Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Understanding the Mechanism and Origins of Stereoconvergent in Nickel-Catalyzed Hydroarylation of 1,3-Dienes with Aryl Boronates

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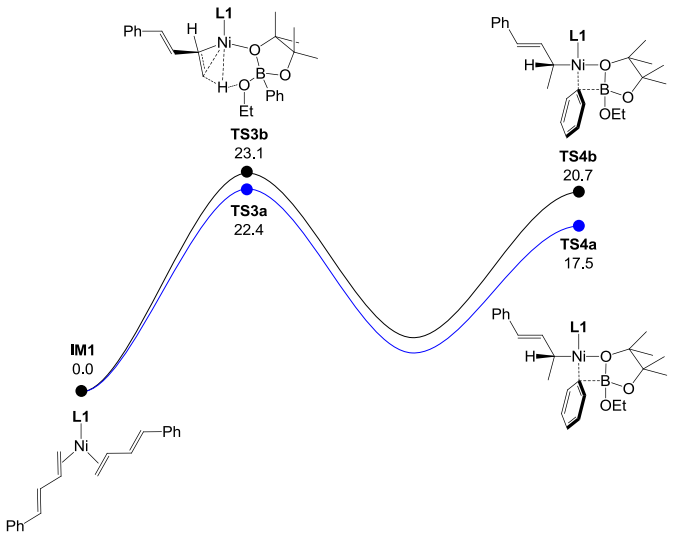


Fig. S1. Free energy profiles of the concerted hydronickelation and the transmetalation for the nickel-catalyzed hydroarylation of (*E*)-1,3-diene. Energies were obtained from B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-311++G**//B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-31G** calculations.

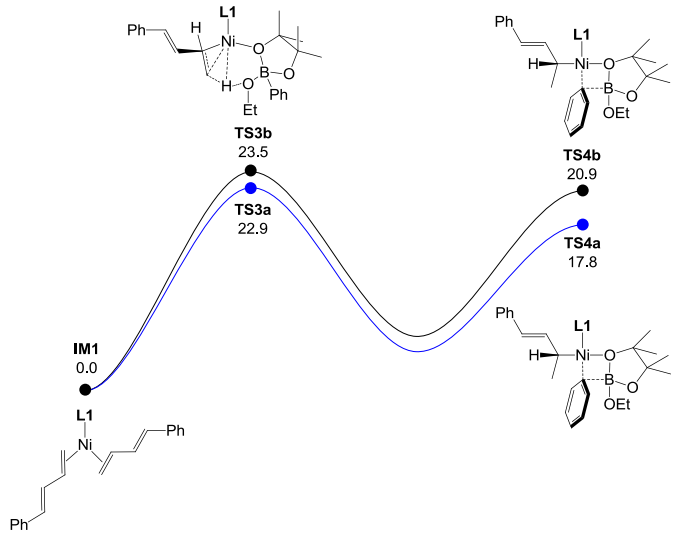


Fig. S2. Free energy profiles of the concerted hydronickelation and the transmetalation for the nickel-catalyzed hydroarylation of (*E*)-1,3-diene. Energies were obtained from B3LYP-D3(BJ)(SMD,EtOH)/def2-TZVP//B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-31G** calculations.

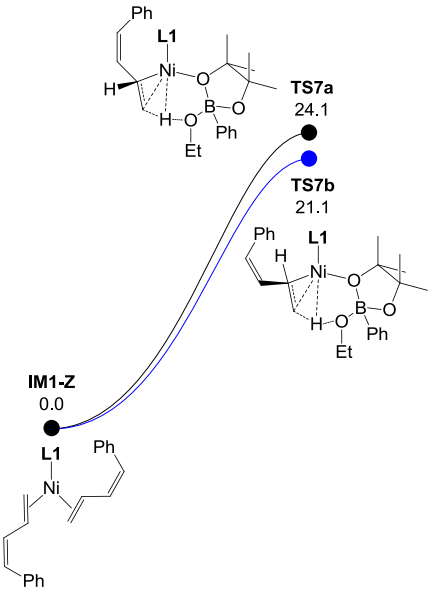


Fig. S3. Free energy profiles for hydronickelation of (*Z*)-diene. Energies were obtained from B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-311++G**//B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-31G** calculations.

