-1.505451
H	2.871615	-3.927445	-1.515777
C	4.207890	-0.094775	-0.743255
H	3.392000	-0.305518	-1.447580
H	5.120280	-0.031984	-1.353725
C	3.948341	1.292799	-0.101587
H	4.337893	2.075952	-0.765881
H	4.535547	1.376367	0.827647

Sum of electronic and zero-point Energies= -1083.732438

Sum of electronic and thermal Energies= -1083.708367

Sum of electronic and thermal Enthalpies= -1083.707423

Sum of electronic and thermal Free Energies= -1083.785681

daec[n=5]-4-E1 (dmf)

C	-1.290339	2.261369	0.818417
H	-1.778980	2.149491	1.782168
C	-2.083638	2.429970	-0.332674
C	-1.449909	2.593555	-1.568538
H	-2.043806	2.732725	-2.469689
C	-0.051186	2.584425	-1.656440
H	0.450372	2.717040	-2.612685
C	0.724086	2.414045	-0.516606
O	2.104479	2.501194	-0.603302
C	0.106197	2.251621	0.744698
O	0.942330	2.105187	1.804271
C	0.363439	1.913655	3.094168

H	1.205457	1.805209	3.783619
H	-0.253478	1.005174	3.125909
O	-0.243300	2.779015	3.394306
C	4.553755	-0.862709	-0.338725
H	5.216905	-1.724229	-0.280398
C	3.181344	-1.054969	-0.547542
C	2.581239	-2.440602	-0.672670
H	3.354602	-3.154047	-0.989325
H	1.822693	-2.424721	-1.466723
C	1.937148	-2.944814	0.638699
H	2.733982	-3.121607	1.375772
C	1.104094	-4.229243	0.463328
H	0.894118	-4.656693	1.455901
H	1.712643	-4.977667	-0.067200
C	-0.227716	-4.031503	-0.287340
H	-0.620587	-5.014268	-0.588569
H	-0.042752	-3.486414	-1.225256
H	1.307754	-2.148059	1.059515
C	2.341138	0.068309	-0.626433
H	1.276575	-0.067852	-0.801262
C	2.865536	1.355959	-0.494556
C	4.238505	1.545780	-0.290332
H	4.628550	2.556520	-0.196729
C	5.073586	0.431434	-0.214044
H	6.141331	0.574416	-0.056711
C	-3.608199	-2.144007	0.474594
C	-1.306515	-3.291695	0.521786
H	-1.676457	-3.952531	1.322031
H	-0.864628	-2.421176	1.029275
C	-4.630314	-1.381606	-0.392462
H	-5.565851	-1.248299	0.172304
C	-2.480649	-2.802003	-0.337342
H	-2.897447	-3.642192	-0.915670
H	-2.092095	-2.088194	-1.079828
H	-4.889327	-2.004277	-1.262509
C	-4.145430	0.000021	-0.877080
H	-4.759526	0.323263	-1.731379
H	-3.117154	-0.081470	-1.259135
H	-3.170712	-1.457446	1.215707
H	-4.127019	-2.921083	1.055901
C	-4.212277	1.085066	0.208428
H	-3.716056	0.735695	1.125225
H	-5.266227	1.252082	0.477078
C	-3.596042	2.440206	-0.205680
H	-3.883663	3.191407	0.544656
H	-4.037521	2.765564	-1.157959

Sum of electronic and zero-point Energies= -1083.753471

Sum of electronic and thermal Energies= -1083.728545

Sum of electronic and thermal Enthalpies= -1083.727600

Sum of electronic and thermal Free Energies= -1083.808878

daec[n=5]-4-E2 (dmf)

C	-1.297478	2.539128	-0.585667
H	-1.801458	2.709097	-1.532663
C	-2.071727	2.356268	0.572523
C	-1.418712	2.152306	1.795773
H	-1.999238	2.021374	2.707104
C	-0.022822	2.122696	1.857112
H	0.493884	1.972591	2.802763
C	0.737052	2.300885	0.705342
O	2.119240	2.359107	0.800586
C	0.104251	2.516461	-0.536682
O	0.923795	2.689950	-1.605129
C	0.325338	2.907655	-2.882000
H	1.156908	3.016337	-3.584013
H	-0.279998	3.824382	-2.890401
H	-0.297561	2.054769	-3.184701
C	4.548364	-0.914720	-0.074253
H	5.206067	-1.753240	-0.296985
C	3.161566	-1.066309	-0.201899

C	2.539340	-2.380982	-0.627469
H	3.295340	-3.006654	-1.121668
H	1.763366	-2.174355	-1.376721
C	1.918163	-3.170518	0.546561
H	2.727842	-3.505016	1.211568
C	1.085475	-4.389790	0.105699
H	0.861273	-5.003665	0.991751
H	1.701718	-5.021011	-0.553046
C	-0.234788	-4.049391	-0.613307
H	-0.636242	-4.964818	-1.073674
H	-0.031828	-3.363413	-1.449352
H	1.296086	-2.492130	1.146874
C	2.326867	0.027309	0.085837
H	1.249481	-0.080859	-0.009808
C	2.872419	1.247809	0.489074
C	4.260847	1.397643	0.612728
H	4.666662	2.356680	0.926051
C	5.088896	0.312282	0.330568
H	6.167605	0.425485	0.424684
C	-3.607056	-2.263568	0.393258
C	-1.315525	-3.434168	0.291999
H	-1.702421	-4.208293	0.973883
H	-0.872431	-2.659345	0.935085
C	-4.599432	-1.358344	-0.364366
H	-5.553052	-1.313409	0.183670
C	-2.472535	-2.801615	-0.493939
H	-2.888924	-3.535516	-1.202546
H	-2.065912	-1.985043	-1.110297
H	-4.830998	-1.823350	-1.334804
C	-4.090291	0.080237	-0.590308
H	-4.642934	0.539920	-1.423692
H	-3.036764	0.053114	-0.905513
H	-3.176666	-1.706742	1.240040
H	-4.146382	-3.114287	0.836196
C	-4.241915	0.978745	0.646672
H	-3.824470	0.478832	1.532789
H	-5.314280	1.117675	0.850560
C	-3.587793	2.373340	0.509231
H	-3.965927	3.011425	1.320627
H	-3.914042	2.836868	-0.432305

Sum of electronic and zero-point Energies= -1083.752900  
Sum of electronic and thermal Energies= -1083.728002  
Sum of electronic and thermal Enthalpies= -1083.727058  
Sum of electronic and thermal Free Energies= -1083.808219

daec[n=5]-5-TS (dmf)

C	-1.272696	3.045767	-0.488412
H	-1.682624	3.930024	-0.973913
C	-2.063790	1.898745	-0.314547
C	-1.465589	0.806843	0.328373
H	-2.016935	-0.106349	0.496512
C	-0.138260	0.842804	0.742742
H	0.278374	-0.029391	1.230227
C	0.659914	1.959741	0.497867
O	2.014855	1.982836	0.819804
C	0.076516	3.089961	-0.105254
O	0.805202	4.212442	-0.409943
C	1.293694	4.955118	0.714650
H	1.805792	5.830718	0.302353
H	2.000743	4.366891	1.311213
H	0.462328	5.289157	1.352457
C	4.190268	-1.188465	-0.819536
H	4.731541	-2.012724	-1.281177
C	3.394636	-1.425312	0.314280
C	3.181881	-2.822982	0.865555
H	2.611331	-2.754312	1.800830
H	4.150419	-3.276309	1.123551
C	2.465825	-3.781201	-0.120531
H	3.132023	-3.946459	-0.979771
C	1.092745	-3.338539	-0.663842

H	0.824279	-4.029330	-1.478145
H	1.188087	-2.348030	-1.133547
C	-0.072603	-3.309630	0.340987
H	0.124913	-2.568416	1.130515
H	-0.142516	-4.285489	0.848101
H	2.363570	-4.758661	0.374973
C	2.731976	-0.337680	0.898572
H	2.162258	-0.487068	1.810887
C	2.770207	0.926700	0.302800
C	3.557411	1.157998	-0.825117
H	3.580160	2.149534	-1.270460
C	4.285737	0.093545	-1.368081
H	4.910304	0.263138	-2.243253
C	-3.984625	-2.692897	-0.061563
C	-1.418579	-2.989379	-0.337785
H	-1.328266	-2.027853	-0.863887
H	-1.611100	-3.744373	-1.117189
C	-4.220146	-1.267758	-0.609955
H	-5.063936	-1.294597	-1.316443
C	-2.621629	-2.950005	0.621309
H	-2.444857	-2.196542	1.404103
H	-2.679925	-3.915763	1.147057
H	-3.347996	-0.961350	-1.203468
C	-4.523877	-0.219021	0.476346
H	-3.794185	-0.300194	1.291474
H	-5.492559	-0.468065	0.936738
H	-4.787790	-2.931216	0.653152
H	-4.095063	-3.412145	-0.887799
C	-4.607239	1.249583	-0.003792
H	-4.727202	1.892835	0.880684
H	-5.531352	1.367467	-0.589769
C	-3.469175	1.819737	-0.888083
H	-3.423941	1.231654	-1.817837
H	-3.771939	2.828946	-1.198943

Sum of electronic and zero-point Energies= -1083.731265  
Sum of electronic and thermal Energies= -1083.707319  
Sum of electronic and thermal Enthalpies= -1083.706374  
Sum of electronic and thermal Free Energies= -1083.783724

daec[n=5]-5-E1 (dmf)

C	1.497097	2.218726	0.867865
H	2.060170	2.257294	1.798488
C	2.166154	2.173917	-0.356919
C	1.392083	2.133561	-1.530838
H	1.871414	2.110482	-2.507018
C	0.001826	2.133697	-1.450913
H	-0.604477	2.113981	-2.354391
C	-0.658692	2.176510	-0.216944
O	-2.044654	2.278838	-0.194557
C	0.093857	2.228922	0.972561
O	-0.375194	2.339329	2.244800
C	-1.707803	1.952605	2.596770
H	-1.718628	1.933966	3.691414
H	-1.948687	0.950906	2.220642
H	-2.449834	2.673722	2.239610
C	-4.569298	-0.987235	-0.764697
H	-5.254012	-1.822776	-0.900245
C	-3.185482	-1.210231	-0.817465
C	-2.641751	-2.609637	-1.031787
H	-1.768502	-2.569418	-1.696527
H	-3.403462	-3.202633	-1.555329
C	-2.264987	-3.359149	0.272875
H	-3.114662	-3.294718	0.968215
C	-0.986904	-2.872105	0.980258
H	-0.942473	-3.333287	1.978689
H	-1.048612	-1.787778	1.153359
C	0.309299	-3.202169	0.224112
H	0.232861	-2.856796	-0.817893
H	0.422410	-4.297003	0.170871
H	-2.148893	-4.425966	0.028304

C	-2.316020	-0.117871	-0.649312
H	-1.242588	-0.270911	-0.703348
C	-2.828178	1.163047	-0.418273
C	-4.210791	1.381228	-0.373441
H	-4.586607	2.386873	-0.200893
C	-5.073338	0.299963	-0.549715
H	-6.148993	0.464228	-0.518557
C	4.149905	-2.330869	0.581294
C	1.573159	-2.586493	0.843351
H	1.471143	-1.490774	0.841982
H	1.655491	-2.884493	1.901095
C	4.230509	-0.800614	0.409642
H	5.228944	-0.472204	0.739215
C	2.850291	-2.998199	0.094971
H	2.716606	-2.795428	-0.978205
H	2.969628	-4.089694	0.177872
H	3.514999	-0.311966	1.085990
C	3.988676	-0.318853	-1.029754
H	2.934440	-0.476696	-1.296789
H	4.572000	-0.946238	-1.722074
H	4.991774	-2.786433	0.036671
H	4.307520	-2.576532	1.643263
C	4.361254	1.149866	-1.296954
H	4.139288	1.380895	-2.348970
H	5.448937	1.273995	-1.184134
C	3.684114	2.199933	-0.390330
H	4.056557	2.094156	0.636603
H	4.015164	3.194616	-0.728002

Sum of electronic and zero-point Energies= -1083.746252  
Sum of electronic and thermal Energies= -1083.721430  
Sum of electronic and thermal Enthalpies= -1083.720486  
Sum of electronic and thermal Free Energies= -1083.801069

#### daec[n=5]-5-E2 (dmf)

C	1.731794	2.702179	-0.071528
H	2.406957	3.304552	-0.676865
C	2.234344	1.819861	0.897739
C	1.310280	1.085934	1.654895
H	1.665557	0.408320	2.429135
C	-0.065502	1.221537	1.449627
H	-0.769598	0.658572	2.057500
C	-0.547843	2.089062	0.467591
O	-1.897839	2.311564	0.274823
C	0.360434	2.846300	-0.297629
O	-0.067123	3.772118	-1.216997
C	-0.646672	3.229592	-2.410004
H	-0.887379	4.085590	-3.048810
H	-1.564487	2.667642	-2.198551
H	0.069812	2.578217	-2.931329
C	-4.649760	-0.817980	0.265331
H	-5.389849	-1.616686	0.255478
C	-3.416424	-1.009417	-0.381220
C	-3.102498	-2.323512	-1.069178
H	-2.368800	-2.154018	-1.867822
H	-4.014665	-2.695936	-1.555586
C	-2.587521	-3.428179	-0.113356
H	-3.326689	-3.563559	0.689895
C	-1.204293	-3.178645	0.512706
H	-1.039903	-3.932051	1.298329
H	-1.201269	-2.204425	1.024428
C	-0.032319	-3.239129	-0.478976
H	-0.185800	-2.508973	-1.287885
H	-0.020607	-4.229430	-0.962317
H	-2.563078	-4.376424	-0.671623
C	-2.481895	0.035573	-0.367113
H	-1.527062	-0.082948	-0.873908
C	-2.772009	1.235936	0.292541
C	-3.999471	1.424518	0.930181
H	-4.206100	2.368883	1.427737
C	-4.937577	0.388224	0.907952

H	-5.899177	0.526899	1.398731
C	3.895285	-2.823929	-0.208420
C	1.332995	-2.973338	0.173154
H	1.312931	-1.979431	0.644309
H	1.496710	-3.695783	0.989281
C	4.150974	-1.426307	0.388588
H	5.167797	-1.415778	0.812214
C	2.501210	-3.057663	-0.820610
H	2.331000	-2.342819	-1.639790
H	2.494574	-4.054566	-1.288418
H	3.471530	-1.255016	1.235224
C	4.022729	-0.277257	-0.623601
H	2.980865	-0.195187	-0.964197
H	4.614150	-0.525719	-1.518958
H	4.651609	-3.014941	-0.985964
H	4.069137	-3.578038	0.575244
C	4.493506	1.093935	-0.108903
H	4.427642	1.818919	-0.933490
H	5.559018	1.034960	0.161045
C	3.727417	1.658052	1.110336
H	3.893085	1.013268	1.982912
H	4.168681	2.634389	1.360835

Sum of electronic and zero-point Energies= -1083.749456  
Sum of electronic and thermal Energies= -1083.724425  
Sum of electronic and thermal Enthalpies= -1083.723481  
Sum of electronic and thermal Free Energies= -1083.804995

#### daec[n=5]-6-TS (dmf)

C	1.860750	2.953199	0.085390
H	2.545285	3.750745	-0.190225
C	2.381860	1.672606	0.350954
C	1.477237	0.667480	0.694078
H	1.818858	-0.333031	0.923839
C	0.105469	0.909693	0.738932
H	-0.554363	0.088910	0.984382
C	-0.411783	2.167708	0.451771
O	-1.768919	2.463851	0.460738
C	0.482478	3.218015	0.136384
O	-0.082456	4.428423	-0.123716
C	0.780469	5.512365	-0.455481
H	1.345643	5.312270	-1.376762
H	1.482361	5.734824	0.360591
H	0.125970	6.374534	-0.614034
C	-4.329015	-0.579142	-0.815983
H	-4.965686	-1.383192	-1.182127
C	-3.689830	-0.710011	0.427894
C	-3.755884	-1.999184	1.223266
H	-4.798326	-2.337698	1.309852
H	-3.396875	-1.811546	2.244398
C	-2.929310	-3.152165	0.595540
H	-3.019235	-4.027087	1.257315
C	-1.440909	-2.850997	0.340338
H	-0.967638	-2.497441	1.268936
H	-1.361183	-2.023571	-0.379627
C	-0.680160	-4.072249	-0.214918
H	-1.333879	-4.581718	-0.940136
H	-0.507109	-4.799436	0.594100
H	-3.395141	-3.442072	-0.358424
C	-2.897242	0.352020	0.884767
H	-2.436526	0.293590	1.867235
C	-2.647123	1.458893	0.067028
C	-3.282729	1.584681	-1.169479
H	-3.089918	2.459579	-1.785560
C	-4.144931	0.567816	-1.593431
H	-4.652955	0.660872	-2.551578
C	3.071674	-2.983439	-0.916161
C	0.648310	-3.763842	-0.934520
H	0.974462	-4.676908	-1.456992
H	0.452054	-3.021304	-1.724885
C	4.345027	-2.555028	-0.155883

H	5.186577	-2.568344	-0.866580
C	1.817906	-3.266187	-0.065957
H	2.054420	-4.022662	0.699864
H	1.517549	-2.360864	0.477988
H	4.578377	-3.321227	0.599850
C	4.312730	-1.179044	0.540183
H	5.231820	-1.069842	1.136307
H	3.494888	-1.164351	1.270227
H	3.313562	-3.897602	-1.480814
H	2.820854	-2.227815	-1.675819
C	4.219107	0.023899	-0.423344
H	3.481464	-0.175367	-1.212175
H	5.187852	0.118840	-0.935437
C	3.872845	1.386288	0.234967
H	4.343916	1.435069	1.230338
H	4.332259	2.195413	-0.348248

Sum of electronic and zero-point Energies= -1083.737069  
Sum of electronic and thermal Energies= -1083.713035  
Sum of electronic and thermal Enthalpies= -1083.712091  
Sum of electronic and thermal Free Energies= -1083.790010

#### daec[n=5]-6-E1 (dmf)

C	-1.346396	2.024085	0.771117
H	-1.892552	1.792955	1.681124
C	-2.065825	2.347491	-0.395543
C	-1.353796	2.664036	-1.556712
H	-1.889277	2.920330	-2.468832
C	0.048144	2.663788	-1.555216
H	0.608664	2.922942	-2.450873
C	0.750443	2.343281	-0.400449
O	2.131162	2.454633	-0.376484
C	0.051688	2.015357	0.784933
O	0.818078	1.727531	1.868325
C	0.158854	1.381315	3.085070
H	-0.459121	0.480757	2.964925
H	-0.465689	2.207294	3.452208
H	0.955702	1.181076	3.806836
C	4.609928	-0.888627	-0.173976
H	5.282541	-1.743637	-0.126939
C	3.357897	-1.026228	-0.792855
C	2.937810	-2.353751	-1.394258
H	3.838992	-2.899088	-1.706038
H	2.349096	-2.170983	-2.304851
C	2.115607	-3.269798	-0.457272
H	1.999122	-4.240201	-0.963676
C	0.726776	-2.725683	-0.096496
H	0.227028	-2.402056	-1.021052
H	0.829182	-1.824477	0.526552
C	-0.159106	-3.749030	0.630662
H	0.385290	-4.144848	1.502259
H	-0.333720	-4.609189	-0.035461
H	2.690504	-3.467709	0.460247
C	2.507733	0.090574	-0.852707
H	1.541435	0.011188	-1.344525
C	2.903621	1.311469	-0.298737
C	4.157524	1.447257	0.306388
H	4.447811	2.409432	0.721388
C	5.004923	0.340187	0.364781
H	5.982192	0.438491	0.834321
C	-3.777436	-2.155675	0.467717
C	-1.513498	-3.191565	1.105696
H	-2.064173	-3.992876	1.622965
H	-1.336540	-2.408267	1.860488
C	-4.615164	-1.444989	-0.614081
H	-5.648213	-1.331359	-0.249832
C	-2.392284	-2.613347	-0.013861
H	-2.517203	-3.366425	-0.809233
H	-1.870202	-1.765803	-0.477031
H	-4.676145	-2.099835	-1.497226
C	-4.090621	-0.063667	-1.053519

H	-4.630545	0.249270	-1.960415
H	-3.034505	-0.143161	-1.347664
H	-4.337153	-3.031774	0.829879
H	-3.658619	-1.495565	1.340339
C	-4.248004	1.032315	0.010869
H	-3.838696	0.690454	0.971491
H	-5.319738	1.211403	0.184940
C	-3.584343	2.375069	-0.363857
H	-3.957600	2.707964	-1.342351
H	-3.908627	3.133205	0.365147

Sum of electronic and zero-point Energies= -1083.753955  
Sum of electronic and thermal Energies= -1083.729117  
Sum of electronic and thermal Enthalpies= -1083.728172  
Sum of electronic and thermal Free Energies= -1083.808597

#### daec[n=5]-6-E2 (dmf)

C	-1.142450	2.643393	-0.510513
H	-1.589536	3.028262	-1.422540
C	-1.982896	2.255476	0.546080
C	-1.402079	1.763233	1.723496
H	-2.031771	1.467624	2.560348
C	-0.013606	1.664901	1.839638
H	0.446673	1.299403	2.755282
C	0.813185	2.058040	0.790758
O	2.188765	2.061009	0.970064
C	0.254527	2.554958	-0.404008
O	1.133689	2.917637	-1.373483
C	0.609758	3.428569	-2.598294
H	0.032880	4.349307	-2.435360
H	-0.021126	2.686653	-3.106837
H	1.480195	3.652291	-3.221600
C	4.574523	-1.232754	0.066895
H	5.221275	-2.079482	-0.157296
C	3.292065	-1.172706	-0.498372
C	2.804330	-2.279146	-1.414534
H	3.677393	-2.771219	-1.863938
H	2.229434	-1.840359	-2.243130
C	1.930946	-3.361698	-0.736327
H	1.784996	-4.172457	-1.466433
C	0.558208	-2.862767	-0.265718
H	0.090322	-2.306865	-1.091000
H	0.683757	-2.141269	0.555252
C	-0.384268	-3.987273	0.190082
H	0.120174	-4.594504	0.957843
H	-0.573940	-4.664534	-0.658138
H	2.481712	-3.802577	0.108533
C	2.472974	-0.068561	-0.205104
H	1.481798	-0.000201	-0.644177
C	2.930420	0.946394	0.640696
C	4.215584	0.885828	1.194521
H	4.553267	1.689860	1.844138
C	5.030478	-0.207363	0.902169
H	6.030141	-0.259061	1.330139
C	-3.917964	-2.207566	0.328311
C	-1.728202	-3.490476	0.755235
H	-2.321517	-4.360292	1.078050
H	-1.539207	-2.896437	1.663839
C	-4.688416	-1.249553	-0.602387
H	-5.724092	-1.151376	-0.241270
C	-2.555521	-2.648267	-0.227583
H	-2.712433	-3.218995	-1.157659
H	-1.977545	-1.759167	-0.511151
H	-4.758454	-1.711108	-1.599601
C	-4.078037	0.159108	-0.744709
H	-4.545373	0.665995	-1.602849
H	-3.009839	0.078297	-0.991218
H	-4.536597	-3.099516	0.511752
H	-3.773540	-1.735376	1.312042
C	-4.254966	1.043951	0.498201
H	-3.936475	0.502404	1.399753

H	-5.325678	1.258407	0.634062
C	-3.492002	2.385293	0.429737
H	-3.744062	2.903197	-0.506075
H	-3.852031	3.027833	1.246951

Sum of electronic and zero-point Energies= -1083.753124  
Sum of electronic and thermal Energies= -1083.728187  
Sum of electronic and thermal Enthalpies= -1083.727243  
Sum of electronic and thermal Free Energies= -1083.808706

daec[n=5]-7-TS (dmf)

C	-3.090936	1.883750	0.103926
H	-3.919586	2.552776	-0.111447
C	-1.791295	2.418101	0.192082
C	-0.749000	1.531482	0.463512
H	0.269317	1.881541	0.564289
C	-0.979046	0.164541	0.608080
H	-0.128932	-0.476140	0.792134
C	-2.259292	-0.368557	0.501064
O	-2.553385	-1.722440	0.621551
C	-3.342099	0.510716	0.260719
O	-4.572717	-0.063361	0.174724
C	-5.690920	0.783899	-0.073208
H	-5.603192	1.297620	-1.040999
H	-6.563680	0.124551	-0.093019
H	-5.817767	1.529683	0.724127
C	0.343748	-4.318303	-0.901070
H	1.113767	-4.941115	-1.353936
C	0.645075	-3.556198	0.236791
C	2.060089	-3.375453	0.748056
H	2.656451	-4.286957	0.607040
H	2.038131	-3.163752	1.826398
C	2.735818	-2.189331	0.006387
H	2.986311	-2.512487	-1.015700
C	3.988343	-1.635382	0.700197
H	4.656511	-2.470013	0.963897
H	3.695472	-1.170525	1.654117
C	4.796639	-0.637719	-0.154871
H	5.140340	-1.165712	-1.058239
H	5.708526	-0.367456	0.400454
H	1.999357	-1.381648	-0.104422
C	-0.373012	-2.779984	0.810319
H	-0.172967	-2.236573	1.729088
C	-1.603295	-2.630700	0.166718
C	-1.903457	-3.392083	-0.966652
H	-2.873959	-3.283799	-1.444819
C	-0.932443	-4.260789	-1.474087
H	-1.159851	-4.863536	-2.351492
C	3.459136	3.091757	0.047504
C	4.100320	0.665955	-0.602896
H	4.787103	1.174866	-1.297624
H	3.202739	0.429879	-1.192719
C	2.157611	3.284928	-0.778322
H	1.718799	2.305327	-1.014367
C	3.746886	1.651487	0.527341
H	4.592697	1.692417	1.231882
H	2.888593	1.276297	1.106325
H	2.389907	3.740799	-1.751725
C	1.094595	4.154383	-0.074871
H	1.506368	5.165259	0.060063
H	0.934205	3.775113	0.943846
H	4.325891	3.434349	-0.537057
H	3.422207	3.747055	0.930723
C	-0.261677	4.245254	-0.835183
H	-0.234250	3.593290	-1.720283
H	-0.383564	5.265795	-1.222620
C	-1.532874	3.903307	-0.016551
H	-1.473599	4.412538	0.959268
H	-2.406016	4.336591	-0.523291

Sum of electronic and zero-point Energies= -1083.726560  
Sum of electronic and thermal Energies= -1083.702481

Sum of electronic and thermal Enthalpies= -1083.701537  
Sum of electronic and thermal Free Energies= -1083.779888

daec[n=5]-7-E1 (dmf)

C	-1.311432	2.370976	0.661582
H	-1.816937	2.383033	1.622472
C	-2.079592	2.382533	-0.518130
C	-1.417179	2.393077	-1.750684
H	-1.991803	2.408777	-2.674767
C	-0.017182	2.393284	-1.807937
H	0.503944	2.411233	-2.762762
C	0.733059	2.375891	-0.639242
O	2.115627	2.461701	-0.696022
C	0.086882	2.360872	0.617948
O	0.900318	2.348046	1.704977
C	0.295626	2.310528	2.996449
H	-0.322479	1.411385	3.124573
H	1.123866	2.286275	3.710315
H	-0.315863	3.204675	3.179753
C	4.515717	-0.890814	-0.079818
H	5.164106	-1.750763	0.079237
C	3.181866	-1.088463	-0.460569
C	2.611704	-2.478214	-0.671397
H	3.412592	-3.222921	-0.567531
H	2.243306	-2.559920	-1.705894
C	1.451515	-2.823947	0.283411
H	1.823536	-2.846023	1.319438
C	0.776184	-4.158531	-0.059231
H	1.517551	-4.969208	0.013276
H	0.458672	-4.136069	-1.112516
C	-0.426869	-4.513208	0.835087
H	-0.075919	-4.645406	1.870479
H	-0.816265	-5.493540	0.518757
H	0.709597	-2.015692	0.241696
C	2.360985	0.034335	-0.660685
H	1.327273	-0.099573	-0.968932
C	2.865154	1.323014	-0.477793
C	4.202025	1.518338	-0.107710
H	4.576906	2.530521	0.024368
C	5.018860	0.405465	0.088627
H	6.057749	0.549908	0.380339
C	-3.448950	-2.322011	-0.519038
C	-1.584424	-3.495447	0.837917
H	-2.368280	-3.869350	1.515457
H	-1.239040	-2.548634	1.275491
C	-3.178667	-0.865795	-0.105240
H	-2.411976	-0.438051	-0.767415
C	-2.209375	-3.234428	-0.542094
H	-2.492139	-4.200649	-0.989342
H	-1.458544	-2.796676	-1.217057
H	-2.758040	-0.837820	0.910924
C	-4.451621	-0.004787	-0.140119
H	-5.230478	-0.526788	0.437832
H	-4.830728	0.047060	-1.173524
H	-4.204011	-2.754500	0.157420
H	-3.904793	-2.323541	-1.521624
C	-4.332251	1.422506	0.425764
H	-3.876412	1.384987	1.426358
H	-5.351294	1.807030	0.578027
C	-3.595622	2.461103	-0.450117
H	-3.998386	2.415842	-1.471698
H	-3.861762	3.458753	-0.066683

Sum of electronic and zero-point Energies= -1083.752124  
Sum of electronic and thermal Energies= -1083.727173  
Sum of electronic and thermal Enthalpies= -1083.726229  
Sum of electronic and thermal Free Energies= -1083.807424

daec[n=5]-7-E2 (dmf)

C	0.019775	2.858460	-0.688261
H	-0.389974	3.151864	-1.650483

C	-0.770241	3.016220	0.462315
C	-0.235569	2.651211	1.705484
H	-0.822276	2.783421	2.612403
C	1.044943	2.098665	1.787698
H	1.463852	1.793296	2.744272
C	1.810182	1.919392	0.639800
O	3.083471	1.378641	0.745232
C	1.313175	2.320739	-0.616699
O	2.137184	2.128557	-1.678492
C	1.668600	2.513051	-2.970313
H	1.449719	3.588799	-3.013831
H	2.483592	2.280742	-3.661638
H	0.773494	1.945319	-3.259057
C	3.701141	-2.700475	0.136993
H	3.888167	-3.762800	-0.010270
C	2.437109	-2.170547	-0.153869
C	1.318105	-3.038746	-0.698584
H	1.686139	-4.066148	-0.824960
H	1.049293	-2.681948	-1.705399
C	0.040118	-3.055808	0.164507
H	0.274741	-3.472978	1.155970
C	-1.088228	-3.867530	-0.486646
H	-0.731131	-4.894751	-0.658957
H	-1.299321	-3.452770	-1.483996
C	-2.390734	-3.940171	0.330465
H	-2.169469	-4.381552	1.314947
H	-3.071121	-4.645682	-0.171672
H	-0.295385	-2.023854	0.336115
C	2.215950	-0.797906	0.045083
H	1.240152	-0.375918	-0.175727
C	3.238617	0.026193	0.520012
C	4.504945	-0.504874	0.800361
H	5.289549	0.151936	1.686605
C	4.724918	-1.868032	0.607168
H	5.705274	-2.286879	0.827972
C	-4.714035	-0.889222	-0.588581
C	-3.145528	-2.612718	0.542601
H	-4.046108	-2.834058	1.136899
H	-2.541643	-1.931172	1.158661
C	-4.448972	0.304442	0.346870
H	-4.184563	-0.059673	1.351402
C	-3.570377	-1.907761	-0.758712
H	-3.908484	-2.668889	-1.479663
H	-2.700670	-1.421391	-1.223623
H	-5.394774	0.855386	0.468729
C	-3.370783	1.288602	-0.133098
H	-3.598615	1.607368	-1.163189
H	-2.394639	0.784490	-0.177033
H	-5.599391	-1.427994	-0.215781
H	-4.991670	-0.502812	-1.581985
C	-3.271496	2.527591	0.769326
H	-3.088726	2.208999	1.806597
H	-4.242772	3.044955	0.776234
C	-2.187155	3.548539	0.358079
H	-2.375949	3.886952	-0.669996
H	-2.289303	4.434260	1.002544

Sum of electronic and zero-point Energies= -1083.753448  
Sum of electronic and thermal Energies= -1083.728523  
Sum of electronic and thermal Enthalpies= -1083.727579  
Sum of electronic and thermal Free Energies= -1083.808838

#### daec[n=5]-8-TS (dmf)

C	1.347718	-3.279181	0.219293
H	1.565534	-4.338687	0.324765
C	-0.000629	-2.862561	0.160148
C	-0.215093	-1.490893	0.019881
H	-1.200387	-1.066216	0.027569
C	0.830404	-0.584095	-0.094034
H	0.580384	0.455729	-0.248812
C	2.151362	-0.984451	0.029776

O	3.217311	-0.099240	0.011295
C	2.419064	-2.367606	0.178503
O	3.733675	-2.712993	0.267377
C	4.056625	-4.093119	0.407514
H	5.148626	-4.139125	0.455976
H	3.707090	-4.679671	-0.453956
H	3.634469	-4.515769	1.330199
C	2.213241	3.892286	-0.691092
H	1.923492	4.916913	-0.919360
C	1.642827	3.240860	0.418289
C	0.569331	3.923193	1.249712
H	0.899910	4.947559	1.472848
H	0.468579	3.409746	2.215981
C	-0.830252	4.025058	0.576576
H	-1.381702	4.824214	1.094156
C	-1.706701	2.755634	0.598989
H	-1.832021	2.430831	1.644354
H	-1.193850	1.933633	0.079634
C	-3.100025	2.998134	-0.026918
H	-2.987082	3.161940	-1.110489
H	-3.492662	3.943629	0.378646
H	-0.703530	4.369381	-0.461017
C	2.058776	1.934533	0.704835
H	1.650526	1.419011	1.570511
C	2.917766	1.249593	-0.167857
C	3.481586	1.901259	-1.263297
H	4.156416	1.360628	-1.922497
C	3.141922	3.238545	-1.502779
H	3.583937	3.759037	-2.350336
C	-4.915125	-0.552744	-0.103229
C	-4.168875	1.906854	0.220365
H	-4.237552	1.722428	1.304651
H	-5.149282	2.308173	-0.079947
C	-4.568147	-1.981595	-0.612655
H	-4.736438	-2.053091	-1.698350
C	-3.923454	0.567786	-0.497596
H	-2.901435	0.253958	-0.261528
H	-3.949593	0.722731	-1.588437
H	-5.255157	-2.699559	-0.139535
C	-3.103475	-2.291872	-0.279611
H	-2.936834	-1.971824	0.761045
H	-2.527568	-1.617220	-0.910297
H	-5.926773	-0.279643	-0.439901
H	-4.961947	-0.594070	0.996767
C	-2.473129	-3.686446	-0.448112
H	-3.157946	-4.470098	-0.090284
H	-2.296218	-3.892552	-1.514295
C	-1.145923	-3.860060	0.355407
H	-0.760846	-4.871606	0.165538
H	-1.416784	-3.847217	1.424369

Sum of electronic and zero-point Energies= -1083.722570  
Sum of electronic and thermal Energies= -1083.698522  
Sum of electronic and thermal Enthalpies= -1083.697577  
Sum of electronic and thermal Free Energies= -1083.775280

#### daec[n=5]-8-E1 (dmf)

C	1.531251	-2.354178	0.466646
H	2.098995	-2.369554	1.392140
C	2.220082	-2.294053	-0.760127
C	1.479161	-2.294770	-1.946164
H	1.991446	-2.251193	-2.905378
C	0.078699	-2.347087	-1.912913
H	-0.502666	-2.359230	-2.832312
C	-0.594426	-2.385170	-0.698392
O	-1.972717	-2.522294	-0.663772
C	0.134355	-2.394644	0.513825
O	-0.604997	-2.452925	1.651342
C	0.082111	-2.445110	2.901209
H	-0.697184	-2.485470	3.667541
H	0.672305	-1.527439	3.029786

H	0.738917	-3.319848	3.004180
C	-4.487226	0.649574	0.327462
H	-5.177998	1.456152	0.568646
C	-3.410136	0.899478	-0.539144
C	-3.238488	2.277937	-1.150961
H	-4.238162	2.697437	-1.328535
H	-2.758683	2.187046	-2.135909
C	-2.435814	3.290297	-0.298718
H	-2.653889	4.299561	-0.679089
C	-0.917128	3.074782	-0.326641
H	-0.577523	3.112812	-1.374584
H	-0.681775	2.063959	0.034439
C	-0.139521	4.121023	0.490574
H	-0.334393	3.966353	1.563761
H	-0.533024	5.121345	0.251486
H	-2.803193	3.266850	0.738624
C	-2.535796	-0.155722	-0.847174
H	-1.705489	0.006566	-1.530887
C	-2.749534	-1.430151	-0.309007
C	-3.829348	-1.674749	0.542835
H	-3.975170	-2.674945	0.942739
C	-4.693929	-0.625402	0.860438
H	-5.537710	-0.807206	1.523843
C	3.589451	2.805727	0.275565
C	1.378925	4.123844	0.234916
H	1.557669	4.344609	-0.829902
H	1.835941	4.952417	0.798198
C	4.278965	1.458062	0.562072
H	4.068904	1.165812	1.603616
C	2.086593	2.811585	0.598571
H	1.598085	1.985371	0.066411
H	1.946561	2.606724	1.672603
H	5.370475	1.584346	0.496247
C	3.840168	0.324008	-0.378030
H	4.187480	0.539876	-1.401094
H	2.744192	0.300530	-0.429871
H	4.085780	3.596988	0.858339
H	3.735555	3.070725	-0.784116
C	4.331518	-1.064385	0.051904
H	5.428769	-1.114579	-0.012064
H	4.082682	-1.220921	1.112014
C	3.738123	-2.220516	-0.783128
H	4.155967	-3.167826	-0.408931
H	4.070509	-2.127801	-1.826214
Sum of electronic and zero-point Energies= -1083.752678			
Sum of electronic and thermal Energies= -1083.727644			
Sum of electronic and thermal Enthalpies= -1083.726700			
Sum of electronic and thermal Free Energies= -1083.808342			

daec[n=5]-8-E2 (dmf)

C	1.510319	-2.481959	-0.839775
H	2.026031	-2.565962	-1.792048
C	2.270110	-2.309716	0.328672
C	1.601809	-2.203008	1.556572
H	2.166937	-2.080762	2.478381
C	0.206859	-2.250945	1.607149
H	-0.320258	-2.174006	2.555998
C	-0.541007	-2.409584	0.442928
O	-1.921116	-2.540127	0.524329
C	0.108553	-2.538799	-0.800781
O	-0.692022	-2.699461	-1.887955
C	-0.069738	-2.845035	-3.163610
H	-0.887645	-2.969512	-3.879034
H	0.578998	-3.731126	-3.194947
H	0.514596	-1.953981	-3.431219
C	-4.404736	0.795278	0.811037
H	-5.083770	1.643707	0.881756
C	-3.404735	0.791597	-0.176758
C	-3.294748	1.955462	-1.144514
H	-4.310965	2.292660	-1.391257

H	-2.842000	1.611407	-2.085218
C	-2.495978	3.173394	-0.621736
H	-2.736519	4.036413	-1.260626
C	-0.974742	2.974625	-0.615911
H	-0.646989	2.741397	-1.642158
H	-0.721275	2.095693	-0.007020
C	-0.203779	4.205645	-0.109340
H	-0.397724	4.340624	0.966698
H	-0.604170	5.103839	-0.604975
H	-2.846935	3.432016	0.389015
C	-2.546137	-0.315287	-0.261293
H	-1.784098	-0.356459	-1.035367
C	-2.695145	-1.394762	0.618903
C	-3.696607	-1.388286	1.593003
H	-3.797998	-2.241477	2.259383
C	-4.549519	-0.285081	1.683708
H	-5.333646	-0.273444	2.438781
C	3.537627	2.916476	0.039761
C	1.314844	4.150725	-0.357792
H	1.494167	4.085330	-1.443200
H	1.765266	5.101341	-0.031958
C	4.239017	1.693894	0.661997
H	4.021593	1.669389	1.742003
C	2.031131	2.985224	0.337900
H	1.556857	2.043767	0.032576
H	1.881263	3.062081	1.427252
H	5.329603	1.815018	0.574143
C	3.824309	0.354474	0.033026
H	4.165862	0.320127	-1.014011
H	2.729052	0.295678	-0.004299
H	4.018941	3.835567	0.408087
H	3.693234	2.907558	-1.051222
C	4.347513	-0.875480	0.786023
H	5.446063	-0.911833	0.734809
H	4.094377	-0.779663	1.852392
C	3.784619	-2.213309	0.255156
H	4.232461	-3.033578	0.836047
H	4.104754	-2.358373	-0.785713
Sum of electronic and zero-point Energies= -1083.752176			
Sum of electronic and thermal Energies= -1083.727091			
Sum of electronic and thermal Enthalpies= -1083.726147			
Sum of electronic and thermal Free Energies= -1083.808831			

daec[n=6]-1-TS (dmf)

C	-1.488662	3.406533	-0.047365
H	-2.044365	4.323835	0.127876
C	-2.199333	2.194692	-0.164940
C	-1.461832	1.034583	-0.396921
H	-1.951031	0.075986	-0.526096
C	-0.065021	1.064546	-0.478410
H	0.458885	0.130449	-0.628373
C	0.634271	2.259479	-0.359601
O	2.009879	2.395386	-0.452520
C	-0.093738	3.458818	-0.149644
O	0.646924	4.595846	-0.052965
C	-0.039436	5.824858	0.165516
H	-0.731239	6.053459	-0.657383
H	0.736947	6.594450	0.208760
H	-0.593807	5.815699	1.114544
C	4.605349	-0.659823	0.721920
H	5.272059	-1.449442	1.064730
C	3.689062	-0.919375	-0.309417
C	3.481596	-2.314817	-0.864128
H	4.432961	-2.756821	-1.192533
H	2.840016	-2.250050	-1.752690
C	2.823915	-3.250813	0.187657
H	3.611740	-3.655735	0.837614
C	2.002869	-4.406637	-0.418769
H	1.932304	-5.221443	0.317809
H	2.547015	-4.823862	-1.279834



C	0.573449	-4.020167	-0.854627
H	0.159355	-4.837136	-1.465370
C	-0.386956	-3.743613	0.315883
H	-0.002952	-2.911473	0.924931
H	-0.402448	-4.622941	0.979893
H	0.610567	-3.139057	-1.514860
H	2.175344	-2.654256	0.842780
C	2.858997	0.122779	-0.747695
H	2.200071	-0.047078	-1.593322
C	2.856561	1.358275	-0.091079
C	3.767272	1.610035	0.938969
H	3.766158	2.581719	1.426594
C	4.655420	0.601374	1.323474
H	5.373309	0.794893	2.118470
C	-4.234313	-2.876228	0.717770
C	-1.826390	-3.415163	-0.115253
H	-1.807221	-2.562124	-0.810212
H	-2.239678	-4.263163	-0.685135
C	-4.538419	-1.647632	-0.160987
H	-5.582475	-1.708207	-0.505418
C	-2.750786	-3.103567	1.075306
H	-2.356961	-2.230363	1.617298
H	-2.698505	-3.942662	1.786558
H	-3.923563	-1.693435	-1.072362
C	-4.316734	-0.285739	0.520100
H	-3.333598	-0.274572	1.005593
H	-5.048161	-0.155108	1.332508
H	-4.812485	-2.800111	1.652072
H	-4.609332	-3.774928	0.203584
C	-4.429664	0.897701	-0.467042
H	-5.492844	1.123223	-0.631712
H	-4.035112	0.595209	-1.448467
C	-3.718178	2.193347	-0.031787
H	-4.115703	3.032902	-0.620638
H	-3.985480	2.421615	1.013086

Sum of electronic and zero-point Energies= -1123.021391

Sum of electronic and thermal Energies= -1122.996028

Sum of electronic and thermal Enthalpies= -1122.995083

Sum of electronic and thermal Free Energies= -1123.076513

daec[n=6]-1-E1 (dmf)

C	-0.465725	2.998299	-0.626438
H	-0.793573	3.332492	-1.606955
C	-1.403161	2.944479	0.422185
C	-0.974656	2.533851	1.689136
H	-1.680617	2.497227	2.516385
C	0.360079	2.166919	1.901934
H	0.703703	1.846760	2.883218
C	1.277560	2.214345	0.859808
O	2.610728	1.932130	1.111701
C	0.872994	2.643540	-0.424607
O	1.842587	2.680612	-1.374207
C	1.477859	3.092177	-2.690679
H	0.726110	2.420634	-3.127489
H	2.396597	3.041828	-3.281792
H	1.096513	4.122490	-2.697416
C	4.403847	-1.627135	-0.113886
H	4.897859	-2.545330	-0.427569
C	3.016701	-1.495756	-0.269071
C	2.173622	-2.623459	-0.828910
H	2.769993	-3.218530	-1.535005
H	1.341482	-2.193074	-1.401015
C	1.616508	-3.558547	0.267362
H	2.461345	-4.060221	0.761713
C	0.637023	-4.625246	-0.257917
H	0.437235	-5.344874	0.551143
H	1.132330	-5.197371	-1.057721
C	-0.707252	-4.088387	-0.787335
H	-1.249458	-4.916379	-1.269275
C	-1.610616	-3.461941	0.286141

H	-1.048269	-2.705418	0.853295
H	-1.897848	-4.236408	1.015599
H	-0.525565	-3.349971	-1.582737
H	1.130401	-2.951409	1.043798
C	2.396149	-0.302143	0.134535
H	1.320662	-0.191717	0.020121
C	3.151654	0.740868	0.676607
C	4.537298	0.606101	0.832326
H	5.108057	1.429554	1.255041
C	5.153484	-0.580686	0.435633
H	6.230820	-0.686932	0.551166
C	-4.985962	-1.401173	0.266121
C	-2.870557	-2.796068	-0.285957
H	-2.560158	-2.015200	-0.996294
H	-3.447507	-3.529237	-0.872564
C	-4.662287	-0.132312	-0.546434
H	-5.611341	0.302387	-0.897150
C	-3.773240	-2.187683	0.798000
H	-3.167901	-1.536869	1.446710
H	-4.140648	-2.996788	1.448111
H	-4.103349	-0.401308	-1.455397
C	-3.879399	0.939953	0.226588
H	-2.905725	0.537099	0.537756
H	-4.418701	1.187036	1.155582
H	-5.619461	-1.117495	1.121107
H	-5.600235	-2.070104	-0.356930
C	-3.658332	2.224268	-0.583869
H	-4.634309	2.650486	-0.861164
H	-3.149520	1.980326	-1.529090
C	-2.849875	3.314952	0.156911
H	-2.881125	4.234899	-0.444215
H	-3.346615	3.544191	1.109976

Sum of electronic and zero-point Energies= -1123.039892

Sum of electronic and thermal Energies= -1123.013673

Sum of electronic and thermal Enthalpies= -1123.012729

Sum of electronic and thermal Free Energies= -1123.097064

daec[n=6]-1-E2 (dmf)

C	-0.972651	2.526105	0.788638
H	-1.584924	2.382796	1.674111
C	-1.592666	2.920070	-0.410323
C	-0.797300	3.126123	-1.544774
H	-1.255973	3.443293	-2.479565
C	0.586946	2.934992	-1.484661
H	1.214653	3.103184	-2.357177
C	1.191839	2.538574	-0.296769
O	2.573163	2.446489	-0.226550
C	0.413133	2.329466	0.861669
O	1.089095	1.952994	1.977287
C	0.339662	1.711480	3.167089
H	-0.179796	2.618460	3.505453
H	1.071604	1.410421	3.921889
H	-0.390574	0.903039	3.024483
C	4.579373	-1.204392	-0.389178
H	5.130942	-2.141742	-0.441187
C	3.200325	-1.193604	-0.643869
C	2.448379	-2.471847	-0.954313
H	3.085916	-3.143620	-1.546895
H	1.578043	-2.229710	-1.577654
C	1.983533	-3.219572	0.315046
H	2.872600	-3.544171	0.875169
C	1.095452	-4.444736	0.025746
H	0.986411	-5.026863	0.953930
H	1.620387	-5.101791	-0.684854
C	-0.307727	-4.126533	-0.526781
H	-0.774947	-5.064755	-0.863096
C	-1.242915	-3.439773	0.480346
H	-0.741630	-2.563955	0.918517
H	-1.439214	-4.127463	1.318754
H	-0.220008	-3.498830	-1.426441

H	1.453081	-2.516049	0.972147
C	2.505610	0.025264	-0.581465
H	1.438553	0.046280	-0.788567
C	3.179568	1.209258	-0.268053
C	4.557002	1.195254	-0.014618
H	5.064427	2.127660	0.221412
C	5.247617	-0.015220	-0.077653
H	6.319110	-0.028678	0.114668
C	-4.798411	-1.719084	0.310532
C	-2.573059	-2.976840	-0.131224
H	-2.355897	-2.273465	-0.949062
H	-3.089783	-3.832658	-0.594961
C	-4.616545	-0.544677	-0.670634
H	-5.613771	-0.228515	-1.014580
C	-3.504391	-2.314714	0.895193
H	-2.948873	-1.530497	1.431338
H	-3.777500	-3.060235	1.658025
H	-4.083782	-0.884956	-1.571327
C	-3.883251	0.670342	-0.081774
H	-2.851359	0.392025	0.172773
H	-4.363946	0.963055	0.866012
H	-5.433059	-1.381648	1.144887
H	-5.363474	-2.517088	-0.196288
C	-3.865191	1.879309	-1.026753
H	-4.900821	2.188954	-1.233259
H	-3.432115	1.586893	-1.995655
C	-3.096350	3.106626	-0.481804
H	-3.314829	3.965351	-1.131568
H	-3.485406	3.358185	0.514996
Sum of electronic and zero-point Energies= -1123.039771			
Sum of electronic and thermal Energies= -1123.013454			
Sum of electronic and thermal Enthalpies= -1123.012510			
Sum of electronic and thermal Free Energies= -1123.097538			

daec[n=6]-2-TS (dmf)

C	2.141307	2.961956	-0.022300
H	2.859386	3.742633	0.214262
C	2.616425	1.662174	-0.291718
C	1.675435	0.679403	-0.596601
H	1.981461	-0.332810	-0.836710
C	0.304003	0.963939	-0.605316
H	-0.390908	0.161712	-0.819013
C	-0.160749	2.244841	-0.335759
O	-1.490373	2.628728	-0.343210
C	0.777076	3.269641	-0.048747
O	0.255680	4.502293	0.195305
C	1.158393	5.560538	0.502735
H	1.731068	5.350566	1.417165
H	0.535027	6.445295	0.662379
H	1.854443	5.751879	-0.326131
C	-4.598132	0.004931	0.595343
H	-5.410876	-0.666716	0.865685
C	-3.811834	-0.270401	-0.535702
C	-4.024056	-1.521918	-1.369650
H	-3.260184	-1.552352	-2.156961
H	-4.993772	-1.463352	-1.887111
C	-4.000847	-2.845120	-0.565236
H	-4.907524	-2.895589	0.054767
C	-2.785427	-3.071403	0.352219
H	-2.965347	-3.991779	0.929074
H	-2.739982	-2.259605	1.093390
C	-1.416888	-3.188186	-0.337924
H	-1.220582	-2.287852	-0.939771
C	-0.275910	-3.372323	0.676928
H	-0.473481	-4.269669	1.285064
H	-0.291578	-2.523173	1.378918
H	-1.429270	-4.033446	-1.044639
H	-4.081281	-3.674409	-1.284190
C	-2.786666	0.626404	-0.871672
H	-2.208544	0.460353	-1.776271

C	-2.499431	1.723157	-0.050529
C	-3.280767	1.986598	1.077047
H	-3.050740	2.850446	1.695784
C	-4.341683	1.129839	1.383585
H	-4.960455	1.333775	2.255558
C	3.673932	-3.677847	0.587249
C	1.128464	-3.477396	0.061482
H	1.184769	-4.367697	-0.585546
H	1.295354	-2.611463	-0.595950
C	4.163120	-2.535406	-0.323185
H	3.512218	-2.474885	-1.208313
C	2.235740	-3.543937	1.127542
H	2.038253	-4.402533	1.788254
H	2.162974	-2.653535	1.769970
H	5.161657	-2.795495	-0.707820
C	4.224353	-1.148584	0.338402
H	4.972107	-1.153544	1.146560
H	3.264763	-0.934420	0.823942
H	3.755282	-4.623677	0.029013
H	4.358833	-3.773254	1.444459
C	4.559187	-0.023789	-0.665471
H	4.105915	-0.255246	-1.640880
H	5.644384	-0.008420	-0.839966
C	4.115445	1.387083	-0.238037
H	4.476060	1.588226	0.783767
H	4.625192	2.126721	-0.873620

Sum of electronic and zero-point Energies= -1123.025619

Sum of electronic and thermal Energies= -1123.000371

Sum of electronic and thermal Enthalpies= -1122.999427

Sum of electronic and thermal Free Energies= -1123.080206

daec[n=6]-2-E1 (dmf)

C	0.860399	2.797455	-0.589363
H	1.153761	3.194986	-1.557134
C	1.854875	2.558876	0.377301
C	1.470210	2.067084	1.630127
H	2.220076	1.889658	2.398252
C	0.122889	1.809353	1.907709
H	-0.186978	1.437456	2.881910
C	-0.854497	2.049100	0.948464
O	-2.185567	1.915942	1.306197
C	-0.493041	2.559788	-0.318639
O	-1.514448	2.796724	-1.181446
C	-1.196377	3.299343	-2.478324
H	-0.703892	4.279505	-2.418823
H	-2.153081	3.405564	-2.997331
H	-0.555662	2.600819	-3.033731
C	-4.726785	-1.060335	-0.118622
H	-5.416972	-1.821044	-0.480021
C	-3.378895	-1.106123	-0.507749
C	-2.887004	-2.220617	-1.411980
H	-2.000892	-1.882701	-1.964195
H	-3.660788	-2.429045	-2.163932
C	-2.571645	-3.547490	-0.678028
H	-3.464555	-3.854097	-0.113606
C	-1.362024	-3.509864	0.271453
H	-1.330853	-4.455246	0.834604
H	-1.506719	-2.715947	1.019950
C	-0.014090	-3.301661	-0.433926
H	-0.046797	-2.374385	-1.024878
C	1.181436	-3.218814	0.525612
H	1.299050	-4.173294	1.062892
H	0.968644	-2.459315	1.295036
H	0.148282	-4.116228	-1.158046
H	-2.406603	-4.325379	-1.439129
C	-2.502337	-0.111038	-0.043198
H	-1.456410	-0.131749	-0.338325
C	-2.973184	0.911027	0.788527
C	-4.318924	0.951712	1.172911
H	-4.662231	1.756693	1.818379

C	-5.188372	-0.038684	0.716250
H	-6.236341	-0.006690	1.009367
C	4.950279	-2.082513	0.106550
C	2.491617	-2.847425	-0.184000
H	2.757254	-3.630290	-0.912591
H	2.312944	-1.935455	-0.771907
C	4.791468	-0.769773	-0.686987
H	4.173952	-0.950874	-1.579375
C	3.667466	-2.614414	0.775436
H	3.906378	-3.555461	1.294555
H	3.349993	-1.913357	1.561676
H	5.780906	-0.469572	-1.065489
C	4.179757	0.390206	0.111879
H	4.804945	0.601628	0.994609
H	3.198279	0.087790	0.500232
H	5.351423	-2.852002	-0.571383
H	5.713212	-1.938978	0.887490
C	4.012800	1.673851	-0.711795
H	3.443975	1.450612	-1.627580
H	5.000547	2.029831	-1.041429
C	3.311264	2.825976	0.046115
H	3.862839	3.029710	0.974748
H	3.378733	3.735409	-0.567129

Sum of electronic and zero-point Energies= -1123.039036

Sum of electronic and thermal Energies= -1123.012807

Sum of electronic and thermal Enthalpies= -1123.011863

Sum of electronic and thermal Free Energies= -1123.095829

daec[n=6]-2-E2 (dmf)

C	1.338325	2.185710	0.742389
H	1.972111	1.949289	1.591860
C	1.938823	2.596047	-0.461798
C	1.115540	2.922375	-1.546926
H	1.558929	3.250674	-2.485244
C	-0.277048	2.851492	-1.429146
H	-0.924038	3.130800	-2.257982
C	-0.863065	2.449282	-0.233654
O	-2.237417	2.525684	-0.076956
C	-0.054501	2.100835	0.870333
O	-0.712201	1.724624	1.996969
C	0.062920	1.372140	3.141629
H	0.717629	0.514316	2.934936
H	-0.659655	1.098746	3.915721
H	0.669170	2.218613	3.492438
C	-4.791198	-0.757470	-0.285660
H	-5.490870	-1.588959	-0.353293
C	-3.499331	-0.891953	-0.819338
C	-3.086368	-2.187668	-1.493285
H	-2.182179	-2.017590	-2.091148
H	-3.874789	-2.480131	-2.201744
C	-2.861599	-3.372236	-0.523658
H	-3.777591	-3.519879	0.066838
C	-1.664767	-3.227713	0.431216
H	-1.695857	-4.055047	1.156794
H	-1.773610	-2.303602	1.019603
C	-0.296896	-3.224949	-0.266071
H	-0.256331	-2.402840	-0.995881
C	0.885565	-3.072348	0.700533
H	0.925355	-3.935955	1.383293
H	0.713003	-2.189046	1.336433
H	-0.181621	-4.153645	-0.847866
H	-2.733888	-4.285225	-1.125043
C	-2.613433	0.194854	-0.735269
H	-1.614031	0.113332	-1.156179
C	-3.020840	1.392718	-0.135808
C	-4.310181	1.521539	0.392288
H	-4.605257	2.462958	0.849457
C	-5.188683	0.440231	0.314342
H	-6.194069	0.537795	0.720456
C	4.730828	-2.263678	0.236763

C	2.232368	-2.905966	-0.017627
H	2.457026	-3.809993	-0.606204
H	2.132275	-2.088035	-0.745820
C	4.683481	-1.073043	-0.742227
H	4.096100	-1.347187	-1.631280
C	3.399495	-2.604929	0.933369
H	3.560967	-3.468756	1.596589
H	3.112725	-1.772670	1.593573
H	5.704845	-0.882520	-1.106881
C	4.106784	0.219836	-0.147455
H	4.670086	0.493702	0.759514
H	3.073554	0.040670	0.178069
H	5.093593	-3.149107	-0.308211
H	5.482927	-2.056797	1.013973
C	4.124553	1.400490	-1.126976
H	3.634176	1.108034	-2.068217
H	5.166502	1.643275	-1.384538
C	3.448794	2.683817	-0.586881
H	3.885859	2.931352	0.391107
H	3.696481	3.514492	-1.261727

Sum of electronic and zero-point Energies= -1123.038727

Sum of electronic and thermal Energies= -1123.012503

Sum of electronic and thermal Enthalpies= -1123.011559

Sum of electronic and thermal Free Energies= -1123.095668

daec[n=6]-3-TS (dmf)

C	3.032553	-2.113514	-0.134141
H	3.964543	-2.641054	0.050971
C	3.058032	-0.708260	-0.240208
C	1.850468	-0.052148	-0.475344
H	1.815333	1.026461	-0.581338
C	0.648797	-0.763604	-0.586729
H	-0.268781	-0.213252	-0.752872
C	0.626716	-2.148843	-0.481050
O	-0.506196	-2.935247	-0.615752
C	1.843883	-2.841056	-0.256978
O	1.752725	-4.195334	-0.168490
C	2.950533	-4.932158	0.058714
H	2.650253	-5.983656	0.090510
H	3.417938	-4.659931	1.015521
H	3.675450	-4.786527	-0.754484
C	-4.222941	-1.750009	0.875226
H	-5.186494	-1.452554	1.285872
C	-3.658618	-1.014497	-0.179297
C	-4.292480	0.266695	-0.684439
H	-5.338715	0.096610	-0.975916
H	-3.762883	0.585717	-1.591087
C	-4.240284	1.396464	0.380869
H	-3.363245	1.245034	1.023178
C	-4.198675	2.821984	-0.202590
H	-4.452206	3.535052	0.596926
H	-4.987376	2.925979	-0.963708
C	-2.845557	3.236499	-0.817024
H	-2.970404	4.215852	-1.304272
C	-1.688208	3.323262	0.192155
H	-1.547083	2.345548	0.675644
H	-1.959012	4.023777	0.998470
H	-2.570165	2.535283	-1.620162
H	-5.112421	1.299444	1.042135
C	-2.426933	-1.432514	-0.705176
H	-2.009960	-0.911733	-1.562327
C	-1.732591	-2.502937	-0.131062
C	-2.295856	-3.226854	0.923132
H	-1.748410	-4.065421	1.346335
C	-3.552380	-2.854221	1.409126
H	-4.001436	-3.419891	2.223518
C	2.186526	4.027731	-0.074582
C	-0.349357	3.751379	-0.429875
H	-0.429878	4.780129	-0.815837
H	-0.140222	3.114713	-1.304689

C	3.408298	3.749417	0.826405
H	3.238113	4.221190	1.806650
C	0.832087	3.650966	0.548960
H	0.874117	2.621609	0.933756
H	0.644122	4.294111	1.423632
H	4.288323	4.253838	0.397412
C	3.748674	2.260225	1.041690
H	2.855208	1.725532	1.389746
H	4.479960	2.177823	1.860023
H	2.173560	5.098542	-0.329710
H	2.304703	3.496609	-1.031186
C	4.334274	1.562159	-0.201698
H	5.358131	1.932028	-0.357838
H	3.776319	1.850315	-1.103246
C	4.388421	0.025837	-0.116277
H	4.869119	-0.269154	0.830022
H	5.058974	-0.345399	-0.906565
Sum of electronic and zero-point Energies= -1123.024189			
Sum of electronic and thermal Energies= -1122.998857			
Sum of electronic and thermal Enthalpies= -1122.997912			
Sum of electronic and thermal Free Energies= -1123.079131			

daec[n=6]-3-E1 (dmf)

C	1.718729	-2.305452	0.582209
H	2.355904	-2.232776	1.458301
C	2.309339	-2.287359	-0.694104
C	1.483026	-2.408281	-1.819285
H	1.920620	-2.406402	-2.815899
C	0.099890	-2.555828	-1.673710
H	-0.543849	-2.677331	-2.542400
C	-0.476096	-2.572799	-0.407668
O	-1.827437	-2.843191	-0.255229
C	0.331421	-2.435547	0.741473
O	-0.315939	-2.458384	1.934534
C	0.462911	-2.327457	3.122590
H	-0.251585	-2.361044	3.950015
H	1.002587	-1.370738	3.146079
H	1.179041	-3.154172	3.226913
C	-4.773739	0.104062	-0.352491
H	-5.566226	0.849788	-0.389947
C	-3.440941	0.495340	-0.543286
C	-3.072968	1.949003	-0.761878
H	-3.838334	2.438832	-1.381120
H	-2.133372	1.993940	-1.326607
C	-2.919519	2.734058	0.559375
H	-2.261215	2.169896	1.234265
C	-2.383668	4.168128	0.385912
H	-2.357359	4.644936	1.378001
H	-3.100370	4.750943	-0.213199
C	-0.989480	4.283803	-0.262570
H	-0.713887	5.348608	-0.309694
C	0.112940	3.502598	0.465741
H	-0.190569	2.450285	0.562566
H	0.215615	3.882713	1.495017
H	-1.038035	3.942528	-1.307555
H	-3.897264	2.777905	1.061110
C	-2.430632	-0.480579	-0.502789
H	-1.395160	-0.189075	-0.659674
C	-2.752125	-1.822574	-0.278571
C	-4.084988	-2.209033	-0.084506
H	-4.314563	-3.258322	0.085147
C	-5.087310	-1.240141	-0.123071
H	-6.124146	-1.539093	0.021419
C	3.828875	2.476722	-0.324341
C	1.478229	3.535224	-0.236284
H	1.870032	4.564460	-0.258732
H	1.346546	3.234514	-1.288154
C	4.834244	1.511605	0.333632
H	5.045037	1.868492	1.353831
C	2.496006	2.596639	0.427542

H	2.034863	1.601972	0.515180
H	2.688580	2.932959	1.459285
H	5.790192	1.566990	-0.210423
C	4.391584	0.037497	0.413244
H	3.423719	-0.031038	0.928079
H	5.107028	-0.508119	1.047892
H	4.295050	3.471718	-0.395125
H	3.632084	2.163110	-1.360798
C	4.312240	-0.676665	-0.944022
H	5.315697	-0.682169	-1.395994
H	3.666161	-0.119884	-1.637582
C	3.810445	-2.140300	-0.863056
H	4.329631	-2.650384	-0.038812
H	4.104078	-2.657423	-1.786352
Sum of electronic and zero-point Energies= -1123.037537			
Sum of electronic and thermal Energies= -1123.011324			
Sum of electronic and thermal Enthalpies= -1123.010380			
Sum of electronic and thermal Free Energies= -1123.094960			

daec[n=6]-3-E2 (dmf)

C	-1.322653	2.554571	-0.804338
H	-1.697142	2.670416	-1.817687
C	-2.246148	2.416791	0.248849
C	-1.760002	2.290919	1.555463
H	-2.453830	2.202412	2.388775
C	-0.381373	2.288346	1.801983
H	0.005521	2.197253	2.814625
C	0.524447	2.425489	0.756347
O	1.873755	2.542920	1.047154
C	0.057099	2.572665	-0.569521
O	1.008037	2.736150	-1.524714
C	0.584453	2.867977	-2.880757
H	1.501150	2.970399	-3.468255
H	-0.039549	3.761201	-3.020964
H	0.032997	1.979506	-3.217378
C	4.702491	-0.333599	-0.004478
H	5.462612	-1.064974	-0.274357
C	3.345620	-0.651599	-0.159544
C	2.906231	-2.012858	-0.659909
H	3.651617	-2.410740	-1.363209
H	1.971370	-1.896270	-1.222654
C	2.695381	-3.032201	0.481201
H	2.060440	-2.575792	1.252993
C	2.084412	-4.372649	0.029773
H	2.015225	-5.029841	0.910426
H	2.777910	-4.868872	-0.666693
C	0.697516	-4.280619	-0.637939
H	0.363525	-5.298861	-0.890167
C	-0.373255	-3.589226	0.217600
H	-0.012920	-2.594748	0.517679
H	-0.517972	-4.152362	1.153713
H	0.784424	-3.749945	-1.597975
H	3.663525	-3.226978	0.965553
C	2.377712	0.305809	0.186366
H	1.322453	0.070180	0.071358
C	2.762743	1.559243	0.668812
C	4.118813	1.872816	0.825598
H	4.398147	2.854128	1.201772
C	5.080523	0.920476	0.487855
H	6.135495	1.163195	0.603573
C	-4.009992	-2.219085	-0.404685
C	-1.723405	-3.406766	-0.490894
H	-2.172338	-4.388140	-0.711644
H	-1.552580	-2.922101	-1.465666
C	-4.979367	-1.339592	0.408916
H	-5.233240	-1.868574	1.340772
C	-2.701788	-2.551064	0.326694
H	-2.189843	-1.617660	0.603252
H	-2.933850	-3.061694	1.275393
H	-5.923313	-1.240146	-0.149651

C	-4.465190	0.067449	0.770928
H	-3.513663	-0.013235	1.314218
H	-5.174450	0.526210	1.477208
H	-4.525567	-3.156294	-0.665867
H	-3.774378	-1.729659	-1.361925
C	-4.299369	1.013040	-0.427574
H	-5.281433	1.156075	-0.903407
H	-3.651158	0.559186	-1.190787
C	-3.732015	2.405806	-0.058312
H	-4.288476	2.801275	0.803366
H	-3.922357	3.090066	-0.896502

Sum of electronic and zero-point Energies= -1123.038503

Sum of electronic and thermal Energies= -1123.012250

Sum of electronic and thermal Enthalpies= -1123.011306

Sum of electronic and thermal Free Energies= -1123.095615

daec[n=7]-1-TS (dmf)

C	-3.303695	2.129574	0.002968
H	-4.107749	2.849703	0.127410
C	-1.971522	2.579592	0.092289
C	-0.958895	1.634860	-0.083527
H	0.085690	1.919744	-0.055149
C	-1.254698	0.288363	-0.314241
H	-0.434951	-0.409407	-0.425931
C	-2.569808	-0.154249	-0.393674
O	-2.944369	-1.464849	-0.646771
C	-3.618216	0.785824	-0.240703
O	-4.882546	0.293511	-0.342041
C	-5.968847	1.200345	-0.176860
H	-5.956287	1.990415	-0.940793
H	-5.963735	1.659945	0.821600
H	-6.876220	0.600434	-0.293340
C	-0.648402	-4.622395	0.834483
H	-0.055050	-5.434960	1.251114
C	-0.095326	-3.799248	-0.158605
C	1.361811	-3.916105	-0.557528
H	1.503655	-3.505235	-1.565893
H	1.669063	-4.971008	-0.590312
C	2.259023	-3.161050	0.453636
H	1.881190	-2.134726	0.566368
C	3.757592	-3.130181	0.106614
H	4.092193	-4.153416	-0.124829
H	4.312270	-2.832587	1.008220
C	4.167881	-2.206775	-1.057370
H	3.667634	-2.533399	-1.981617
C	3.903747	-0.698622	-0.864655
H	2.820984	-0.508301	-0.851840
H	4.287062	-0.177408	-1.756213
H	5.245490	-2.349344	-1.233968
H	2.133176	-3.636092	1.437501
C	-0.885318	-2.771514	-0.695634
H	-0.492689	-2.164377	-1.506573
C	-2.156967	-2.507604	-0.175991
C	-2.702360	-3.329095	0.814422
H	-3.700183	-3.119276	1.191818
C	-1.947770	-4.400257	1.300432
H	-2.369234	-5.050535	2.064841
C	3.299281	2.192120	0.233576
C	4.551173	-0.084069	0.390143
H	4.002475	-0.410215	1.286630
H	5.571961	-0.483795	0.498525
C	2.207685	4.502313	-0.164324
H	2.454329	5.573234	-0.222265
H	2.031140	4.179738	-1.524273
C	4.639899	1.455010	0.385469
H	5.310309	1.772304	-0.429516
C	0.905520	4.319961	0.642674
H	0.917174	4.980057	1.523418
H	5.125070	1.778617	1.319855
H	0.867360	3.302688	1.046453

C	-0.362293	4.603153	-0.192580
H	-0.227531	4.196011	-1.205455
H	-0.464103	5.690799	-0.318719
H	2.586818	1.807265	0.978818
C	3.427539	3.723208	0.364238
H	4.312600	4.049953	-0.203634
H	3.625943	3.990107	1.414400
C	-1.684768	4.048860	0.383163
H	-2.522104	4.641300	-0.010393
H	2.868245	1.957719	-0.751527
H	-1.700265	4.212629	1.473488

Sum of electronic and zero-point Energies= -1162.304885

Sum of electronic and thermal Energies= -1162.278231

Sum of electronic and thermal Enthalpies= -1162.277286

Sum of electronic and thermal Free Energies= -1162.361838

daec[n=7]-1-E1 (dmf)

C	-2.072733	2.936811	-0.272319
H	-2.124142	3.762664	-0.976368
C	-1.289336	3.080231	0.887294
C	-1.233062	2.016239	1.794385
H	-0.641897	2.108388	2.703611
C	-1.945281	0.835586	1.552819
H	-1.913718	0.014759	2.266210
C	-2.711218	0.699412	0.398853
O	-3.509123	-0.406250	0.170858
C	-2.782064	1.758562	-0.533681
O	-3.558182	1.544428	-1.628193
C	-3.670282	2.597168	-2.583089
H	-2.695469	2.847842	-3.024191
H	-4.112259	3.499649	-2.138446
H	-4.333795	2.217803	-3.365562
C	-2.099156	-4.322163	0.267209
H	-1.760130	-5.356768	0.280254
C	-1.216624	-3.310994	-0.143064
C	0.205749	-3.649587	-0.543987
H	0.485591	-3.070458	-1.434391
H	0.252187	-4.710075	-0.829293
C	1.229498	-3.390501	0.583199
H	1.290241	-2.309091	0.773298
C	2.629654	-3.968082	0.307709
H	2.544424	-5.063136	0.229055
H	3.259432	-3.779690	1.189377
C	3.347741	-3.453460	-0.954541
H	2.772254	-3.746967	-1.845012
C	3.605264	-1.937086	-1.015086
H	2.645153	-1.401932	-1.019444
H	4.081233	-1.707833	-1.981840
H	4.311976	-3.979512	-1.035109
H	0.850140	-3.840891	1.512321
C	-1.668535	-1.981264	-0.158816
H	-1.003462	-1.184898	-0.485738
C	-2.978228	-1.677808	0.230347
C	-3.855398	-2.690679	0.635521
H	-4.870012	-2.429927	0.926659
C	-3.407735	-4.011797	0.649389
H	-4.085807	-4.804300	0.961230
C	3.738816	1.064639	-0.124212
C	4.494713	-1.395514	0.115549
H	3.977529	-1.507948	1.080518
H	5.403089	-2.015132	0.183400
C	3.051574	3.542411	-0.381989
H	3.467412	4.561750	-0.353330
H	2.704830	3.384499	-1.415989
C	4.912833	0.076372	-0.053260
H	5.528212	0.180535	-0.961356
C	1.844957	3.462186	0.564283
H	2.183268	3.599780	1.604244
H	5.565297	0.353762	0.789628
H	1.408464	2.455437	0.516113

C	0.755991	4.494505	0.245450
H	0.469927	4.410234	-0.814260
H	1.162599	5.508961	0.374469
H	3.046423	0.855341	0.704994
C	4.175787	2.537191	-0.074013
H	4.991752	2.694254	-0.796922
H	4.603085	2.754741	0.917958
C	-0.512665	4.362367	1.119159
H	-1.165355	5.222975	0.913979
H	3.167366	0.893259	-1.048941
H	-0.228954	4.428044	2.178893

Sum of electronic and zero-point Energies= -1162.321758

Sum of electronic and thermal Energies= -1162.294186

Sum of electronic and thermal Enthalpies= -1162.293242

Sum of electronic and thermal Free Energies= -1162.381253

daec[n=7]-1-E2 (dmf)

C	0.597668	2.852271	0.932861
H	1.088754	2.776055	1.898692
C	1.332796	3.329733	-0.165941
C	0.693142	3.439994	-1.407310
H	1.239326	3.816177	-2.270413
C	-0.650963	3.079824	-1.545861
H	-1.161615	3.176757	-2.501573
C	-1.374256	2.613266	-0.452515
O	-2.735621	2.402038	-0.587871
C	-0.752350	2.496726	0.809767
O	-1.536479	2.053682	1.826035
C	-0.947274	1.909644	3.117332
H	-0.588676	2.873210	3.504476
H	-0.118028	1.189321	3.102341
H	-1.743484	1.532913	3.765571
C	-4.551042	-1.338603	-0.383895
H	-5.054398	-2.302956	-0.339794
C	-3.162761	-1.291590	-0.578108
C	-2.364537	-2.575436	-0.696751
H	-1.654371	-2.494738	-1.531139
H	-3.050874	-3.397067	-0.945550
C	-1.599692	-2.935410	0.596522
H	-0.788659	-2.208763	0.749659
C	-1.047461	-4.372356	0.624736
H	-1.898169	-5.071283	0.605545
H	-0.551735	-4.531428	1.593540
C	-0.086146	-4.762478	-0.514016
H	-0.625895	-4.727806	-1.472020
C	1.191684	-3.914537	-0.641668
H	0.919261	-2.875492	-0.874548
H	1.759806	-4.278249	-1.512719
H	0.200468	-5.816118	-0.370263
H	-2.279810	-2.815181	1.452568
C	-2.525623	-0.039695	-0.637254
H	-1.451579	0.016955	-0.800607
C	-3.271017	1.134792	-0.497033
C	-4.658010	1.082498	-0.308419
H	-5.215094	2.011133	-0.210025
C	-5.290329	-0.158232	-0.253763
H	-6.368278	-0.204508	-0.108570
C	3.387156	-1.783925	-0.010818
C	2.106040	-3.944583	0.593448
H	1.596754	-3.465794	1.443554
H	2.273595	-4.992262	0.889871
C	4.722845	0.327465	-0.661389
H	5.745039	0.737057	-0.667826
H	4.426930	0.231802	-1.718582
C	3.471860	-3.265254	0.386457
H	4.039656	-3.812864	-0.382937
C	3.783507	1.327502	0.028223
H	4.070711	1.432099	1.087236
H	4.054392	-3.356008	1.316789
H	2.759606	0.929974	0.027289

C	3.783250	2.709252	-0.637696
H	3.550387	2.598939	-1.707842
H	4.793851	3.141847	-0.585897
H	2.706233	-1.267179	0.682152
C	4.749746	-1.073509	-0.024890
H	5.471645	-1.693795	-0.578985
H	5.135582	-1.004885	1.004831
C	2.792399	3.714810	-0.009261
H	2.955056	4.696701	-0.476530
H	2.930853	-1.695788	-1.008259
H	3.025789	3.832459	1.058090

Sum of electronic and zero-point Energies= -1162.322468

Sum of electronic and thermal Energies= -1162.294920

Sum of electronic and thermal Enthalpies= -1162.293976

Sum of electronic and thermal Free Energies= -1162.381494

daec[n=7]-2-TS (dmf)

C	-1.738115	3.298567	-0.362483
H	-2.388366	4.169101	-0.341729
C	-2.320670	2.015764	-0.414045
C	-1.465001	0.916088	-0.438395
H	-1.862609	-0.090288	-0.499162
C	-0.073606	1.073423	-0.382348
H	0.558196	0.192209	-0.371832
C	0.494878	2.339617	-0.329873
O	1.851536	2.598592	-0.281175
C	-0.351814	3.477464	-0.331905
O	0.274050	4.684916	-0.287116
C	-0.536246	5.856342	-0.280242
H	0.160648	6.699120	-0.248877
H	-1.188258	5.892179	0.603950
H	-1.151336	5.927689	-1.188323
C	4.643497	-0.214664	1.015374
H	5.387207	-0.927244	1.367193
C	3.964543	-0.454780	-0.191690
C	4.230049	-1.709102	-1.006525
H	5.264806	-1.684242	-1.380966
H	3.584609	-1.700641	-1.894052
C	4.044406	-3.034761	-0.230693
H	4.299526	-3.861430	-0.910979
C	2.647674	-3.279965	0.367994
H	2.384998	-2.443845	1.033847
H	2.703278	-4.170960	1.012243
C	1.521494	-3.483559	-0.656286
H	1.772235	-4.334959	-1.309484
C	0.148599	-3.721425	-0.006005
H	-0.074924	-2.877932	0.664361
H	0.193516	-4.616997	0.634622
H	1.452682	-2.605042	-1.315727
H	4.784259	-3.073776	0.581492
C	3.028139	0.493305	-0.630930
H	2.515326	0.348233	-1.578903
C	2.743304	1.623891	0.143987
C	3.415484	1.851823	1.345984
H	3.185933	2.741595	1.927059
C	4.376415	0.929523	1.770185
H	4.913336	1.103387	2.700916
C	-2.849286	-2.824442	0.417319
C	-0.983623	-3.879328	-1.031868
H	-0.975859	-3.004816	-1.702628
H	-0.770802	-4.751535	-1.669615
C	-4.865664	-1.496051	1.377860
H	-5.959839	-1.420963	1.276856
H	-4.678327	-1.787414	2.423160
C	-2.399749	-4.022809	-0.442976
H	-2.471776	-4.951176	0.144806
C	-4.243088	-0.102191	1.156129
H	-3.174433	-0.138640	1.404045
H	-3.101646	-4.142601	-1.282839
H	-4.692885	0.592867	1.882299

C	-4.431028	0.478137	-0.255633
H	-5.508234	0.536186	-0.473139
H	-4.013647	-0.206230	-1.007287
H	-2.384740	-1.914869	0.015080
C	-4.372564	-2.627384	0.452507
H	-4.854412	-3.565077	0.771367
H	-4.724698	-2.446401	-0.574509
C	-3.838818	1.886358	-0.461988
H	-4.188174	2.265907	-1.435414
H	-2.464786	-2.929059	1.443086
H	-4.270728	2.570559	0.284673

Sum of electronic and zero-point Energies= -1162.311898

Sum of electronic and thermal Energies= -1162.285340

Sum of electronic and thermal Enthalpies= -1162.284396

Sum of electronic and thermal Free Energies= -1162.368320

daec[n=7]-2-E1 (dmf)

C	-2.101181	2.575945	-0.493454
H	-2.887559	2.907861	-1.165570
C	-2.462639	2.007547	0.743518
C	-1.440901	1.590586	1.601677
H	-1.684070	1.165431	2.573262
C	-0.092915	1.725131	1.236653
H	0.689292	1.397534	1.916108
C	0.253577	2.291837	0.013607
O	1.548816	2.507804	-0.408520
C	-0.763809	2.728004	-0.869432
O	-0.341746	3.278126	-2.040148
C	-1.332104	3.729591	-2.959470
H	-0.781644	4.127087	-3.817257
H	-1.952734	4.526445	-2.526034
H	-1.979111	2.906144	-3.293568
C	4.799943	0.423564	1.151869
H	5.675719	-0.098223	1.534985
C	4.105855	-0.106504	0.050222
C	4.561236	-1.392324	-0.613416
H	5.648894	-1.347557	-0.767321
H	4.109885	-1.460713	-1.611154
C	4.251044	-2.679783	0.186824
H	4.673112	-3.529841	-0.370512
C	2.764169	-2.945542	0.474078
H	2.363462	-2.131150	1.096787
H	2.689173	-3.857861	1.085898
C	1.875422	-3.099568	-0.769135
H	2.271084	-3.900299	-1.414351
C	0.407019	-3.387195	-0.420295
H	0.092003	-2.682276	0.362668
H	0.319151	-4.392928	0.021480
H	1.918758	-2.177661	-1.367168
H	4.793620	-2.640104	1.142952
C	2.989616	0.593333	-0.429566
H	2.436899	0.225581	-1.291551
C	2.589808	1.791768	0.168322
C	3.286152	2.320244	1.255988
H	2.971256	3.263082	1.696661
C	4.394833	1.620990	1.746191
H	4.951629	2.023092	2.590548
C	-2.583247	-2.648068	-0.171553
C	-0.539509	-3.259653	-1.623170
H	-0.438268	-2.244008	-2.038513
H	-0.214597	-3.947197	-2.419767
C	-4.675840	-2.049320	1.214696
H	-5.775021	-2.014445	1.154161
H	-4.439026	-2.756019	2.025357
C	-2.025478	-3.516054	-1.311709
H	-2.177969	-4.578561	-1.064098
C	-4.142961	-0.663960	1.623153
H	-3.048299	-0.706458	1.701249
H	-2.608080	-3.331787	-2.227973
H	-4.506754	-0.435891	2.637224

C	-4.548539	0.490137	0.696107
H	-5.644814	0.588132	0.709395
H	-4.272244	0.266164	-0.344504
H	-2.207572	-1.620094	-0.285880
C	-4.118097	-2.623310	-0.102657
H	-4.505022	-3.647765	-0.219403
H	-4.507562	-2.056411	-0.961826
C	-3.931015	1.853957	1.095381
H	-4.496550	2.651984	0.595296
H	-2.185811	-3.008825	0.788916
H	-4.070421	2.001985	2.176277

Sum of electronic and zero-point Energies= -1162.317746

Sum of electronic and thermal Energies= -1162.290221

Sum of electronic and thermal Enthalpies= -1162.289276

Sum of electronic and thermal Free Energies= -1162.376532

daec[n=7]-2-E2 (dmf)

C	-1.238235	2.543659	0.358772
H	-1.811129	2.676410	1.271196
C	-1.918588	2.493243	-0.873090
C	-1.167632	2.352147	-2.046322
H	-1.670778	2.316918	-3.010879
C	0.231105	2.295738	-1.996263
H	0.820948	2.234630	-2.908339
C	0.896191	2.365119	-0.777130
O	2.273479	2.506508	-0.744162
C	0.158510	2.471170	0.424022
O	0.888519	2.531599	1.567466
C	0.190369	2.650233	2.805695
H	0.961912	2.660079	3.580836
H	-0.481729	1.797077	2.971398
H	-0.385544	3.584653	2.854007
C	4.971358	-0.482434	0.314192
H	5.716718	-1.237267	0.559791
C	3.831353	-0.849074	-0.420902
C	3.670305	-2.282062	-0.895975
H	4.615395	-2.596968	-1.361384
H	2.910566	-2.323028	-1.686642
C	3.328929	-3.301431	0.216730
H	3.483252	-4.313683	-0.186796
C	1.901913	-3.201358	0.780944
H	1.712448	-2.171841	1.122530
H	1.832050	-3.836764	1.677131
C	0.808261	-3.616364	-0.213952
H	0.982180	-4.656293	-0.534026
C	-0.615790	-3.476478	0.340879
H	-0.730689	-2.464628	0.755847
H	-0.761104	-4.171446	1.183639
H	0.886419	-3.002929	-1.123876
H	4.054354	-3.184218	1.034826
C	2.886314	0.139611	-0.740746
H	2.004044	-0.116800	-1.323647
C	3.096995	1.467912	-0.350653
C	4.235923	1.826738	0.375376
H	4.376696	2.865850	0.662322
C	5.168543	0.842645	0.708538
H	6.058968	1.116105	1.272066
C	-3.371437	-2.068451	0.323684
C	-1.693783	-3.715617	-0.726601
H	-1.489298	-3.050062	-1.580849
H	-1.603117	-4.742571	-1.113643
C	-5.118615	-0.335388	1.103341
H	-6.167962	-0.040626	0.946225
H	-5.023967	-0.560993	2.176998
C	-3.140276	-3.472494	-0.262197
H	-3.433089	-4.231953	0.479703
C	-4.203259	0.863015	0.789790
H	-3.169736	0.611826	1.063505
H	-3.807352	-3.619861	-1.125886
H	-4.494015	1.697558	1.447011