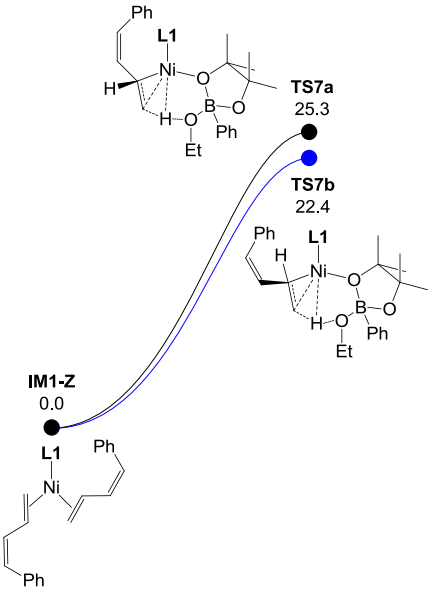
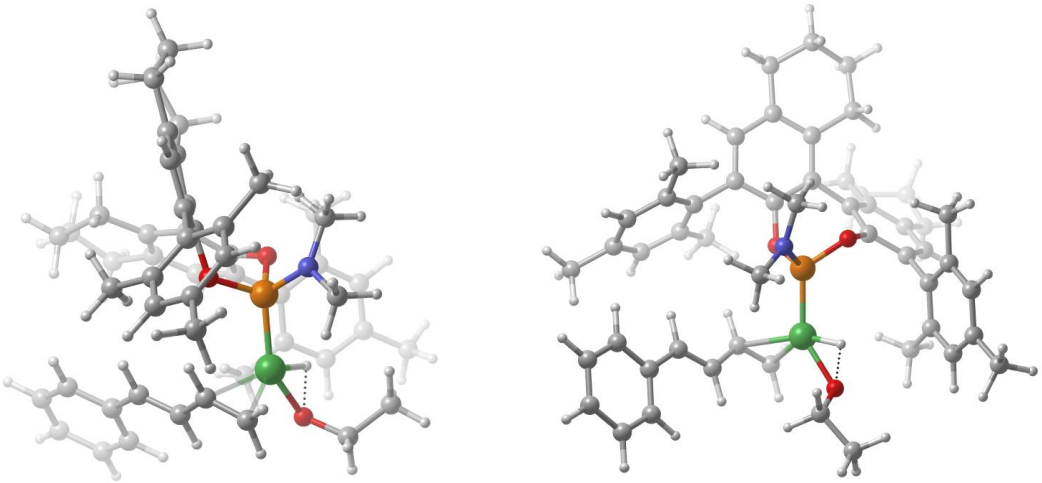


Fig. S4. Free energy profiles for hydronickelation of (*Z*)-diene. Energies were obtained from B3LYP-D3(BJ)(SMD,EtOH)/def2-TZVP//B3LYP-D3(BJ)(SMD,EtOH)/sdd-6-31G** calculations.



TS1c
$\Delta G^{\ddagger}$ = 42.2 kcal/mol

TS1d
$\Delta G^{\ddagger}$ = 42.5 kcal/mol

Fig. S5. Optimized structures for the oxidative addition of EtOH to Ni(0) center with coordinated 1,3-diene substrate.

1a

SCF energy in Ethanol: -387.203133 a.u.

Free energy in Ethanol: -387.070384 a.u.

C	-3.263700	0.382259	0.000007
C	-2.857675	-0.953028	0.000024
C	-1.500542	-1.270257	0.000020
C	-0.513740	-0.265997	-0.000002
C	-0.943055	1.076577	-0.000019
C	-2.297722	1.394055	-0.000015
H	-4.320548	0.634594	0.000011
H	-3.597656	-1.749063	0.000043
H	-1.190831	-2.312992	0.000034
H	-0.211118	1.878950	-0.000033
H	-2.604131	2.436943	-0.000026
C	0.896339	-0.661760	-0.000003
H	1.068661	-1.738836	-0.000016
C	1.981866	0.142643	-0.000024
H	1.863861	1.225691	-0.000046
C	3.346078	-0.351660	-0.000054
H	3.467111	-1.435486	-0.000183
C	4.438935	0.429616	0.000063
H	4.363452	1.514781	0.000192
H	5.440497	0.010721	0.000034

2a

SCF energy in Ethanol: -643.191059 a.u.