C	-4.246705	1.348451	-0.665466
H	-5.292271	1.555475	-0.941217
H	-3.900380	0.555943	-1.344275
H	-2.770427	-1.342331	-0.243767
C	-4.840206	-1.623231	0.304658
H	-5.473543	-2.426378	0.712858
H	-5.157506	-1.494034	-0.741362
C	-3.429703	2.635467	-0.934047
H	-3.698627	3.009180	-1.931161
H	-2.991847	-2.031904	1.355754
H	-3.748874	3.405412	-0.215987

Sum of electronic and zero-point Energies= -1162.317737

Sum of electronic and thermal Energies= -1162.290211

Sum of electronic and thermal Enthalpies= -1162.289267

Sum of electronic and thermal Free Energies= -1162.376856

daec[n=7]-3-TS (dmf)

C	-1.694359	-3.566459	0.228496
H	-2.035631	-4.582427	0.421802
C	-0.325957	-3.252926	0.286120
C	0.031743	-1.927663	0.012012
H	1.071173	-1.621510	0.007534
C	-0.925162	-0.952464	-0.272380
H	-0.592152	0.061032	-0.456357
C	-2.282357	-1.271779	-0.306460
O	-3.290386	-0.364657	-0.594680
C	-2.669178	-2.605911	-0.060942
O	-3.991448	-2.977220	-0.034374
C	-4.639445	-3.017695	-1.311642
H	-5.663232	-3.358520	-1.125097
H	-4.137621	-3.730240	-1.982737
H	-4.666261	-2.027807	-1.783087
C	-3.086138	3.542540	0.865173
H	-3.035483	4.551357	1.271915
C	-2.167176	3.144938	-0.118892
C	-1.012847	4.038280	-0.525391
H	-1.359781	5.067954	-0.693318
H	-0.590015	3.681970	-1.474120
C	0.082315	4.053018	0.568767
H	-0.338557	4.533782	1.463360
C	1.380135	4.778023	0.166196
H	1.911219	5.080710	1.081614
H	1.120595	5.712743	-0.354615
C	2.359256	3.968435	-0.706570
H	3.153505	4.651834	-1.045210
C	3.018426	2.772817	0.007416
H	2.276139	1.979927	0.178176
H	3.358554	3.093747	1.005456
H	1.855167	3.618422	-1.620918
H	0.309670	3.018592	0.862837
C	-2.267144	1.848687	-0.645374
H	-1.605054	1.547123	-1.452095
C	-3.196359	0.942188	-0.125542
C	-4.105139	1.339501	0.857708
H	-4.829980	0.623209	1.236465
C	-4.056439	2.652587	1.334521
H	-4.767321	2.974804	2.093118
C	4.191515	-0.328871	-0.218441
C	4.224074	2.208524	-0.763121
H	3.910914	1.921036	-1.779946
H	4.955274	3.021379	-0.892769
C	4.351522	-2.893521	0.033115
H	4.143523	-2.925304	-1.047956
H	5.090408	-3.687199	0.217894
C	4.933750	1.012137	-0.097791
H	5.119851	1.241425	0.963837
C	3.054744	-3.210804	0.808933
H	2.540608	-2.274852	1.052986
H	5.926465	0.896635	-0.559887
H	3.304265	-3.665720	1.779626

C	2.106638	-4.149905	0.037092
H	2.581331	-5.139635	-0.033291
H	2.006215	-3.791646	-0.998266
H	3.208947	-0.257731	0.270126
C	4.979247	-1.522527	0.353540
H	5.997664	-1.498291	-0.064266
H	5.094778	-1.406586	1.443084
C	0.694763	-4.327741	0.639626
H	0.778897	-4.398605	1.736690
H	3.989766	-0.520908	-1.284831
H	0.288263	-5.296135	0.317652

Sum of electronic and zero-point Energies= -1162.303757

Sum of electronic and thermal Energies= -1162.276648

Sum of electronic and thermal Enthalpies= -1162.275704

Sum of electronic and thermal Free Energies= -1162.361852

daec[n=7]-3-E1 (dmf)

C	0.249444	-3.696994	-0.208744
H	0.708819	-4.432408	-0.867278
C	0.918361	-3.254859	0.942915
C	0.268954	-2.316613	1.757912
H	0.755676	-1.962128	2.664885
C	-1.004093	-1.837238	1.437406
H	-1.502396	-1.123528	2.089089
C	-1.651783	-2.281042	0.282241
O	-2.946688	-1.918778	-0.033326
C	-1.019987	-3.225023	-0.550580
O	-1.648574	-3.747044	-1.654116
C	-1.792065	-2.846349	-2.759183
H	-2.271296	-3.419027	-3.559860
H	-0.810047	-2.491787	-3.104629
H	-2.421950	-1.985117	-2.504870
C	-4.379408	1.981353	0.269367
H	-4.781774	2.991223	0.331265
C	-3.045049	1.791421	-0.125347
C	-2.152144	2.977492	-0.428920
H	-2.755620	3.783402	-0.870870
H	-1.405769	2.689791	-1.180831
C	-1.440417	3.522321	0.828820
H	-2.199833	3.728544	1.597366
C	-0.632013	4.809787	0.587421
H	-0.259432	5.169795	1.559087
H	-1.317317	5.588427	0.217739
C	0.557028	4.699644	-0.384696
H	0.982507	5.706650	-0.517320
C	1.673889	3.748320	0.070758
H	1.280880	2.724468	0.140095
H	1.991445	4.023816	1.089834
H	0.201809	4.392714	-1.380272
H	-0.793656	2.736582	1.245093
C	-2.544178	0.483723	-0.208494
H	-1.517196	0.315944	-0.525242
C	-3.363344	-0.606268	0.107106
C	-4.691117	-0.414163	0.498729
H	-5.309950	-1.277571	0.730275
C	-5.193047	0.887016	0.574161
H	-6.227503	1.044957	0.873761
C	3.756573	1.353419	-0.536645
C	2.897305	3.773750	-0.859206
H	2.584324	3.505095	-1.881221
H	3.269719	4.808281	-0.919177
C	4.710874	-1.042016	-0.311067
H	4.465638	-1.243420	-1.366384
H	5.655127	-1.572640	-0.112522
C	4.055996	2.856312	-0.428604
H	4.343403	3.097984	0.607536
C	3.611035	-1.632763	0.583815
H	2.657868	-1.124776	0.383729
H	4.936813	3.085586	-1.048447
H	3.851762	-1.426790	1.639524



C	3.425075	-3.143654	0.393047
H	4.369153	-3.660069	0.623858
H	3.209072	-3.355593	-0.665391
H	2.883731	1.106386	0.082630
C	4.944292	0.468379	-0.127802
H	5.825529	0.762220	-0.719238
H	5.203451	0.670906	0.923964
C	2.309826	-3.761603	1.267657
H	2.530817	-3.561871	2.325533
H	3.471838	1.117739	-1.575302
H	2.336407	-4.853314	1.140719

Sum of electronic and zero-point Energies= -1162.320629

Sum of electronic and thermal Energies= -1162.292688

Sum of electronic and thermal Enthalpies= -1162.291744

Sum of electronic and thermal Free Energies= -1162.380708

daec[n=7]-3-E2 (dmf)

C	-0.003671	-2.837424	1.031775
H	0.397140	-2.802612	2.043290
C	0.712469	-3.470801	0.005809
C	0.143267	-3.496170	-1.277626
H	0.669331	-3.989649	-2.093075
C	-1.094590	-2.900387	-1.526273
H	-1.538513	-2.924154	-2.519093
C	-1.796422	-2.277027	-0.493123
O	-3.070258	-1.800177	-0.747629
C	-1.251034	-2.247992	0.802501
O	-1.904897	-1.620124	1.834566
C	-2.995465	-2.367820	2.391397
H	-3.422444	-1.744722	3.183615
H	-2.638722	-3.313842	2.823569
H	-3.765996	-2.579682	1.639229
C	-4.127727	2.224708	-0.575108
H	-4.432968	3.269409	-0.545076
C	-2.763460	1.904278	-0.651768
C	-1.719241	3.002860	-0.649694
H	-2.141215	3.900787	-1.123670
H	-0.859052	2.696271	-1.259302
C	-1.243295	3.368846	0.773753
H	-2.127540	3.527685	1.408327
C	-0.370183	4.634901	0.841561
H	-0.134096	4.833979	1.898583
H	-0.971786	5.491071	0.498512
C	0.942104	4.607833	0.037931
H	1.420061	5.595426	0.132941
C	1.944196	3.529054	0.473799
H	1.506847	2.534110	0.311350
H	2.121118	3.612148	1.558678
H	0.721981	4.484871	-1.033531
H	-0.710136	2.510102	1.206545
C	-2.382768	0.553282	-0.697814
H	-1.330115	0.288791	-0.768251
C	-3.354770	-0.451137	-0.657166
C	-4.714479	-0.128259	-0.582839
H	-5.451145	-0.927855	-0.563635
C	-5.092641	1.213833	-0.543245
H	-6.149093	1.470788	-0.489243
C	3.961315	1.139103	-0.322626
C	3.288515	3.634100	-0.263499
H	3.111828	3.587286	-1.350374
H	3.717325	4.629595	-0.069611
C	4.737912	-1.321477	-0.481848
H	4.599245	-1.288284	-1.574587
H	5.622286	-1.953926	-0.307443
C	4.324140	2.563447	0.123338
H	4.473430	2.578791	1.215137
C	3.515652	-1.993080	0.162123
H	2.620706	-1.377445	-0.002845
H	5.295228	2.835054	-0.319248
H	3.659873	-2.037970	1.253874

C	3.259149	-3.407201	-0.374021
H	4.153847	-4.027033	-0.211160
H	3.109879	-3.364286	-1.463669
H	3.003061	0.845521	0.126729
C	5.035169	0.098992	0.030231
H	5.999119	0.429248	-0.387436
H	5.171584	0.071098	1.123400
C	2.054951	-4.124321	0.274744
H	2.215098	-4.187403	1.359889
H	3.801783	1.134996	-1.413485
H	2.028743	-5.158605	-0.098310

Sum of electronic and zero-point Energies= -1162.321399

Sum of electronic and thermal Energies= -1162.293411

Sum of electronic and thermal Enthalpies= -1162.292467

Sum of electronic and thermal Free Energies= -1162.381672

daec[n=7]-4-TS (dmf)

C	0.325295	3.482157	0.277878
H	0.510865	4.440480	0.755585
C	1.390660	2.568245	0.158409
C	1.135025	1.335729	-0.447238
H	1.921564	0.599969	-0.561461
C	-0.142150	1.023286	-0.924970
H	-0.317856	0.067401	-1.409640
C	-1.193012	1.920830	-0.788768
O	-2.464168	1.633890	-1.273711
C	-0.963308	3.175508	-0.178894
O	-2.039928	3.999595	-0.072458
C	-1.849802	5.273246	0.539339
H	-2.827859	5.762452	0.515657
H	-1.125072	5.883399	-0.017441
H	-1.518022	5.174479	1.582356
C	-4.619876	-1.361884	0.681521
H	-5.191301	-2.134262	1.194128
C	-3.680333	-1.728035	-0.297469
C	-3.406999	-3.186161	-0.615142
H	-2.789206	-3.250025	-1.520329
H	-4.354788	-3.693783	-0.846658
C	-2.727299	-3.955147	0.543589
H	-3.390337	-3.911972	1.419817
C	-1.331372	-3.454049	0.956114
H	-1.080426	-3.902861	1.929365
H	-1.367496	-2.367514	1.127737
C	-0.194888	-3.778741	-0.027281
H	-0.134564	-4.871571	-0.155678
C	1.165262	-3.244287	0.450079
H	1.327965	-3.562285	1.492568
H	1.128898	-2.144388	0.472717
H	-0.419634	-3.366445	-1.022778
H	-2.664288	-5.017139	0.261473
C	-2.974311	-0.711089	-0.955303
H	-2.269121	-0.964767	-1.742646
C	-3.168155	0.630419	-0.610744
C	-4.098570	0.988874	0.365713
H	-4.235118	2.038254	0.613342
C	-4.830446	-0.018580	1.003019
H	-5.565297	0.248621	1.760379
C	3.972651	-1.686723	-0.390090
C	2.363263	-3.714304	-0.391480
H	2.199622	-3.460843	-1.451353
H	2.409129	-4.813128	-0.346389
C	5.608526	0.333963	-0.240726
H	6.411427	0.728893	0.401531
H	6.071688	0.145724	-1.221858
C	3.713258	-3.130975	0.074259
H	4.534341	-3.768797	-0.286327
C	4.534461	1.423894	-0.425630
H	3.814070	1.096830	-1.186299
H	3.757748	-3.176210	1.174428
H	5.022335	2.316168	-0.848029

C	3.805722	1.837842	0.864834
H	4.560946	2.187282	1.584705
H	3.326201	0.966369	1.332329
H	3.061288	-1.091675	-0.246074
C	5.139221	-1.011773	0.348542
H	6.003295	-1.694875	0.355408
H	4.857617	-0.879022	1.404111
C	2.761358	2.961664	0.697570
H	2.606614	3.444335	1.673379
H	4.167314	-1.689605	-1.474586
H	3.185139	3.749171	0.053100

Sum of electronic and zero-point Energies= -1162.310875

Sum of electronic and thermal Energies= -1162.284254

Sum of electronic and thermal Enthalpies= -1162.283310

Sum of electronic and thermal Free Energies= -1162.367361

daec[n=7]-4-E1 (dmf)

C	0.897054	2.154831	1.086843
H	1.338052	1.842045	2.029313
C	1.721782	2.756294	1.16835
C	1.145007	3.170498	-1.188081
H	1.760966	3.639545	-1.852818
C	-0.229893	3.018902	-1.306578
H	-0.691977	3.371157	-2.226251
C	-1.045702	2.458854	-0.329725
O	-2.416036	2.529887	-0.502775
C	-0.479935	2.005389	0.885645
O	-1.346267	1.484430	1.792765
C	-0.819713	0.996505	3.025769
H	-1.677206	0.601538	3.577743
H	-0.351525	1.801815	3.608312
H	-0.090223	0.192140	2.860131
C	-5.045732	-0.692656	-0.588955
H	-5.759961	-1.513785	-0.625136
C	-3.690718	-0.943363	-0.861521
C	-3.243555	-2.358117	-1.176014
H	-2.331118	-2.335708	-1.786532
H	-4.017961	-2.839005	-1.789155
C	-3.008080	-3.229656	0.084322
H	-3.847730	-3.075218	0.776789
C	-1.675137	-2.958913	0.804832
H	-1.729712	-3.351932	1.831128
H	-1.525048	-1.872737	0.905128
C	-0.467730	-3.590419	0.094291
H	-0.544268	-4.686935	0.171241
C	0.890522	-3.127915	0.636068
H	0.929695	-3.276656	1.727090
H	0.979668	-2.043234	0.474297
H	-0.507119	-3.361235	-0.981636
H	-3.044450	-4.289278	-0.210325
C	-2.780930	0.126229	-0.823846
H	-1.730423	-0.041515	-1.051213
C	-3.225847	1.414507	-0.506139
C	-4.577189	1.658687	-0.239202
H	-4.896832	2.671211	-0.004700
C	-5.482621	0.598339	-0.283666
H	-6.536010	0.783886	-0.080926
C	3.684031	-1.920681	-0.536495
C	2.077385	-3.858185	-0.014762
H	1.921640	-3.906748	-1.104663
H	2.084247	-4.901402	0.335760
C	5.316049	0.002179	-1.085809
H	6.301500	0.402486	-0.800327
H	5.411677	-0.321288	-2.134117
C	3.447920	-3.213227	0.259591
H	4.243969	-3.932063	0.011750
C	4.282218	1.142298	-1.020372
H	3.313778	0.794523	-1.407192
H	3.547962	-3.008195	1.337806
H	4.608883	1.941058	-1.704492

C	4.093968	1.741577	0.379673
H	5.078552	2.024327	0.783086
H	3.686958	0.986058	1.066830
H	2.857678	-1.220387	-0.351794
C	5.015942	-1.231198	-0.213778
H	5.836636	-1.954055	-0.343256
H	5.029759	-0.949790	0.850096
C	3.191234	2.994040	0.414890
H	3.274552	3.446298	1.413889
H	3.648234	-2.155200	-1.612957
H	3.583594	3.734944	-0.295726

Sum of electronic and zero-point Energies= -1162.320904

Sum of electronic and thermal Energies= -1162.293367

Sum of electronic and thermal Enthalpies= -1162.292423

Sum of electronic and thermal Free Energies= -1162.380357

daec[n=7]-4-E2 (dmf)

C	1.660974	2.859207	0.041335
H	2.472191	3.410325	-0.425358
C	1.939912	2.065003	1.168748
C	0.884740	1.367390	1.765147
H	1.066218	0.755568	2.647365
C	-0.417837	1.460086	1.256828
H	-1.231860	0.930180	1.744132
C	-0.683906	2.246863	0.138239
O	-1.941047	2.442083	-0.392816
C	0.368337	2.958595	-0.484180
O	0.023982	3.708533	-1.565925
C	1.053263	4.443809	-2.221546
H	0.564662	4.962505	-3.051558
H	1.834352	3.779910	-2.618126
H	1.511338	5.184054	-1.550654
C	-5.129123	-0.118880	0.386916
H	-5.984300	-0.768575	0.567129
C	-4.042128	-0.601460	-0.363685
C	-4.051509	-2.020280	-0.898273
H	-3.355898	-2.099326	-1.743705
H	-5.052180	-2.243187	-1.294244
C	-3.708219	-3.090320	0.166778
H	-4.391196	-2.961495	1.019094
C	-2.255526	-3.069074	0.672258
H	-2.190619	-3.685005	1.582069
H	-1.989488	-2.046713	0.981307
C	-1.221737	-3.583207	-0.341554
H	-1.432534	-4.641975	-0.562642
C	0.226040	-3.437849	0.147078
H	0.328470	-3.911744	1.136693
H	0.441580	-2.369461	0.298746
H	-1.328348	-3.046955	-1.296585
H	-3.929232	-4.081764	-0.256855
C	-2.958016	0.256373	-0.596311
H	-2.109450	-0.078107	-1.189860
C	-2.964927	1.559118	-0.084932
C	-4.045029	2.034053	0.659095
H	-4.031654	3.053820	1.035882
C	-5.131517	1.183439	0.889276
H	-5.984479	1.544406	1.460947
C	3.215622	-2.372649	-0.664071
C	1.261375	-4.053977	-0.806829
H	1.101342	-3.665230	-1.825560
H	1.081701	-5.138462	-0.864918
C	5.217286	-0.737946	-0.504542
H	6.212939	-0.643947	-0.043278
H	5.385680	-0.733704	-1.592844
C	2.723755	-3.803646	-0.394366
H	3.378453	-4.507093	-0.931293
C	4.379336	0.502283	-0.141905
H	3.427839	0.478241	-0.691265
H	2.841449	-4.037611	0.676203
H	4.912153	1.395521	-0.504249

C	4.100717	0.668834	1.357889
H	5.055298	0.660402	1.906658
H	3.522977	-0.188069	1.732821
H	2.505600	-1.651068	-0.236397
C	4.618562	-2.099267	-0.103304
H	5.304040	-2.889967	-0.446698
H	4.588489	-2.185770	0.993450
C	3.350954	1.971493	1.719957
H	3.312110	2.050583	2.815958
H	3.213070	-2.194026	-1.751732
H	3.937409	2.830863	1.365030

Sum of electronic and zero-point Energies= -1162.321020

Sum of electronic and thermal Energies= -1162.293524

Sum of electronic and thermal Enthalpies= -1162.292580

Sum of electronic and thermal Free Energies= -1162.379858

daec[n=8]-1-TS (dmf)

C	-4.019484	1.220907	0.057233
H	-4.946449	1.721341	0.324400
C	-2.887662	2.005756	-0.243633
C	-1.711702	1.340488	-0.589792
H	-0.815881	1.889754	-0.858063
C	-1.648925	-0.058970	-0.610922
H	-0.708002	-0.532488	-0.861469
C	-2.765808	-0.828961	-0.310247
O	-2.810589	-2.212775	-0.335381
C	-3.980540	-0.176716	0.021471
O	-5.038220	-0.987833	0.293363
C	-6.279996	-0.375527	0.628732
H	-6.652536	0.257078	-0.189236
H	-6.200671	0.225418	1.545670
H	-6.980898	-1.198571	0.796526
C	0.484379	-4.573251	0.666644
H	1.335902	-5.188625	0.952704
C	0.572305	-3.747348	-0.465106
C	1.871614	-3.585059	-1.227871
H	1.670641	-3.068001	-2.176225
H	2.301394	-4.564279	-1.483304
C	2.907717	-2.775035	-0.410975
H	2.394778	-1.935182	0.077840
C	4.071564	-2.237403	-1.257061
H	3.694223	-1.438537	-1.913225
H	4.432558	-3.032338	-1.928013
C	5.271920	-1.729954	-0.433937
H	6.026041	-1.324226	-1.126385
C	4.976450	-0.683371	0.656802
H	5.906709	-0.517571	1.222488
H	4.260349	-1.099514	1.381515
H	5.744693	-2.597437	0.052629
H	3.294205	-3.409897	0.400544
C	-0.545779	-2.981134	-0.827002
H	-0.511990	-2.386918	-1.735656
C	-1.690658	-2.969097	-0.022825
C	-1.770602	-3.788755	1.106335
H	-2.675382	-3.778578	1.709054
C	-0.683346	-4.603405	1.434355
H	-0.742874	-5.251631	2.306754
C	2.461507	3.233059	0.355182
C	4.459843	0.680513	0.169733
H	5.166378	1.098122	-0.566096
H	3.503851	0.554094	-0.358704
C	0.689877	4.866967	-0.586956
H	0.552042	5.929056	-0.842389
H	0.766847	4.334290	-1.548505
C	4.291363	1.672327	1.334160
H	5.245931	1.727356	1.880734
H	3.558828	1.264423	2.049404
C	-0.557573	4.365685	1.608005
H	-0.752854	5.012684	1.030265
H	-0.362453	3.368054	0.571564

C	-1.810059	4.326116	-0.737067
H	-1.540801	3.918913	-1.723202
H	-2.144385	5.357180	-0.922456
C	2.020303	4.695608	0.168605
H	2.806318	5.231443	-0.386155
H	1.956509	5.186039	1.153221
C	-3.000255	3.525118	-0.177361
H	1.749370	2.707791	1.009355
C	3.872121	3.102705	0.950618
H	3.930445	3.730112	1.854015
H	4.605734	3.522701	0.243731
H	-3.177326	3.822717	0.869087
H	-3.911161	3.822244	-0.717711
H	2.418950	2.720252	-0.618092

Sum of electronic and zero-point Energies= -1201.594547

Sum of electronic and thermal Energies= -1201.566443

Sum of electronic and thermal Enthalpies= -1201.565499

Sum of electronic and thermal Free Energies= -1201.653467

daec[n=8]-1-E1 (dmf)

C	-2.251174	2.758584	-0.479172
H	-2.389958	3.261480	-1.432226
C	-1.419855	3.352543	0.488772
C	-1.259166	2.712736	1.722668
H	-0.629564	3.160159	2.489094
C	-1.907069	1.498787	1.981872
H	-1.793886	0.996742	2.940341
C	-2.724928	0.917444	1.020565
O	-3.444374	-0.221094	1.343885
C	-2.912878	1.550948	-0.228918
O	-3.747985	0.924285	-1.096850
C	-3.952909	1.517027	-2.378442
H	-3.012350	1.591630	-2.941246
H	-4.407582	2.513367	-2.291592
H	-4.640149	0.850079	-2.906548
C	-2.576968	-3.991696	-0.202258
H	-2.376262	-4.986981	-0.595545
C	-1.677615	-2.947878	-0.464251
C	-0.409873	-3.198078	-1.256056
H	-0.164487	-2.305421	-1.849059
H	-0.582594	-4.015358	-1.970486
C	0.804310	-3.554911	-0.372258
H	0.974272	-2.737121	0.342405
C	2.072654	-3.812598	-1.198234
H	2.293433	-2.921979	-1.805305
H	1.867839	-4.621023	-1.917081
C	3.314428	-4.202363	-0.374439
H	4.136741	-4.422103	-1.073195
C	3.800867	-3.159746	0.649810
H	4.678894	-3.572228	1.171054
H	3.033908	-3.014537	1.425696
H	3.107644	-5.144865	0.156235
H	0.565999	-4.446019	0.228785
C	-1.952921	-1.667276	0.043281
H	-1.262724	-0.849975	-0.151896
C	-3.111087	-1.439474	0.792414
C	-4.006052	-2.484928	1.053449
H	-4.901515	-2.284452	1.636954
C	-3.730389	-3.757285	0.553818
H	-4.426244	-4.571077	0.750632
C	3.799316	1.368317	0.042965
C	4.168947	-1.794808	0.049852
H	4.917121	-1.933249	-0.747956
H	3.283755	-1.361659	-0.434937
C	2.913914	3.570207	-0.979314
H	3.252387	4.567438	-1.301225
H	2.609172	3.041788	-1.897073
C	4.715631	-0.806784	1.091702
H	5.628505	-1.229434	1.539565
H	3.989057	-0.713321	1.915149

C	1.691978	3.729417	-0.062194
H	1.995329	4.248264	0.861778
H	1.331094	2.739612	0.248283
C	0.540027	4.500788	-0.719328
H	0.251206	4.001579	-1.657031
H	0.888035	5.506303	-1.000396
C	4.100732	2.824658	-0.342402
H	4.944399	2.839418	-1.050090
H	4.442317	3.374429	0.549373
C	-0.711526	4.656728	0.175397
H	3.025563	1.343749	0.824858
C	5.030189	0.597908	0.545899
H	5.513654	1.183138	1.343781
H	5.771325	0.520750	-0.265903
H	-0.420652	5.146017	1.115455
H	-1.414113	5.335253	-0.328984
H	3.367803	0.854496	-0.829139
Sum of electronic and zero-point Energies= -1201.609837			
Sum of electronic and thermal Energies= -1201.580832			
Sum of electronic and thermal Enthalpies= -1201.579887			
Sum of electronic and thermal Free Energies= -1201.670876			

daec[n=8]-1-E2 (dmf)

C	-0.219416	3.010562	0.907215
H	0.503866	3.020060	1.717359
C	0.038802	3.776032	-0.243954
C	-0.905889	3.778393	-1.277956
H	-0.729688	4.371741	-2.173334
C	-2.084831	3.034205	-1.163358
H	-2.833602	3.045213	-1.952621
C	-2.332807	2.279666	-0.021698
O	-3.556076	1.647346	0.131897
C	-1.393775	2.256284	1.032077
O	-1.722185	1.497533	2.109021
C	-0.793685	1.427991	3.189914
H	-0.629961	2.415316	3.643136
H	0.169135	1.009819	2.865551
H	-1.248463	0.761621	3.928368
C	-4.105487	-2.438984	-0.463706
H	-4.284657	-3.500420	-0.627541
C	-2.888686	-1.869857	-0.868862
C	-1.812660	-2.725971	-1.506207
H	-1.169803	-2.097789	-2.138697
H	-2.283199	-3.465984	-2.169611
C	-0.931236	-3.470239	-0.480783
H	-0.459289	-2.732086	0.183266
C	0.137526	-4.342622	-1.154707
H	0.776654	-3.706356	-1.784919
H	-0.361157	-5.041372	-1.844169
C	1.010391	-5.162580	-0.186224
H	1.694016	-5.786937	-0.782526
C	1.838143	-4.352556	0.828986
H	2.399857	-5.060041	1.458849
H	1.164422	-3.813721	1.512499
H	0.365263	-5.862797	0.367140
H	-1.570770	-4.097402	0.159227
C	-2.675588	-0.497441	-0.660499
H	-1.741950	-0.041381	-0.981215
C	-3.665946	0.287044	-0.060037
C	-4.878768	-0.284965	0.343183
H	-5.636239	0.345072	0.803339
C	-5.089482	-1.648493	0.138174
H	-6.033031	-2.095671	0.446390
C	3.899813	-0.359898	0.015670
C	2.818813	-3.350507	0.202541
H	3.477089	-3.875323	-0.509223
H	2.256529	-2.614841	-0.388227
C	4.160972	1.932822	-1.150290
H	4.927617	2.668302	-1.440153
H	3.744990	1.539942	-2.091973

C	3.678793	-2.620326	1.245329
H	4.275413	-3.362637	1.798116
H	3.017399	-2.147945	1.989779
C	3.048865	2.650236	-0.370207
H	3.447190	2.993181	0.598766
H	2.245261	1.939202	-0.135964
C	2.459219	3.850273	-1.122412
H	2.088342	3.524908	-2.106528
H	3.258519	4.580503	-1.320074
C	4.842277	0.786122	-0.381795
H	5.656173	0.381381	-1.003554
H	5.323454	1.190065	0.523487
C	1.320197	4.578078	-0.369806
H	3.135959	0.014643	0.713616
C	4.621690	-1.548514	0.669637
H	5.259898	-1.171028	1.483935
H	5.304199	-2.010793	-0.061568
H	1.677901	4.860237	0.630614
H	1.099524	5.514001	-0.901338
H	3.355749	-0.698240	-0.878908
Sum of electronic and zero-point Energies= -1201.609431			
Sum of electronic and thermal Energies= -1201.580437			
Sum of electronic and thermal Enthalpies= -1201.579493			
Sum of electronic and thermal Free Energies= -1201.670537			

daec[n=8]-2-TS (dmf)

C	1.930543	-3.324803	0.356439
H	2.324012	-4.280249	0.693343
C	0.563175	-3.047292	0.552874
C	0.076145	-1.816131	0.113553
H	-0.969356	-1.557039	0.231736
C	0.921600	-0.883416	-0.495064
H	0.504696	0.056092	-0.836743
C	2.276435	-1.144133	-0.656726
O	3.154283	-0.248508	-1.257055
C	2.794448	-2.391950	-0.232735
O	4.125905	-2.586672	-0.428810
C	4.688647	-3.828432	-0.014024
H	4.580056	-3.979946	1.069132
H	5.751686	-3.770907	-0.265631
H	4.235047	-4.675522	-0.547308
C	3.508072	3.574114	0.402073
H	3.608333	4.558666	0.856422
C	2.333020	3.241940	-0.290557
C	1.124846	4.156505	-0.319507
H	0.440364	3.809442	-1.104347
H	1.415061	5.182736	-0.584390
C	0.383477	4.174063	1.046744
H	0.534769	3.209428	1.552353
C	-1.132161	4.434745	0.949912
H	-1.328811	5.252394	0.238386
H	-1.493635	4.788345	1.927522
C	-1.940527	3.186024	0.555824
H	-1.596495	2.813493	-0.420156
C	-3.458450	3.423074	0.519523
H	-3.760717	3.906284	1.461927
H	-3.697057	4.142333	-0.280497
H	-1.721341	2.386657	1.282265
H	0.853157	4.929299	1.691975
C	2.242659	1.974687	-0.883611
H	1.366534	1.728805	-1.475308
C	3.256465	1.027855	-0.711693
C	4.422283	1.360714	-0.017643
H	5.206599	0.016860	0.097463
C	4.547043	2.645348	0.521282
H	5.455657	2.915205	1.056697
C	-5.142239	-0.907687	-0.442982
C	-4.312161	2.154247	0.329156
H	-4.111263	1.457916	1.158076
H	-5.373260	2.435770	0.419746

C	-3.950190	-3.153365	0.008731
H	-4.637736	-3.668592	-0.678974
H	-4.428882	-3.193455	1.000475
C	-4.106889	1.441644	-1.017550
H	-3.094311	1.016233	-1.067547
H	-4.155273	2.194893	-1.820086
C	-2.606092	-3.911550	0.051972
H	-1.994955	-3.596818	-0.806723
H	-2.783779	-4.988133	-0.087208
C	-1.815690	-3.720902	1.362681
H	-2.266308	-4.359528	2.135735
H	-1.929138	-2.691752	1.731318
C	-3.818261	-1.691260	-0.454103
H	-3.079462	-1.167739	0.168961
H	-3.407465	-1.692993	-1.476537
C	-0.318198	-4.066682	1.266022
H	-5.949724	-1.567593	-0.797326
C	-5.145853	0.349058	-1.335994
H	-6.150145	0.800331	-1.303193
H	-4.994200	0.024901	-2.377629
H	0.078691	-4.202214	2.284023
H	-0.200893	-5.047350	0.778835
H	-5.404854	-0.643295	0.592560
Sum of electronic and zero-point Energies= -1201.589379			
Sum of electronic and thermal Energies= -1201.561367			
Sum of electronic and thermal Enthalpies= -1201.560423			
Sum of electronic and thermal Free Energies= -1201.648117			

daec[n=8]-2-E1 (dmf)

C	0.819253	-3.218142	-0.034110
H	0.314379	-3.888406	-0.723061
C	0.311605	-3.071341	1.268376
C	0.982343	-2.224650	2.161117
H	0.613843	-2.108874	3.178708
C	2.131739	-1.537875	1.761614
H	2.663740	-0.890720	2.455850
C	2.618305	-1.675651	0.464995
O	3.796038	-1.055054	0.077500
C	1.962010	-2.520718	-0.454092
O	2.506330	-2.597330	-1.695827
C	1.872222	-3.441840	-2.654453
H	1.873501	-4.491582	-2.330007
H	2.463143	-3.345746	-3.569817
H	0.839866	-3.121873	-2.852838
C	4.014215	3.062832	-0.546967
H	4.099426	4.135552	-0.712352
C	2.748794	2.480282	-0.397548
C	1.479191	3.306541	-0.424507
H	0.715713	2.759819	-0.993584
H	1.658043	4.249534	-0.959221
C	0.935453	3.622658	0.988176
H	0.942464	2.702441	1.591600
C	-0.487055	4.211747	0.993430
H	-0.535913	5.064908	0.297971
H	-0.697733	4.620450	1.993557
C	-1.573348	3.186825	0.633271
H	-1.352190	2.754611	-0.351572
C	-2.998782	3.758528	0.627699
H	-3.212565	4.198193	1.614379
H	-3.056260	4.588326	-0.095211
H	-1.524976	2.350981	1.350261
H	1.628917	4.318507	1.482557
C	2.656957	1.093834	-0.189521
H	1.678522	0.633263	-0.081527
C	3.810535	0.308862	-0.120264
C	5.075112	0.893740	-0.274567
H	5.961714	0.266081	-0.224657
C	5.166120	2.268491	-0.489378
H	6.146726	2.725405	-0.611376
C	-5.183261	-0.136184	-0.717218

C	-4.088716	2.721414	0.295588
H	-4.035909	1.900989	1.027746
H	-5.077344	3.187529	0.431332
C	-4.090161	-2.415198	-0.281687
H	-4.662811	-2.916512	-1.076339
H	-4.725417	-2.457786	0.617680
C	-3.997620	2.157729	-1.131110
H	-3.026823	1.664306	-1.275126
H	-4.013949	2.999783	-1.841248
C	-2.786343	-3.195707	-0.015514
H	-2.016803	-2.877225	-0.734947
H	-2.955350	-4.266581	-0.204904
C	-2.265906	-3.045488	1.422296
H	-3.035531	-3.435592	2.104950
H	-2.140713	-1.982587	1.677017
C	-3.877485	-0.949510	-0.695946
H	-3.153522	-0.471671	-0.019556
H	-3.414648	-0.933393	-1.695716
C	-0.942738	-3.798381	1.712878
H	-5.982452	-0.755852	-1.153508
C	-5.118081	1.177521	-1.519765
H	-6.090445	1.688611	-1.438772
H	-4.995938	0.925522	-2.584916
H	-0.873825	-3.968413	2.795624
H	-0.988257	-4.791275	1.242564
H	-5.495719	0.066450	0.318328
Sum of electronic and zero-point Energies= -1201.603742			
Sum of electronic and thermal Energies= -1201.574710			
Sum of electronic and thermal Enthalpies= -1201.573766			
Sum of electronic and thermal Free Energies= -1201.665755			

daec[n=8]-2-E2 (dmf)

C	0.881456	-2.689313	1.215841
H	0.594118	-2.694681	2.263549
C	0.081456	-3.383884	0.289582
C	0.467940	-3.396660	-1.055612
H	-0.121014	-3.945466	-1.787404
C	1.615817	-2.708518	-1.469091
H	1.923385	-2.709573	-2.512585
C	2.396919	-2.019184	-0.548641
O	3.575916	-1.426834	-0.971383
C	2.042689	-2.017171	0.819639
O	2.881974	-1.353763	1.655556
C	2.548306	-1.301062	3.041771
H	1.583318	-0.801513	3.203544
H	3.343074	-0.717866	3.515307
H	2.519726	-2.305389	3.486053
C	4.112029	2.708905	-0.944267
H	4.277928	3.784953	-0.945980
C	2.816615	2.205045	-0.764271
C	1.629058	3.116041	-0.529613
H	0.769715	2.726163	-1.090921
H	1.840442	4.117420	-0.929280
C	1.251972	3.238322	0.965252
H	1.240262	2.234867	1.417017
C	-0.108800	3.913808	1.215496
H	-0.155499	4.866117	0.663356
H	-0.183921	4.175196	2.282140
C	-1.307553	3.032862	0.831655
H	-1.223404	2.745116	-0.224658
C	-2.673398	3.693462	1.070038
H	-2.748194	3.990499	2.127748
H	-2.734368	4.626082	0.486089
H	-1.257688	2.094330	1.407690
H	2.046140	3.796933	1.481740
C	2.620448	0.814570	-0.771034
H	1.617630	0.413678	-0.645599
C	3.701441	-0.053476	-0.936070
C	4.994799	0.451823	-1.120906
H	5.823061	-0.239627	-1.256746

C	5.189302	1.833102	-1.125849
H	6.192689	2.229916	-1.270810
C	-5.304229	0.206273	-0.567356
C	-3.874633	2.795578	0.716977
H	-3.817376	1.871720	1.312918
H	-4.801563	3.302115	1.028916
C	-4.374190	-2.183528	-0.604064
H	-5.067161	-2.509922	-1.393978
H	-4.915297	-2.323812	0.345572
C	-3.976851	2.450311	-0.776950
H	-3.071125	1.918904	-1.099441
H	-3.993967	3.389570	-1.352381
C	-3.123698	-3.086827	-0.610466
H	-2.405061	-2.711675	-1.354932
H	-3.404112	-4.098247	-0.941488
C	-2.448707	-3.209220	0.764263
H	-3.173958	-3.653366	1.462286
H	-2.208203	-2.213150	1.164866
C	-4.077824	-0.689286	-0.814739
H	-3.251357	-0.376381	-0.159718
H	-3.717428	-0.547553	-1.846229
C	-1.171218	-4.086045	0.776497
H	-6.194272	-0.281918	-0.994617
C	-5.210250	1.619971	-1.172841
H	-6.122298	2.178049	-0.908287
H	-5.219880	1.526327	-2.270152
H	-0.998400	-4.430731	1.804971
H	-1.352309	-4.985696	0.171061
H	-5.490139	0.268015	0.515559
Sum of electronic and zero-point Energies= -1201.604514			
Sum of electronic and thermal Energies= -1201.575598			
Sum of electronic and thermal Enthalpies= -1201.574654			
Sum of electronic and thermal Free Energies= -1201.665198			

daec[n=8]-3-TS (dmf)

C	-2.351452	-3.339160	0.576843
H	-2.845948	-4.309865	0.573370
C	-0.948525	-3.255501	0.546101
C	-0.390960	-1.973552	0.573508
H	0.685207	-1.836751	0.584376
C	-1.185261	-0.823578	0.595858
H	-0.689768	0.137293	0.596402
C	-2.577043	-0.917492	0.609634
O	-3.450095	0.156266	0.667610
C	-3.162037	-2.203008	0.620190
O	-4.526527	-2.348438	0.712426
C	-5.213583	-2.275504	-0.540896
H	-6.279783	-2.387815	-0.317538
H	-4.896354	-3.086760	-1.212967
H	-5.046747	-1.310374	-1.037455
C	-2.823349	3.691650	-1.465714
H	-2.668603	4.595316	-2.053066
C	-1.857879	3.305236	-0.525252
C	-0.531333	4.041167	-0.426766
H	-0.612356	4.999942	-0.956027
H	0.194949	3.449079	-1.005006
C	0.050277	4.286908	0.982798
H	-0.393966	5.202509	1.397865
C	1.587782	4.401717	0.978705
H	1.916569	4.888367	1.909123
H	1.903972	5.066509	0.158955
C	2.304181	3.044830	0.854911
H	1.916579	2.495546	-0.015364
C	3.831993	3.168081	0.745437
H	4.189819	3.826812	1.552360
H	4.089518	3.677536	-0.196994
H	2.052807	2.434223	1.737312
H	-0.232834	3.477073	1.668814
C	-2.089131	2.144224	0.231129
H	-1.392889	1.869531	1.014151