Free energy in Ethanol: -642.958135 a.u.

B	0.124331	-0.000098	-0.000392
O	-0.635306	1.127242	0.208511
O	-0.635521	-1.127245	-0.209435
C	-2.018976	0.785717	-0.082499
C	-2.018950	-0.785701	0.082561
C	-2.293455	1.247930	-1.520304
H	-1.653390	0.722857	-2.236386
H	-3.338716	1.087443	-1.805358
H	-2.076124	2.317931	-1.596157
C	-2.919169	1.543042	0.892514
H	-3.970947	1.272104	0.744237
H	-2.649848	1.341058	1.931684
H	-2.820070	2.620030	0.722086
C	-2.292321	-1.247796	1.520629
H	-2.075355	-2.317888	1.596236
H	-1.651354	-0.723006	2.236124
H	-3.337240	-1.086849	1.806652
C	-2.919804	-1.543205	-0.891737
H	-3.971490	-1.272261	-0.742980
H	-2.651023	-1.341505	-1.931111
H	-2.820580	-2.620145	-0.721078
C	1.677468	-0.000175	-0.000281
C	2.399911	1.196397	0.157731
C	2.400261	-1.196540	-0.158070
C	3.794666	1.199782	0.159340
H	1.856612	2.129910	0.280109
C	3.795016	-1.199573	-0.159207
H	1.857255	-2.130201	-0.280664
C	4.493710	0.000187	0.000196
H	4.337722	2.133379	0.283337
H	4.338341	-2.133038	-0.283026
H	5.581029	0.000314	0.000406

3a

SCF energy in Ethanol: -619.569257 a.u.

Free energy in Ethanol: -619.340730 a.u.

C	-5.028273	-0.965684	-0.025981
C	-4.767421	0.128374	0.799603
C	-3.503499	0.717578	0.800234
C	-2.468666	0.231987	-0.019133
C	-2.750924	-0.871484	-0.846973
C	-4.011930	-1.461030	-0.849190
H	-6.011445	-1.428357	-0.030767
H	-5.547589	0.524983	1.444188
H	-3.308109	1.570177	1.447054
H	-1.978479	-1.272122	-1.496873
H	-4.204590	-2.311970	-1.497599
C	-1.155846	0.897730	0.031515
H	-1.116615	1.754502	0.702390
C	-0.047563	0.560821	-0.646459
H	-0.068450	-0.299691	-1.314971
C	1.295801	1.255677	-0.587883
H	1.516952	1.599102	-1.610990
C	2.406557	0.271980	-0.213995
C	3.602145	0.236000	-0.942664
C	2.268146	-0.588939	0.883965
C	4.636638	-0.630591	-0.583743
H	3.724603	0.894085	-1.800777
C	3.299368	-1.456078	1.246622
H	1.340353	-0.583218	1.450496
C	4.488417	-1.479986	0.513836

H	5.555641	-0.644069	-1.164265
H	3.172488	-2.117058	2.100323
H	5.290563	-2.157621	0.793981
C	1.334058	2.494619	0.325207
H	0.589106	3.237151	0.017635
H	1.141199	2.224957	1.369603
H	2.322324	2.963304	0.280811

L1

SCF energy in Ethanol: -2099.336257 a.u.

Free energy in Ethanol: -2098.645475 a.u.