C	-3.200816	1.336392	-0.023553
C	-4.160129	1.728926	-0.963677
H	-5.033335	1.103615	-1.131574
C	-3.972363	2.919486	-1.667712
H	-4.717334	3.235781	-2.395516
C	5.206347	-1.391945	-1.372173
C	4.603783	1.838382	0.835496
H	4.349473	1.340460	1.785217
H	5.679306	2.067614	0.895054
C	3.366816	-2.954684	-0.427362
H	4.147290	-3.678425	-0.141939
H	3.218236	-2.309805	0.451596
C	4.383921	0.851016	-0.324084
H	4.602260	1.357236	-1.278683
H	3.325933	0.555216	-0.368597
C	2.049159	-3.694725	-0.714314
H	2.214509	-4.475686	-1.471926
H	1.343795	-2.986751	-1.169940
C	1.417975	-4.325207	0.547308
H	1.654361	-3.706412	1.425598
H	1.886910	-5.300656	0.738220
C	3.856811	-2.098051	-1.604509
H	3.951284	-2.733643	-2.498859
H	3.083384	-1.353127	-1.847059
C	-0.107031	-4.524923	0.482323
H	5.979961	-2.160294	-1.216406
C	5.273973	-0.397477	-0.196574
H	5.035230	-0.915697	0.744478
H	6.319659	-0.067081	-0.095358
H	-0.364772	-5.072375	-0.438512
H	-0.414160	-5.186074	1.306457
H	5.488051	-0.863944	-2.296771
Sum of electronic and zero-point Energies= -1201.585910			
Sum of electronic and thermal Energies= -1201.557648			
Sum of electronic and thermal Enthalpies= -1201.556704			
Sum of electronic and thermal Free Energies= -1201.645218			

daec[n=8]-3-E1 (dmf)

C	1.362037	-3.060301	0.365382
H	1.013575	-3.554398	1.267688
C	0.763386	-3.388787	-0.863371
C	1.228810	-2.765846	-2.028650
H	0.787982	-3.015724	-2.991995
C	2.260723	-1.824162	-1.965135
H	2.633410	-1.338777	-2.864654
C	2.841781	-1.497493	-0.744394
O	3.921398	-0.628835	-0.710892
C	2.399646	-2.121010	0.442093
O	3.034097	-1.751799	1.584291
C	2.606797	-2.341377	2.811238
H	3.234261	-1.895360	3.588079
H	2.753583	-3.430146	2.805621
H	1.552213	-2.114921	3.019910
C	3.556209	3.314648	0.593056
H	3.489195	4.346111	0.935324
C	2.384615	2.568882	0.397847
C	1.015889	3.183133	0.609913
H	1.054525	3.896316	1.445645
H	0.312064	2.925333	0.900176
C	0.481173	3.916487	-0.641041
H	1.131928	4.779167	-0.845093
C	-0.978389	4.388375	-0.506753
H	-1.192660	5.114603	-1.305631
H	-1.100538	4.934096	0.442629
C	-2.004654	3.247734	-0.585404
H	-1.763184	2.485931	0.167912
C	-3.459332	3.705642	-0.399723
H	-3.670137	4.522101	-1.108060
H	-3.580313	4.137320	0.606872
H	-1.906048	2.750163	-1.564004

H	0.568034	3.252769	-1.514869
C	2.489391	1.237281	-0.034967
H	1.587265	0.650801	-0.190287
C	3.743144	0.663275	-0.264097
C	4.911317	1.411534	-0.071956
H	5.877470	0.946682	-0.253807
C	4.807637	2.735455	0.355735
H	5.714056	3.317903	0.512080
C	-5.414519	-0.826514	1.165373
C	-4.502047	2.591611	-0.607853
H	-4.389266	2.183039	-1.625192
H	-5.509706	3.033880	-0.568611
C	-3.600033	-2.295247	0.031890
H	-4.356617	-3.036788	-0.271826
H	-3.526064	-1.578183	-0.799238
C	-4.421927	1.440685	0.407061
H	-4.573089	1.840530	1.423312
H	-3.409676	1.015433	0.395277
C	-2.240228	-2.987835	0.205886
H	-2.291095	-3.692604	1.051397
H	-1.488945	-2.233043	0.482976
C	-1.776762	-3.740505	-1.048376
H	-1.781303	-3.057535	-1.911582
H	-2.502452	-4.534579	-1.280334
C	-4.075741	-1.576545	1.303428
H	-4.176583	-2.317499	2.111676
H	-3.293260	-0.878292	1.636236
C	-0.376759	-4.387314	-0.928060
H	-6.202599	-1.549404	0.902111
C	-5.441680	0.323791	0.140217
H	-5.278960	-0.075690	-0.872278
H	-6.454805	0.755380	0.131683
H	-0.353704	-5.032333	-0.038524
H	-0.225494	-5.043082	-1.796983
H	-5.689931	-0.424899	2.153155
Sum of electronic and zero-point Energies= -1201.609165			
Sum of electronic and thermal Energies= -1201.580158			
Sum of electronic and thermal Enthalpies= -1201.579214			
Sum of electronic and thermal Free Energies= -1201.670379			

daec[n=8]-3-E2 (dmf)

C	1.263460	-2.747811	-1.117079
H	0.912419	-2.868332	-2.140648
C	0.678288	-3.481353	-0.071563
C	1.181117	-3.300118	1.224455
H	0.754154	-3.863750	2.051937
C	2.223385	-2.400933	1.472995
H	2.611168	-2.258201	2.479315
C	2.784191	-1.672771	0.425963
O	3.861491	-0.837157	0.675555
C	2.306841	-1.849201	-0.886518
O	2.816744	-1.119510	-1.931647
C	4.109878	-1.543917	-2.386264
H	4.377637	-0.878283	-3.212905
H	4.073213	-2.580617	-2.750690
H	4.863546	-1.462281	-1.593221
C	3.473111	3.310256	0.860780
H	3.400453	4.394541	0.928100
C	2.304118	2.537383	0.792518
C	0.935607	3.187408	0.769734
H	0.908286	4.019148	1.488610
H	0.188252	2.456312	1.103161
C	0.546036	3.730188	-0.623643
H	1.240008	4.540762	-0.889080
C	-0.903642	4.242939	-0.705423
H	-1.014116	4.856065	-1.612786
H	-1.101593	4.916558	0.143797
C	-1.954084	3.122185	-0.735640
H	-1.809317	2.460460	0.128949
C	-3.403905	3.630506	-0.752920

H	-3.513079	4.371984	-1.559855
H	-3.612671	4.169166	0.185389
H	-1.779780	2.499543	-1.628321
H	0.694577	2.940025	-1.375460
C	2.415359	1.139992	0.717943
H	1.515798	0.531324	0.675834
C	3.673866	0.531249	0.706377
C	4.838858	1.304138	0.771930
H	5.807783	0.810563	0.768673
C	4.728025	2.693082	0.850339
H	5.631492	3.297785	0.906907
C	-5.628445	-0.706191	1.003407
C	-4.457073	2.525824	-0.956549
H	-4.261604	2.020961	-1.916521
H	-5.449464	2.992552	-1.056182
C	-3.723430	-2.245174	0.147417
H	-4.461912	-2.974684	-0.222781
H	-3.524158	-1.561959	-0.691560
C	-4.509289	1.472321	0.160733
H	-4.742600	1.966392	1.118284
H	-3.514354	1.024446	0.284035
C	-2.419511	-2.971568	0.509007
H	-2.604388	-3.670102	1.340813
H	-1.692591	-2.235649	0.884867
C	-1.808649	-3.739820	-0.670347
H	-1.665078	-3.054640	-1.519760
H	-2.520443	-4.506566	-1.011335
C	-4.325226	-1.463119	1.324335
H	-4.526805	-2.162665	2.150472
H	-3.572839	-0.758124	1.708462
C	-0.465591	-4.436343	-0.353673
H	-6.403812	-1.435556	0.720989
C	-5.534030	0.359853	-0.105224
H	-5.295605	-0.123469	-1.064747
H	-6.529874	0.810970	-0.237657
H	-0.599517	-5.106419	0.506896
H	-0.197964	-5.072856	-1.209313
H	-5.986683	-0.226091	1.927540
Sum of electronic and zero-point Energies= -1201.605348			
Sum of electronic and thermal Energies= -1201.576135			
Sum of electronic and thermal Enthalpies= -1201.575191			
Sum of electronic and thermal Free Energies= -1201.667026			

daec[n=8]-4-TS (dmf)

C	1.032222	-3.607559	0.094818
H	1.013293	-4.657347	0.384532
C	-0.164600	-2.883125	-0.038273
C	-0.056635	-1.538678	-0.411430
H	-0.942048	-0.925821	-0.541198
C	1.183181	-0.933600	-0.614719
H	1.210788	0.113770	-0.886564
C	2.366073	-1.650669	-0.444728
O	3.627827	-1.088302	-0.603748
C	2.286336	-3.016347	-0.099083
O	3.412062	-3.767915	0.133260
C	4.198383	-4.066075	-1.026971
H	3.606682	-4.623869	-1.767620
H	5.027041	-4.693173	-0.681970
H	4.599176	-3.155728	-1.488699
C	4.193531	2.654639	1.166168
H	4.304620	3.615324	1.666728
C	3.436432	2.570644	-0.010953
C	2.606854	3.733309	-0.519582
H	3.028762	4.688317	-0.178291
H	2.610231	3.748428	-1.618960
C	1.150663	3.587403	-0.014391
H	0.802982	2.578799	-0.275360
C	0.156567	4.625137	-0.553989
H	0.145172	4.589407	-1.655038
H	0.503744	5.633918	-0.283145

C	-1.276903	4.428589	-0.015243
H	-1.877167	5.317283	-0.262930
C	-2.002981	3.178712	-0.544443
H	-1.363185	2.293011	-0.418316
H	-2.161675	3.286913	-1.629440
H	-1.237700	4.386753	1.085194
H	1.156494	3.629886	1.085740
C	3.321167	1.323236	-0.645287
H	2.783569	1.248354	-1.586664
C	3.839883	0.173413	-0.047522
C	4.594411	0.259059	1.125688
H	5.004339	-0.646286	1.566526
C	4.788455	1.511810	1.713504
H	5.379962	1.591513	2.623688
C	-6.173102	0.138635	-0.208730
C	-3.347900	2.902450	0.148233
H	-3.168318	2.758178	1.225747
H	-3.999433	3.786912	0.064550
C	-5.093849	-1.965840	0.870881
H	-4.702952	-1.260191	1.619427
H	-6.013213	-2.387118	1.304793
C	-4.082255	1.671424	-0.410726
H	-4.377557	1.866927	-1.454300
H	-3.377138	0.827835	-0.447892
C	-4.049526	-3.087411	0.682827
H	-4.371319	-3.771216	-0.118774
H	-3.998449	-3.689993	1.602434
C	-2.661600	-2.516774	0.364849
H	-2.393575	-1.798204	1.154639
H	-2.731043	-1.935760	-0.562773
C	-5.457775	-1.210252	-0.422725
H	-4.556738	-1.038336	-1.025627
H	-6.103628	-1.857654	-1.035506
C	-1.520099	-3.533558	0.218134
H	-6.556207	0.484697	-1.181437
C	-5.321722	1.269351	0.406964
H	-5.003327	0.990084	1.422830
H	-5.969031	2.151830	0.529816
H	-1.752742	-4.231818	-0.601909
H	-1.451459	-4.154669	1.123823
H	-7.059324	-0.018757	0.426239

Sum of electronic and zero-point Energies= -1201.591048

Sum of electronic and thermal Energies= -1201.562626

Sum of electronic and thermal Enthalpies= -1201.561682

Sum of electronic and thermal Free Energies= -1201.650430

daec[n=8]-4-E1 (dmf)

C	0.335628	-3.331804	-0.520981
H	-0.129988	-3.950442	-1.286293
C	-0.368960	-2.984776	0.638365
C	0.285983	-2.188435	1.592229
H	-0.229019	-1.911694	2.510797
C	1.593975	-1.751460	1.387703
H	2.096552	-1.145787	2.138362
C	2.281014	-2.097438	0.219264
O	3.606312	-1.748610	0.026034
C	1.650245	-2.902888	-0.745182
O	2.295956	-3.339241	-1.874764
C	2.633470	-2.328109	-2.832819
H	1.740934	-1.760759	-3.133595
H	3.033836	-2.857273	-3.703774
H	3.394368	-1.638650	-2.449107
C	4.902582	2.158854	0.676379
H	5.262239	3.172447	0.845175
C	3.672503	1.961319	0.030857
C	2.836870	3.134608	-0.447311
H	3.378620	4.068970	-0.246214
H	2.719687	3.073106	-1.540428
C	1.434240	3.200698	0.188599
H	0.912897	2.254893	-0.010106

C	0.592582	4.378440	-0.327840
H	0.610878	4.384400	-1.429556
H	1.066240	5.319844	-0.010689
C	-0.872613	4.358246	0.149477
H	-1.331062	5.337546	-0.056379
C	-1.722131	3.260840	-0.509610
H	-1.234650	2.284404	-0.371888
H	-1.749057	3.434365	-1.597472
H	-0.896477	4.234658	1.244147
H	1.532422	3.273314	1.282508
C	3.227155	0.646014	-0.176471
H	2.283185	0.462644	-0.684622
C	3.992396	-0.437766	0.262818
C	5.222249	-0.238374	0.896648
H	5.803367	-1.097499	1.222658
C	5.671635	1.068419	1.096489
H	6.626105	1.236648	1.591949
C	-6.107610	0.592204	-0.643337
C	-3.158027	3.158573	0.025089
H	-3.125942	3.008589	1.116233
H	-3.689528	4.109636	-0.137866
C	-5.201584	-1.354647	0.809389
H	-4.796996	-0.578130	1.475380
H	-6.182884	-1.628141	1.226713
C	-3.939236	2.003262	-0.619050
H	-4.045635	2.190134	-1.700024
H	-3.332942	1.090390	-0.529024
C	-4.262667	-2.574827	0.872327
H	-4.590405	-3.338765	0.149319
H	-4.349877	-3.037598	1.867422
C	-2.788602	-2.220202	0.623529
H	-2.502456	-1.399440	1.298788
H	-2.655144	-1.837034	-0.397993
C	-5.409619	-0.781619	-0.603350
H	-4.445188	-0.709158	-1.123362
H	-6.008189	-1.497257	-1.187898
C	-1.813889	-3.396788	0.839347
H	-6.317288	0.844004	-1.694672
C	-5.324819	1.757989	-0.004300
H	-5.210875	1.583313	1.076107
H	-5.929781	2.673418	-0.096390
H	-2.065481	-4.215628	0.151482
H	-1.948567	-3.786231	1.859468
H	-7.088651	0.513563	-0.148870

Sum of electronic and zero-point Energies= -1201.602987

Sum of electronic and thermal Energies= -1201.573616

Sum of electronic and thermal Enthalpies= -1201.572672

Sum of electronic and thermal Free Energies= -1201.665142

daec[n=8]-4-E2 (dmf)

C	0.409805	-2.642573	0.745325
H	-0.016117	-2.714924	1.744838
C	-0.344626	-3.016481	-0.378954
C	0.257831	-2.918611	-1.640657
H	-0.300699	-3.208356	-2.529120
C	1.568537	-2.448410	-1.778466
H	2.036144	-2.373281	-2.757785
C	2.300617	-2.073279	-0.653349
O	3.624052	-1.690302	-0.796516
C	1.719588	-2.176291	0.625604
O	2.408671	-1.787770	1.748353
C	3.393610	-2.728386	2.198714
H	2.920620	-3.676948	2.491364
H	3.872833	-2.276650	3.072972
H	4.149539	-2.922307	1.427456
C	4.892153	2.198489	-0.001732
H	5.249405	3.206580	0.201424
C	3.567972	2.006182	-0.421392
C	2.637103	3.188583	-0.621033
H	3.180583	4.113780	-0.384557



H	2.363642	3.256408	-1.685783
C	1.339916	3.127678	0.207868
H	0.790176	2.215195	-0.058856
C	0.442669	4.358826	0.000358
H	0.333591	4.553442	-1.078732
H	0.950521	5.241237	0.418066
C	-0.958180	4.227459	0.628518
H	-1.430064	5.221005	0.669682
C	-1.882598	3.266475	-0.133832
H	-1.383769	2.293258	-0.253720
H	-2.036729	3.654107	-1.153765
H	-0.858909	3.893345	1.673809
H	1.590522	3.034651	1.275518
C	3.123821	0.697409	-0.677457
H	2.105142	0.523140	-1.015181
C	3.989423	-0.386033	-0.510284
C	5.314875	-0.189227	-0.106277
H	5.974031	-1.046846	0.004126
C	5.757560	1.108907	0.146435
H	6.785335	1.271482	0.466266
C	-6.247573	0.578663	-0.319410
C	-3.246073	3.027310	0.530142
H	-3.087742	2.657702	1.555995
H	-3.790573	3.979959	0.628005
C	-5.164260	-1.599412	0.579697
H	-4.700876	-0.966057	1.350596
H	-6.087464	-1.994966	1.030142
C	-4.097736	2.011769	-0.245907
H	-4.329325	2.415182	-1.245110
H	-3.484572	1.115409	-0.417513
C	-4.204415	-2.765195	0.273593
H	-4.576555	-3.338248	-0.590701
H	-4.204877	-3.462140	1.125648
C	-2.758785	-2.313219	0.014837
H	-2.411173	-1.723631	0.876865
H	-2.717068	-1.641086	-0.854120
C	-5.540349	-0.750876	-0.647642
H	-4.643636	-0.542825	-1.246601
H	-6.198202	-1.348110	-1.297671
C	-1.777879	-3.481533	-0.215593
H	-6.580180	1.036945	-1.263877
C	-5.401843	1.609012	0.456965
H	-5.163188	1.218486	1.457628
H	-6.016605	2.506832	0.625595
H	-2.085245	-4.046539	-1.106355
H	-1.843648	-4.172969	0.637317
H	-7.163626	0.368886	0.255004

Sum of electronic and zero-point Energies= -1201.603967

Sum of electronic and thermal Energies= -1201.574621

Sum of electronic and thermal Enthalpies= -1201.573677

Sum of electronic and thermal Free Energies= -1201.665904

daec[n=8]-5-TS (dmf)

C	2.043499	-3.403951	-0.027151
H	2.290882	-4.427243	0.251999
C	0.703918	-3.002390	-0.150262
C	0.479049	-1.670902	-0.516637
H	-0.524464	-1.288104	-0.658522
C	1.530792	-0.781234	-0.709626
H	1.287967	0.236033	-0.979030
C	2.859500	-1.175849	-0.559868
O	3.930920	-0.306539	-0.759416
C	3.120662	-2.525485	-0.229722
O	4.376263	-3.064368	-0.138732
C	5.335572	-2.419391	0.709542
H	4.869118	-2.069084	1.640126
H	5.823400	-1.580666	0.203110
H	6.082675	-3.183515	0.950922
C	3.385813	3.528243	0.822713
H	3.196504	4.491864	1.293363

C	2.639867	3.144760	-0.300580
C	1.409717	3.907058	-0.756393
H	1.275121	3.789219	-1.840874
H	1.509198	4.981459	-0.551593
C	0.171514	3.334592	-0.016815
H	0.230933	2.237042	-0.054274
C	-1.206186	3.749784	-0.553079
H	-1.286630	3.457855	-1.612163
H	-1.318031	4.844841	-0.523857
C	-2.340111	3.088347	0.253836
H	-2.306747	3.466533	1.288291
C	-3.749640	3.311205	-0.317386
H	-3.822186	2.836651	-1.307877
H	-3.896986	4.388936	-0.489179
H	-2.138241	2.008594	0.321010
H	0.248130	3.601503	1.048347
C	2.919565	1.904905	-0.897256
H	2.399386	1.626576	-1.808930
C	3.790121	1.000341	-0.284645
C	4.534096	1.385350	0.834777
H	5.227934	0.684210	1.291001
C	4.349568	2.667408	1.360894
H	4.930551	2.978441	2.227200
C	-5.644516	-1.023760	-0.148417
C	-4.892162	2.816867	0.595651
H	-4.787441	3.315138	1.572157
H	-5.849980	3.167775	0.180275
C	-4.369518	-3.273563	0.014226
H	-5.229990	-3.724946	0.531569
H	-4.535954	-3.445702	-1.061095
C	-4.991358	1.294804	0.832670
H	-5.704154	1.122686	1.654736
H	-4.024935	0.911570	1.189599
C	-3.075541	-4.011007	0.439658
H	-3.105282	-5.039685	0.049543
H	-3.039206	-4.096331	1.537008
C	-1.823573	-3.273699	-0.048586
H	-1.798165	-2.313689	0.477295
H	-1.944223	-3.031273	-1.115907
C	-4.351508	-1.752448	0.259631
H	-4.124068	-1.551567	1.317673
H	-3.525962	-1.311919	-0.315779
C	-0.458527	-3.948026	0.150289
H	-6.028038	-1.471135	-1.078778
C	-5.456993	0.488417	-0.391092
H	-6.410359	0.909871	-0.747248
H	-4.739818	0.620493	-1.216190
H	-0.379897	-4.848680	-0.477474
H	-0.365061	-4.302023	1.189109
H	-6.425145	-1.186735	0.611378

Sum of electronic and zero-point Energies= -1201.581975

Sum of electronic and thermal Energies= -1201.553654

Sum of electronic and thermal Enthalpies= -1201.552710

Sum of electronic and thermal Free Energies= -1201.640853

daec[n=8]-5-E1 (dmf)

C	1.736218	-2.985939	-0.462161
H	1.520589	-3.627187	-1.315199
C	0.928055	-3.027816	0.682807
C	1.257962	-2.189026	1.759008
H	0.656851	-2.214697	2.666390
C	2.336342	-1.307645	1.675824
H	2.582744	-0.647936	2.505129
C	3.103878	-1.246168	0.511623
O	4.171296	-0.363761	0.422891
C	2.817316	-2.102416	-0.565068
O	3.521074	-2.045062	-1.741101
C	4.869104	-2.530284	-1.672684
H	4.888405	-3.585030	-1.362286
H	5.478392	-1.933789	-0.983207

H	5.275830	-2.444264	-2.685417
C	3.481283	3.733290	0.060657
H	3.324759	4.807336	-0.023415
C	2.454191	2.852398	-0.304546
C	1.120138	3.359365	-0.820319
H	0.936360	2.936660	-1.820120
H	1.169903	4.449360	-0.947652
C	-0.074599	2.998329	0.086038
H	-0.088050	1.909741	0.243331
C	-1.427800	3.435003	-0.493376
H	-1.514141	3.056022	-1.524281
H	-1.462845	4.533374	-0.567932
C	-2.626140	2.928910	0.323810
H	-2.567057	3.322430	1.351413
C	-3.984666	3.302199	-0.289014
H	-4.013697	2.956333	-1.333125
H	-4.065690	4.399271	-0.336416
H	-2.546998	1.835429	0.412241
H	0.070986	3.450212	1.079005
C	2.675547	1.469713	-0.188045
H	1.893869	0.772780	-0.478192
C	3.893655	0.985609	0.294993
C	4.921675	1.867677	0.649962
H	5.863978	1.469964	1.019067
C	4.706148	3.240076	0.526518
H	5.499417	3.932210	0.803392
C	-5.484252	-1.035292	-0.685789
C	-5.210174	2.758264	0.472479
H	-5.208979	3.177685	1.490789
H	-6.120821	3.143310	-0.012826
C	-4.062904	-3.161415	-0.368384
H	-4.989545	-3.680998	-0.078557
H	-3.956978	-3.311214	-1.454677
C	-5.311220	1.223386	0.576679
H	-6.184401	0.972910	1.199639
H	-4.437431	0.838481	1.119782
C	-2.877015	-3.828727	0.354939
H	-2.818333	-4.883573	0.045005
H	-3.071779	-3.838678	1.439160
C	-1.526603	-3.143444	0.103505
H	-1.554360	-2.123990	0.511090
H	-1.355686	-3.035619	-0.978908
C	-4.210467	-1.657499	-0.088261
H	-4.185461	-1.486980	0.998622
H	-3.338045	-1.128021	-0.498829
C	-0.322693	-3.880844	0.731049
H	-5.633124	-1.433430	-1.701753
C	-5.442367	0.501671	-0.773874
H	-6.351885	0.859208	-1.282107
H	-4.601262	0.781782	-1.425615
H	-0.160767	-4.833126	0.206968
H	-0.555733	-4.125578	1.776896
H	-6.361651	-1.356053	-0.101948

Sum of electronic and zero-point Energies= -1201.603253

Sum of electronic and thermal Energies= -1201.573958

Sum of electronic and thermal Enthalpies= -1201.573013

Sum of electronic and thermal Free Energies= -1201.665492

daec[n=8]-5-E2 (dmf)

C	1.227383	-2.540974	0.961442
H	0.729221	-2.578089	1.928804
C	0.714660	-3.259148	-0.130068
C	1.406209	-3.196140	-1.348347
H	1.040679	-3.755880	-2.207665
C	2.545822	-2.396645	-1.485326
H	3.069262	-2.325931	-2.436327
C	3.018298	-1.657602	-0.401789
O	4.150252	-0.871052	-0.549973
C	2.370725	-1.748760	0.844859
O	2.800036	-1.023041	1.927797

C	4.015857	-1.495106	2.525631
H	4.850173	-1.479978	1.813622
H	3.886483	-2.515372	2.914529
H	4.232980	-0.815394	3.355541
C	3.853265	3.286676	-0.382637
H	3.800470	4.372996	-0.334138
C	2.706540	2.550532	-0.711637
C	1.382463	3.231799	-1.004182
H	1.043795	2.944145	-2.011493
H	1.529778	4.320217	-1.024239
C	0.267825	2.878520	0.001801
H	0.163311	1.784576	0.049545
C	-1.092317	3.492923	-0.358618
H	-1.334195	3.237983	-1.402841
H	-1.026154	4.591719	-0.320157
C	-2.232647	3.006592	0.548662
H	-2.018049	3.282326	1.593743
C	-3.610081	3.556522	0.147897
H	-3.794104	3.324522	-0.911829
H	-3.588605	4.655496	0.212697
H	-2.250146	1.907113	0.522405
H	0.570039	3.202017	1.009464
C	2.796179	1.149941	-0.769761
H	1.920201	0.563763	-1.035001
C	4.001900	0.504611	-0.486993
C	5.148936	1.241970	-0.170753
H	6.081561	0.721686	0.034171
C	5.064134	2.633688	-0.122745
H	5.950665	3.214395	0.126132
C	-5.577324	-0.566810	-0.461080
C	-4.785442	3.043420	1.003966
H	-4.622905	3.351547	2.048709
H	-5.704419	3.554680	0.676616
C	-4.353080	-2.833190	-0.533103
H	-5.286570	-3.294495	-0.174780
H	-4.394916	-2.876493	-1.633153
C	-5.024639	1.520653	0.975215
H	-5.835921	1.281798	1.680933
H	-4.133635	1.005997	1.359804
C	-3.163803	-3.677726	-0.035648
H	-3.251837	-4.694895	-0.447726
H	-3.226844	-3.784503	1.058966
C	-1.790072	-3.094378	-0.394897
H	-1.664699	-2.124917	0.105705
H	-1.739419	-2.889639	-1.475646
C	-4.310390	-1.359963	-0.097203
H	-4.135242	-1.307897	0.987972
H	-3.445240	-0.870298	-0.568160
C	-0.601030	-3.998142	0.000916
H	-5.888281	-0.839838	-1.481690
C	-5.390743	0.960998	-0.408554
H	-6.314206	1.449717	-0.757416
H	-4.610744	1.233333	-1.135296
H	-0.598897	-4.900024	-0.626975
H	-0.732402	-4.330562	1.040309
H	-6.405266	-0.868661	0.199976

Sum of electronic and zero-point Energies= -1201.603769

Sum of electronic and thermal Energies= -1201.574570

Sum of electronic and thermal Enthalpies= -1201.573625

Sum of electronic and thermal Free Energies= -1201.664839

daec[n=8]-6-TS (dmf)

C	0.403926	3.398632	0.366918
H	0.759909	4.276342	0.904287
C	1.311628	2.435655	-0.101476
C	0.782903	1.337661	-0.793499
H	1.433659	0.567566	-1.195576
C	-0.590257	1.192563	-0.985285
H	-0.958197	0.330698	-1.529564
C	-1.485688	2.130287	-0.471535

O	-2.862676	2.004383	-0.617951
C	-0.979746	3.258758	0.202068
O	-1.809231	4.196455	0.765761
C	-2.516832	5.025568	-0.165063
H	-1.815367	5.584346	-0.801715
H	-3.098820	5.731943	0.435952
H	-3.195272	4.437449	-0.794487
C	-4.622229	-1.494348	0.842999
H	-5.076325	-2.398012	1.245483
C	-3.923232	-1.546077	-0.374722
C	-3.733213	-2.842108	-1.143165
H	-3.092478	-2.641729	-2.011612
H	-4.700711	-3.175240	-1.549341
C	-3.145550	-4.011270	-0.318916
H	-3.005878	-4.862003	-1.002942
C	-1.831757	-3.742976	0.437203
H	-1.610510	-4.639749	1.036732
H	-1.989166	-2.931718	1.163625
C	-0.590545	-3.415147	-0.411770
H	-0.470305	-4.173397	-1.202123
C	0.679801	-3.371183	0.455006
H	0.800714	-4.352988	0.940606
H	0.527431	-2.650208	1.274206
H	-0.725282	-2.451039	-0.925081
H	-3.896788	-4.337040	0.415114
C	-3.369758	-0.358614	-0.873747
H	-2.872517	-0.366714	-1.839400
C	-3.445685	0.829543	-0.141199
C	-4.135041	0.875447	1.070990
H	-4.186220	1.809779	1.624250
C	-4.735961	-0.293533	1.549286
H	-5.282517	-0.268932	2.490272
C	4.919081	-1.406114	-0.289374
C	1.989368	-3.021162	-0.272868
H	2.119992	-3.684479	-1.142980
H	1.927705	-1.996937	-0.671636
C	5.471195	0.918627	0.782038
H	5.227309	1.502177	1.682199
H	6.556396	0.738837	0.831469
C	3.203423	-3.164184	0.662193
H	3.215520	-4.198283	1.040598
H	3.050661	-2.529313	1.547831
C	5.195224	1.777005	-0.471361
H	5.723699	1.339293	-1.331228
H	5.647927	2.768399	-0.314861
C	3.719275	1.931804	-0.872679
H	3.658804	2.530968	-1.793480
H	3.346235	0.937568	-1.139682
C	4.738107	-0.434742	0.891268
H	5.097047	-0.925010	1.810102
H	3.665582	-0.256364	1.052806
C	2.800808	2.556266	0.192463
H	4.312101	-1.074753	-1.143945
C	4.590052	-2.874268	0.054759
H	5.346460	-3.228005	0.772929
H	4.722596	-3.489703	-0.849022
H	2.992029	2.073436	1.162986
H	3.059174	3.615315	0.334774
H	5.964875	-1.371745	-0.633224

Sum of electronic and zero-point Energies= -1201.586852  
Sum of electronic and thermal Energies= -1201.558708  
Sum of electronic and thermal Enthalpies= -1201.557764  
Sum of electronic and thermal Free Energies= -1201.645550

daec[n=8]-6-E1 (dmf)

C	0.107875	3.346807	-0.149925
H	0.451040	4.170968	-0.773178
C	1.026494	2.557229	0.554552
C	0.526331	1.517177	1.353866
H	1.214544	0.897741	1.926708

C	-0.843719	1.266502	1.432946
H	-1.223580	0.464544	2.062086
C	-1.745256	2.046585	0.703587
O	-3.112542	1.864511	0.811076
C	-1.269374	3.107560	-0.087085
O	-2.120743	3.953296	-0.753799
C	-2.771195	3.391457	-1.900199
H	-2.033218	3.041051	-2.636402
H	-3.364910	4.199053	-2.340573
H	-3.436266	2.562637	-1.628632
C	-4.914994	-1.826049	0.098136
H	-5.417612	-2.773518	-0.089106
C	-3.697555	-1.544877	-0.544965
C	-3.072831	-2.550083	-1.494487
H	-2.270321	-2.063405	-2.063474
H	-3.829806	-2.862037	-2.228731
C	-2.530411	-3.824148	-0.805689
H	-2.250744	-4.542817	-1.590988
C	-1.331166	-3.621814	0.136339
H	-1.160010	-4.566613	0.675002
H	-1.585267	-2.877297	0.906432
C	-0.022029	-3.213236	-0.558107
H	0.184840	-3.917410	-1.380164
C	1.179739	-3.189015	0.398366
H	1.290632	-4.183825	0.859046
H	0.971188	-2.493000	1.226804
H	-0.134269	-2.223121	-1.025050
H	-3.350907	-4.291937	-0.242209
C	-3.074323	-0.313325	-0.299466
H	-2.140388	-0.073640	-0.801223
C	-3.652898	0.612275	0.578643
C	-4.863563	0.329291	1.216128
H	-5.298505	1.063977	1.889373
C	-5.489752	-0.894496	0.965985
H	-6.435407	-1.119778	1.455854
C	5.234976	-1.060018	-0.440785
C	2.505371	-2.793660	-0.269868
H	2.697692	-3.463256	-1.123883
H	2.407308	-1.782019	-0.691768
C	5.442051	1.444191	0.203061
H	5.346083	2.111446	1.072389
H	6.502539	1.486927	-0.090516
C	3.700753	-2.851006	0.694156
H	3.764291	-3.868542	1.110373
H	3.506322	-2.190440	1.552512
C	4.602026	1.999276	-0.964809
H	4.858559	1.455166	-1.885520
H	4.900270	3.044433	-1.141232
C	3.076270	1.932324	-0.785660
H	2.595252	2.280009	-1.711903
H	2.763843	0.885916	-0.659844
C	5.104790	0.010448	0.653922
H	5.774003	-0.252794	1.488392
H	4.088087	-0.009654	1.070802
C	2.518552	2.759034	0.394245
H	4.510755	-0.863484	-1.243912
C	5.065108	-2.504851	0.067600
H	5.850082	-2.707113	0.813281
H	5.255644	-3.196915	-0.767755
H	3.024832	2.466398	1.323374
H	2.742283	3.822474	0.228584
H	6.229768	-0.974054	-0.906098

Sum of electronic and zero-point Energies= -1201.601179  
Sum of electronic and thermal Energies= -1201.572131  
Sum of electronic and thermal Enthalpies= -1201.571187  
Sum of electronic and thermal Free Energies= -1201.662721

daec[n=8]-6-E2 (dmf)

C	0.591726	1.912539	0.794264
H	1.239727	1.419975	1.517319

C	1.140372	2.664176	-0.256364
C	0.261903	3.295090	-1.149009
H	0.659759	3.894807	-1.965922
C	-1.121972	3.151917	-1.013807
H	-1.805774	3.631382	-1.710916
C	-1.650353	2.382552	0.022140
O	-3.025550	2.294841	0.164952
C	-0.788456	1.765979	0.947971
O	-1.273835	0.977639	1.962105
C	-1.888349	1.695654	3.042098
H	-1.161690	2.362343	3.528084
H	-2.225016	0.940755	3.759482
H	-2.749276	2.282780	2.699252
C	-5.110150	-1.233352	-0.598815
H	-5.682307	-2.138126	-0.797746
C	-3.773785	-1.148597	-1.022379
C	-3.115630	-2.317480	-1.730375
H	-2.215196	-1.970565	-2.253613
H	-3.799925	-2.696378	-2.502931
C	-2.757925	-3.496693	-0.794012
H	-2.461476	-4.352825	-1.419045
C	-1.648156	-3.221627	0.235737
H	-1.630657	-4.057886	0.951567
H	-1.899756	-2.325678	0.823368
C	-0.241918	-3.063473	-0.363465
H	-0.014479	-3.946053	-0.983001
C	0.853742	-2.898984	0.700284
H	0.822974	-3.760820	1.386237
H	0.632181	-2.012236	1.315692
H	-0.216009	-2.198979	-1.043871
H	-3.670302	-3.806361	-0.263656
C	-3.056627	0.030256	-0.769835
H	-2.026510	0.115196	-1.105311
C	-3.661638	1.094743	-0.092393
C	-4.992625	1.007680	0.327647
H	-5.446920	1.850315	0.843407
C	-5.710397	-0.161287	0.066832
H	-6.748562	-0.232430	0.386615
C	5.137803	-1.330995	-0.196211
C	2.268079	-2.769310	0.115043
H	2.478947	-3.642449	-0.523695
H	2.300805	-1.892141	-0.548568
C	5.473936	1.240341	-0.220982
H	5.412738	2.113822	0.444855
H	6.537733	1.143264	-0.488546
C	3.360151	-2.657454	1.190016
H	3.292675	-3.535662	1.850967
H	3.151703	-1.786836	1.829935
C	4.680737	1.524567	-1.512919
H	4.910427	0.748705	-2.257689
H	5.045087	2.470372	-1.943141
C	3.151967	1.594697	-1.358950
H	2.700232	1.718866	-2.354229
H	2.774216	0.636411	-0.975228
C	5.040280	-0.005363	0.574218
H	5.668586	-0.073829	1.476397
H	4.012982	0.136180	0.937986
C	2.641417	2.730102	-0.444508
H	4.486914	-1.298647	-1.081126
C	4.800090	-2.575833	0.647089
H	5.496959	-2.622724	1.498744
H	4.999479	-3.474778	0.042819
H	3.131751	2.664750	0.535374
H	2.924278	3.699042	-0.879945
H	6.163455	-1.442473	-0.582284

Sum of electronic and zero-point Energies= -1201.602680  
Sum of electronic and thermal Energies= -1201.573756  
Sum of electronic and thermal Enthalpies= -1201.572812  
Sum of electronic and thermal Free Energies= -1201.663322

daec[n=8]-7-TS (dmf)

C	0.407125	3.365551	-0.526514
H	0.834013	4.350966	-0.691241
C	1.268648	2.287267	-0.258228
C	0.697263	1.029262	-0.049417
H	1.325389	0.163268	0.143870
C	-0.686734	0.851999	-0.072526
H	-1.096761	-0.132420	0.120574
C	-1.539096	1.923014	-0.328659
O	-2.920518	1.817254	-0.366531
C	-0.985831	3.201372	-0.574050
O	-1.875803	4.199374	-0.827710
C	-1.362600	5.503819	-1.081505
H	-0.809959	5.896780	-0.216452
H	-0.710258	5.516516	-1.966020
H	-2.236340	6.135122	-1.268279
C	-4.525394	-1.387756	1.749666
H	-4.909400	-2.226320	2.329327
C	-3.956001	-1.631166	0.484882
C	-3.833042	-3.072320	0.012028
H	-4.840097	-3.516770	0.010710
H	-3.285859	-3.624066	0.791264
C	-3.193923	-3.380968	-1.355404
H	-3.314571	-4.464550	-1.501296
C	-1.706374	-3.031095	-1.590757
H	-1.595791	-1.964110	-1.825696
H	-1.396639	-3.560384	-2.505484
C	-0.708042	-3.368247	-0.469405
H	-0.863260	-4.397749	-0.110247
C	0.743116	-3.206063	-0.959162
H	0.817546	-2.278505	-1.548949
H	0.967525	-4.023594	-1.662828
H	-0.886461	-2.710974	0.395312
H	-3.788201	-2.907986	-2.151760
C	-3.485928	-0.533141	-0.245732
H	-3.065443	-0.659826	-1.237395
C	-3.489747	0.748131	0.319200
C	-4.052416	0.983681	1.571325
H	-4.051227	1.989383	1.984431
C	-4.593944	-0.098081	2.275715
H	-5.044811	0.066970	3.252559
C	4.655277	-1.515387	0.913407
C	1.827816	-3.166576	0.131011
H	1.710044	-2.246328	0.723798
H	1.691373	-4.003300	0.834527
C	5.504123	0.805337	0.030723
H	6.556953	0.614430	0.290941
H	5.532032	1.377181	-0.908865
C	3.240064	-3.239569	-0.477745
H	3.367534	-4.241695	-0.915339
H	3.301426	-2.540885	-1.325245
C	4.899913	1.689939	1.142507
H	5.398399	2.670994	1.103929
H	5.157162	1.263494	2.123682
C	3.374265	1.878015	1.113628
H	2.908155	0.906610	1.315473
H	3.080041	2.526640	1.952412
C	4.814210	-0.541564	-0.268992
H	3.828876	-0.351678	-0.716772
H	5.404092	-1.038251	-1.055837
C	2.778270	2.455015	-0.189540
H	5.567201	-1.493231	1.530589
C	4.419490	-2.979621	0.480785
H	4.302406	-3.604982	1.379836
H	5.337671	-3.332765	-0.014143
H	3.043370	3.516745	-0.288443
H	3.230879	1.945226	-1.052510
H	3.840505	-1.178065	1.570037

Sum of electronic and zero-point Energies= -1201.585971  
Sum of electronic and thermal Energies= -1201.558114

Sum of electronic and thermal Enthalpies= -1201.557170  
Sum of electronic and thermal Free Energies= -1201.643954

daec[n=8]-7-E1 (dmf)

C	0.554807	2.021909	-0.898115
H	1.232789	1.579891	-1.622875
C	1.091945	2.731391	0.190744
C	0.218279	3.318173	1.113588
H	0.614297	3.881740	1.956367
C	-1.166000	3.173633	0.966751
H	-1.855597	3.620548	1.679758
C	-1.689064	2.453297	-0.101209
O	-3.062321	2.375651	-0.268564
C	-0.828104	1.878467	-1.061544
O	-1.428611	1.218963	-2.085241
C	-0.598396	0.636295	-3.088575
H	0.010064	1.396834	-3.596814
H	0.058693	-0.137313	-2.667919
H	-1.282159	0.178124	-3.808708
C	-5.181107	-1.121482	0.538041
H	-5.763465	-2.016542	0.750974
C	-3.847820	-1.039558	0.971333
C	-3.211125	-2.194501	1.721534
H	-3.909615	-2.539250	2.497407
H	-2.313341	-1.841771	2.245485
C	-2.855922	-3.409456	0.831374
H	-2.596102	-4.252063	1.490149
C	-1.711437	-3.192512	-0.173782
H	-1.928246	-2.313532	-0.800175
H	-1.689928	-4.054195	-0.858691
C	-0.320325	-3.038771	0.461529
H	-0.135574	-3.892044	1.133988
C	0.811470	-2.959497	-0.573602
H	0.619530	-2.116441	-1.257137
H	0.793763	-3.866750	-1.198631
H	-0.292266	-2.139766	1.095515
H	-3.760201	-3.715585	0.285324
C	-3.117898	0.127393	0.699166
H	-2.090235	0.211306	1.042770
C	-3.708854	1.187457	0.001323
C	-5.037884	1.102046	-0.427029
H	-5.480643	1.938920	-0.961896
C	-5.766462	-0.056770	-0.152841
H	-6.802529	-0.125557	-0.480122
C	5.065949	-1.334124	0.346500
C	2.207967	-2.797378	0.045108
H	2.223734	-1.881314	0.654589
H	2.397446	-3.630153	0.741744
C	5.408895	1.232450	0.222081
H	6.472132	1.149282	0.496480
H	5.349626	2.067417	-0.491666
C	3.330384	-2.751252	-1.003197
H	3.282735	-3.669743	-1.608786
H	3.138902	-1.923455	-1.702542
C	4.614284	1.587950	1.495165
H	4.987999	2.548991	1.881439
H	4.832675	0.845992	2.276908
C	3.087157	1.669191	1.331171
H	2.701056	0.705103	0.970865
H	2.631892	1.824145	2.320374
C	4.976417	-0.056415	-0.502273
H	3.951907	0.065647	-0.881008
H	5.610928	-0.179004	-1.394327
C	2.593250	2.786992	0.385976
H	6.084075	-1.415073	0.759203
C	4.754386	-2.629946	-0.427154
H	4.939928	-3.488849	0.236820
H	5.474283	-2.726214	-1.255164
H	2.883537	3.762285	0.802432
H	3.089812	2.695753	-0.588705