P	0.211955	-1.862544	-0.233618
N	-0.432658	-2.728501	1.057320
C	-0.899264	-4.084771	0.792877
H	-0.473506	-4.784036	1.526004
H	-1.995535	-4.151580	0.844380
H	-0.583544	-4.402232	-0.205945
C	-0.708938	-2.240402	2.403800
H	-0.392435	-1.202114	2.498210
H	-1.778983	-2.314239	2.635780
H	-0.157899	-2.840723	3.141944
O	1.098099	-0.792984	0.729025
O	-0.931799	-0.743493	-0.834168
C	1.634557	0.295436	0.053012
C	0.796182	1.383254	-0.220073
C	2.984898	0.267369	-0.327745
C	1.284405	2.443412	-1.026000
C	-0.613260	1.359782	0.287954
C	3.461270	1.372151	-1.035645
C	2.635842	2.437468	-1.416795
C	-1.461306	0.311805	-0.117294
C	-1.120183	2.368020	1.143072
H	4.509155	1.386930	-1.329328
C	-2.846625	0.337092	0.137986
C	-2.498074	2.401167	1.423937
C	-3.330615	1.414685	0.885605
C	-3.778702	-0.716280	-0.374355
C	-4.524905	-1.515328	0.519278
C	-3.953937	-0.892228	-1.770030
C	-5.384409	-2.498607	0.008921
C	-4.831963	-1.875046	-2.231323
C	-5.552246	-2.699325	-1.360177
H	-5.940967	-3.119742	0.708902
H	-4.958627	-1.998824	-3.305563
C	-4.461797	-1.344336	2.023506
H	-5.236874	-0.651165	2.377998
H	-4.636698	-2.300651	2.529078
H	-3.503494	-0.944082	2.360000
C	-6.498006	-3.751632	-1.891753
H	-7.397057	-3.297621	-2.329429
H	-6.027982	-4.353118	-2.679016
H	-6.825905	-4.432035	-1.098955
C	-3.232892	-0.025730	-2.778136
H	-3.293491	1.035929	-2.512498
H	-2.170275	-0.284703	-2.834235
H	-3.668088	-0.150456	-3.774935
C	3.881621	-0.885283	0.002284
C	4.277379	-1.788311	-1.007596
C	4.352959	-1.059068	1.321115
C	5.140621	-2.840143	-0.680154
C	5.218323	-2.120793	1.602410
C	5.628719	-3.021885	0.616069
H	5.435188	-3.538445	-1.461517
H	5.580071	-2.246694	2.621441
C	3.932744	-0.122725	2.431371
H	4.104469	0.926387	2.164280
H	2.863397	-0.227770	2.650107
H	4.487625	-0.334161	3.351077
C	3.769432	-1.660416	-2.427882
H	2.673658	-1.656438	-2.462691
H	4.104740	-0.731567	-2.903505
H	4.122688	-2.495631	-3.040902
C	6.589160	-4.144096	0.936996
H	6.434588	-5.005120	0.277528
H	7.633020	-3.824450	0.813580
H	6.476184	-4.485625	1.971855
C	3.233928	3.531347	-2.290355
C	2.334257	4.762165	-2.442786
C	0.895664	4.317567	-2.716740
C	0.345412	3.539458	-1.514356
H	0.248796	5.179399	-2.920943
H	2.358357	5.362388	-1.521849
H	2.712273	5.403287	-3.248323
H	3.432006	3.112116	-3.288654
H	4.214965	3.819351	-1.890107
H	0.144928	4.256981	-0.706571
H	-0.626664	3.097565	-1.760493
H	0.874440	3.684675	-3.615266

H	-4.400101	1.471581	1.076631
C	-3.122942	3.510102	2.259104
H	-3.577636	4.248033	1.579579
H	-3.951790	3.101800	2.851098
C	-0.175933	3.327547	1.857073
C	-2.123104	4.232614	3.168550
H	-1.848126	3.582104	4.011043
H	-2.589063	5.127695	3.598671
C	-0.861225	4.595099	2.380701
H	0.253838	2.784857	2.714155
H	0.678221	3.585564	1.227800
H	-1.131977	5.249218	1.538817
H	-0.159284	5.160043	3.006383

IM1

SCF energy in Ethanol: -3044.797090 a.u.

Free energy in Ethanol: -3043.793463 a.u.