H 4.396810 -1.254169 1.214629  
Sum of electronic and zero-point Energies= -1201.606082  
Sum of electronic and thermal Energies= -1201.577366  
Sum of electronic and thermal Enthalpies= -1201.576421  
Sum of electronic and thermal Free Energies= -1201.666337

daec[n=8]-7-E2 (dmf)

C	-0.029162	2.977916	0.317380
H	0.235796	3.578357	1.183224
C	0.994488	2.510160	-0.526262
C	0.652235	1.748711	-1.649618
H	1.430630	1.387913	-2.319251
C	-0.686555	1.439392	-1.913905
H	-0.964694	0.846488	-2.782706
C	-1.690690	1.887727	-1.064512
O	-3.017436	1.621841	-1.365525
C	-1.372926	2.675864	0.063178
O	-2.421785	3.078963	0.825129
C	-2.145849	3.866777	1.982092
H	-1.515576	3.322005	2.698346
H	-1.660352	4.815530	1.715242
H	-3.118016	4.073166	2.438629
C	-5.041984	-1.606148	0.323168
H	-5.596073	-2.440068	0.751193
C	-3.691325	-1.423986	0.658624
C	-2.991927	-2.396468	1.588883
H	-3.686163	-2.678014	2.392927
H	-2.140861	-1.898241	2.071200
C	-2.512815	-3.697205	0.898494
H	-2.212733	-4.408946	1.682653
C	-1.353067	-3.539475	-0.100514
H	-1.612845	-2.781582	-0.855199
H	-1.242542	-4.487159	-0.649783
C	-0.001214	-3.185154	0.538964
H	0.237769	-3.934769	1.310582
C	1.151470	-3.118740	-0.474036
H	0.916592	-2.364633	-1.242287
H	1.223688	-4.081783	-1.004579
H	-0.073004	-2.220754	1.064116
H	-3.371825	-4.152213	0.383798
C	-2.995807	-0.336756	0.106168
H	-1.951651	-0.181492	0.363257
C	-3.639744	0.546697	-0.767941
C	-4.987213	0.361138	-1.098998
H	-5.470153	1.060973	-1.776880
C	-5.679729	-0.717779	-0.548252
H	-6.729239	-0.862195	-0.799186
C	5.239724	-1.085729	0.400756
C	2.510454	-2.786537	0.160450
H	2.434767	-1.817987	0.677113
H	2.739706	-3.530675	0.940500
C	5.388015	1.477971	0.043550
H	6.426787	1.512295	0.407476
H	5.326794	2.232113	-0.754906
C	3.662234	-2.751370	-0.855966
H	3.704228	-3.722915	-1.372682
H	3.435181	-2.009086	-1.635932
C	4.460377	1.885928	1.206656
H	4.715709	2.912546	1.512155
H	4.673969	1.251994	2.079440
C	2.952008	1.802980	0.917557
H	2.686584	0.774761	0.634253
H	2.399978	2.010682	1.845888
C	5.118062	0.093814	-0.576353
H	4.120649	0.091740	-1.037748
H	5.829133	-0.057977	-1.403803
C	2.447062	2.765901	-0.180098
H	6.236525	-1.056230	0.868651
C	5.051799	-2.468996	-0.252122
H	5.272619	-3.244626	0.497971

H 5.807736 -2.589785 -1.044036  
H 2.581812 3.802171 0.162781  
H 3.055250 2.648956 -1.086021  
H 4.520062 -0.966777 1.222728  
Sum of electronic and zero-point Energies= -1201.605717  
Sum of electronic and thermal Energies= -1201.576990  
Sum of electronic and thermal Enthalpies= -1201.576045  
Sum of electronic and thermal Free Energies= -1201.666363

jugcathanin-1-TS (dmf)

C 1.300427 2.727002 -0.143885  
O 1.719651 3.991430 -0.426464  
H 0.946636 4.570609 -0.296955  
C 2.180136 1.635287 -0.284737  
C 1.629124 0.415792 0.045883  
H 2.247463 -0.446273 0.005051  
C 0.332553 0.210495 0.424662  
H 0.055177 -0.805979 0.589051  
C -0.562066 1.262133 0.554073  
O -1.889612 1.037945 0.945722  
C -0.054782 2.547515 0.277388  
O -0.813206 3.701508 0.311066  
C -1.333849 4.059500 1.604219  
H -1.822863 5.030308 1.476970  
H -2.066392 3.320574 1.947780  
H -0.523780 4.148557 2.341082  
C -2.447220 -2.859689 -0.345987  
H -2.448133 -3.835321 -0.830611  
C -1.586696 -2.618852 0.734453  
C -0.397520 -3.534105 1.033530  
H -0.722635 -4.581727 1.044417  
H 0.015276 -3.314243 2.025527  
C 0.756280 -3.400855 -0.033563  
H 0.374750 -2.958801 -0.962077  
H 1.094598 -4.409658 -0.319520  
C 2.050936 -2.658898 0.370218  
C 3.016158 -2.267403 -0.784538  
H 2.418429 -2.022854 -1.671648  
H 3.524926 -3.211621 -1.036889  
C 4.107680 -1.159611 -0.518740  
H 4.136452 -0.937021 0.556127  
C 4.027204 0.172383 -1.374915  
H 3.366818 -0.005452 -2.236026  
C 3.629067 1.558241 -0.745258  
H 4.306937 1.783805 0.094029  
H 3.834635 2.326337 -1.503421  
H 5.027005 0.330820 -1.799747  
H 5.079140 -1.616207 -0.741828  
O 2.332660 -2.452778 1.535960  
C -1.673798 -1.351304 1.338361  
H -1.055025 -1.128854 2.203980  
C -2.301511 -0.283465 0.687546  
C -3.155729 -0.529336 -0.404989  
O -3.762715 0.546781 -0.966507  
C -4.592971 0.325156 -2.105436  
H -4.025374 -0.112574 -2.938163  
H -4.963437 1.311815 -2.397882  
H -5.444850 -0.324674 -1.861932  
C -3.275626 -1.854228 -0.860795  
H -3.936761 -2.085203 -1.690465  
Sum of electronic and zero-point Energies= -1190.270240  
Sum of electronic and thermal Energies= -1190.246838  
Sum of electronic and thermal Enthalpies= -1190.245894  
Sum of electronic and thermal Free Energies= -1190.321771

jugcathanin-1-E1 (dmf)

C -1.742472 1.904246 0.407508  
O -2.252524 2.252326 1.621181  
H -1.489142 2.411766 2.204971  
C -2.610652 1.545868 -0.638090

C -2.036408 1.248318 -1.881211  
H -2.691684 1.002842 -2.714753  
C -0.651393 1.197453 -2.066693  
H -0.219365 0.904801 -3.020344  
C 0.190106 1.442244 -0.983031  
O 1.557472 1.233648 -1.095905  
C -0.346737 1.849036 0.245839  
O 0.397957 2.096143 1.375506  
C 1.376424 3.151392 1.278405  
H 1.733055 3.322157 2.298663  
H 2.211591 2.851722 0.637831  
H 0.916820 4.070215 0.890756  
C 3.015328 -2.353459 0.457594  
H 3.423574 -3.269049 0.882558  
C 1.669013 -2.297095 0.089870  
C 0.743508 -3.489307 0.265984  
H 1.285951 -4.275157 0.805253  
H 0.473363 -3.911038 -0.712898  
C -0.569650 -3.178702 1.019423  
H -0.390971 -2.512831 1.872535  
H -0.969558 -4.115367 1.440437  
C -1.700209 -2.628081 0.145367  
C -2.605867 -1.594047 0.794004  
H -1.958717 -0.723970 0.983740  
H -2.881556 -1.955176 1.796962  
C -3.850962 -1.189432 -0.010125  
H -3.587875 -1.135852 -1.073994  
C -4.477838 0.149266 0.454002  
H -4.209396 0.339061 1.501534  
C -4.096507 1.389560 -0.401353  
H -4.591794 1.307982 -1.378118  
H -4.506381 2.283515 0.089183  
H -5.573456 0.070917 0.430025  
H -4.594429 -1.993800 0.073065  
O -1.852106 -3.007557 -1.003694  
C 1.190834 -1.089516 -0.447865  
H 0.157327 -1.012649 -0.766893  
C 2.011996 0.025110 -0.587284  
C 3.375877 -0.042747 -0.224812  
O 4.106069 1.092828 -0.402497  
C 5.483279 1.058792 -0.035479  
H 5.609924 0.848028 1.035661  
H 5.874450 2.055883 -0.257127  
H 6.037107 0.312440 -0.621869  
C 3.862789 -1.246796 0.293578  
H 4.903470 -1.328167 0.592285  
Sum of electronic and zero-point Energies= -1190.340650  
Sum of electronic and thermal Energies= -1190.316464  
Sum of electronic and thermal Enthalpies= -1190.315520  
Sum of electronic and thermal Free Energies= -1190.393949

jugcathanin-1-E2 (dmf)

C -2.139357 1.852628 -0.316820  
O -2.992714 2.142305 -1.337611  
H -2.438146 2.464762 -2.071083  
C -2.636246 1.378407 0.906750  
C -1.708630 1.159310 1.936799  
H -2.071173 0.832717 2.910118  
C -0.336168 1.290118 1.732272  
H 0.374511 1.061707 2.522726  
C 0.144767 1.660302 0.471995  
O 1.509042 1.654847 0.220257  
C -0.753490 1.999348 -0.543657  
O -0.400350 2.497752 -1.779302  
C 0.276632 1.603641 -2.684161  
H 0.292538 2.115981 -3.651082  
H 1.303435 1.412600 -2.357284  
H -0.268618 0.656041 -2.780957  
C 3.324456 -2.092178 -0.066692  
H 3.827300 -3.056077 -0.126995

C	1.949392	-2.008703	-0.300972
C	1.126422	-3.233459	-0.666742
H	1.746976	-4.125733	-0.520032
H	0.866445	-3.207639	-1.735054
C	-0.186492	-3.402130	0.128742
H	-0.036726	-3.188295	1.194166
H	-0.502700	-4.456265	0.070694
C	-1.379430	-2.604104	-0.407393
C	-2.352513	-2.084072	0.636941
H	-1.767444	-1.393822	1.263026
H	-2.608149	-2.917113	1.310747
C	-3.619376	-1.394784	0.106358
H	-3.359107	-0.782901	-0.766158
C	-4.333743	-0.528001	1.177328
H	-4.029630	-0.864240	2.178891
C	-4.096042	1.003633	1.062133
H	-4.657303	1.387422	0.203429
H	-4.517340	1.485597	1.956215
H	-5.418986	-0.690857	1.124911
H	-4.307619	-2.165232	-0.266403
O	-1.526406	-2.409135	-1.602568
C	1.351376	-0.741621	-0.201374
H	0.289190	-0.630635	-0.386726
C	2.085378	0.394849	0.127959
C	3.477783	0.305736	0.348968
O	4.118790	1.465680	0.653508
C	5.524596	1.405402	0.879945
H	5.768018	0.762773	1.737790
H	5.834807	2.431546	1.097711
H	6.061034	1.044607	-0.008877
C	4.081372	-0.952678	0.245713
H	5.147678	-1.058392	0.421414
Sum of electronic and zero-point Energies= -1190.336297			
Sum of electronic and thermal Energies= -1190.312051			
Sum of electronic and thermal Enthalpies= -1190.311106			
Sum of electronic and thermal Free Energies= -1190.389968			

jugcathanin-2-TS (dmf)

C	-1.049271	2.847427	-0.175626
O	-1.332883	4.168941	-0.009010
H	-0.523324	4.654322	-0.251731
C	-2.032130	1.868703	0.072330
C	-1.612720	0.573787	-0.146662
H	-2.315179	-0.212270	-0.020974
C	-0.354153	0.203188	-0.527744
H	-0.184839	-0.846725	-0.607953
C	0.631839	1.143613	-0.784631
O	1.910264	0.752817	-1.208521
C	0.268671	2.492889	-0.603901
O	1.117722	3.555829	-0.843621
C	2.250136	3.639862	0.045033
H	2.811774	4.527333	-0.263123
H	1.917694	3.758450	1.085793
H	2.881058	2.748936	-0.041162
C	2.143662	-3.038995	0.443814
H	2.070424	-3.959666	1.021449
C	1.268582	-2.817752	-0.629179
C	-0.013660	-3.634584	-0.802074
H	0.208114	-4.705179	-0.712835
H	-0.437990	-3.475112	-1.800705
C	-1.110957	-3.280989	0.274490
H	-0.656125	-2.789673	1.143393
H	-1.535327	-4.217386	0.670521
C	-2.341172	-2.456629	-0.169226
C	-3.226220	-1.864780	0.964224
H	-2.579722	-1.597184	1.809453
H	-3.814242	-2.726401	1.318989
C	-4.215248	-0.685886	0.616235
H	-4.257494	-0.565423	-0.474385
C	-3.981181	0.707991	1.334410

H	-4.948353	1.005258	1.760339
C	-3.468959	1.980231	0.563047
H	-3.579425	2.834855	1.244459
H	-4.144179	2.188546	-0.282808
H	-3.316624	0.549574	2.196124
H	-5.217995	-1.021705	0.905625
O	-2.640421	-2.334377	-1.342330
C	1.452780	-1.628385	-1.357306
H	0.823940	-1.427584	-2.220940
C	2.205593	-0.571559	-0.833630
C	3.073157	-0.795932	0.252417
O	3.801791	0.265237	0.687229
C	4.633147	0.082147	1.832762
H	5.101126	1.053240	2.016844
H	5.414206	-0.667571	1.646354
H	4.044657	-0.212685	2.712439
C	3.083814	-2.076136	0.833440
H	3.751781	-2.292802	1.661524
Sum of electronic and zero-point Energies= -1190.270924			
Sum of electronic and thermal Energies= -1190.247629			
Sum of electronic and thermal Enthalpies= -1190.246685			
Sum of electronic and thermal Free Energies= -1190.322011			

jugcathanin-2-E1 (dmf)

C	-1.821016	1.720376	-0.541946
O	-2.372261	1.817163	-1.784286
H	-1.627701	1.850865	-2.411663
C	-2.643037	1.580959	0.588738
C	-2.016739	1.538953	1.842904
H	-2.635486	1.467703	2.736012
C	-0.625519	1.514739	1.975640
H	-0.151616	1.414473	2.948886
C	0.170981	1.550197	0.830263
O	1.543249	1.379567	0.930742
C	-0.419084	1.715019	-0.428022
O	0.281925	1.749802	-1.611523
C	1.223685	2.831759	-1.758032
H	1.580230	2.780025	-2.791027
H	0.731603	3.798196	-1.585557
H	2.065796	2.714565	-1.068377
C	3.098186	-2.306326	-0.250344
H	3.537663	-3.253742	-0.559198
C	1.719011	-2.215586	-0.032354
C	0.813650	-3.417601	-0.264297
H	1.328450	-4.318477	0.094628
H	0.672621	-3.560968	-1.345559
C	-0.580420	-3.351132	0.382654
H	-0.526553	-3.021005	1.427733
H	-1.002448	-4.368543	0.410550
C	-1.613061	-2.516181	-0.381920
C	-2.672278	-1.830160	0.466926
H	-2.131798	-1.122076	1.112842
H	-3.082772	-2.577528	1.164448
C	-3.796865	-1.118843	-0.301241
H	-3.375723	-0.618755	-1.181371
C	-4.583886	-0.103302	0.566043
H	-5.649720	-0.140505	0.301218
C	-4.136015	1.379458	0.435585
H	-4.670422	1.967450	1.194820
H	-4.453479	1.759108	-0.542131
H	-4.525981	-0.404258	1.622322
H	-4.486997	-1.879400	-0.691239
O	-1.583989	-2.430754	-1.597489
C	1.208081	-0.974495	0.373727
H	0.149314	-0.861750	0.570516
C	2.026586	0.142080	0.530593
C	3.414797	0.045954	0.302324
O	4.138262	1.186812	0.476072
C	5.542901	1.121892	0.243193
H	5.922201	2.130668	0.430447

H	5.767162	0.836300	-0.794145
H	6.032828	0.416801	0.929241
C	3.935741	-1.195418	-0.083519
H	5.001145	-1.303914	-0.263022

Sum of electronic and zero-point Energies= -1190.339450  
Sum of electronic and thermal Energies= -1190.315390  
Sum of electronic and thermal Enthalpies= -1190.314446  
Sum of electronic and thermal Free Energies= -1190.392141

jugcathanin-2-E2 (dmf)

C	-2.093328	1.952548	0.192876
O	-2.878739	2.430787	1.197109
H	-2.274471	2.805203	1.863150
C	-2.684051	1.302143	-0.900444
C	-1.837758	0.876296	-1.934522
H	-2.276210	0.408466	-2.813702
C	-0.452417	0.992703	-1.841782
H	0.196909	0.607957	-2.624192
C	0.125184	1.545857	-0.695683
O	1.504798	1.529681	-0.541639
C	-0.691239	2.077771	0.311348
O	-0.276668	2.751942	1.434135
C	0.779895	2.199771	2.240047
H	0.709585	2.708281	3.206537
H	0.641270	1.121193	2.384334
H	1.758704	2.395522	1.792327
C	3.304511	-2.147940	0.274989
H	3.808437	-3.089352	0.488944
C	1.908580	-2.077713	0.316193
C	1.063404	-3.305686	0.622979
H	1.623171	-3.952106	1.310872
H	0.919592	-3.892852	-0.296153
C	-0.329995	-3.026804	1.218927
H	-0.288553	-2.254158	1.996934
H	-0.687987	-3.940507	1.719911
C	-1.420722	-2.689759	0.196450
C	-2.500933	-1.724500	0.663729
H	-1.988475	-0.765171	0.834159
H	-2.832699	-2.039941	1.665218
C	-3.697754	-1.544926	-0.283012
H	-3.338866	-1.551739	-1.319865
C	-4.519888	-0.260176	-0.012581
H	-5.586510	-0.468129	-0.175522
C	-4.156507	0.958632	-0.905749
H	-4.756334	1.817768	-0.576766
H	-4.456165	0.735209	-1.938544
H	-4.423820	0.026319	1.043715
H	-4.350119	-2.423734	-0.188123
O	-1.416260	-3.183443	-0.917973
C	1.314538	-0.837572	0.038826
H	0.237616	-0.738381	0.069282
C	2.069614	0.288629	-0.281949
C	3.478425	0.211738	-0.318113
O	4.140478	1.361565	-0.619826
C	5.564162	1.314178	-0.661645
H	5.887783	2.326863	-0.919318
H	5.922446	0.612460	-1.428085
H	5.987298	1.034718	0.313539
C	4.079174	-1.021268	-0.036034
H	5.161158	-1.111687	-0.052218

Sum of electronic and zero-point Energies= -1190.337666  
Sum of electronic and thermal Energies= -1190.313559  
Sum of electronic and thermal Enthalpies= -1190.312615  
Sum of electronic and thermal Free Energies= -1190.391019

jugcathanin-3-TS (dmf)

C	0.283144	2.927269	-0.144518
O	0.255048	4.262931	-0.407635
H	-0.676624	4.538747	-0.334941
C	1.490790	2.206649	-0.242744

C	1.380049	0.864959	0.054555
H	2.256197	0.265949	0.024104
C	0.220675	0.220244	0.384330
H	0.303912	-0.829393	0.553968
C	-0.983647	0.900139	0.467295
O	-2.171715	0.230574	0.795321
C	-0.943281	2.283064	0.205995
O	-2.065783	3.090408	0.197343
C	-2.671608	3.299574	1.487808
H	-3.066256	2.359764	1.890218
H	-1.947505	3.729357	2.193342
H	-3.492949	4.004866	1.327992
C	-1.244984	-3.539907	-0.656854
H	-0.860646	-4.423463	-1.164921
C	-0.615606	-3.076332	0.513605
C	0.792976	-3.536258	0.895466
H	0.851468	-4.631466	0.871736
H	1.034029	-3.222377	1.918161
C	1.897624	-2.973855	-0.078965
H	1.447792	-2.637471	-1.021289
H	2.573198	-3.794707	-0.367725
C	2.834644	-1.858464	0.436907
C	3.713254	-1.142922	-0.628124
H	3.172292	-1.133457	-1.582704
H	4.554633	-1.836887	-0.784112
C	4.293893	0.286357	-0.297387
H	4.143862	0.493887	0.770334
C	3.801555	1.499664	-1.190728
H	4.703839	2.003688	-1.560619
C	2.897172	2.651263	-0.618090
H	2.861432	3.442024	-1.380103
H	3.395171	3.105543	0.253901
H	3.303326	1.096489	-2.084202
H	5.380573	0.221705	-0.426704
O	2.930245	-1.597199	1.621459
C	-1.193992	-1.962947	1.139687
H	-0.758535	-1.580548	2.059751
C	-2.113951	-1.140632	0.464272
C	-2.741600	-1.611080	-0.700944
O	-3.657089	-0.934021	-1.443284
C	-4.506364	0.034763	-0.813523
H	-5.358788	0.159158	-1.489399
H	-3.996945	0.994363	-0.680968
H	-4.864203	-0.327789	0.158983
C	-2.333628	-2.862710	-1.203247
H	-2.827617	-3.232547	-2.099197

Sum of electronic and zero-point Energies= -1190.268694  
Sum of electronic and thermal Energies= -1190.245251  
Sum of electronic and thermal Enthalpies= -1190.244307  
Sum of electronic and thermal Free Energies= -1190.320019

jugcathanin-3-E1 (dmf)

C	1.707520	1.892241	-0.456446
O	2.287434	2.200006	-1.649196
H	1.560342	2.329768	-2.284376
C	2.514024	1.587477	0.653386
C	1.869157	1.330791	1.870937
H	2.475717	1.127719	2.751379
C	0.476388	1.268123	1.974288
H	-0.010172	1.008468	2.911054
C	-0.298858	1.458783	0.832291
O	-1.670026	1.234722	0.870139
C	0.304683	1.823079	-0.378338
O	-0.369556	2.013231	-1.560925
C	-1.395978	3.026780	-1.567034
H	-2.282949	2.689450	-1.021824
H	-1.019053	3.960823	-1.130132
H	-1.647112	3.189402	-2.619551
C	-2.994370	-2.431786	-0.633117
H	-3.359091	-3.368191	-1.051518



C	-1.671967	-2.337735	-0.180861
C	-0.723184	-3.522287	-0.261016
H	-1.222335	-4.332987	-0.804780
H	-0.509884	-3.905513	0.747120
C	0.629320	-3.217622	-0.943480
H	0.494950	-2.582387	-1.827427
H	1.063812	-4.162067	-1.308872
C	1.698566	-2.623425	-0.021783
C	2.631829	-1.602638	-0.651371
H	1.988251	-0.748548	-0.912483
H	2.972576	-1.996174	-1.621567
C	3.820731	-1.152401	0.211305
H	3.492351	-1.061219	1.254304
C	4.460821	0.175304	-0.266230
H	5.553554	0.112749	-0.171131
C	4.013386	1.443249	0.513272
H	4.441561	2.322607	0.012198
H	4.449164	1.407899	1.520664
H	4.256238	0.320020	-1.335139
H	4.576087	-1.949912	0.204981
O	1.782504	-2.959738	1.147496
C	-1.238766	-1.110051	0.343324
H	-0.226343	-1.010337	0.718264
C	-2.082911	0.000311	0.391664
C	-3.415563	-0.105974	-0.049808
O	-4.255307	0.982602	-0.065126
C	-4.738469	1.389994	1.222564
H	-5.403894	2.241016	1.045084
H	-3.918209	1.700520	1.881361
H	-5.305578	0.578169	1.700438
C	-3.855974	-1.331630	-0.552138
H	-4.882683	-1.401364	-0.905602

Sum of electronic and zero-point Energies= -1190.337851

Sum of electronic and thermal Energies= -1190.313422

Sum of electronic and thermal Enthalpies= -1190.312477

Sum of electronic and thermal Free Energies= -1190.391726

#### jugcathanin-3-E2 (dmf)

C	1.991371	1.901209	0.301926
O	2.773760	2.264515	1.355184
H	2.168660	2.599332	2.041552
C	2.575419	1.406965	-0.874744
C	1.717645	1.113033	-1.945540
H	2.148045	0.768850	-2.884475
C	0.331281	1.192771	-1.823154
H	-0.323563	0.908592	-2.643095
C	-0.232780	1.584815	-0.605526
O	-1.610152	1.530629	-0.430815
C	0.590312	1.995018	0.446472
O	0.140896	2.518082	1.639956
C	-0.489753	1.605476	2.560443
H	-1.479358	1.302960	2.203573
H	0.135009	0.718269	2.725232
H	-0.595886	2.156834	3.499807
C	-3.285300	-2.284714	-0.090575
H	-3.742791	-3.270372	-0.025471
C	-1.927453	-2.123639	0.215530
C	-1.072733	-3.299028	0.662133
H	-1.646853	-4.221742	0.516378
H	-0.869439	-3.225037	1.740256
C	0.284257	-3.434327	-0.062068
H	0.180287	-3.258009	-1.139696
H	0.639570	-4.472094	0.044007
C	1.414760	-2.571459	0.507733
C	2.424087	-2.050456	-0.500904
H	1.848488	-1.406625	-1.182751
H	2.748301	-2.895429	-1.128698
C	3.631974	-1.292511	0.071905
H	3.301025	-0.666214	0.909549
C	4.366327	-0.428851	-0.987733

H	5.452981	-0.540388	-0.870742
C	4.056362	1.093310	-0.937608
H	4.505258	1.565502	-1.823382
H	4.551794	1.528987	-0.063310
H	4.133336	-0.810030	-1.992204
H	4.330246	-2.021537	0.504480
O	1.486582	-2.328201	1.700891
C	-1.378083	-0.837963	0.106381
H	-0.332418	-0.677533	0.342161
C	-2.143526	0.255685	-0.305029
C	-3.512686	0.090484	-0.590199
O	-4.290316	1.126762	-1.043204
C	-4.601575	2.129732	-0.067284
H	-5.257266	2.849862	-0.567634
H	-3.699526	2.644313	0.285654
H	-5.132630	1.690233	0.789637
C	-4.064880	-1.187568	-0.473208
H	-5.119591	-1.310907	-0.710633

Sum of electronic and zero-point Energies= -1190.333276

Sum of electronic and thermal Energies= -1190.308829

Sum of electronic and thermal Enthalpies= -1190.307884

Sum of electronic and thermal Free Energies= -1190.387266

#### jugcathanin-4-TS (dmf)

C	-1.165117	2.769539	0.207667
O	-1.557194	4.044083	0.483172
H	-0.776444	4.608350	0.335354
C	-2.078722	1.702858	0.339408
C	-1.550351	0.467993	0.028754
H	-2.181169	-0.388341	0.041002
C	-0.246868	0.231528	-0.301254
H	0.011254	-0.793944	-0.419908
C	0.668132	1.258269	-0.465901
O	1.981453	0.992091	-0.880998
C	0.185456	2.559165	-0.215163
O	0.962753	3.699448	-0.279393
C	1.470123	4.024060	-1.586756
H	2.179860	3.262744	-1.929513
H	0.650280	4.119224	-2.311960
H	1.983140	4.985312	-1.484007
C	2.294998	-2.978171	0.246481
H	2.226487	-3.964073	0.704785
C	1.427797	-2.632954	-0.799537
C	0.136650	-3.409887	-1.074897
H	0.342379	-4.486509	-1.118386
H	-0.275323	-3.120978	-2.049124
C	-0.978204	-3.175325	0.021392
H	-0.592503	-2.597273	0.873342
H	-1.266060	-4.142432	0.460478
C	-2.305812	-2.522075	-0.426362
C	-3.428869	-2.320597	0.639620
H	-3.270271	-3.068410	1.427993
H	-4.352199	-2.595978	0.112514
C	-3.702888	-0.956653	1.392795
H	-4.476455	-1.216641	2.127171
C	-4.219028	0.286036	0.570412
H	-4.181595	0.061691	-0.504299
C	-3.529600	1.675580	0.803776
H	-4.125830	2.439003	0.283498
H	-3.584931	1.937313	1.872629
H	-5.282784	0.423156	0.803107
H	-2.821383	-0.691332	1.988096
O	-2.522113	-2.261808	-1.596848
C	1.607278	-1.358041	-1.370193
H	0.972581	-1.053829	-2.198806
C	2.326730	-0.363130	-0.698815
C	3.186298	-0.712451	0.360780
O	3.883489	0.294526	0.945043
C	4.711870	-0.026017	2.061686
H	5.510197	-0.727455	1.782491

H	4.125802	-0.449384	2.888986
H	5.157979	0.920464	2.380179
C	3.216766	-2.059236	0.765985
H	3.880063	-2.370325	1.567296

Sum of electronic and zero-point Energies= -1190.263110  
Sum of electronic and thermal Energies= -1190.239944  
Sum of electronic and thermal Enthalpies= -1190.239000  
Sum of electronic and thermal Free Energies= -1190.313958

jugcathanin-4-E1 (dmf)

C	-1.935570	2.095313	-0.183467
O	-2.790755	2.483022	-1.168740
H	-2.234597	2.825111	-1.892090
C	-2.442820	1.533587	0.999435
C	-1.523227	1.217785	2.009704
H	-1.894749	0.834622	2.958129
C	-0.147652	1.307009	1.800923
H	0.558091	0.979769	2.560407
C	0.338414	1.729785	0.561523
O	1.690449	1.600536	0.275023
C	-0.548213	2.200837	-0.413697
O	-0.190371	2.771117	-1.615780
C	0.523461	1.955021	-2.564763
H	1.558884	1.796480	-2.248542
H	0.021771	0.989842	-2.708515
H	0.511286	2.515676	-3.504537
C	3.031771	-2.323771	-0.211754
H	3.411950	-3.338165	-0.322027
C	1.679210	-2.058023	-0.443009
C	0.718876	-3.151112	-0.882159
H	1.257761	-4.105993	-0.861279
H	0.427319	-2.982109	-1.928860
C	-0.575699	-3.304177	-0.053654
H	-0.418338	-3.046696	1.004837
H	-0.882804	-4.361733	-0.040535
C	-1.796477	-2.534798	-0.551186
C	-3.080546	-2.708557	0.258334
H	-2.986642	-3.588565	0.905999
H	-3.904525	-2.894771	-0.444247
C	-3.399799	-1.464481	1.129922
H	-4.069568	-1.777169	1.942962
C	-4.044024	-0.292602	0.365058
H	-3.605218	-0.220731	-0.637664
C	-3.884419	1.084135	1.070950
H	-4.544599	1.811657	0.583474
H	-4.203119	1.004250	2.119400
H	-5.114331	-0.502871	0.223067
H	-2.471184	-1.136352	1.614308
O	-1.761920	-1.827098	-1.545664
C	1.239666	-0.734051	-0.280646
H	0.197809	-0.497557	-0.465463
C	2.108207	0.283836	0.109371
C	3.477064	0.011843	0.325887
O	4.255339	1.066144	0.690796
C	5.639476	0.817966	0.921804
H	6.138574	0.442259	0.017531
H	5.789811	0.103770	1.743678
H	6.072485	1.783640	1.198644
C	3.921681	-1.304648	0.159201
H	4.965718	-1.549524	0.329587

Sum of electronic and zero-point Energies= -1190.335075  
Sum of electronic and thermal Energies= -1190.311009  
Sum of electronic and thermal Enthalpies= -1190.310065  
Sum of electronic and thermal Free Energies= -1190.388033

jugcathanin-4-E2 (dmf)

C	-1.511468	2.077304	0.435884
O	-2.006052	2.373532	1.670577
H	-1.236321	2.444394	2.263358
C	-2.383889	1.822469	-0.633942

C	-1.814975	1.597826	-1.896373
H	-2.475695	1.438861	-2.747083
C	-0.435446	1.474907	-2.074175
H	-0.009971	1.215432	-3.040377
C	0.402677	1.572302	-0.963203
O	1.738020	1.207705	-1.059681
C	-0.118931	1.946645	0.279943
O	0.622768	2.060290	1.432474
C	1.709967	3.006577	1.405643
H	2.526160	2.645935	0.772044
H	1.361841	3.984866	1.048651
H	2.054045	3.095357	2.440541
C	2.673601	-2.596707	0.378521
H	2.949844	-3.574881	0.769075
C	1.355645	-2.351005	-0.014385
C	0.289950	-3.430859	0.070593
H	0.741288	-4.320714	0.525391
H	-0.020351	-3.721506	-0.943264
C	-0.984385	-3.066598	0.863797
H	-0.773261	-2.354462	1.675668
H	-1.375611	-3.961976	1.372476
C	-2.154743	-2.524598	0.047822
C	-3.406637	-2.142289	0.834863
H	-3.355039	-2.582240	1.838082
H	-4.278545	-2.572863	0.323363
C	-3.570877	-0.603675	0.956468
H	-4.219858	-0.392366	1.817373
C	-4.155162	0.071356	-0.299347
H	-3.753005	-0.418883	-1.195047
C	-3.863056	1.593235	-0.407202
H	-4.436796	1.998659	-1.251503
H	-4.206444	2.109528	0.497131
H	-5.243651	-0.087690	-0.317748
H	-2.594624	-0.169999	1.204953
O	-2.105262	-2.410428	-1.166718
C	1.048416	-1.071467	-0.508968
H	0.037627	-0.859777	-0.840238
C	2.013706	-0.070223	-0.588975
C	3.347254	-0.329610	-0.201422
O	4.223755	0.706315	-0.320119
C	5.574417	0.478094	0.074021
H	6.040147	-0.315389	-0.527007
H	5.645210	0.217458	1.139433
H	6.099261	1.421304	-0.103078
C	3.661090	-1.604672	0.279031
H	4.674992	-1.832441	0.593975

Sum of electronic and zero-point Energies= -1190.338006  
Sum of electronic and thermal Energies= -1190.313944  
Sum of electronic and thermal Enthalpies= -1190.313000  
Sum of electronic and thermal Free Energies= -1190.390833

jugcathanin-5-TS (dmf)

C	-1.496225	2.641912	0.228945
O	-2.018715	3.866505	0.513552
H	-1.294436	4.507261	0.392053
C	-2.295101	1.483917	0.318615
C	-1.636029	0.317765	0.002748
H	-2.205240	-0.577067	-0.045604
C	-0.302676	0.208052	-0.273388
H	0.068306	-0.786327	-0.379333
C	0.497795	1.330731	-0.417928
O	1.833510	1.220680	-0.825356
C	-0.124021	2.572247	-0.169692
O	0.537302	3.785126	-0.214928
C	0.981214	4.188842	-1.523465
H	0.139583	4.222942	-2.228974
H	1.403022	5.191953	-1.406307
H	1.751848	3.507087	-1.900800
C	2.663946	-2.723920	0.133605
H	2.741939	-3.729342	0.545662

C	1.722960	-2.452038	-0.870250
C	0.551346	-3.397368	-1.150913
H	0.918269	-4.422201	-1.286445
H	0.042926	-3.114629	-2.080834
C	-0.508831	-3.420608	0.022081
H	-0.066408	-3.034569	0.947668
H	-0.758524	-4.471239	0.239844
C	-1.889677	-2.752556	-0.201226
C	-2.633260	-2.288670	1.075024
H	-1.910373	-1.761112	1.709725
H	-2.849013	-3.219754	1.627242
C	-4.000880	-1.515293	1.003239
H	-4.725279	-2.209316	0.554781
C	-4.313292	-0.135557	0.294459
H	-4.147005	-0.242895	-0.785789
C	-3.742214	1.261555	0.738392
H	-3.836901	1.370554	1.830903
H	-4.401475	2.029297	0.309036
H	-5.402550	-0.045965	0.411183
H	-4.307969	-1.414745	2.054515
O	-2.378925	-2.659317	-1.312359
C	1.714554	-1.142881	-1.385736
H	1.023611	-0.892273	-2.186347
C	2.329300	-0.091423	-0.695792
C	3.262391	-0.369142	0.321523
O	3.851057	0.694187	0.925001
C	4.752191	0.436915	2.001053
H	5.622295	-0.145149	1.667251
H	5.086605	1.418947	2.347606
H	4.253534	-0.090389	2.825983
C	3.476219	-1.715589	0.667840
H	4.201131	-1.969863	1.434883

Sum of electronic and zero-point Energies= -1190.262303

Sum of electronic and thermal Energies= -1190.239003

Sum of electronic and thermal Enthalpies= -1190.238059

Sum of electronic and thermal Free Energies= -1190.313745

#### jugcathanin-5-E1 (dmf)

C	-1.903425	2.018530	-0.161874
O	-2.710971	2.477565	-1.158339
H	-2.122677	2.836086	-1.846684
C	-2.469553	1.367401	0.943508
C	-1.606668	0.986541	1.981285
H	-2.026241	0.535966	2.878782
C	-0.224765	1.102513	1.853312
H	0.444639	0.725454	2.622657
C	0.330013	1.626156	0.681123
O	1.701119	1.512315	0.475613
C	-0.504390	2.158559	-0.309728
O	-0.136974	2.823411	-1.451654
C	1.023624	2.420880	-2.198833
H	1.031453	1.336786	-2.362321
H	0.938476	2.932979	-3.161988
H	1.944233	2.731821	-1.696553
C	3.036580	-2.347108	-0.401668
H	3.414152	-3.348740	-0.601192
C	1.676454	-2.070148	-0.555774
C	0.676991	-3.127050	-0.994299
H	1.195280	-4.091037	-1.062791
H	0.303069	-2.899479	-2.003028
C	-0.546588	-3.280736	-0.063892
H	-0.264840	-3.172023	0.991416
H	-0.945508	-4.304401	-0.157683
C	-1.746861	-2.378518	-0.372377
C	-2.696150	-2.143074	0.792975
H	-2.160633	-1.486602	1.493633
H	-2.791869	-3.099913	1.328971
C	-4.102890	-1.604774	0.472205
H	-4.559327	-2.276171	-0.270012
C	-4.278266	-0.160483	-0.044466

H	-3.715752	-0.028060	-0.974655
C	-3.937150	1.000523	0.934228
H	-4.255120	0.734034	1.951741
H	-4.531028	1.874947	0.636279
H	-5.340622	-0.058150	-0.310987
H	-4.705018	-1.717523	1.386438
O	-1.934544	-1.921012	-1.487488
C	1.243127	-0.763935	-0.276837
H	0.196051	-0.515808	-0.403823
C	2.118933	0.223583	0.167353
C	3.496875	-0.057451	0.304693
O	4.284908	0.969376	0.723194
C	5.678159	0.713472	0.879463
H	6.142562	0.414952	-0.070952
H	6.117769	1.656843	1.216150
H	5.863209	-0.063386	1.634665
C	3.937723	-1.352873	0.011786
H	4.988807	-1.603853	0.118217

Sum of electronic and zero-point Energies= -1190.334370

Sum of electronic and thermal Energies= -1190.310352

Sum of electronic and thermal Enthalpies= -1190.309408

Sum of electronic and thermal Free Energies= -1190.387189

#### jugcathanin-5-E2 (dmf)

C	-1.586123	1.839643	0.501673
O	-2.110211	1.976982	1.753378
H	-1.351695	2.046301	2.360958
C	-2.430382	1.641283	-0.600698
C	-1.831696	1.559138	-1.867492
H	-2.471042	1.451581	-2.742140
C	-0.445673	1.525504	-2.031117
H	0.005624	1.372807	-3.008336
C	0.372851	1.582096	-0.903018
O	1.728046	1.298583	-1.008816
C	-0.186501	1.810982	0.358835
O	0.532195	1.864089	1.530013
C	1.564840	2.867033	1.605296
H	1.164337	3.854199	1.339272
H	1.897960	2.874742	2.647403
H	2.403569	2.615324	0.948698
C	2.806628	-2.527902	0.267203
H	3.115074	-3.507338	0.629461
C	1.471694	-2.298051	-0.072806
C	0.402551	-3.367638	0.067973
H	0.859943	-4.266246	0.499045
H	0.016206	-3.653631	-0.920741
C	-0.802213	-2.950281	0.940975
H	-0.485495	-2.341715	1.797953
H	-1.264584	-3.851885	1.375974
C	-1.953008	-2.251531	0.208851
C	-2.868194	-1.411707	1.087759
H	-2.296125	-0.523135	1.389829
H	-3.011976	-1.971637	2.024943
C	-4.248810	-1.031414	0.521734
H	-4.759661	-1.960292	0.228333
C	-4.357446	-0.054298	-0.668334
H	-3.817316	-0.462546	-1.530521
C	-3.920537	1.420603	-0.441074
H	-4.256940	1.762521	0.544894
H	-4.445553	2.037604	-1.183740
H	-5.420323	-0.034692	-0.951082
H	-4.834455	-0.619972	1.357494
O	-2.136638	-2.405597	-0.987304
C	1.126808	-1.016202	-0.530889
H	0.102789	-0.815474	-0.823447
C	2.061952	0.011561	-0.606559
C	3.412606	-0.228230	-0.269981
O	4.259776	0.832434	-0.378479
C	5.626955	0.625151	-0.032646
H	6.093876	-0.133836	-0.675812

H	6.122803	1.587321	-0.190265
H	5.736164	0.328216	1.019908
C	3.769254	-1.511568	0.157689
H	4.798142	-1.725169	0.431340

Sum of electronic and zero-point Energies= -1190.337635  
Sum of electronic and thermal Energies= -1190.313572  
Sum of electronic and thermal Enthalpies= -1190.312628  
Sum of electronic and thermal Free Energies= -1190.390629

jugcathanin-6-TS (dmf)

C	-0.938389	2.872198	-0.115133
O	-1.206183	4.197609	0.046586
H	-0.394914	4.673888	-0.207989
C	-1.943637	1.911315	0.122132
C	-1.535786	0.609211	-0.076223
H	-2.242446	-0.179471	0.023936
C	-0.269114	0.223410	-0.408994
H	-0.108492	-0.828206	-0.442486
C	0.724103	1.143586	-0.700910
O	1.986267	0.723533	-1.147172
C	0.374291	2.500084	-0.544653
O	1.229027	3.551971	-0.810777
C	2.388372	3.622463	0.042852
H	3.005661	2.723727	-0.062097
H	2.952051	4.502148	-0.283086
H	2.089454	3.745162	1.093173
C	2.004445	-3.129575	0.360926
H	1.870299	-4.056931	0.916562
C	1.129736	-2.811280	-0.687498
C	-0.232357	-3.493642	-0.846594
H	-0.120929	-4.583192	-0.785474
H	-0.652529	-3.267632	-1.833876
C	-1.283791	-3.054032	0.249283
H	-1.641572	-3.944295	0.788097
H	-0.819048	-2.435164	1.030247
C	-2.562768	-2.327042	-0.226695
C	-3.629343	-1.926370	0.841392
H	-3.509298	-2.605729	1.695853
H	-4.589032	-2.169943	0.366098
C	-3.763103	-0.477248	1.461869
H	-4.534845	-0.596170	2.233636
C	-4.193359	0.722176	0.532518
H	-4.208644	0.393314	-0.515481
C	-3.378225	2.060112	0.613388
H	-3.919029	2.819839	0.030775
H	-3.381523	2.428566	1.651744
H	-5.233408	0.976422	0.773737
H	-2.845502	-0.234903	2.010537
O	-2.792748	-2.157551	-1.411152
C	1.394535	-1.618182	-1.386902
H	0.755920	-1.339166	-2.221423
C	2.223305	-0.632052	-0.840687
C	3.089872	-0.952164	0.221759
O	3.892857	0.042203	0.681395
C	4.730999	-0.238759	1.801887
H	4.140372	-0.523313	2.683552
H	5.269125	0.690429	2.009272
H	5.453836	-1.033781	1.573147
C	3.021035	-2.250387	0.758618
H	3.685816	-2.540640	1.566488

Sum of electronic and zero-point Energies= -1190.263706  
Sum of electronic and thermal Energies= -1190.240594  
Sum of electronic and thermal Enthalpies= -1190.239649  
Sum of electronic and thermal Free Energies= -1190.314397

jugcathanin-6-E1 (dmf)

C	-1.784897	2.020713	-0.321607
O	-2.530952	2.312519	-1.421987
H	-1.900661	2.481062	-2.145300
C	-2.418882	1.628796	0.870061

C	-1.608356	1.393663	1.989263
H	-2.082091	1.133906	2.934122
C	-0.214106	1.395256	1.902262
H	0.405208	1.126182	2.754293
C	0.391003	1.644243	0.670807
O	1.750134	1.416370	0.507118
C	-0.382358	2.030327	-0.428955
O	0.126323	2.276305	-1.683429
C	1.053357	3.374711	-1.780812
H	1.976651	3.155387	-1.234462
H	1.272620	3.489870	-2.846530
H	0.601669	4.298488	-1.395170
C	2.887015	-2.509488	-0.336621
H	3.219294	-3.527398	-0.534459
C	1.532340	-2.186173	-0.443465
C	0.507188	-3.222870	-0.873729
H	0.992659	-4.206109	-0.861587
H	0.216440	-3.034358	-1.917505
C	-0.787974	-3.302182	-0.037286
H	-1.134831	-4.346215	0.013262
H	-0.620264	-3.013350	1.011345
C	-1.978197	-2.505197	-0.564854
C	-3.265622	-2.586525	0.253703
H	-3.204634	-3.434225	0.946980
H	-4.097121	-2.777968	-0.438698
C	-3.538611	-1.287728	1.057672
H	-4.245419	-1.526161	1.864652
C	-4.096659	-0.122895	0.218522
H	-3.622497	-0.120750	-0.769999
C	-3.888959	1.275705	0.863877
H	-4.466840	2.015592	0.296045
H	-4.277922	1.276351	1.891330
H	-5.171562	-0.284549	0.049600
H	-2.606639	-0.985736	1.553248
O	-1.916496	-1.847573	-1.591385
C	1.152445	-0.860891	-0.168940
H	0.108847	-0.581479	-0.256999
C	2.086063	0.103759	0.204834
C	3.457627	-0.226777	0.293924
O	4.299349	0.780657	0.653045
C	5.686799	0.475326	0.761415
H	5.873110	-0.288789	1.529324
H	6.175005	1.409146	1.055312
H	6.101737	0.135215	-0.197924
C	3.840069	-1.543340	0.019956
H	4.884659	-1.830929	0.092057

Sum of electronic and zero-point Energies= -1190.337839  
Sum of electronic and thermal Energies= -1190.313691  
Sum of electronic and thermal Enthalpies= -1190.312747  
Sum of electronic and thermal Free Energies= -1190.391323

jugcathanin-6-E2 (dmf)

C	-1.827959	2.151383	0.236253
O	-2.524767	2.587380	1.322597
H	-1.860040	2.856974	1.981682
C	-2.507687	1.615829	-0.865476
C	-1.744578	1.251064	-1.985638
H	-2.254633	0.875144	-2.870913
C	-0.353251	1.270127	-1.955496
H	0.233554	0.906440	-2.795420
C	0.311415	1.661629	-0.789202
O	1.680814	1.458290	-0.682615
C	-0.415128	2.177717	0.290238
O	0.089025	2.728725	1.443289
C	1.160003	2.075179	2.147622
H	2.118223	2.238170	1.646025
H	1.181107	2.536484	3.139700
H	0.965178	1.000691	2.249136
C	2.971046	-2.402369	0.248723
H	3.345870	-3.392376	0.503938

C	1.596775	-2.191231	0.112534
C	0.606307	-3.334137	0.273325
H	1.112162	-4.150601	0.802778
H	0.345358	-3.727850	-0.720176
C	-0.713261	-3.010214	1.004315
H	-1.036305	-3.883909	1.592138
H	-0.589574	-2.206856	1.746013
C	-1.905905	-2.662723	0.115819
C	-3.208857	-2.314760	0.834699
H	-3.145475	-2.640928	1.879965
H	-4.021343	-2.878751	0.355886
C	-3.527425	-0.796319	0.792387
H	-4.244565	-0.573856	1.594516
C	-4.095683	-0.304000	-0.552139
H	-3.579036	-0.817865	-1.372531
C	-3.968571	1.227304	-0.779988
H	-4.482987	1.482841	-1.716580
H	-4.470901	1.774236	0.026127
H	-5.155499	-0.590978	-0.621804
H	-2.613593	-0.243448	1.044938
O	-1.834101	-2.679599	-1.102364
C	1.163341	-0.894356	-0.211492
H	0.103157	-0.705430	-0.327855
C	2.064087	0.154539	-0.394381
C	3.452828	-0.068315	-0.256988
O	4.257730	1.014634	-0.437326
C	5.663428	0.823542	-0.303076
H	5.930371	0.486159	0.708356
H	6.115643	1.802309	-0.488119
H	6.044571	0.102436	-1.039782
C	3.888980	-1.357788	0.063180
H	4.949738	-1.557081	0.182010

Sum of electronic and zero-point Energies= -1190.334183

Sum of electronic and thermal Energies= -1190.310103

Sum of electronic and thermal Enthalpies= -1190.309158

Sum of electronic and thermal Free Energies= -1190.387586

jugcathanin-7-TS (dmf)

C	0.447999	2.965108	-0.160892
O	0.484118	4.302806	0.093135
H	-0.402272	4.645563	-0.123104
C	1.594162	2.171082	0.051937
C	1.420602	0.837606	-0.254671
H	2.229364	0.157236	-0.128863
C	0.257282	0.284028	-0.697778
H	0.281926	-0.769100	-0.834826
C	-0.893231	1.026381	-0.892213
O	-2.072810	0.386110	-1.313566
C	-0.787140	2.405496	-0.624404
O	-1.814793	3.311829	-0.796595
C	-2.945793	3.120067	0.077394
H	-2.642830	3.218438	1.129158
H	-3.659654	3.910652	-0.173850
H	-3.401009	2.137515	-0.083481
C	-1.297219	-3.268675	0.441981
H	-0.944474	-4.104156	1.044259
C	-0.619599	-2.931431	-0.736077
C	0.754468	-3.525640	-1.059342
H	0.751606	-3.937110	-2.079122
H	0.926768	-4.373547	-0.384848
C	2.026796	-2.598761	-1.005160
H	1.946647	-1.770891	-1.724961
H	2.864866	-3.200864	-1.388196
C	2.500781	-2.019745	0.344703
C	3.922368	-1.363062	0.435389
H	4.572441	-1.928927	-0.246256
H	4.248004	-1.593809	1.458085
C	4.262480	0.160502	0.173187
H	5.359109	0.186965	0.218960
C	3.718443	1.252008	1.175812

H	3.061736	0.775229	1.916168
C	2.970038	2.511769	0.610316
H	3.592785	2.996541	-0.158752
H	2.884323	3.243920	1.425146
H	4.577453	1.631709	1.743713
H	4.019643	0.421140	-0.864217
O	1.845797	-2.172586	1.360022
C	-1.152616	-1.861403	-1.483499
H	-0.671206	-1.561309	-2.412239
C	-2.065287	-0.968481	-0.906975
C	-2.742327	-1.319483	0.277187
O	-3.643311	-0.423826	0.759034
C	-4.271163	-0.713042	2.007702
H	-3.532147	-0.811655	2.814613
H	-4.875830	-1.628413	1.950860
H	-4.924514	0.139085	2.214821
C	-2.393875	-2.528046	0.901744
H	-2.897760	-2.836544	1.812650

Sum of electronic and zero-point Energies= -1190.260022

Sum of electronic and thermal Energies= -1190.236874

Sum of electronic and thermal Enthalpies= -1190.235929

Sum of electronic and thermal Free Energies= -1190.310851

jugcathanin-7-E1 (dmf)

C	1.511364	2.077339	-0.435741
O	2.005910	2.373692	-1.670442
H	1.236127	2.444950	-2.263106
C	2.383768	1.822419	0.634026
C	1.814886	1.597442	1.896449
H	2.475672	1.438397	2.747093
C	0.435394	1.474468	2.074231
H	0.009830	1.214785	3.040339
C	-0.402747	1.572180	0.963260
O	-1.738105	1.207665	1.059749
C	0.118790	1.946690	-0.279822
O	-0.622866	2.060568	-1.432340
C	-1.710242	3.006681	-1.405340
H	-1.362311	3.984878	-1.047924
H	-2.054135	3.095773	-2.440273
H	-2.526479	2.645677	-0.772016
C	-2.673586	-2.596849	-0.378319
H	-2.949760	-3.575072	-0.768799
C	-1.355540	-2.351013	0.014410
C	-0.289764	-3.430748	-0.070850
H	-0.741036	-4.320491	-0.525914
H	0.020595	-3.721670	0.942914
C	0.984532	-3.066180	-0.864000
H	0.773355	-2.353895	-1.675714
H	1.375725	-3.961449	-1.372928
C	2.154984	-2.524534	-0.047978
C	3.406760	-2.141964	-0.835117
H	3.355013	-2.581805	-1.838383
H	4.278745	-2.572652	-0.323830
C	3.571030	-0.603392	-0.956595
H	4.220182	-0.392035	-1.817360
C	4.155180	0.071577	0.299339
H	3.752957	-0.418727	1.194973
C	3.862970	1.593410	0.407220
H	4.206208	2.109780	-0.497124
H	4.436715	1.998907	1.251487
H	5.243668	-0.087470	0.317828
H	2.594843	-0.169643	-1.205223
O	2.105703	-2.410909	1.166619
C	-1.048398	-1.071497	0.508940
H	-0.037593	-0.859638	0.840046
C	-2.013793	-0.070316	0.589076
C	-3.347300	-0.329759	0.201639
O	-4.223909	0.706078	0.320297
C	-5.574341	0.478002	-0.074700
H	-6.040626	-0.315267	0.526187

H	-5.644462	0.217150	-1.140102
H	-6.099140	1.421336	0.101866
C	-3.661100	-1.604928	-0.278722
H	-4.675038	-1.832742	-0.593528

Sum of electronic and zero-point Energies= -1190.338005  
Sum of electronic and thermal Energies= -1190.313944  
Sum of electronic and thermal Enthalpies= -1190.313000  
Sum of electronic and thermal Free Energies= -1190.390835

jugcathanin-7-E2 (dmf)

C	1.933798	2.095165	0.189520
O	2.782931	2.479332	1.181569
H	2.221287	2.800111	1.910385
C	2.448955	1.539086	-0.991956
C	1.536262	1.221933	-2.008322
H	1.913931	0.842308	-2.955710
C	0.159940	1.304984	-1.804812
H	-0.541635	0.976789	-2.567759
C	-0.335055	1.724843	-0.567581
O	-1.689330	1.589291	-0.292761
C	0.544369	2.196970	0.414049
O	0.191847	2.763578	1.617858
C	-0.641614	2.009804	2.518990
H	-0.274294	0.981743	2.625934
H	-0.573182	2.523554	3.482823
H	-1.681974	2.003987	2.180705
C	-3.022773	-2.335569	0.210272
H	-3.401505	-3.349969	0.325350
C	-1.669546	-2.067769	0.434801
C	-0.707389	-3.158340	0.876212
H	-1.242487	-4.115224	0.849669
H	-0.423066	-2.991091	1.925231
C	0.592870	-3.304443	0.055785
H	0.440602	-3.047923	-1.003719
H	0.905654	-4.360322	0.044760
C	1.806162	-2.528016	0.560596
C	3.096998	-2.698327	-0.238870
H	3.011847	-3.580872	-0.884289
H	3.916646	-2.878588	0.470311
C	3.417075	-1.455557	-1.112044
H	4.092162	-1.768223	-1.920680
C	4.053605	-0.280006	-0.346450
H	3.609641	-0.207488	0.653919
C	3.892557	1.094732	-1.055718
H	4.216329	1.014067	-2.102554
H	4.548004	1.825415	-0.566592
H	5.123914	-0.486390	-0.198816
H	2.490153	-1.131261	-1.602288
O	1.760245	-1.817329	1.552498
C	-1.231634	-0.743966	0.265849
H	-0.189347	-0.505959	0.445584
C	-2.103062	0.272023	-0.122461
C	-3.472760	-0.001873	-0.331380
O	-4.253949	1.051117	-0.694054
C	-5.639327	0.801492	-0.915764
H	-6.132305	0.426807	-0.007700
H	-5.794384	0.085870	-1.735521
H	-6.074885	1.766380	-1.191364
C	-3.915289	-1.318340	-0.159718
H	-4.959899	-1.564604	-0.324547

Sum of electronic and zero-point Energies= -1190.335099  
Sum of electronic and thermal Energies= -1190.311005  
Sum of electronic and thermal Enthalpies= -1190.310061  
Sum of electronic and thermal Free Energies= -1190.388377

jugcathanin-8-TS (dmf)

C	0.737443	2.909200	-0.176983
O	0.888830	4.255990	-0.044719
H	0.022884	4.652238	-0.251086
C	1.836002	2.045960	0.007282

C	1.544009	0.710416	-0.169180
H	2.333372	0.005719	-0.081877
C	0.310997	0.200356	-0.464741
H	0.254030	-0.862049	-0.531596
C	-0.786575	1.025165	-0.652986
O	-2.045073	0.495972	-0.980795
C	-0.561402	2.407125	-0.500098
O	-1.552588	3.356829	-0.662583
C	-2.499071	3.407013	0.424332
H	-3.257530	4.141820	0.137130
H	-2.967962	2.429244	0.579586
H	-2.008320	3.728222	1.353696
C	-1.744358	-3.275726	0.714654
H	-1.521651	-4.168901	1.296768
C	-0.973349	-2.970785	-0.419929
C	0.375798	-3.646447	-0.674786
H	0.708960	-3.460118	-1.702695
H	0.278230	-4.732560	-0.557519
C	1.498786	-3.153589	0.316248
H	2.044045	-4.029715	0.701712
H	1.055426	-2.686370	1.204252
C	2.600779	-2.218301	-0.231850
C	3.508955	-1.522520	0.820912
H	4.218904	-2.310164	1.120063
H	2.913586	-1.321819	1.720502
C	4.325000	-0.243200	0.389182
H	5.379786	-0.459104	0.595778
C	3.991219	1.122851	1.120835
H	3.414183	0.900189	2.030032
C	3.284234	2.321327	0.386976
H	3.349709	3.191013	1.054970
H	3.865803	2.593322	-0.508831
H	4.947852	1.530340	1.472809
H	4.263914	-0.132183	-0.701526
O	2.790723	-2.084094	-1.426227
C	-1.336954	-1.827930	-1.152567
H	-0.787056	-1.576345	-2.055759
C	-2.172232	-0.850822	-0.589144
C	-2.949697	-1.167620	0.535601
O	-3.792867	-0.262761	1.125272
C	-4.878215	0.186586	0.299615
H	-4.518284	0.715302	-0.590956
H	-5.467154	0.871978	0.917020
H	-5.507697	-0.661649	-0.004770
C	-2.769636	-2.423304	1.135175
H	-3.377619	-2.668440	2.003420

Sum of electronic and zero-point Energies= -1190.267671  
Sum of electronic and thermal Energies= -1190.244173  
Sum of electronic and thermal Enthalpies= -1190.243229  
Sum of electronic and thermal Free Energies= -1190.319115

jugcathanin-8-E1 (dmf)

C	1.846033	1.751841	-0.424638
O	2.527248	1.930969	-1.590504
H	1.855663	2.004523	-2.292480
C	2.540036	1.501321	0.770774
C	1.781544	1.362521	1.942532
H	2.300175	1.202101	2.886373
C	0.384686	1.355944	1.925110
H	-0.191202	1.184481	2.831051
C	-0.283010	1.513248	0.709705
O	-1.663387	1.367974	0.648247
C	0.439219	1.766502	-0.459402
O	-0.146179	1.907820	-1.698161
C	-0.875008	3.136900	-1.888854
H	-1.234296	3.118762	-2.922056
H	-1.727073	3.196291	-1.202610
H	-0.218724	4.005020	-1.740723
C	-3.161400	-2.470204	-0.059972
H	-3.577526	-3.463928	-0.216188

C	-1.787601	-2.253273	-0.227375
C	-0.860160	-3.382667	-0.647375
H	-0.652076	-3.313701	-1.725235
H	-1.381994	-4.334944	-0.494492
C	0.496091	-3.427193	0.088102
H	0.900004	-4.450308	0.023521
H	0.378304	-3.214298	1.157662
C	1.588119	-2.536515	-0.512795
C	2.561592	-1.915769	0.475681
H	2.902173	-2.706037	1.163041
H	1.955887	-1.246479	1.105627
C	3.754372	-1.163606	-0.134218
H	4.478403	-1.902132	-0.504443
C	4.453993	-0.208710	0.866646
H	4.277050	-0.561895	1.892954
C	4.038918	1.285186	0.765011
H	4.495927	1.826994	1.604955
H	4.461380	1.708097	-0.153226
H	5.541899	-0.250129	0.718136
H	3.419051	-0.606876	-1.017395
O	1.660838	-2.350894	-1.715676
C	-1.290577	-0.960763	-0.003041
H	-0.232921	-0.763487	-0.128376
C	-2.125921	0.089471	0.383533
C	-3.507849	-0.134819	0.539794
O	-4.347124	0.860334	0.979880
C	-4.723705	1.812596	-0.021463
H	-3.851417	2.346930	-0.419937
H	-5.392564	2.527739	0.468732
H	-5.258609	1.322920	-0.848466
C	-4.006900	-1.417946	0.308368
H	-5.073539	-1.583661	0.446550

Sum of electronic and zero-point Energies= -1190.335955

Sum of electronic and thermal Energies= -1190.311404

Sum of electronic and thermal Enthalpies= -1190.310460

Sum of electronic and thermal Free Energies= -1190.390855

#### jugcathanin-8-E2 (dmf)

C	2.038411	1.925211	0.270732
O	2.866450	2.354562	1.262501
H	2.292297	2.692576	1.973098
C	2.581488	1.332373	-0.878628
C	1.691787	0.956280	-1.895456
H	2.092276	0.534673	-2.815118
C	0.311766	1.063605	-1.737604
H	-0.370276	0.716135	-2.509589
C	-0.214648	1.557104	-0.541207
O	-1.588673	1.526918	-0.327431
C	0.642356	2.040052	0.456143
O	0.276008	2.654177	1.628191
C	-0.753531	2.066899	2.444564
H	-0.638401	2.519804	3.434101
H	-1.747569	2.296264	2.049341
H	-0.621217	0.980795	2.522908
C	-3.349502	-2.202986	0.362606
H	-3.836142	-3.158350	0.552107
C	-1.949518	-2.117519	0.362596
C	-1.091132	-3.352863	0.593174
H	-0.993322	-3.908406	-0.351190
H	-1.620808	-4.020956	1.284012
C	0.327705	-3.094746	1.134014
H	0.707495	-4.027310	1.581163
H	0.321690	-2.354511	1.943925
C	1.370981	-2.714292	0.077686
C	2.473231	-1.771417	0.538698
H	2.853766	-2.136394	1.505425
H	1.969701	-0.823470	0.783022
C	3.622412	-1.539818	-0.454418
H	4.278663	-2.420663	-0.437958
C	4.456178	-0.268805	-0.155350

H	4.408330	-0.038089	0.917758
C	4.052721	0.994354	-0.966089
H	4.665432	1.836982	-0.618820
H	4.307032	0.826664	-2.021321
H	5.514276	-0.465312	-0.377183
H	3.213801	-1.492445	-1.471636
O	1.314137	-3.158139	-1.056062
C	-1.369044	-0.865875	0.124217
H	-0.292324	-0.760776	0.135324
C	-2.143282	0.271330	-0.123650
C	-3.546567	0.178067	-0.124648
O	-4.345191	1.283626	-0.287533
C	-4.390648	1.808544	-1.620837
H	-3.404433	2.155815	-1.952443
H	-5.082598	2.656652	-1.592573
H	-4.769856	1.054206	-2.325499
C	-4.130031	-1.069254	0.118359
H	-5.216460	-1.130511	0.124396

Sum of electronic and zero-point Energies= -1190.334892

Sum of electronic and thermal Energies= -1190.310550

Sum of electronic and thermal Enthalpies= -1190.309606

Sum of electronic and thermal Free Energies= -1190.388807

#### pterocaraine-1-TS (dmf)

C	-2.099523	1.921335	0.077427
C	-1.288700	3.066132	-0.050111
H	-1.683783	4.071073	0.092782
C	0.090970	2.960365	-0.362772
O	0.815075	4.113361	-0.477352
H	1.736564	3.884961	-0.678371
C	0.687773	1.692665	-0.528262
O	2.066743	1.555354	-0.820988
C	-0.130825	0.589466	-0.392023
H	0.235862	-0.409713	-0.471522
C	-1.465489	0.712900	-0.129194
H	-2.025945	-0.186308	-0.083987
C	2.788531	-2.225048	0.713621
H	2.822602	-3.172314	1.250119
C	3.502206	-1.137116	1.221631
H	4.115881	-1.238317	2.114031
C	3.318246	0.142201	0.674598
O	3.844123	1.224026	1.308479
H	3.570009	2.019638	0.822595
C	2.544965	0.266249	-0.485997
C	2.025569	-0.875319	-1.112594
H	1.451346	-0.746792	-2.026636
C	1.987918	-2.106097	-0.437884
C	0.887465	-3.121360	-0.755160
H	1.281479	-4.141627	-0.671793
H	0.535369	-2.994293	-1.785986
C	-0.349189	-3.003521	0.217776
H	-0.068823	-2.478561	1.139441
H	-0.639931	-4.013884	0.547041
C	-1.657516	-2.381472	-0.323785
C	-2.739941	-2.007113	0.729680
H	-2.237912	-1.688934	1.652088
H	-3.209417	-2.972030	0.979799
C	-3.873318	-0.986075	0.323759
H	-3.835333	-0.825393	-0.761847
C	-3.940927	0.395229	1.100598
H	-3.342806	0.310243	2.019381
H	-4.979520	0.512089	1.436419
C	-3.578054	1.765308	0.415715
H	-3.908871	2.565269	1.092839
H	-4.182250	1.881717	-0.498486
H	-4.828910	-1.491994	0.504971
O	-1.859264	-2.254892	-1.517017

Sum of electronic and zero-point Energies= -1036.513189

Sum of electronic and thermal Energies= -1036.494033

Sum of electronic and thermal Enthalpies= -1036.493089

Sum of electronic and thermal Free Energies= -1036.559020

pterocaraine-1-E1 (dmf)

C	-2.578598	1.587061	0.294383
C	-2.002644	1.771856	-0.968228
H	-2.608957	1.707434	-1.869326
C	-0.624854	1.976761	-1.108075
O	-0.089438	2.101497	-2.351018
H	0.868875	2.232985	-2.254104
C	0.178272	1.985391	0.038854
O	1.565866	2.000593	-0.144267
C	-0.388854	1.895235	1.308383
H	0.258114	1.927356	2.182498
C	-1.765927	1.711277	1.436544
H	-2.203392	1.609309	2.427767
C	3.535820	-1.652533	0.279095
H	4.076036	-2.587534	0.417700
C	4.199018	-0.443350	0.518902
H	5.238318	-0.429817	0.839752
C	3.526683	0.772180	0.376940
O	4.166424	1.946118	0.635446
H	3.521351	2.665712	0.534265
C	2.182170	0.748460	-0.026018
C	1.533362	-0.453825	-0.287528
H	0.499662	-0.431958	-0.615197
C	2.193982	-1.681637	-0.125610
C	1.462506	-2.991441	-0.367673
H	2.124673	-3.818459	-0.085114
H	1.243794	-3.116117	-1.437882
C	0.129747	-3.131388	0.403255
H	0.226893	-2.765978	1.432844
H	-0.126641	-4.200425	0.479295
C	-1.080127	-2.483971	-0.278066
C	-2.097461	-1.828776	0.641133
H	-1.566666	-0.982162	1.103924
H	-2.302395	-2.515531	1.476946
C	-3.401735	-1.359612	-0.021995
H	-3.170273	-0.934891	-1.006710
C	-4.194068	-0.335555	0.830441
H	-3.917563	-0.445588	1.888806
H	-5.267765	-0.561725	0.776124
C	-4.024362	1.151020	0.412357
H	-4.552541	1.775838	1.146910
H	-4.523603	1.305024	-0.553516
H	-4.029121	-2.239730	-0.217452
O	-1.203647	-2.500290	-1.491422

Sum of electronic and zero-point Energies= -1036.584686

Sum of electronic and thermal Energies= -1036.564709

Sum of electronic and thermal Enthalpies= -1036.563765

Sum of electronic and thermal Free Energies= -1036.633035

pterocaraine-1-E2 (dmf)

C	-2.596777	1.519881	-0.431496
C	-2.044034	1.983651	0.771202
H	-2.667929	2.132512	1.650687
C	-0.665669	2.189828	0.893047
O	-0.148207	2.581108	2.087478
H	0.816032	2.653315	1.986493
C	0.161090	1.939148	-0.212673
O	1.543685	1.987056	-0.006652
C	-0.382290	1.573866	-1.439839
H	0.279307	1.400317	-2.285723
C	-1.758917	1.370388	-1.549181
H	-2.179572	1.050782	-2.500063
C	3.581780	-1.651751	-0.076971
H	4.143854	-2.583852	-0.111786
C	4.248661	-0.449140	-0.324727
H	5.313239	-0.436106	-0.548245
C	3.555030	0.765526	-0.305860
O	4.208898	1.932118	-0.566838

H	3.554619	2.650178	-0.559991
C	2.184881	0.742843	-0.016228
C	1.527270	-0.456999	0.247272
H	0.469749	-0.421681	0.476523
C	2.206132	-1.680013	0.206939
C	1.484340	-3.003541	0.421889
H	2.099087	-3.639120	1.073218
H	1.415228	-3.534133	-0.538703
C	0.067550	-2.914909	1.013549
H	0.038566	-2.265565	1.897723
H	-0.225510	-3.916134	1.367893
C	-1.030082	-2.507680	0.023928
C	-2.194516	-1.722757	0.610121
H	-1.768532	-0.774615	0.971521
H	-2.526326	-2.239148	1.524611
C	-3.378614	-1.459533	-0.332894
H	-2.997063	-1.242493	-1.338392
C	-4.303408	-0.312868	0.148226
H	-4.231759	-0.217418	1.241367
H	-5.350157	-0.571139	-0.063218
C	-4.042494	1.074950	-0.501249
H	-4.694601	1.810834	-0.009966
H	-4.348780	1.030838	-1.555019
H	-3.961824	-2.385379	-0.428562
O	-0.966531	-2.813699	-1.154075

Sum of electronic and zero-point Energies= -1036.584502

Sum of electronic and thermal Energies= -1036.564640

Sum of electronic and thermal Enthalpies= -1036.563695

Sum of electronic and thermal Free Energies= -1036.632105

pterocaraine-2-TS (dmf)

C	-2.182611	1.823913	0.086942
C	-1.427716	3.011789	-0.007679
H	-1.876644	3.991659	0.149652
C	-0.044294	2.987584	-0.319643
O	0.611817	4.180808	-0.432750
H	1.544937	4.007574	-0.634838
C	0.622586	1.754587	-0.482995
O	2.005840	1.675435	-0.779063
C	-0.136124	0.611422	-0.352815
H	0.295934	-0.362305	-0.388743
C	-1.485081	0.655728	-0.143516
H	-1.991579	-0.277726	-0.139223
C	2.731082	-2.148308	0.616692
H	2.751100	-3.115233	1.116767
C	3.396975	-1.072248	1.207817
H	3.955679	-1.200258	2.132266
C	3.222337	0.222297	0.699562
O	3.686231	1.288408	1.403615
H	3.420635	2.096070	0.932918
C	2.509901	0.379988	-0.495888
C	2.039612	-0.741489	-1.194768
H	1.487615	-0.573889	-2.117183
C	1.997164	-2.002496	-0.573674
C	1.021760	-3.089971	-1.034673
H	1.131143	-3.951882	-0.365079
H	1.299655	-3.442919	-2.038585
C	-0.499533	-2.726322	-1.137342
H	-1.003039	-3.270303	-1.635500
H	-0.650514	-1.883822	-1.828015
C	-1.326085	-2.428586	0.130045
C	-2.852375	-2.187773	-0.080596
H	-3.294548	-3.181080	0.094998
H	-3.042707	-1.969412	-1.139138
C	-3.596433	-1.143404	0.845620
H	-4.444975	-1.670744	1.296734
C	-4.180811	0.156644	0.148596
H	-5.251948	0.192740	0.385148
H	-4.127773	0.024366	-0.941785
C	-3.635958	1.591500	0.485895



H -4.303230 2.317356 -0.001073  
H -3.744185 1.772631 1.567334  
H -2.938435 -0.881375 1.684148  
O -0.836825 -2.425974 1.243662  
Sum of electronic and zero-point Energies= -1036.511534  
Sum of electronic and thermal Energies= -1036.492497  
Sum of electronic and thermal Enthalpies= -1036.491553  
Sum of electronic and thermal Free Energies= -1036.557040

pterocaraine-2-E1 (dmf)

C -2.596779 1.519833 0.431540  
C -2.044045 1.983693 -0.771127  
H -2.667957 2.132634 -1.650585  
C -0.665683 2.189877 -0.892973  
O -0.148243 2.581321 -2.087356  
H 0.816004 2.653460 -1.986398  
C 0.161082 1.939115 0.212725  
O 1.543676 1.987037 0.006698  
C -0.382283 1.573703 1.439857  
H 0.279335 1.400051 2.285704  
C -1.758912 1.370213 1.549200  
H -2.179545 1.050493 2.500052  
C 3.581817 -1.651753 0.076910  
H 4.143910 -2.583843 0.111681  
C 4.248696 -0.449129 0.324631  
H 5.313288 -0.436082 0.548079  
C 3.555047 0.765525 0.305816  
O 4.208911 1.932127 0.566764  
H 3.554637 2.650192 0.559895  
C 2.184875 0.742826 0.016269  
C 1.527268 -0.457027 -0.247185  
H 0.469735 -0.421735 -0.476387  
C 2.206154 -1.680031 -0.206908  
C 1.484347 -3.003552 -0.421839  
H 1.415187 -3.534107 0.538772  
H 2.099107 -3.639168 -1.073119  
C 0.067578 -2.914891 -1.013541  
H -0.225497 -3.916109 -1.367897  
H 0.038638 -2.265550 -1.897719  
C -1.030078 -2.507625 -0.023962  
C -2.194508 -1.722725 -0.610212  
H -2.526257 -2.239130 -1.524719  
H -1.768539 -0.774571 -0.971593  
C -3.378648 -1.459564 0.332768  
H -3.961862 -2.385417 0.428340  
C -4.303434 -0.312864 -0.148289  
H -5.350180 -0.571141 0.063155  
H -4.231808 -0.217368 -1.241430  
C -4.042505 1.074919 0.501250  
H -4.694589 1.810851 0.010010  
H -4.348796 1.030758 1.555018  
H -2.997133 -1.242608 1.338297  
O -0.966546 -2.813594 1.154053

Sum of electronic and zero-point Energies= -1036.584502  
Sum of electronic and thermal Energies= -1036.564640  
Sum of electronic and thermal Enthalpies= -1036.563695  
Sum of electronic and thermal Free Energies= -1036.632106

pterocaraine-2-E2 (dmf)

C -2.578602 1.587129 -0.294285  
C -2.002641 1.771626 0.968373  
H -2.608944 1.706975 1.869460  
C -0.624860 1.976487 1.108254  
O -0.089431 2.100918 2.351224  
H 0.868848 2.232670 2.254322  
C 0.178287 1.985399 -0.038674  
O 1.565880 2.000604 0.144440  
C -0.388854 1.895594 -1.308219  
H 0.258064 1.927991 -2.182361  
C -1.765942 1.711661 -1.436410

H -2.203387 1.609883 -2.427666  
C 3.535787 -1.652515 -0.279297  
H 4.075966 -2.587514 -0.418068  
C 4.198931 -0.443316 -0.519186  
H 5.238162 -0.429748 -0.840255  
C 3.526633 0.772210 -0.377019  
O 4.166343 1.946147 -0.635582  
H 3.521262 2.665728 -0.534346  
C 2.182201 0.748483 0.026217  
C 1.533465 -0.453814 0.287822  
H 0.499838 -0.431981 0.615719  
C 2.194053 -1.681624 0.125728  
C 1.462489 -2.991377 0.367791  
H 1.243516 -3.115934 1.437958  
H 2.124656 -3.818476 0.085467  
C 0.129844 -3.131278 -0.403381  
H -0.126511 -4.200313 -0.479590  
H 0.227127 -2.765741 -1.432906  
C -1.080153 -2.483989 0.277893  
C -2.097311 -1.828579 -0.641318  
H -2.302080 -2.515097 -1.477372  
H -1.566417 -0.981845 -1.103771  
C -3.401708 -1.359651 0.021700  
H -4.029015 -2.239901 0.216802  
C -4.194056 -0.335505 -0.830595  
H -5.267752 -0.561674 -0.776194  
H -3.917629 -0.445475 -1.888988  
C -4.024334 1.151031 -0.412370  
H -4.552513 1.775908 -1.146873  
H -4.523632 1.304916 0.553495  
H -3.170487 -0.935133 1.006568  
O -1.203848 -2.500552 1.491226

Sum of electronic and zero-point Energies= -1036.584687  
Sum of electronic and thermal Energies= -1036.564709  
Sum of electronic and thermal Enthalpies= -1036.563765  
Sum of electronic and thermal Free Energies= -1036.633040

pterocaraine-3-TS (dmf)

C -1.927996 2.036204 0.121028  
C -1.053377 3.135149 -0.011352  
H -1.398150 4.161068 0.111699  
C 0.318504 2.958342 -0.325187  
O 1.093556 4.073278 -0.477165  
H 2.002628 3.797974 -0.675608  
C 0.854244 1.659197 -0.456554  
O 2.218638 1.437444 -0.768534  
C -0.019339 0.605988 -0.287101  
H 0.297530 -0.410587 -0.317085  
C -1.354011 0.795216 -0.069865  
H -1.949417 -0.085084 -0.047504  
C 2.600921 -2.435332 0.638984  
H 2.540190 -3.392517 1.155163  
C 3.432310 -1.440640 1.160143  
H 4.043806 -1.628343 2.039997  
C 3.368032 -0.132943 0.653033  
O 3.997083 0.874265 1.315058  
H 3.793052 1.707334 0.858127  
C 2.599454 0.100334 -0.493563  
C 1.962001 -0.966668 -1.142629  
H 1.375989 -0.749642 -2.032386  
C 1.798753 -2.202624 -0.493860  
C 0.565025 -3.057843 -0.799986  
H 0.818843 -4.123911 -0.752352  
H 0.211854 -2.855577 -1.818142  
C -0.634956 -2.801877 0.197986  
H -0.335948 -2.153085 1.033703  
H -0.914352 -3.750321 0.681022  
C -1.953169 -2.241764 -0.385796  
C -3.159335 -2.018468 0.581861  
H -3.034612 -2.712511 1.423823

H	-4.030342	-2.359794	0.006611
C	-3.537605	-0.625254	1.230392
H	-4.354313	-0.875326	1.920186
C	-4.036152	0.549873	0.302905
H	-5.116402	0.663765	0.459820
H	-3.922744	0.265437	-0.752066
C	-3.406406	1.974019	0.496998
H	-3.995151	2.688158	-0.096709
H	-3.531846	2.286917	1.545742
H	-2.713553	-0.291383	1.871628
O	-2.095332	-2.075990	-1.584394

Sum of electronic and zero-point Energies= -1036.505595

Sum of electronic and thermal Energies= -1036.486629

Sum of electronic and thermal Enthalpies= -1036.485685

Sum of electronic and thermal Free Energies= -1036.550991

#### pterocaraine-3-E1 (dmf)

C	-2.294038	1.895169	0.379180
C	-1.705834	2.169601	-0.863645
H	-2.313675	2.230560	-1.764526
C	-0.316974	2.255331	-0.994049
O	0.232616	2.443272	-2.222919
H	1.199604	2.439540	-2.122866
C	0.482276	2.060029	0.141543
O	1.855243	1.878068	-0.060197
C	-0.089020	1.919592	1.401756
H	0.556901	1.793961	2.268105
C	-1.478735	1.853321	1.522654
H	-1.925938	1.691359	2.501062
C	3.199965	-2.066068	0.167370
H	3.581231	-3.082337	0.252140
C	4.049004	-0.995494	0.470164
H	5.074697	-1.167730	0.789106
C	3.583631	0.318585	0.390898
O	4.403531	1.358756	0.708622
H	3.882764	2.176816	0.647215
C	2.256317	0.534821	-0.011216
C	1.419049	-0.530901	-0.331542
H	0.401420	-0.337827	-0.654341
C	1.873774	-1.855523	-0.236793
C	0.953732	-3.018968	-0.567819
H	1.505678	-3.950758	-0.396326
H	0.700485	-2.997088	-1.637211
C	-0.368658	-3.080654	0.228151
H	-0.249953	-2.691105	1.250307
H	-0.672513	-4.131158	0.362842
C	-1.573530	-2.393822	-0.408391
C	-2.872335	-2.423612	0.395303
H	-2.786533	-3.163085	1.200546
H	-3.681036	-2.748850	-0.273819
C	-3.216696	-1.038162	1.004798
H	-3.904784	-1.193888	1.847203
C	-3.847718	-0.045406	0.010185
H	-4.908707	-0.300763	-0.126800
H	-3.369811	-0.158849	-0.970888
C	-3.738100	1.445218	0.437254
H	-4.357494	2.048807	-0.239850
H	-4.140972	1.575099	1.451152
H	-2.301737	-0.613022	1.437546
O	-1.514676	-1.859850	-1.504931

Sum of electronic and zero-point Energies= -1036.582852

Sum of electronic and thermal Energies= -1036.563061

Sum of electronic and thermal Enthalpies= -1036.562117

Sum of electronic and thermal Free Energies= -1036.630342

#### pterocaraine-3-E2 (dmf)

C	-2.310124	1.933347	-0.240316
C	-1.547953	2.151324	0.914295
H	-2.022379	2.203998	1.892063
C	-0.151658	2.201507	0.849339

O	0.562640	2.327394	1.999346
H	1.506200	2.363087	1.771138
C	0.476294	2.040414	-0.393542
O	1.858091	1.833992	-0.400025
C	-0.271134	1.961064	-1.565212
H	0.244497	1.861019	-2.517823
C	-1.663749	1.918419	-1.489154
H	-2.247045	1.791959	-2.399140
C	3.214524	-2.079190	0.109992
H	3.607339	-3.082969	0.263146
C	4.098606	-0.993802	0.128428
H	5.163438	-1.142216	0.294622
C	3.624946	0.305839	-0.052378
O	4.487324	1.361334	-0.020096
H	3.977648	2.173360	-0.174225
C	2.247543	0.496375	-0.253571
C	1.372362	-0.586619	-0.290940
H	0.317847	-0.416664	-0.473757
C	1.841515	-1.897083	-0.103172
C	0.891919	-3.083267	-0.158663
H	1.430092	-3.967038	0.204382
H	0.629028	-3.290090	-1.206348
C	-0.424938	-2.947967	0.635010
H	-0.302378	-2.323078	1.532511
H	-0.728465	-3.934028	1.020683
C	-1.630801	-2.430888	-0.145158
C	-2.934042	-2.283367	0.638485
H	-2.856410	-2.835205	1.583044
H	-3.740071	-2.740321	0.047818
C	-3.277036	-0.800119	0.939950
H	-3.984063	-0.774647	1.780702
C	-3.876675	-0.030843	-0.252230
H	-4.937132	-0.302652	-0.358164
H	-3.379561	-0.346624	-1.177945
C	-3.761119	1.514987	-0.138547
H	-4.348540	1.968969	-0.948136
H	-4.196129	1.855153	0.811165
H	-2.367071	-0.300247	1.296506
O	-1.567769	-2.160538	-1.333968