P	-0.592789	0.997705	-1.145745
N	-1.411942	1.804367	-2.375337
C	-2.396573	1.236094	-3.291008
H	-3.339217	1.795264	-3.244659
H	-2.021900	1.286519	-4.324122
H	-2.592719	0.194876	-3.043337
C	-1.153982	3.225559	-2.582634
H	-0.332335	3.556853	-1.940714
H	-0.870991	3.413749	-3.628309
H	-2.040068	3.829916	-2.346147
O	-0.803863	-0.541446	-1.789474
O	-1.611182	0.874203	0.205124
C	-0.808647	-1.668848	-0.976560
C	-1.906132	-1.887558	-0.131105
C	0.252244	-2.585896	-1.075025
C	-1.861843	-2.959080	0.797994
C	-3.090292	-0.970830	-0.184456
C	0.205935	-3.691527	-0.222689
C	-0.793731	-3.870532	0.738745
C	-2.906670	0.391906	0.098200
C	-4.392485	-1.446009	-0.476769
H	1.003006	-4.428496	-0.291247
C	-3.991080	1.265705	0.308281
C	-5.489975	-0.584056	-0.301241
C	-5.269525	0.729019	0.128750
C	-3.812371	2.688854	0.737865
C	-4.259018	3.755481	-0.071788
C	-3.239226	2.974720	2.002123
C	-4.067257	5.074748	0.362572
C	-3.076111	4.304193	2.397033
C	-3.468107	5.374592	1.585094
H	-4.404496	5.888674	-0.277132
H	-2.639329	4.510004	3.372601
C	-4.977274	3.540118	-1.387774
H	-6.066274	3.511615	-1.245736
H	-4.769300	4.360168	-2.083885
H	-4.696084	2.599862	-1.864739
C	-3.244376	6.803710	2.022104
H	-3.478470	6.939811	3.084286
H	-2.197146	7.104023	1.883242
H	-3.863930	7.500212	1.447517
C	-2.843043	1.870996	2.957249
H	-3.664630	1.161386	3.111870
H	-1.990620	1.299132	2.576939
H	-2.565635	2.284360	3.931976
C	1.383363	-2.442253	-2.044488
C	2.700061	-2.242949	-1.569236
C	1.155544	-2.573665	-3.431726
C	3.752366	-2.168045	-2.488654
C	2.239110	-2.490520	-4.313829
C	3.546557	-2.289446	-3.866087
H	4.763257	-2.009895	-2.116490
H	2.053562	-2.593533	-5.381402
C	-0.229119	-2.821079	-3.987420
H	-0.732496	-3.642675	-3.464900
H	-0.863958	-1.934336	-3.881103
H	-0.180099	-3.075865	-5.050920
C	3.000241	-2.093923	-0.093057
H	2.328869	-1.377338	0.390983
H	2.892355	-3.039692	0.450111
H	4.029210	-1.751623	0.058370
C	4.706458	-2.232377	-4.833132
H	5.447695	-1.486026	-4.526249
H	5.225581	-3.198779	-4.891032
H	4.372061	-1.980563	-5.845004
C	-0.654533	-5.027503	1.716189
C	-1.925844	-5.308223	2.523835
C	-2.502302	-3.989541	3.045503
C	-2.933074	-3.097539	1.873602
H	-3.361431	-4.166402	3.704002
H	-2.674153	-5.806806	1.890890