Sum of electronic and zero-point Energies= -1036.582349

Sum of electronic and thermal Energies= -1036.562531

Sum of electronic and thermal Enthalpies= -1036.561586

Sum of electronic and thermal Free Energies= -1036.629810

#### myricatomentogenin-1-TS (dmf)

C	2.949679	-0.002294	-0.166099
O	4.286501	0.051374	-0.416690
H	4.536688	0.992382	-0.377560
C	2.262801	-1.232380	-0.215564
C	0.916241	-1.144097	0.063975
H	0.341699	-2.036329	0.074560
C	0.236349	0.011581	0.326082
H	-0.814603	-0.092681	0.473431
C	0.883452	1.234889	0.365724
O	0.164518	2.418177	0.633046
C	2.270242	1.222189	0.124699
O	3.050558	2.360442	0.075261
C	3.207840	3.048078	1.331411
H	2.250312	3.455203	1.676004
H	3.620472	2.375725	2.095745
H	3.908934	3.867108	1.144041
C	-3.599405	1.347823	-0.722320
H	-4.486018	0.941761	-1.207559
C	-3.115706	0.747367	0.455479
C	-3.556999	-0.656710	0.874333
H	-4.650508	-0.734459	0.834199
H	-3.256642	-0.859471	1.909423
C	-2.964888	-1.786539	-0.052547
H	-2.683166	-1.377154	-1.030446
H	-3.760246	-2.517175	-0.270714

C	-1.792741	-2.641511	0.482380
C	-1.038828	-3.516910	-0.558952
H	-1.015835	-2.979501	-1.515496
H	-1.716289	-4.368854	-0.729529
C	0.391813	-4.072472	-0.191500
H	0.340478	-5.163042	-0.290752
C	1.614979	-3.593819	-1.080186
H	2.142947	-4.501318	-1.400617
C	2.740484	-2.644082	-0.526075
H	3.188917	-3.097322	0.372843
H	3.542777	-2.624516	-1.276402
H	1.220915	-3.142238	-2.002101
H	0.582562	-3.890103	0.874298
O	-1.518984	-2.680611	1.667358
C	-2.000940	1.347042	1.062977
H	-1.610140	0.939428	1.991882
C	-1.213800	2.264618	0.354389
C	-1.687357	2.834265	-0.833309
O	-0.941730	3.722515	-1.542858
H	-0.091377	3.827033	-1.082734
C	-2.936891	2.422289	-1.321048
H	-3.316743	2.874381	-2.234565

Sum of electronic and zero-point Energies= -1150.998748  
Sum of electronic and thermal Energies= -1150.976817  
Sum of electronic and thermal Enthalpies= -1150.975872  
Sum of electronic and thermal Free Energies= -1151.048648

#### myricatomentogenin-1-E1 (dmf)

C	1.773321	1.737969	-0.388334
O	2.370491	2.011077	-1.580357
H	1.660039	2.270771	-2.194182
C	2.542833	1.246016	0.680521
C	1.890678	1.030318	1.901736
H	2.474672	0.684048	2.752204
C	0.508337	1.185900	2.043801
H	0.006042	0.953041	2.979198
C	-0.247574	1.563754	0.936943
O	-1.637753	1.540956	1.001072
C	0.380345	1.890009	-0.271415
O	-0.291301	2.243600	-1.419249
C	-1.009105	3.491999	-1.368737
H	-1.870140	3.422725	-0.695308
H	-0.349757	4.307877	-1.044860
H	-1.356744	3.681049	-2.388612
C	-3.596616	-1.853462	-0.415711
H	-4.140767	-2.714199	-0.800890
C	-2.227367	-1.965445	-0.140202
C	-1.480951	-3.272223	-0.355442
H	-2.123010	-3.948018	-0.933104
H	-1.296915	-3.767891	0.609009
C	-0.121768	-3.133358	-1.075642
H	-0.183966	-2.424183	-1.910119
H	0.146081	-4.105921	-1.519128
C	1.058442	-2.779172	-0.165724
C	2.114602	-1.865814	-0.766426
H	1.598623	-0.912351	-0.957044
H	2.367990	-2.245587	-1.768578
C	3.379370	-1.648753	0.077918
H	3.999244	-2.553298	0.014156
C	4.209633	-0.416511	-0.362054
H	5.280527	-0.655927	-0.309144
C	3.994462	0.866776	0.488066
H	4.441949	0.711114	1.478689
H	4.548769	1.688583	0.013881
H	4.000855	-0.188020	-1.415405
H	3.094754	-1.557119	1.133756
O	1.132950	-3.214521	0.970913
C	-1.561323	-0.829736	0.348506
H	-0.505682	-0.877392	0.589792
C	-2.236009	0.372789	0.534870

C	-3.611549	0.474671	0.267356
O	-4.280335	1.648180	0.454367
H	-3.648756	2.302262	0.795608
C	-4.284554	-0.651600	-0.206696
H	-5.347477	-0.570653	-0.423888

Sum of electronic and zero-point Energies= -1151.068202  
Sum of electronic and thermal Energies= -1151.045405  
Sum of electronic and thermal Enthalpies= -1151.044460  
Sum of electronic and thermal Free Energies= -1151.120132

#### myricatomentogenin-1-E2 (dmf)

C	-2.122733	-1.657210	0.298395
O	-2.979614	-1.859588	1.336481
H	-2.459431	-2.289097	2.039608
C	-2.579251	-1.067127	-0.890261
C	-1.661019	-0.945450	-1.944399
H	-2.000433	-0.531458	-2.892297
C	-0.316766	-1.281057	-1.792964
H	0.396310	-1.124419	-2.598546
C	0.137645	-1.765208	-0.563251
O	1.502496	-1.940168	-0.346239
C	-0.766840	-2.011435	0.472511
O	-0.450858	-2.601600	1.676332
C	0.366834	-1.844318	2.590962
H	1.402024	-1.785665	2.240439
H	-0.038229	-0.834724	2.735869
H	0.334726	-2.390135	3.538832
C	3.813383	1.522420	-0.112163
H	4.444626	2.408611	-0.072907
C	2.462048	1.616836	0.249518
C	1.848207	2.930387	0.706846
H	2.589297	3.727440	0.572668
H	1.623934	2.890108	1.782515
C	0.548560	3.329842	-0.027735
H	0.634831	3.158717	-1.107779
H	0.388235	4.412687	0.099594
C	-0.728411	2.676014	0.511072
C	-1.786499	2.328410	-0.522242
H	-1.313391	1.588466	-1.185585
H	-1.943646	3.210878	-1.162378
C	-3.121054	1.795991	0.022729
H	-3.686706	2.636909	0.445872
C	-3.977090	1.077413	-1.054531
H	-5.024304	1.399526	-0.973988
C	-3.970771	-0.474904	-0.983377
H	-4.555770	-0.794732	-0.114408
H	-4.487725	-0.862658	-1.873053
H	-3.644142	1.391944	-2.053876
H	-2.922816	1.120010	0.863659
O	-0.871133	2.453879	1.702105
C	1.685150	0.450456	0.178338
H	0.638601	0.474031	0.460451
C	2.231603	-0.754052	-0.255441
C	3.587202	-0.842994	-0.610913
O	4.129843	-2.018407	-1.034728
H	3.418905	-2.680133	-1.064434
C	4.372827	0.308547	-0.529501
H	5.421068	0.245385	-0.813422

Sum of electronic and zero-point Energies= -1151.064355  
Sum of electronic and thermal Energies= -1151.041649  
Sum of electronic and thermal Enthalpies= -1151.040705  
Sum of electronic and thermal Free Energies= -1151.115632

#### myricatomentogenin-2-TS (dmf)

C	0.104496	2.954427	-0.067549
O	0.192753	4.304284	0.086254
H	1.128450	4.537744	-0.051619
C	-1.141856	2.309686	0.062558
C	-1.093196	0.942539	-0.112096
H	-1.995816	0.379277	-0.095090

C	0.048470	0.222416	-0.312653
H	-0.077171	-0.834440	-0.328014
C	1.278295	0.829783	-0.501460
O	2.409329	0.047138	-0.828146
C	1.303515	2.233772	-0.379561
O	2.406419	3.037996	-0.567215
C	3.615769	2.672870	0.118506
H	4.249179	3.565315	0.112209
H	3.406753	2.379747	1.155764
H	4.130941	1.860315	-0.406209
C	1.190726	-3.624561	0.647767
H	0.752761	-4.468715	1.178824
C	0.540680	-3.102579	-0.486374
C	-0.936574	-3.389655	-0.770909
H	-1.135415	-4.466605	-0.708057
H	-1.192188	-3.073433	-1.789266
C	-1.912854	-2.657767	0.233643
H	-1.361979	-2.183456	1.058454
H	-2.551575	-3.404054	0.729760
C	-2.890136	-1.607779	-0.341754
C	-3.876782	-0.901616	0.640106
H	-4.014450	-1.567450	1.502365
H	-4.829333	-0.877506	0.093796
C	-3.640503	0.540100	1.245438
H	-4.462962	0.659260	1.962855
C	-3.656117	1.789561	0.283936
H	-3.680101	1.454274	-0.761850
C	-2.515576	2.856111	0.430386
H	-2.499356	3.235966	1.464401
H	-2.778718	3.720704	-0.195911
H	-4.602867	2.322113	0.440718
H	-2.729163	0.528808	1.854434
O	-2.969368	-1.402563	-1.540272
C	1.183033	-2.047757	-1.156585
H	0.726642	-1.623951	-2.047694
C	2.204058	-1.321457	-0.527051
C	2.822355	-1.829491	0.621651
O	3.810139	-1.152252	1.265990
H	3.961205	-0.317818	0.791459
C	2.357498	-3.043955	1.150983
H	2.849180	-3.450806	2.031891

Sum of electronic and zero-point Energies= -1150.990850  
Sum of electronic and thermal Energies= -1150.969223  
Sum of electronic and thermal Enthalpies= -1150.968279  
Sum of electronic and thermal Free Energies= -1151.039590

#### myricatomentogenin-2-E1 (dmf)

C	-1.683104	1.929592	-0.304859
O	-2.445546	2.173478	-1.404956
H	-1.829633	2.407673	-2.122342
C	-2.286257	1.459036	0.874303
C	-1.465614	1.276593	1.995917
H	-1.920150	0.957728	2.931930
C	-0.076393	1.402441	1.920420
H	0.558644	1.171023	2.771872
C	0.508543	1.727017	0.697671
O	1.884775	1.595963	0.527366
C	-0.285992	2.064051	-0.402131
O	0.208248	2.373327	-1.647587
C	1.020220	3.560893	-1.724026
H	1.233657	3.711412	-2.786428
H	0.475806	4.429272	-1.329876
H	1.958460	3.429092	-1.174608
C	3.333053	-2.253584	-0.150158
H	3.746761	-3.249307	-0.301064
C	1.975309	-2.020824	-0.408147
C	1.068895	-3.130441	-0.915894
H	1.641555	-4.065545	-0.914953
H	0.796715	-2.932922	-1.962681
C	-0.238712	-3.354945	-0.125873

H	-0.116265	-3.126808	0.943580
H	-0.511864	-4.421878	-0.154606
C	-1.470707	-2.611723	-0.634823
C	-2.758482	-2.809179	0.162824
H	-2.642200	-3.665703	0.837802
H	-3.564954	-3.046946	-0.544741
C	-3.136987	-1.551880	0.990190
H	-3.819797	-1.862106	1.793368
C	-3.792132	-0.423815	0.171602
H	-3.312679	-0.357182	-0.812031
C	-3.717739	0.973404	0.848734
H	-4.111203	0.915792	1.872780
H	-4.357288	1.669700	0.292044
H	-4.846731	-0.678270	-0.010367
H	-2.232169	-1.181460	1.489954
O	-1.440007	-1.907610	-1.631770
C	1.477435	-0.724514	-0.197333
H	0.434325	-0.512230	-0.404298
C	2.307776	0.291643	0.269523
C	3.669201	0.052161	0.521959
O	4.482711	1.044062	0.982494
H	3.936738	1.835950	1.118614
C	4.174158	-1.229711	0.302611
H	5.225996	-1.418339	0.506611

Sum of electronic and zero-point Energies= -1151.065972  
Sum of electronic and thermal Energies= -1151.043270  
Sum of electronic and thermal Enthalpies= -1151.042326  
Sum of electronic and thermal Free Energies= -1151.117783

#### myricatomentogenin-2-E2 (dmf)

C	-1.787300	2.023041	0.231732
O	-2.527179	2.383466	1.316246
H	-1.897200	2.729636	1.973775
C	-2.404358	1.411133	-0.867534
C	-1.607017	1.127909	-1.987255
H	-2.073386	0.693981	-2.869941
C	-0.226021	1.299490	-1.959828
H	0.396433	0.997182	-2.798264
C	0.388898	1.767701	-0.795698
O	1.774658	1.690620	-0.681292
C	-0.385679	2.202414	0.285245
O	0.061564	2.802968	1.436478
C	1.159363	2.226572	2.167657
H	1.111230	2.669912	3.166932
H	1.052154	1.138147	2.245435
H	2.117519	2.478658	1.703308
C	3.471142	-2.021015	0.176143
H	3.955073	-2.967703	0.410955
C	2.072640	-1.955253	0.103094
C	1.221977	-3.200636	0.303441
H	1.819890	-3.934777	0.857125
H	1.011993	-3.654270	-0.676544
C	-0.126564	-3.013712	1.027577
H	-0.088328	-2.203436	1.771091
H	-0.359618	-3.917429	1.612741
C	-1.345532	-2.790254	0.134923
C	-2.678993	-2.573129	0.849432
H	-2.585890	-2.886477	1.896374
H	-3.428946	-3.218598	0.371522
C	-3.148781	-1.094590	0.798941
H	-3.880552	-0.938954	1.603575
C	-3.770425	-0.671663	-0.545420
H	-3.203074	-1.129060	-1.365747
C	-3.813199	0.863744	-0.778426
H	-4.371754	1.354641	0.026670
H	-4.353416	1.057906	-1.715127
H	-4.792774	-1.072676	-0.611058
H	-2.293304	-0.451296	1.042055
O	-1.268944	-2.803176	-1.082988
C	1.487368	-0.714916	-0.194994

H	0.409409	-0.633064	-0.262151
C	2.274169	0.415267	-0.414802
C	3.674840	0.339610	-0.345007
O	4.449641	1.443083	-0.548697
H	3.861586	2.188010	-0.754687
C	4.264442	-0.889986	-0.048879
H	5.349203	-0.946375	0.011932

Sum of electronic and zero-point Energies= -1151.062284

Sum of electronic and thermal Energies= -1151.039601

Sum of electronic and thermal Enthalpies= -1151.038656

Sum of electronic and thermal Free Energies= -1151.113894

myricatomentogenin-3-TS (dmf)

C	0.215265	2.922966	-0.213750
O	0.288294	4.261491	-0.448899
H	-0.622441	4.602645	-0.386251
C	1.381960	2.130608	-0.255527
C	1.165580	0.793136	-0.001838
H	1.995221	0.129290	0.043643
C	-0.056736	0.218683	0.198620
H	-0.052374	-0.842027	0.287204
C	-1.213004	0.973999	0.277261
O	-2.449678	0.359407	0.566182
C	-1.067841	2.360216	0.075168
O	-2.122193	3.251827	0.064792
C	-2.775422	3.439329	1.335028
H	-3.269002	2.516204	1.660076
H	-2.056697	3.763527	2.099836
H	-3.524948	4.221254	1.178973
C	-1.605404	-3.514956	-0.615809
H	-1.244507	-4.436082	-1.071560
C	-0.958831	-3.003324	0.525051
C	0.454193	-3.446256	0.917426
H	0.523116	-4.541003	0.917022
H	0.685233	-3.108730	1.934804
C	1.573531	-2.892936	-0.052172
H	1.138011	-2.422860	-0.945745
H	2.159113	-3.735832	-0.449193
C	2.618571	-1.914150	0.531242
C	3.755282	-1.399206	-0.408173
H	3.881854	-2.141874	-1.207007
H	4.657817	-1.438251	0.216537
C	3.741326	0.008040	-1.131614
H	4.627707	-0.024887	-1.778484
C	3.829105	1.322064	-0.263615
H	4.837919	1.736615	-0.385464
C	2.828457	2.490464	-0.571166
H	3.150573	3.370553	0.003649
H	2.918045	2.781405	-1.630008
H	3.743574	1.069950	0.802149
H	2.888225	0.050950	-1.818863
O	2.627453	-1.626295	1.715109
C	-1.504252	-1.840416	1.095464
H	-1.048951	-1.418561	1.988009
C	-2.394730	-1.041646	0.364840
C	-3.007597	-1.543516	-0.789167
O	-3.868452	-0.790881	-1.524549
H	-3.923038	0.086710	-1.109378
C	-2.665233	-2.834479	-1.221266
H	-3.153158	-3.235111	-2.107049

Sum of electronic and zero-point Energies= -1150.991331

Sum of electronic and thermal Energies= -1150.969612

Sum of electronic and thermal Enthalpies= -1150.968668

Sum of electronic and thermal Free Energies= -1151.040367

myricatomentogenin-3-E1 (dmf)

C	1.414931	2.011275	-0.420506
O	1.966037	2.266058	-1.639391
H	1.223142	2.384322	-2.258259
C	2.235138	1.689531	0.672552

C	1.616630	1.507718	1.918216
H	2.239191	1.297050	2.786176
C	0.227410	1.490176	2.058136
H	-0.243067	1.261105	3.010917
C	-0.567342	1.655359	0.924615
O	-1.928560	1.370630	0.982800
C	0.012608	1.985764	-0.304139
O	-0.688638	2.145288	-1.476866
C	-1.650044	3.217015	-1.506307
H	-2.525290	2.976136	-0.893929
H	-1.199169	4.154855	-1.157053
H	-1.954069	3.320328	-2.552106
C	-3.122202	-2.381900	-0.384429
H	-3.470764	-3.343286	-0.758056
C	-1.775306	-2.222009	-0.031428
C	-0.792665	-3.377374	-0.133877
H	-1.302758	-4.216341	-0.622077
H	-0.525070	-3.721271	0.875688
C	0.520317	-3.092294	-0.894695
H	0.375971	-2.358919	-1.702365
H	0.859738	-4.007262	-1.405752
C	1.707548	-2.641429	-0.048157
C	3.000124	-2.338516	-0.803385
H	2.941166	-2.763632	-1.812567
H	3.828367	-2.833421	-0.277749
C	3.272891	-0.813854	-0.904022
H	3.955930	-0.640070	-1.746754
C	3.871884	-0.193150	0.372571
H	4.943754	-0.436444	0.419736
C	3.697486	1.346509	0.484455
H	4.276689	1.700435	1.347835
H	4.105515	1.839651	-0.405736
H	3.407834	-0.655520	1.253005
H	2.335189	-0.311681	-1.171167
O	1.639193	-2.536355	1.166362
C	-1.363187	-0.965416	0.441736
H	-0.331612	-0.816982	0.740765
C	-2.265376	0.091400	0.539448
C	-3.617457	-0.080727	0.199025
O	-4.506520	0.948632	0.305264
H	-4.031485	1.718361	0.658877
C	-4.036729	-1.328393	-0.262748
H	-5.081242	-1.459555	-0.537142

Sum of electronic and zero-point Energies= -1151.065652

Sum of electronic and thermal Energies= -1151.042960

Sum of electronic and thermal Enthalpies= -1151.042016

Sum of electronic and thermal Free Energies= -1151.116982

myricatomentogenin-3-E2 (dmf)

C	1.867883	1.965583	0.193202
O	2.712509	2.280767	1.212068
H	2.164128	2.693350	1.903863
C	2.367351	1.331352	-0.956166
C	1.468722	1.093575	-2.005646
H	1.842158	0.655160	-2.928915
C	0.101150	1.326825	-1.865125
H	-0.598509	1.056927	-2.652214
C	-0.391252	1.821057	-0.656478
O	-1.764394	1.812278	-0.419216
C	0.489775	2.217264	0.355546
O	0.134749	2.842444	1.529673
C	-0.691303	2.114956	2.460629
H	-1.725617	2.056259	2.108178
H	-0.294481	1.106737	2.632277
H	-0.656689	2.685038	3.394043
C	-3.503258	-1.953580	0.017754
H	-3.989245	-2.923340	0.111778
C	-2.145339	-1.823771	0.343200
C	-1.335622	-3.006518	0.849663
H	-1.971886	-3.898710	0.807954

H	-1.084937	-2.852951	1.909144
C	-0.022757	-3.309890	0.094833
H	-0.104899	-3.078200	-0.977942
H	0.182861	-4.391474	0.131863
C	1.240883	-2.641582	0.629891
C	2.535921	-2.947662	-0.120467
H	2.387248	-3.825754	-0.760320
H	3.308562	-3.198248	0.619428
C	3.007018	-1.753081	-0.992946
H	3.672466	-2.141267	-1.776443
C	3.734991	-0.639250	-0.216824
H	4.769588	-0.957191	-0.020917
C	3.755039	0.731954	-0.951070
H	4.464960	1.395986	-0.443429
H	4.111472	0.597717	-1.981589
H	3.260842	-0.501381	0.762668
H	2.133589	-1.342635	-1.515924
O	1.229677	-1.912236	1.609276
C	-1.556777	-0.557547	0.204640
H	-0.511554	-0.423556	0.460109
C	-2.295754	0.529847	-0.256848
C	-3.656686	0.394807	-0.574611
O	-4.383907	1.455444	-1.025097
H	-3.782840	2.214944	-1.102747
C	-4.253478	-0.859023	-0.428383
H	-5.305357	-0.968873	-0.683249

Sum of electronic and zero-point Energies= -1151.063290

Sum of electronic and thermal Energies= -1151.040706

Sum of electronic and thermal Enthalpies= -1151.039762

Sum of electronic and thermal Free Energies= -1151.114161

#### myricatomentogenin-4-TS (dmf)

C	0.689332	2.905077	-0.118355
O	0.931597	4.235597	0.036856
H	0.077000	4.687346	-0.084687
C	1.734583	1.972222	0.015878
C	1.357495	0.660472	-0.178073
H	2.106385	-0.091443	-0.149764
C	0.080873	0.236998	-0.410973
H	-0.053977	-0.819358	-0.466887
C	-0.967713	1.130993	-0.561404
O	-2.265191	0.657208	-0.857613
C	-0.651287	2.497166	-0.421850
O	-1.528439	3.547392	-0.587440
C	-2.772521	3.497992	0.129980
H	-3.146749	4.526110	0.161204
H	-3.499846	2.867789	-0.395018
H	-2.622442	3.134161	1.155003
C	-2.109877	-3.180002	0.709885
H	-1.934285	-4.109408	1.250068
C	-1.356196	-2.893897	-0.443980
C	-0.066712	-3.654151	-0.758587
H	0.256643	-3.452736	-1.786868
H	-0.240144	-4.734585	-0.680331
C	1.113831	-3.290374	0.221097
H	1.647247	-4.217527	0.485862
H	0.724340	-2.905561	1.171342
C	2.226238	-2.344984	-0.287823
C	3.140077	-1.698940	0.790724
H	3.775717	-2.529251	1.138018
H	2.519481	-1.440620	1.658233
C	4.061192	-0.488761	0.373532
H	5.092929	-0.789286	0.591055
C	3.833206	0.899985	1.103348
H	3.254210	0.721494	2.021047
C	3.203829	2.145210	0.374631
H	3.339324	3.009270	1.039182
H	3.791611	2.372721	-0.529435
H	4.821210	1.239468	1.440829
H	4.022269	-0.369988	-0.717409

O	2.418503	-2.173040	-1.477212
C	-1.663736	-1.706284	-1.126711
H	-1.129965	-1.458968	-2.040872
C	-2.425021	-0.704306	-0.507596
C	-3.149213	-0.989823	0.656352
O	-3.901195	-0.047814	1.285829
H	-3.825651	0.781192	0.784925
C	-3.044602	-2.273530	1.213766
H	-3.620174	-2.501959	2.108089

Sum of electronic and zero-point Energies= -1150.997825

Sum of electronic and thermal Energies= -1150.976102

Sum of electronic and thermal Enthalpies= -1150.975158

Sum of electronic and thermal Free Energies= -1151.046595

#### myricatomentogenin-4-E1 (dmf)

C	1.776421	1.591511	-0.521704
O	2.361346	1.631433	-1.751011
H	1.641242	1.761015	-2.394270
C	2.549564	1.331191	0.622190
C	1.897533	1.350558	1.863753
H	2.483398	1.186187	2.766560
C	0.512416	1.503020	1.970935
H	0.009388	1.447537	2.932936
C	-0.245586	1.660439	0.810950
O	-1.634728	1.641206	0.879379
C	0.382774	1.763800	-0.434014
O	-0.288777	1.896797	-1.627306
C	-1.033418	3.119026	-1.798103
H	-1.384998	3.114433	-2.833908
H	-1.891958	3.154393	-1.118929
H	-0.389980	3.992344	-1.629113
C	-3.620931	-1.866402	-0.179742
H	-4.176729	-2.762968	-0.449923
C	-2.223826	-1.923070	-0.063643
C	-1.467389	-3.212237	-0.351340
H	-1.326693	-3.320046	-1.437027
H	-2.091598	-4.060189	-0.041550
C	-0.084054	-3.341678	0.313031
H	0.204353	-4.405003	0.318591
H	-0.112218	-3.031864	1.365207
C	1.058547	-2.627754	-0.417446
C	2.171510	-2.077665	0.461785
H	2.481909	-2.876405	1.154070
H	1.702321	-1.321963	1.109669
C	3.383365	-1.487214	-0.275402
H	3.988818	-2.315051	-0.668792
C	4.265465	-0.582334	0.622787
H	4.141679	-0.880194	1.674170
C	4.008376	0.945203	0.495009
H	4.596399	1.457861	1.269019
H	4.389778	1.287965	-0.473351
H	5.325526	-0.748700	0.386276
H	3.037610	-0.928070	-1.152860
O	1.067806	-2.527736	-1.632249
C	-1.550598	-0.747621	0.296189
H	-0.473831	-0.745354	0.406629
C	-2.241149	0.441610	0.514781
C	-3.637909	0.492911	0.391981
O	-4.324878	1.651567	0.607105
H	-3.683738	2.340655	0.846168
C	-4.319991	-0.675740	0.045870
H	-5.403574	-0.638053	-0.044116

Sum of electronic and zero-point Energies= -1151.067176

Sum of electronic and thermal Energies= -1151.044495

Sum of electronic and thermal Enthalpies= -1151.043551

Sum of electronic and thermal Free Energies= -1151.118251

#### myricatomentogenin-4-E2 (dmf)

C	2.121786	1.730178	0.165281
O	2.983447	2.094768	1.153830

H	2.454968	2.575816	1.815878
C	2.589743	0.972714	-0.918806
C	1.675813	0.666521	-1.937565
H	2.025160	0.117989	-2.809909
C	0.327394	1.001874	-1.837286
H	-0.382895	0.706979	-2.605526
C	-0.139326	1.664121	-0.699545
O	-1.509207	1.845858	-0.521630
C	0.758419	2.079064	0.291875
O	0.462534	2.828080	1.404103
C	-0.634687	2.432064	2.248001
H	-0.467066	2.934952	3.205413
H	-1.591207	2.756258	1.827200
H	-0.640671	1.346123	2.402328
C	-3.824263	-1.568549	0.090463
H	-4.460192	-2.440305	0.237177
C	-2.442743	-1.667620	0.322531
C	-1.812465	-2.989846	0.739044
H	-1.790330	-3.668100	-0.126334
H	-2.462097	-3.470958	1.482175
C	-0.385027	-2.908218	1.308565
H	-0.164141	-3.851446	1.833589
H	-0.296692	-2.118073	2.064975
C	0.729614	-2.768174	0.265428
C	1.954999	-1.975140	0.699138
H	2.252690	-2.326822	1.699390
H	1.603909	-0.945063	0.864310
C	3.147552	-1.993649	-0.269415
H	3.656118	-2.962895	-0.176208
C	4.164575	-0.850816	-0.024241
H	4.126216	-0.540408	1.028958
C	3.989176	0.400194	-0.929932
H	4.719613	1.157578	-0.615671
H	4.240443	0.121015	-1.962005
H	5.183451	-1.225739	-0.193553
H	2.773527	-1.952184	-1.300099
O	0.632399	-3.279702	-0.836476
C	-1.667838	-0.518667	0.126567
H	-0.601036	-0.540649	0.306221
C	-2.238406	0.675595	-0.310960
C	-3.617626	0.767689	-0.542631
O	-4.190792	1.930732	-0.963118
H	-3.483154	2.584101	-1.089502
C	-4.404708	-0.368817	-0.331792
H	-5.475564	-0.299164	-0.510801
Sum of electronic and zero-point Energies= -1151.065801			
Sum of electronic and thermal Energies= -1151.043066			
Sum of electronic and thermal Enthalpies= -1151.042122			
Sum of electronic and thermal Free Energies= -1151.117575			

myricatomentogenin-5-TS (dmf)

C	-2.806066	1.209788	-0.160944
O	-4.057459	1.715951	0.015359
H	-4.667289	0.956292	0.000550
C	-1.686097	2.063860	-0.179212
C	-0.485302	1.415533	-0.372442
H	0.399447	1.995035	-0.483990
C	-0.326725	0.063338	-0.411290
H	0.679542	-0.282538	-0.403745
C	-1.406745	-0.800008	-0.475879
O	-1.173614	-2.176461	-0.702903
C	-2.679218	-0.210184	-0.348417
O	-3.883502	-0.876976	-0.406494
C	-4.022153	-2.049868	0.413895
H	-3.648870	-1.864107	1.429681
H	-5.093855	-2.267747	0.451736
H	-3.494499	-2.901795	-0.029763
C	2.800266	-2.334739	0.438833
H	3.792715	-2.203363	0.866215
C	2.481906	-1.703335	-0.776988

C	3.368405	-0.597473	-1.355477
H	3.469371	-0.728300	-2.441325
H	4.373493	-0.677951	-0.926788
C	2.870055	0.884822	-1.147112
H	1.861443	1.019211	-1.544399
H	3.510617	1.517349	-1.783915
C	3.030981	1.493235	0.263139
C	2.042697	2.508334	0.932191
H	2.633111	2.927340	1.755196
H	1.315545	1.842838	1.421036
C	1.263540	3.687819	0.229622
H	1.853355	4.595461	0.409292
C	-0.194522	3.969314	0.796844
H	-0.247279	3.546220	1.810440
C	-1.520658	3.563278	0.040178
H	-2.354826	3.968975	0.627489
H	-1.554835	4.088150	-0.928039
H	-0.271822	5.056790	0.928002
H	1.246084	3.582194	-0.862776
O	3.980589	1.136788	0.940219
C	1.196816	-1.941454	-1.300919
H	0.898070	-1.457744	-2.228707
C	0.192868	-2.502596	-0.497872
C	0.520557	-3.107531	0.722494
O	-0.430114	-3.646048	1.530959
H	-1.294422	-3.512379	1.106831
C	1.857876	-3.088478	1.143511
H	2.116841	-3.567893	2.084923

Sum of electronic and zero-point Energies= -1150.979512

Sum of electronic and thermal Energies= -1150.957959

Sum of electronic and thermal Enthalpies= -1150.957014

Sum of electronic and thermal Free Energies= -1151.028600

myricatomentogenin-5-E1 (dmf)

C	1.628452	1.840973	-0.563739
O	2.145893	2.005246	-1.812614
H	1.391929	2.192517	-2.400232
C	2.460906	1.477926	0.507713
C	1.874476	1.374482	1.778200
H	2.507366	1.135931	2.631208
C	0.493160	1.469540	1.964698
H	0.040054	1.290653	2.936515
C	-0.326168	1.703814	0.860333
O	-1.704490	1.548065	0.973629
C	0.237512	1.973045	-0.390581
O	-0.492406	2.195176	-1.534575
C	-1.346421	3.355862	-1.525990
H	-0.772482	4.256908	-1.273097
H	-1.742755	3.443868	-2.541725
H	-2.172409	3.230921	-0.817751
C	-3.347570	-2.022972	-0.426601
H	-3.816319	-2.935747	-0.791620
C	-1.955112	-1.867331	-0.521146
C	-1.094110	-2.944667	-1.172771
H	-1.456942	-3.100432	-2.198650
H	-1.243353	-3.901483	-0.654535
C	0.423829	-2.670901	-1.234209
H	0.638977	-1.659329	-1.594463
H	0.861043	-3.356718	-1.975871
C	1.157022	-2.973156	0.076673
C	2.166854	-1.980150	0.639744
H	2.642332	-2.472691	1.497439
H	1.569997	-1.150744	1.046898
C	3.252405	-1.404457	-0.296456
H	3.845523	-2.238548	-0.695709
C	4.199881	-0.417987	0.441706
H	4.199007	-0.659861	1.513892
C	3.906908	1.098187	0.264121
H	4.563354	1.650518	0.951720
H	4.189809	1.399155	-0.750142

H	5.230742	-0.582909	0.099287
H	2.795572	-0.909928	-1.163960
O	0.904131	-4.001293	0.683699
C	-1.400574	-0.677477	-0.036776
H	-0.333222	-0.516742	-0.092648
C	-2.198598	0.333404	0.496430
C	-3.588352	0.174316	0.583508
O	-4.384183	1.152867	1.102974
H	-3.814094	1.888194	1.380774
C	-4.152013	-1.019102	0.121358
H	-5.230600	-1.144120	0.190466

Sum of electronic and zero-point Energies= -1151.058671  
Sum of electronic and thermal Energies= -1151.035920  
Sum of electronic and thermal Enthalpies= -1151.034976  
Sum of electronic and thermal Free Energies= -1151.110862

#### myricatomentogenin-5-E2 (dmf)

C	-2.065280	-1.723790	0.202202
O	-2.872204	-1.940137	1.275748
H	-2.310222	-2.332113	1.968529
C	-2.583368	-1.090203	-0.938041
C	-1.737788	-0.966175	-2.049059
H	-2.131218	-0.525959	-2.963193
C	-0.391533	-1.324743	-1.987873
H	0.274986	-1.149264	-2.828478
C	0.142022	-1.803301	-0.789949
O	1.524511	-1.901871	-0.646573
C	-0.699702	-2.070584	0.298276
O	-0.344299	-2.661604	1.485874
C	0.780248	-2.147954	2.224441
H	0.774928	-1.051482	2.238020
H	0.660478	-2.525756	3.244428
H	1.723991	-2.514946	1.809623
C	3.644298	1.643070	-0.025759
H	4.232421	2.543224	0.147152
C	2.268881	1.745967	-0.288067
C	1.584457	3.106432	-0.374271
H	2.002810	3.654337	-1.231130
H	1.838812	3.699988	0.513734
C	0.046486	3.098703	-0.517428
H	-0.282820	2.441045	-1.328925
H	-0.267671	4.114208	-0.802060
C	-0.690523	2.790524	0.790413
C	-1.808015	1.753744	0.811023
H	-2.208814	1.747427	1.832465
H	-1.320494	0.781594	0.652573
C	-2.967779	1.907634	-0.199241
H	-3.427660	2.894286	-0.049874
C	-4.059812	0.818027	-0.023332
H	-4.083608	0.503812	1.028109
C	-3.950682	-0.444145	-0.925967
H	-4.717860	-1.157998	-0.594796
H	-4.203728	-0.163444	-1.956917
H	-5.042513	1.264259	-0.229485
H	-2.586038	1.898532	-1.229448
O	-0.356067	3.358620	1.817280
C	1.558257	0.559636	-0.500905
H	0.501067	0.598541	-0.716222
C	2.185609	-0.684799	-0.463843
C	3.559463	-0.780432	-0.202866
O	4.188365	-1.989655	-0.146845
H	3.530937	-2.679635	-0.333512
C	4.280410	0.398062	0.014305
H	5.345882	0.322483	0.221191

Sum of electronic and zero-point Energies= -1151.057028  
Sum of electronic and thermal Energies= -1151.034407  
Sum of electronic and thermal Enthalpies= -1151.033463  
Sum of electronic and thermal Free Energies= -1151.108641

#### myricatomentogenin-6-TS (dmf)

C	1.022617	2.803055	-0.048465
O	1.433803	4.090355	0.114349
H	0.647204	4.649840	-0.017790
C	1.944861	1.743297	0.052614
C	1.396683	0.494050	-0.131182
H	2.052930	-0.340254	-0.165786
C	0.066522	0.233963	-0.295289
H	-0.207433	-0.796584	-0.305124
C	-0.853012	1.255224	-0.472040
O	-2.192451	0.953922	-0.802049
C	-0.359481	2.570322	-0.348679
O	-1.097268	3.721524	-0.525740
C	-2.324939	3.837957	0.213019
H	-2.582129	4.901778	0.209295
H	-3.128059	3.271993	-0.273299
H	-2.195929	3.495738	1.248249
C	-2.509471	-2.959490	0.529038
H	-2.454414	-3.929039	1.022330
C	-1.666642	-2.686971	-0.565475
C	-0.425362	-3.538579	-0.844258
H	-0.004309	-3.294826	-1.827267
H	-0.694260	-4.601873	-0.865923
C	0.699209	-3.353420	0.251053
H	1.087449	-4.349736	0.516366
H	0.270464	-2.957068	1.178725
C	1.972906	-2.547261	-0.109699
C	2.721946	-1.895161	1.077196
H	3.061149	-2.744277	1.695536
H	1.976676	-1.388557	1.703185
C	3.993221	-0.995564	0.860897
H	4.340925	-0.771587	1.879999
C	4.119463	0.340774	0.023764
H	5.197734	0.550023	0.063923
C	3.429280	1.705947	0.389841
H	3.976158	2.496905	-0.142780
H	3.574306	1.918681	1.461299
H	3.907637	0.123719	-1.031733
H	4.764020	-1.648816	0.428767
O	2.385611	-2.488984	-1.253920
C	-1.823039	-1.440488	-1.192787
H	-1.211533	-1.196601	-2.057626
C	-2.512620	-0.401421	-0.550319
C	-3.319410	-0.674117	0.560383
O	-3.997039	0.306813	1.213745
H	-3.796083	1.151722	0.777653
C	-3.376806	-1.992120	1.040430
H	-4.019295	-2.210192	1.890657

Sum of electronic and zero-point Energies= -1150.990111  
Sum of electronic and thermal Energies= -1150.968425  
Sum of electronic and thermal Enthalpies= -1150.967480  
Sum of electronic and thermal Free Energies= -1151.039058

#### myricatomentogenin-6-E1 (dmf)

C	1.576238	1.879824	-0.341795
O	2.244728	2.193036	-1.484752
H	1.570610	2.456312	-2.136839
C	2.280517	1.372738	0.764585
C	1.557050	1.140909	1.942155
H	2.090963	0.797702	2.826421
C	0.164738	1.255331	1.987770
H	-0.395506	0.983922	2.878963
C	-0.522808	1.624422	0.833017
O	-1.906675	1.479284	0.768977
C	0.175560	2.003712	-0.317393
O	-0.421369	2.358791	-1.503678
C	-1.256432	3.532337	-1.465048
H	-1.535547	3.736394	-2.502936
H	-2.157854	3.352245	-0.869744
H	-0.703890	4.388188	-1.055563
C	-3.343946	-2.265432	-0.375337



H	-3.757093	-3.234921	-0.648864
C	-1.958796	-2.061241	-0.420616
C	-0.997367	-3.157431	-0.850643
H	-0.659629	-2.980894	-1.882537
H	-1.538536	-4.111228	-0.861390
C	0.258839	-3.300055	0.035444
H	0.630872	-4.335692	-0.032108
H	0.022733	-3.140479	1.095209
C	1.464632	-2.441345	-0.363977
C	2.435765	-2.119662	0.762623
H	2.535346	-3.031928	1.371081
H	1.918516	-1.405423	1.419648
C	3.838683	-1.620596	0.370605
H	4.461514	-1.660743	1.277020
C	4.004870	-0.226664	-0.271554
H	5.050736	-0.163723	-0.606690
C	3.743908	1.015214	0.627084
H	4.285218	1.863547	0.186114
H	4.175059	0.849482	1.623977
H	3.389527	-0.158517	-1.174466
H	4.273883	-2.354869	-0.323108
O	1.639383	-2.084600	-1.517021
C	-1.469132	-0.799409	-0.051581
H	-0.403928	-0.606552	-0.085509
C	-2.328024	0.215779	0.359153
C	-3.716886	0.006629	0.397928
O	-4.567213	0.993575	0.800872
H	-4.034542	1.766655	1.048853
C	-4.214135	-1.242319	0.023527
H	-5.288926	-1.406601	0.061604

Sum of electronic and zero-point Energies= -1151.065188  
Sum of electronic and thermal Energies= -1151.042459  
Sum of electronic and thermal Enthalpies= -1151.041515  
Sum of electronic and thermal Free Energies= -1151.117277

#### myricatomentogenin-6-E2 (dmf)

C	1.786969	1.881665	0.245649
O	2.575244	2.184343	1.315318
H	1.981724	2.531625	2.004952
C	2.344034	1.275408	-0.886500
C	1.495965	1.036801	-1.980173
H	1.915623	0.614077	-2.891028
C	0.125960	1.256993	-1.898475
H	-0.537426	0.990886	-2.717678
C	-0.432323	1.739031	-0.710525
O	-1.818615	1.698648	-0.557653
C	0.394555	2.119042	0.352178
O	0.027158	2.709777	1.533760
C	-1.174738	2.310012	2.215192
H	-1.082621	2.716550	3.226760
H	-2.061602	2.729668	1.731173
H	-1.254109	1.217818	2.267036
C	-3.491805	-2.076516	0.044138
H	-3.965224	-3.044761	0.199257
C	-2.100306	-1.952492	0.172118
C	-1.219080	-3.151304	0.490162
H	-0.957534	-3.674415	-0.441780
H	-1.802174	-3.865298	1.085359
C	0.093226	-2.832884	1.232080
H	0.427268	-3.737254	1.766442
H	-0.055920	-2.072093	2.009003
C	1.290495	-2.453323	0.351706
C	2.358858	-1.608578	1.033224
H	2.478239	-2.009431	2.051798
H	1.925254	-0.609298	1.182916
C	3.741053	-1.536474	0.358081
H	4.440127	-1.113208	1.094758
C	3.906726	-0.760840	-0.966132
H	4.919321	-0.984939	-1.332837
C	3.777695	0.786099	-0.914853

H	4.268517	1.187223	-1.813417
H	4.332403	1.177716	-0.054411
H	3.214092	-1.160862	-1.716231
H	4.081031	-2.567155	0.180662
O	1.388657	-2.852209	-0.796050
C	-1.538041	-0.685751	-0.028939
H	-0.468704	-0.547828	0.068583
C	-2.327070	0.414724	-0.359295
C	-3.717875	0.284003	-0.488253
O	-4.503587	1.352716	-0.803399
H	-3.924885	2.120406	-0.941620
C	-4.290167	-0.973958	-0.281020
H	-5.369051	-1.075586	-0.377666

Sum of electronic and zero-point Energies= -1151.061524  
Sum of electronic and thermal Energies= -1151.038943  
Sum of electronic and thermal Enthalpies= -1151.037999  
Sum of electronic and thermal Free Energies= -1151.112700

#### galeon-1-TS (dmf)

C	0.438890	3.062977	0.006503
H	0.610544	4.122897	0.174727
C	-0.864873	2.530419	0.121602
C	-0.981130	1.177712	-0.102245
H	-1.934718	0.715030	-0.057522
C	0.081198	0.364172	-0.386302
H	-0.150340	-0.672421	-0.489976
C	1.366143	0.846723	-0.511801
O	2.434480	-0.027552	-0.818364
C	1.552622	2.239167	-0.312750
O	2.833129	2.688737	-0.428223
C	3.084010	4.077181	-0.226122
H	4.160360	4.208133	-0.371236
H	2.813807	4.392102	0.791574
H	2.541403	4.695029	-0.955159
C	0.975492	-3.583212	0.722101
H	0.488613	-4.395780	1.259853
C	0.375897	-3.061019	-0.439482
C	-1.096517	-3.322592	-0.765255
H	-1.317825	-4.393464	-0.677693
H	-1.316852	-3.030649	-1.799181
C	-2.078839	-2.549386	0.196535
H	-1.565386	-2.257400	1.121039
H	-2.874801	-3.237860	0.522632
C	1.076362	-2.049768	-1.117108
H	0.668364	-1.637990	-2.037003
C	2.122742	-1.363315	-0.485621
C	2.692383	-1.872209	0.687742
O	3.702665	-1.219425	1.321750
H	3.878268	-0.402813	0.822947
C	2.156356	-3.045014	1.240704
H	2.606793	-3.452281	2.143219
C	-2.833599	-1.317300	-0.353728
C	-3.557908	-0.421440	0.692071
H	-2.985458	-0.440078	1.627969
H	-4.485315	-0.973053	0.914859
C	-3.934540	1.058359	0.292715
H	-3.781377	1.185640	-0.787076
C	-3.254137	2.237099	1.106811
H	-4.066970	2.893671	1.443487
C	-2.192075	3.200739	0.459290
H	-2.622421	3.652447	-0.449227
H	-2.040343	4.034292	1.159667
H	-2.813883	1.820318	2.024230
H	-5.015975	1.158201	0.442598
O	-2.916192	-1.096727	-1.547498

Sum of electronic and zero-point Energies= -1075.787011  
Sum of electronic and thermal Energies= -1075.766460  
Sum of electronic and thermal Enthalpies= -1075.765516  
Sum of electronic and thermal Free Energies= -1075.834915

## galeon-1-E1 (dmf)

C	-1.809646	1.647066	-0.723835
H	-2.285421	1.575662	-1.697289
C	-2.599085	1.506965	0.430113
C	-1.993368	1.643477	1.686397
H	-2.592349	1.571948	2.592295
C	-0.606000	1.797226	1.785982
H	-0.113332	1.833683	2.755272
C	0.175443	1.845565	0.637414
O	1.563144	1.844558	0.741956
C	-0.423280	1.825087	-0.638792
O	0.416819	1.928563	-1.698474
C	-0.134243	1.790203	-3.008348
H	0.711635	1.879763	-3.695672
H	-0.862943	2.583504	-3.223178
H	-0.609428	0.808445	-3.138686
C	3.586381	-1.718102	-0.021580
H	4.151070	-2.628486	-0.217074
C	2.188186	-1.773885	0.078228
C	1.437683	-3.082197	-0.127874
H	2.054567	-3.904876	0.256094
H	1.318518	-3.270056	-1.205219
C	0.041594	-3.163266	0.517377
H	0.052074	-2.785402	1.547467
H	-0.251850	-4.222993	0.588073
C	1.505085	-0.578858	0.340948
H	0.427207	-0.576064	0.438100
C	2.183005	0.629684	0.477326
C	3.581421	0.679196	0.367773
O	4.256596	1.856897	0.500770
H	3.600065	2.560919	0.630760
C	4.274890	-0.507939	0.121826
H	5.359348	-0.469543	0.042429
C	-1.087068	-2.495870	-0.276107
C	-2.215835	-1.896703	0.550281
H	-1.762230	-1.081699	1.134463
H	-2.515979	-2.639625	1.305776
C	-3.434451	-1.389146	-0.235862
H	-3.092605	-0.920620	-1.167107
C	-4.317314	-0.401677	0.567716
H	-5.376146	-0.585578	0.339019
C	-4.053494	1.105575	0.295779
H	-4.398117	1.342841	-0.719712
H	-4.674867	1.691326	0.987887
H	-4.202772	-0.598646	1.643490
H	-4.037758	-2.254600	-0.541721
O	-1.073824	-2.465557	-1.494756

Sum of electronic and zero-point Energies= -1075.857843

Sum of electronic and thermal Energies= -1075.836463

Sum of electronic and thermal Enthalpies= -1075.835519

Sum of electronic and thermal Free Energies= -1075.907551

## galeon-1-E2 (dmf)

C	-1.665469	1.936674	0.499241
H	-2.049523	2.165277	1.489583
C	-2.556226	1.485212	-0.493374
C	-2.068532	1.238283	-1.780789
H	-2.749799	0.923053	-2.568243
C	-0.695942	1.322849	-2.047771
H	-0.296526	1.066298	-3.026488
C	0.185386	1.662751	-1.032719
O	1.560401	1.574033	-1.240038
C	-0.293183	2.029496	0.244700
O	0.650045	2.405807	1.145627
C	0.223096	2.727633	2.469279
H	1.131192	2.996709	3.015899
H	-0.254671	1.866603	2.956199
H	-0.469253	3.580407	2.470066
C	3.413432	-1.752695	0.453760
H	3.920258	-2.596295	0.919610

C	2.113375	-1.914695	-0.043800
C	1.365859	-3.230769	0.085057
H	2.027208	-3.967895	0.556028
H	1.104844	-3.626965	-0.906232
C	0.061403	-3.132225	0.912142
H	0.211194	-2.523704	1.812168
H	-0.215945	-4.139807	1.261746
C	1.495393	-0.802464	-0.638804
H	0.497389	-0.891634	-1.055405
C	2.138464	0.429575	-0.692801
C	3.436926	0.588298	-0.181059
O	4.054672	1.800712	-0.219510
H	3.399127	2.444916	-0.537295
C	4.074927	-0.519978	0.378155
H	5.078962	-0.399097	0.779254
C	-1.159048	-2.636118	0.130200
C	-2.093466	-1.690719	0.866628
H	-1.508452	-0.769238	1.016493
H	-2.255858	-2.082934	1.882324
C	-3.428912	-1.383629	0.171416
H	-3.254061	-1.276509	-0.906222
C	-4.140166	-0.122650	0.727140
H	-5.216417	-0.318870	0.827655
C	-3.991785	1.159204	-0.138324
H	-4.564535	1.026488	-1.065899
H	-4.454816	1.995608	0.404934
H	-3.777242	0.086608	1.743658
H	-4.086559	-2.256484	0.281651
O	-1.353829	-2.988892	-1.021222

Sum of electronic and zero-point Energies= -1075.858098

Sum of electronic and thermal Energies= -1075.836713

Sum of electronic and thermal Enthalpies= -1075.835769

Sum of electronic and thermal Free Energies= -1075.908115

## galeon-2-TS (dmf)

C	0.322710	3.062215	0.054620
H	0.430375	4.133452	0.203625
C	-0.952830	2.459561	0.163858
C	-0.986339	1.099390	-0.043919
H	-1.908797	0.570349	-0.037982
C	0.132988	0.345283	-0.263378
H	-0.034492	-0.705562	-0.309882
C	1.384739	0.897533	-0.418130
O	2.493706	0.079197	-0.737995
C	1.484083	2.304730	-0.258674
O	2.730204	2.833696	-0.407420
C	2.890819	4.241736	-0.257289
H	2.617764	4.573760	0.754158
H	2.295325	4.796103	-0.996077
H	3.953341	4.438523	-0.427620
C	1.090292	-3.568854	0.618608
H	0.607464	-4.404953	1.122922
C	0.482078	-2.992705	-0.512475
C	-1.001747	-3.206447	-0.828045
H	-1.251084	-4.273835	-0.785028
H	-1.222288	-2.864393	-1.846295
C	-1.965029	-2.444604	0.167815
H	-1.410024	-2.002810	1.007795
H	-2.642715	-3.169044	0.644008
C	1.180502	-1.951083	-1.147398
H	0.756230	-1.487882	-2.035005
C	2.220726	-1.284246	-0.484675
C	2.796900	-1.846243	0.660819
O	3.799257	-1.217143	1.330314
H	3.965209	-0.371580	0.879027
C	2.273004	-3.051283	1.154384
H	2.730636	-3.499030	2.033828
C	-2.886825	-1.347534	-0.413119
C	-3.873767	-0.620279	0.554734
H	-4.078778	-1.306302	1.387471

H	-4.801170	-0.529935	-0.026586
C	-3.593828	0.787151	1.220948
H	-4.442069	0.922729	1.904735
C	-3.503481	2.069558	0.307031
H	-3.511809	1.774012	-0.750908
C	-2.307790	3.060892	0.528794
H	-2.508204	3.968898	-0.058390
H	-2.295650	3.386282	1.581290
H	-4.422577	2.650952	0.454957
H	-2.713374	0.709420	1.869329
O	-2.927737	-1.120472	-1.609454

Sum of electronic and zero-point Energies= -1075.779513

Sum of electronic and thermal Energies= -1075.759143

Sum of electronic and thermal Enthalpies= -1075.758198

Sum of electronic and thermal Free Energies= -1075.826931

#### galeon-2-E1 (dmf)

C	-1.664189	2.041657	-0.492531
H	-2.247656	2.142714	-1.403391
C	-2.323027	1.701072	0.702538
C	-1.580498	1.607911	1.885265
H	-2.079763	1.386711	2.826305
C	-0.184280	1.691872	1.844177
H	0.413835	1.522176	2.737021
C	0.463849	1.897480	0.634012
O	1.844016	1.734137	0.553533
C	-0.269372	2.147027	-0.544590
O	0.455889	2.397264	-1.663113
C	-0.246960	2.555534	-2.895487
H	-0.936493	3.409921	-2.857369
H	-0.803854	1.645626	-3.157752
H	0.520731	2.742566	-3.651559
C	3.286809	-2.123120	-0.083691
H	3.702113	-3.119669	-0.224799
C	1.915096	-1.909470	-0.272913
C	0.994983	-3.040270	-0.705211
H	1.551624	-3.981820	-0.626260
H	0.741412	-2.919050	-1.768506
C	-0.328437	-3.183364	0.076677
H	-0.223829	-2.863264	1.124248
H	-0.611363	-4.246324	0.136924
C	1.416327	-0.611521	-0.074081
H	0.360522	-0.417222	-0.224125
C	2.259163	0.429833	0.309049
C	3.636034	0.208104	0.488644
O	4.463995	1.224371	0.864691
H	3.919505	2.020324	0.981485
C	4.140671	-1.076217	0.287021
H	5.204450	-1.248387	0.437006
C	-1.544288	-2.478290	-0.518876
C	-2.848511	-2.595961	0.268396
H	-2.756118	-3.399849	1.008704
H	-3.646013	-2.876373	-0.433662
C	-3.224142	-1.275331	0.991922
H	-3.930599	-1.514611	1.798889
C	-3.842205	-0.201722	0.076511
H	-3.335950	-0.217437	-0.896725
C	-3.764745	1.242791	0.644491
H	-4.355987	1.904256	-0.003550
H	-4.217340	1.277327	1.645042
H	-4.895349	-0.454950	-0.114561
H	-2.325586	-0.882166	1.485077
O	-1.489143	-1.865594	-1.573408

Sum of electronic and zero-point Energies= -1075.855703

Sum of electronic and thermal Energies= -1075.834380

Sum of electronic and thermal Enthalpies= -1075.833436

Sum of electronic and thermal Free Energies= -1075.905398

#### galeon-2-E2 (dmf)

C	-1.343477	2.126691	0.583960
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H	-1.731107	2.269635	1.588435
C	-2.244347	1.881487	-0.466798
C	-1.749000	1.756297	-1.771175
H	-2.435843	1.605089	-2.601837
C	-0.369784	1.708238	-1.998535
H	0.029974	1.514297	-2.991500
C	0.510985	1.806882	-0.929394
O	1.859836	1.505428	-1.105988
C	0.039500	2.094230	0.367667
O	0.986682	2.246412	1.328313
C	0.552626	2.466432	2.670036
H	-0.037804	1.619110	3.044505
H	-0.036459	3.389714	2.753951
H	1.465693	2.563479	3.263999
C	3.040664	-2.225949	0.329647
H	3.380476	-3.182368	0.723922
C	1.729817	-2.100516	-0.150711
C	0.760329	-3.270579	-0.124278
H	1.290695	-4.148716	0.263203
H	0.446717	-3.518585	-1.147895
C	-0.514921	-3.058952	0.722139
H	-0.318929	-2.432621	1.605053
H	-0.853875	-4.023910	1.133015
C	1.330152	-0.851316	-0.653901
H	0.327057	-0.729180	-1.048980
C	2.202461	0.233892	-0.645465
C	3.511826	0.103274	-0.153860
O	4.355462	1.172421	-0.132090
H	3.839248	1.949559	-0.405728
C	3.926788	-1.140957	0.322483
H	4.938777	-1.242881	0.708683
C	-1.728049	-2.491621	-0.009534
C	-2.964420	-2.216350	0.844834
H	-2.848808	-2.701728	1.821357
H	-3.832748	-2.669588	0.346639
C	-3.207225	-0.696970	1.051120
H	-3.826138	-0.565529	1.949498
C	-3.885510	0.005480	-0.140360
H	-3.495142	-0.409407	-1.078021
C	-3.691300	1.547565	-0.171680
H	-4.346118	1.964718	-0.948770
H	-4.004099	1.984467	0.786803
H	-4.962209	-0.218882	-0.122322
H	-2.244423	-0.219939	1.275856
O	-1.725433	-2.281796	-1.212365

Sum of electronic and zero-point Energies= -1075.856087

Sum of electronic and thermal Energies= -1075.834801

Sum of electronic and thermal Enthalpies= -1075.833856

Sum of electronic and thermal Free Energies= -1075.905688

#### galeon-3-TS (dmf)

C	-0.652788	3.039822	0.084865
H	-0.871736	4.092903	0.240619
C	-1.686342	2.078180	0.162757
C	-1.305747	0.775641	-0.051407
H	-2.047907	0.019301	-0.096961
C	-0.008459	0.383508	-0.233959
H	0.151860	-0.670717	-0.276168
C	1.016971	1.292967	-0.377208
O	2.321713	0.858797	-0.703336
C	0.685543	2.664454	-0.214891
O	1.718066	3.543200	-0.347968
C	1.447950	4.933269	-0.190249
H	2.404285	5.440765	-0.347253
H	1.078303	5.160861	0.819483
H	0.720989	5.289568	-0.933447
C	2.186261	-3.102261	0.498748
H	2.019402	-4.073785	0.962293
C	1.387901	-2.704845	-0.590977
C	0.060184	-3.400981	-0.904001

H	0.205142	-4.487393	-0.949251
H	-0.315850	-3.087107	-1.885451
C	-1.052505	-3.112506	0.181578
H	-0.596391	-2.775714	1.119695
H	-1.547026	-4.065310	0.429541
C	1.687514	-1.464712	-1.178251
H	1.113087	-1.127975	-2.037575
C	2.482967	-0.528993	-0.501038
C	3.245622	-0.923687	0.604341
O	4.017928	-0.035029	1.284411
H	3.889111	0.836881	0.872661
C	3.152247	-2.253154	1.044715
H	3.757967	-2.567685	1.891749
C	-2.230009	-2.170775	-0.180266
C	-2.947106	-1.491042	1.012718
H	-2.176742	-1.113912	1.696827
H	-3.417410	-2.322539	1.565787
C	-4.089525	-0.430252	0.799582
H	-4.914289	-0.959920	0.302869
C	-4.019025	0.954621	0.035831
H	-3.803074	0.767087	-1.024434
C	-3.171394	2.200382	0.491420
H	-3.612092	3.085783	0.010920
H	-3.299691	2.357584	1.574502
H	-5.063590	1.295811	0.062024
H	-4.451099	-0.218767	1.816501
O	-2.603309	-2.031160	-1.330705

Sum of electronic and zero-point Energies= -1075.778717

Sum of electronic and thermal Energies= -1075.758259

Sum of electronic and thermal Enthalpies= -1075.757315

Sum of electronic and thermal Free Energies= -1075.826461

#### galeon-3-E1 (dmf)

C	-1.558695	1.950614	-0.514815
H	-2.055447	2.083531	-1.471718
C	-2.326010	1.586721	0.607212
C	-1.694684	1.467225	1.849833
H	-2.278007	1.227770	2.336678
C	-0.299640	1.556870	1.941463
H	0.213517	1.366387	2.881738
C	0.457031	1.796161	0.802946
O	1.839750	1.633825	0.840893
C	-0.167308	2.061875	-0.434421
O	0.657154	2.337652	-1.475374
C	0.070880	2.520690	-2.764175
H	0.904759	2.722884	-3.442173
H	-0.620224	3.374519	-2.772590
H	-0.458256	1.616726	-3.095124
C	3.314678	-2.097585	-0.298516
H	3.738825	-3.060134	-0.580019
C	1.923514	-1.938630	-0.240307
C	0.971073	-3.071641	-0.590843
H	1.506243	-4.023330	-0.484383
H	0.679958	-3.000467	-1.649560
C	-0.322766	-3.125570	0.246843
H	-0.131077	-2.880376	1.299321
H	-0.703540	-4.160108	0.250045
C	1.423426	-0.684690	0.137762
H	0.353736	-0.528719	0.194997
C	2.274025	0.375177	0.441329
C	3.667525	0.211372	0.371325
O	4.511481	1.241905	0.664970
H	3.968685	2.019276	0.875798
C	4.176755	-1.034391	0.000800
H	5.256338	-1.161695	-0.044940
C	-1.500925	-2.293560	-0.274474
C	-2.520971	-1.882520	0.778049
H	-2.031236	-1.125330	1.407670
H	-2.659096	-2.747965	1.444497
C	-3.898077	-1.403719	0.283085

H	-4.297723	-2.170158	-0.396832
C	-4.022914	-0.041590	-0.432506
H	-3.365222	-0.024442	-1.309702
C	-3.788897	1.240058	0.414700
H	-4.291242	2.072063	-0.099899
H	-4.280172	1.133673	1.391797
H	-5.051182	0.012241	-0.818993
H	-4.570534	-1.396340	1.154022
O	-1.620538	-2.026783	-1.458285

Sum of electronic and zero-point Energies= -1075.855002

Sum of electronic and thermal Energies= -1075.833660

Sum of electronic and thermal Enthalpies= -1075.832716

Sum of electronic and thermal Free Energies= -1075.904599

#### galeon-3-E2 (dmf)

C	-1.462553	1.927454	0.607644
H	-1.895167	2.014752	1.600232
C	-2.305474	1.652250	-0.481920
C	-1.754620	1.600231	-1.769468
H	-2.398517	1.434121	-2.630920
C	-0.369557	1.664198	-1.946599
H	0.078455	1.530385	-2.928921
C	0.463971	1.804251	-0.844679
O	1.837024	1.608788	-0.984054
C	-0.073234	2.006626	0.442985
O	0.823402	2.197553	1.443684
C	0.324233	2.359850	2.771050
H	1.204620	2.516146	3.400684
H	-0.212202	1.463512	3.111083
H	-0.337230	3.233558	2.846105
C	3.220653	-2.143335	0.199502
H	3.611701	-3.102047	0.536335
C	1.871648	-2.029920	-0.160063
C	0.905698	-3.198390	-0.062770
H	1.447358	-4.073328	0.316256
H	0.527142	-3.468238	-1.058908
C	-0.313226	-2.930757	0.849374
H	-0.025738	-2.357486	1.739962
H	-0.700527	-3.891455	1.227878
C	1.408602	-0.775595	-0.586902
H	0.374783	-0.661774	-0.892522
C	2.250398	0.332061	-0.612903
C	3.602046	0.212798	-0.247415
O	4.427632	1.297069	-0.264592
H	3.885057	2.073026	-0.483728
C	4.080523	-1.037435	0.146654
H	5.125319	-1.128395	0.436193
C	-1.525785	-2.274838	0.178807
C	-2.432653	-1.482278	1.108120
H	-1.885131	-0.559619	1.351163
H	-2.482341	-2.033491	2.059459
C	-3.864270	-1.181810	0.626653
H	-4.329906	-2.135553	0.337976
C	-4.097991	-0.187074	-0.530584
H	-3.563395	-0.528528	-1.424722
C	-3.767613	1.310773	-0.273833
H	-4.375364	1.906799	-0.969526
H	-4.084104	1.593067	0.739822
H	-5.169519	-0.243948	-0.771805
H	-4.429346	-0.826893	1.501606
O	-1.754398	-2.419532	-1.010740

Sum of electronic and zero-point Energies= -1075.854857

Sum of electronic and thermal Energies= -1075.833532

Sum of electronic and thermal Enthalpies= -1075.832588

Sum of electronic and thermal Free Energies= -1075.904599

#### galeon-4-TS (dmf)

C	-0.080578	3.143428	-0.249871
H	-0.046111	4.209508	-0.470683
C	-1.287309	2.416475	-0.289682

C	-1.172901	1.075573	0.012968
H	-2.040533	0.464598	0.024678
C	0.009630	0.454808	0.299154
H	-0.055346	-0.596495	0.470390
C	1.211308	1.137972	0.332859
O	2.412679	0.449280	0.615410
C	1.159838	2.524492	0.055311
O	2.295781	3.294828	-0.005246
C	2.989866	3.460846	1.238670
H	3.839602	4.118309	1.028588
H	3.358649	2.503961	1.628317
H	2.339776	3.934851	1.988211
C	1.448807	-3.361874	-0.686784
H	1.068002	-4.266245	-1.159563
C	0.835377	-2.879504	0.484924
C	-0.556328	-3.353312	0.909902
H	-0.767279	-3.044824	1.940952
H	-0.604811	-4.448926	0.884051
C	-1.700006	-2.802237	-0.025015
H	-2.401913	-3.621481	-0.248805
H	-1.293813	-2.506814	-1.000362
C	1.402960	-1.739420	1.076121
H	0.984432	-1.348153	2.000223
C	2.297429	-0.935465	0.356381
C	2.878845	-1.408997	-0.825667
O	3.743323	-0.646468	-1.546281
H	3.820700	0.213045	-1.097607
C	2.502923	-2.676502	-1.295945
H	2.964689	-3.055284	-2.205066
C	-2.595705	-1.656974	0.500429
C	-3.509770	-0.954374	-0.544194
H	-4.352139	-1.653287	-0.669848
H	-2.997121	-0.952307	-1.514445
C	-4.086637	0.475845	-0.209010
H	-5.176958	0.403047	-0.296738
C	-3.636866	1.684916	-1.131483
H	-3.172641	1.278188	-2.041538
C	-2.716957	2.845137	-0.600104
H	-2.728275	3.642633	-1.356350
H	-3.175578	3.284535	0.300419
H	-4.556211	2.181195	-1.468244
H	-3.897777	0.696219	0.849919
O	-2.635896	-1.365298	1.681081

Sum of electronic and zero-point Energies= -1075.784483  
Sum of electronic and thermal Energies= -1075.763665  
Sum of electronic and thermal Enthalpies= -1075.762721  
Sum of electronic and thermal Free Energies= -1075.832991

#### galeon-4-E1 (dmf)

C	-1.697739	1.958505	-0.634629
H	-2.119829	2.153467	-1.618949
C	-2.527104	1.605516	0.442105
C	-1.936359	1.408986	1.698145
H	-2.560332	1.170461	2.557134
C	-0.547193	1.451305	1.850792
H	-0.082010	1.232047	2.809401
C	0.264630	1.694607	0.747059
O	1.645074	1.547017	0.862562
C	-0.307322	1.999033	-0.502589
O	0.453520	2.223307	-1.619191
C	1.277166	3.397800	-1.591106
H	1.736981	3.468545	-2.581694
H	2.063808	3.325309	-0.830978
H	0.670124	4.294970	-1.406096
C	3.329242	-2.096957	-0.256359
H	3.805619	-3.027210	-0.561396
C	1.944809	-2.063822	-0.043402
C	1.088974	-3.309251	-0.211617
H	0.833944	-3.729463	0.772374
H	1.683532	-4.072152	-0.728590

C	-0.231262	-3.094219	-0.983146
H	-0.573332	-4.064256	-1.378383
H	-0.082046	-2.445081	-1.854582
C	1.369155	-0.841932	0.341718
H	0.304170	-0.776940	0.531512
C	2.146334	0.302646	0.491808
C	3.536117	0.258508	0.287945
O	4.305239	1.373920	0.441329
H	3.723224	2.104216	0.707904
C	4.118664	-0.952789	-0.085290
H	5.192999	-0.984632	-0.253660
C	-1.399694	-2.582130	-0.135187
C	-2.350384	-1.616179	-0.822937
H	-2.610186	-2.032363	-1.808864
H	-1.745963	-0.725011	-1.051417
C	-3.611959	-1.233271	-0.034460
H	-4.315855	-2.075588	-0.071005
C	-4.304289	0.047495	-0.566604
H	-4.031662	0.202344	-1.620414
C	-4.004240	1.345041	0.232626
H	-4.470718	2.188972	-0.295714
H	-4.493067	1.275734	1.213619
H	-5.394255	-0.089262	-0.555869
H	-3.350011	-1.110385	1.023956
O	-1.545134	-2.938879	1.021861

Sum of electronic and zero-point Energies= -1075.854361  
Sum of electronic and thermal Energies= -1075.832536  
Sum of electronic and thermal Enthalpies= -1075.831592  
Sum of electronic and thermal Free Energies= -1075.906259

#### galeon-4-E2 (dmf)

C	-1.809786	1.647066	0.723645
H	-2.285680	1.575758	1.697046
C	-2.599096	1.506790	-0.430371
C	-1.993257	1.643100	-1.686614
H	-2.592147	1.571391	-2.592559
C	-0.605881	1.796885	-1.786067
H	-0.113093	1.833220	-2.755301
C	0.175427	1.845455	-0.637422
O	1.563144	1.844558	-0.741805
C	-0.423413	1.825108	0.638729
O	0.416575	1.928730	1.698477
C	-0.134702	1.791053	3.008329
H	0.711055	1.881040	3.695746
H	-0.609844	0.809331	3.139125
H	-0.863489	2.584421	3.222605
C	3.586461	-1.718082	0.021647
H	4.151173	-2.628444	0.217176
C	2.188261	-1.773871	-0.078051
C	1.437788	-3.082185	0.128157
H	1.318705	-3.269989	1.205520
H	2.054657	-3.904876	-0.255812
C	0.041681	-3.163344	-0.517022
H	-0.251759	-4.223086	-0.587534
H	0.052132	-2.785656	-1.547177
C	1.505128	-0.578860	-0.340776
H	0.427242	-0.576103	-0.437835
C	2.183030	0.629678	-0.477280
C	3.581464	0.679189	-0.367880
O	4.256632	1.856876	-0.501054
H	3.600074	2.560919	-0.630820
C	4.274952	-0.507923	-0.121898
H	5.359416	-0.469518	-0.042578
C	-1.086981	-2.495831	0.276354
C	-2.215756	-1.896837	-0.550153
H	-2.515815	-2.639859	-1.305582
H	-1.762148	-1.081875	-1.134401
C	-3.434434	-1.389227	0.235850
H	-4.037752	-2.254646	0.541788
C	-4.317256	-0.401871	-0.567925

H	-4.202576	-0.598927	-1.643668
C	-4.053520	1.105418	-0.296129
H	-4.674816	1.691078	-0.988385
H	-4.398251	1.342815	0.719292
H	-5.376106	-0.585807	-0.339342
H	-3.092642	-0.920583	1.167053
O	-1.073725	-2.465273	1.494996
Sum of electronic and zero-point Energies= -1075.857842			
Sum of electronic and thermal Energies= -1075.836463			
Sum of electronic and thermal Enthalpies= -1075.835518			
Sum of electronic and thermal Free Energies= -1075.907550			

galeon-5-TS (dmf)

C	-3.084631	0.629031	-0.003052
H	-4.136922	0.843326	0.164572
C	-2.137613	1.681791	0.001023
C	-0.833548	1.306286	-0.218142
H	-0.065615	2.036060	-0.288085
C	-0.433115	0.002316	-0.313424
H	0.621707	-0.146275	-0.313868
C	-1.325056	-1.043403	-0.385106
O	-0.857485	-2.359080	-0.619582
C	-2.699585	-0.720515	-0.231970
O	-3.568995	-1.768183	-0.293343
C	-4.957734	-1.505663	-0.114497
H	-5.341774	-0.822371	-0.884956
H	-5.164675	-1.085951	0.880080
H	-5.457410	-2.474317	-0.208577
C	3.144762	-1.851912	0.328302
H	4.123035	-1.571924	0.716132
C	2.638792	-1.218796	-0.821803
C	3.234941	0.060055	-1.412020
H	2.638964	0.342935	-2.288434
H	4.255591	-0.117715	-1.780120
C	3.382855	1.328934	-0.475516
H	3.782928	2.123266	-1.119043
H	4.157435	1.100110	0.268544
C	1.392192	-1.662063	-1.293976
H	0.961814	-1.193726	-2.175938
C	0.548515	-2.436262	-0.485946
C	1.051399	-3.033353	0.675334
O	0.256792	-3.772227	1.494394
H	-0.642520	-3.751997	1.124145
C	2.391157	-2.798782	1.026673
H	2.785731	-3.274631	1.921783
C	2.212201	1.906565	0.365441
C	1.593972	3.271433	-0.042505
H	1.398049	3.254352	-1.125003
H	2.424930	3.986964	0.066968
C	0.348515	3.787825	0.777449
H	0.193049	3.105084	1.621633
C	-1.013765	4.029262	0.000990
H	-1.313339	5.068769	0.186663
C	-2.291412	3.167299	0.315553
H	-3.131591	3.612227	-0.238127
H	-2.548222	3.283620	1.380779
H	-0.823054	3.970960	-1.080625
H	0.638184	4.747157	1.222883
O	1.878020	1.344962	1.392498

Sum of electronic and zero-point Energies= -1075.775744  
Sum of electronic and thermal Energies= -1075.755416  
Sum of electronic and thermal Enthalpies= -1075.754471  
Sum of electronic and thermal Free Energies= -1075.822849

galeon-5-E1 (dmf)

C	2.130684	1.810053	-0.275497
H	2.799559	2.034316	-1.101853
C	2.606137	1.030649	0.794350
C	1.757266	0.778581	1.878782
H	2.121592	0.217898	2.736767

C	0.417686	1.174417	1.829086
H	-0.273766	0.906872	2.625474
C	-0.071773	1.843825	0.714828
O	-1.450461	2.016082	0.562834
C	0.793832	2.229343	-0.329410
O	0.234249	2.925052	-1.351285
C	1.068656	3.287873	-2.450889
H	1.467655	2.401195	-2.962348
H	1.899947	3.930021	-2.129193
H	0.425615	3.844480	-3.138450
C	-3.444458	-1.504916	-0.467281
H	-3.980702	-2.425700	-0.691721
C	-2.129097	-1.332221	-0.922761
C	-1.368338	-2.403177	-1.681893
H	-0.673928	-1.929750	-2.388106
H	-2.067018	-2.999999	-2.282662
C	-0.586204	-3.397941	-0.781447
H	-0.124070	-4.150719	-1.439944
H	-1.281942	-3.923415	-0.116460
C	-1.484404	-0.127477	-0.618282
H	-0.477151	0.040651	-0.981432
C	-2.095986	0.848745	0.162214
C	-3.412839	0.672289	0.614587
O	-4.027497	1.620185	1.376324
H	-3.379469	2.323414	1.549829
C	-4.083823	-0.508301	0.279843
H	-5.103418	-0.644190	0.634241
C	0.534908	-2.844855	0.101885
C	1.669024	-2.056248	-0.551896
H	1.292124	-1.033350	-0.690713
H	1.844825	-2.440986	-1.566444
C	2.974924	-2.023605	0.264145
H	2.722227	-1.913261	1.325211
C	3.971779	-0.916618	-0.164097
H	4.994455	-1.317118	-0.130396
C	3.964400	0.368004	0.711527
H	4.706519	1.066260	0.299460
H	4.300186	0.103526	1.723479
H	3.792072	-0.637295	-1.212531
C	3.460735	-3.004946	0.172790
O	0.526173	-3.063624	1.301906

Sum of electronic and zero-point Energies= -1075.852422  
Sum of electronic and thermal Energies= -1075.830983  
Sum of electronic and thermal Enthalpies= -1075.830038  
Sum of electronic and thermal Free Energies= -1075.902479

galeon-5-E2 (dmf)

C	1.691278	1.623029	0.740561
H	2.082606	1.456612	1.739681
C	2.563057	1.525192	-0.357903
C	2.071559	1.800515	-1.640556
H	2.740093	1.768718	-2.498935
C	0.704027	2.027487	-1.838493
H	0.295118	2.155748	-2.838435
C	-0.167419	1.996858	-0.757023
O	-1.548399	1.968285	-0.964342
C	0.324507	1.859065	0.557350
O	-0.601811	1.906129	1.548732
C	-0.184581	1.567541	2.872282
H	0.553560	2.284285	3.256778
H	0.232372	0.552218	2.905967
H	-1.087481	1.613830	3.487584
C	-3.158084	-1.799046	-0.155638
H	-3.588166	-2.767255	0.096450
C	-1.908817	-1.733015	-0.791257
C	-1.065121	-2.959287	-1.083999
H	-0.415175	-2.759186	-1.945482
H	-1.709944	-3.802333	-1.365390
C	-0.199628	-3.436414	0.114625
H	0.346454	-4.338545	-0.204105

H	-0.848376	-3.720174	0.951805
C	-1.403376	-0.466486	-1.109606
H	-0.453333	-0.383396	-1.626650
C	-2.077837	0.694407	-0.745866
C	-3.317877	0.625173	-0.095220
O	-3.973996	1.757051	0.279856
H	-3.368066	2.502160	0.127111
C	-3.862216	-0.635022	0.174474
H	-4.825066	-0.689493	0.678114
C	0.841365	-2.464382	0.673864
C	1.903858	-1.900265	-0.267804
H	1.434676	-1.050434	-0.783121
H	2.121923	-2.634336	-1.056110
C	3.195962	-1.440369	0.433638
H	2.928068	-0.936889	1.369843
C	4.104357	-0.522833	-0.423578
H	5.155768	-0.784121	-0.239548
C	3.969031	1.002589	-0.155319
H	4.667498	1.528175	-0.821389
H	4.292966	1.206839	0.874390
C	3.928013	-0.715673	-1.491872
H	3.761503	-2.335668	0.727193
O	0.825547	-2.173904	1.859370

Sum of electronic and zero-point Energies= -1075.853850

Sum of electronic and thermal Energies= -1075.832509

Sum of electronic and thermal Enthalpies= -1075.831564

Sum of electronic and thermal Free Energies= -1075.903675

#### galeon-6-TS (dmf)

C	0.186027	3.187852	-0.080758
H	0.169636	4.267853	0.058465
C	1.374444	2.445597	0.030223
C	1.235885	1.086009	-0.163249
H	2.095418	0.463322	-0.149426
C	0.036760	0.472476	-0.380561
H	0.072849	-0.592591	-0.440177
C	-1.148819	1.173656	-0.524485
O	-2.340508	0.471688	-0.834610
C	-1.067495	2.581056	-0.377235
O	-2.116441	3.445784	-0.537545
C	-3.376381	3.102924	0.048947
H	-3.913392	2.357764	-0.549775
H	-3.958826	4.029814	0.070719
H	-3.248327	2.739421	1.078225
C	-1.531030	-3.298784	0.693323
H	-1.201827	-4.190732	1.224793
C	-0.830875	-2.873441	-0.451342
C	0.570414	-3.399191	-0.766393
H	0.855929	-3.141300	-1.793289
H	0.585076	-4.493594	-0.692246
C	1.669339	-2.840508	0.216206
H	2.348624	-3.664393	0.487891
H	1.217390	-2.521879	1.163286
C	-1.333241	-1.747293	-1.122551
H	-0.844614	-1.401878	-2.030334
C	-2.260410	-0.898790	-0.499593
C	-2.933731	-1.320951	0.653377
O	-3.845068	-0.531578	1.282098
H	-3.910407	0.302578	0.788097
C	-2.611836	-2.573423	1.198589
H	-3.146047	-2.909348	2.084627
C	2.609894	-1.724064	-0.293276
C	3.400834	-0.931780	0.785206
H	4.170097	-1.640480	1.131539
H	2.746055	-0.783316	1.653291
C	4.099542	0.418356	0.366498
H	5.168266	0.299011	0.580327
C	3.640085	1.748589	1.095940
H	3.105374	1.476796	2.017591
C	2.802513	2.861359	0.362624

H	2.807701	3.751791	1.006611
H	3.328644	3.157641	-0.559223
H	4.556914	2.254099	1.426297
H	4.037138	0.528733	-0.724277
O	2.772870	-1.524295	-1.482687

Sum of electronic and zero-point Energies= -1075.783922

Sum of electronic and thermal Energies= -1075.763311

Sum of electronic and thermal Enthalpies= -1075.762367

Sum of electronic and thermal Free Energies= -1075.831657

#### galeon-6-E1 (dmf)

C	1.751445	1.793555	-0.780042
H	2.201259	1.818997	-1.770510
C	2.549613	1.630068	0.357901
C	1.928188	1.662254	1.618340
H	2.527181	1.580195	2.523440
C	0.538243	1.728235	1.717406
H	0.041760	1.678870	2.684249
C	-0.248297	1.789842	0.565671
O	-1.630760	1.662014	0.682097
C	0.354877	1.885887	-0.699973
O	-0.332081	1.962247	-1.875338
C	-1.435243	2.876157	-1.965256
H	-2.362208	2.440204	-1.577802
H	-1.557346	3.090238	-3.032036
H	-1.217793	3.810173	-1.431282
C	-3.359429	-2.072298	0.025104
H	-3.850424	-3.030991	-0.134400
C	-1.959346	-1.997469	0.006106
C	-1.114744	-3.232051	-0.272552
H	-0.981276	-3.352205	-1.357968
H	-1.669650	-4.116434	0.064878
C	0.284818	-3.241593	0.372112
H	0.644545	-4.281950	0.418642
H	0.251670	-2.886299	1.409512
C	-1.367203	-0.744850	0.226531
H	-0.289326	-0.641910	0.226612
C	-2.143638	0.389606	0.447924
C	-3.545559	0.307841	0.457407
O	-4.313472	1.414668	0.672314
H	-3.717702	2.168815	0.812416
C	-4.144414	-0.935084	0.246726
H	-5.230314	-0.999337	0.261836
C	1.364832	-2.487683	-0.410409
C	2.438572	-1.807135	0.424239
H	2.805182	-2.534691	1.165439
H	1.916409	-1.046377	1.023955
C	3.604373	-1.181796	-0.356348
H	4.274080	-1.986466	-0.688566
C	4.408423	-0.144230	0.466419
H	4.307979	-0.366518	1.538624
C	4.029458	1.341190	0.215943
H	4.606249	1.963870	0.914636
H	4.350809	1.618396	-0.796916
H	5.478637	-0.242192	0.238129
H	3.216884	-0.720049	-1.273220
O	1.356758	-2.454805	-1.628968

Sum of electronic and zero-point Energies= -1075.854148

Sum of electronic and thermal Energies= -1075.832419

Sum of electronic and thermal Enthalpies= -1075.831475

Sum of electronic and thermal Free Energies= -1075.905634

#### galeon-6-E2 (dmf)

C	1.684144	2.006487	0.638154
H	2.107275	2.226729	1.616686
C	2.512680	1.639948	-0.431931
C	1.922506	1.420930	-1.685640
H	2.546066	1.175585	-2.542844
C	0.534103	1.453366	-1.832129
H	0.065448	1.215464	-2.784677

C	-0.280338	1.709149	-0.731354
O	-1.658447	1.536335	-0.850285
C	0.289925	2.044849	0.511766
O	-0.431234	2.317260	1.637132
C	-1.544410	3.217629	1.537440
H	-1.338484	4.024253	0.822309
H	-1.672980	3.645934	2.537005
H	-2.464842	2.698422	1.250002
C	-3.287155	-2.141592	0.238700
H	-3.750068	-3.080950	0.536379
C	-1.902801	-2.086225	0.030340
C	-1.029897	-3.320075	0.195403
H	-0.764113	-3.730844	-0.789713
H	-1.615847	-4.094367	0.705156
C	0.283299	-3.089937	0.974403
H	0.636461	-4.056548	1.368210
H	0.121094	-2.445610	1.847085
C	-1.343556	-0.853585	-0.345542
H	-0.279012	-0.771097	-0.530711
C	-2.138120	0.279391	-0.492518
C	-3.527154	0.213000	-0.289980
O	-4.310049	1.321965	-0.430678
H	-3.739035	2.056126	-0.710830

C	-4.093479	-1.008409	0.073496
H	-5.167449	-1.057227	0.239870
C	1.448364	-2.559712	0.133278
C	2.380417	-1.579672	0.826303
H	2.637126	-1.989279	1.815752
H	1.762544	-0.695575	1.046660
C	3.643460	-1.183135	0.047289
H	4.358426	-2.015598	0.094201
C	4.313297	0.109139	0.579349
H	4.035979	0.260787	1.632437
C	3.993452	1.400012	-0.222432
H	4.448057	2.251908	0.303370
H	4.482832	1.335237	-1.203506
H	5.405408	-0.009800	0.570745
H	3.389381	-1.068617	-1.013980
O	1.605143	-2.913596	-1.023165

Sum of electronic and zero-point Energies= -1075.854171  
Sum of electronic and thermal Energies= -1075.832554  
Sum of electronic and thermal Enthalpies= -1075.831610  
Sum of electronic and thermal Free Energies= -1075.904393