H	-1.700313	-5.995344	3.348341	C	3.147262	-1.105891	3.550237
H	0.162125	-4.790890	2.414687	C	3.656133	-2.181964	4.271891
H	-0.334985	-5.926750	1.173449	H	3.205389	-3.853169	5.566426
H	-3.851796	-3.520207	1.443507	H	0.756519	-3.390680	5.573944
H	-3.212281	-2.102363	2.238002	H	-0.147919	-1.483384	4.286798
H	-1.739377	-3.474818	3.646224	H	3.832093	-0.469954	2.996996
H	-6.128568	1.372354	0.306331	H	4.726952	-2.369267	4.268767
C	-6.922554	-1.051921	-0.515488	C	1.165346	0.278151	2.789021
H	-7.367506	-1.281912	0.465234	H	0.084644	0.369781	2.891881
H	-7.519881	-0.228668	-0.927203	C	1.800061	1.182247	2.008254
C	-4.596529	-2.825022	-1.092223	H	2.879791	1.122303	1.874474
C	-7.035815	-2.292485	-1.408462	C	1.143468	2.290280	1.320150
H	-6.832480	-2.019093	-2.453652	H	0.088551	2.445167	1.532686
H	-8.060460	-2.682408	-1.376666	C	1.879744	3.285934	0.676396
C	-6.029051	-3.355824	-0.960871	H	1.400556	4.224061	0.400766
H	-4.351393	-2.745083	-2.163305	H	2.963091	3.313446	0.761694
H	-3.882119	-3.546361	-0.690811				
H	-6.231283	-3.631477	0.084523	**IM2**			
H	-6.136906	-4.271140	-1.555451	SCF energy in Ethanol: -2425.428828 a.u.			
Ni	1.337855	1.893817	-0.719686	Free energy in Ethanol: -2424.661780 a.u.			
C	8.811530	0.997082	1.218268	P	-0.378031	-1.172706	-0.628036
C	8.571816	2.363460	1.063060	N	0.348928	-1.669750	-2.070885
C	7.406119	2.804444	0.439427	C	0.395912	-3.095150	-2.371925
C	6.443217	1.898346	-0.047468	H	-0.101350	-3.303311	-3.331047
C	6.705043	0.522088	0.117849	H	1.433430	-3.453415	-2.432665
C	7.869172	0.080770	0.739959	H	-0.121435	-3.657428	-1.588848
H	9.719112	0.648694	1.703625	C	0.859670	-0.818347	-3.138120
H	9.294158	3.089233	1.428252	H	0.871750	0.223729	-2.824968
H	7.228803	3.871585	0.324068	H	1.878792	-1.117055	-3.416341
H	5.991130	-0.209816	-0.248854	H	0.227358	-0.906606	-4.035584
H	8.044456	-0.986464	0.852310	O	-0.783037	0.380685	-1.192253
C	5.237111	2.423201	-0.692001	O	0.859479	-0.688134	0.448473
H	5.190732	3.511354	-0.757825	C	-0.965351	1.401906	-0.281751
C	4.204005	1.718344	-1.211136	C	0.173661	2.025144	0.250351
H	4.218532	0.629558	-1.179797	C	-2.267707	1.811734	0.061883
C	3.030303	2.310855	-1.838699	C	0.021168	3.037270	1.232867
H	3.065863	3.390314	-1.987049	C	1.531013	1.539317	-0.156688
C	2.078865	1.556148	-2.551389	C	-2.378067	2.892653	0.939298
H	2.232835	0.488880	-2.701515	C	-1.271068	3.495514	1.545217
H	1.471501	2.040580	-3.313410	C	1.856584	0.188776	0.074951
C	2.803260	-3.016260	5.001938	C	2.504579	2.398039	-0.721909
C	1.431221	-2.757240	5.003297	H	-3.372563	3.256245	1.190583
C	0.921722	-1.680748	4.278665	C	3.181799	-0.280695	-0.026034
C	1.763590	-0.832882	3.532268	C	3.826163	1.938106	-0.862292

C	4.142718	0.633466	-0.468312
C	3.569851	-1.677120	0.350022
C	4.145955	-2.549875	-0.598915
C	3.407199	-2.120690	1.686412
C	4.504456	-3.848273	-0.211377
C	3.790085	-3.419471	2.028431
C	4.330099	-4.308013	1.092998
H	4.935458	-4.515256	-0.956334
H	3.665984	-3.745291	3.059859
C	4.418907	-2.138026	-2.030770
H	5.425371	-1.711874	-2.141381
H	4.365160	-3.004775	-2.698833
H	3.714271	-1.383890	-2.385978
C	4.701224	-5.719313	1.485901
H	5.232181	-5.742921	2.445007
H	3.809600	-6.350880	1.597444
H	5.343559	-6.188898	0.733433
C	2.851264	-1.217613	2.764419
H	3.318084	-0.226143	2.741388
H	1.773060	-1.071929	2.637680
H	3.023680	-1.649770	3.755549
C	-3.498182	1.112341	-0.426784
C	-4.316956	0.420156	0.494624
C	-3.871333	1.156118	-1.788941
C	-5.468589	-0.235879	0.030686
C	-5.025217	0.485628	-2.208093
C	-5.838737	-0.221755	-1.318830
H	-6.115117	-0.735665	0.752395
H	-5.299872	0.526858	-3.260590
C	-3.052846	1.924547	-2.800035
H	-2.835203	2.939833	-2.449212
H	-2.091324	1.431278	-2.977263
H	-3.582374	1.999309	-3.755168
C	-3.980638	0.345067	1.969715
H	-2.955302	-0.010366	2.125331
H	-4.061841	1.318979	2.464070
H	-4.664275	-0.338252	2.485634
C	-7.085761	-0.926988	-1.800629
H	-6.848098	-1.696635	-2.545525
H	-7.616392	-1.413178	-0.975299
H	-7.782432	-0.225504	-2.276362
C	-1.523385	4.588016	2.574917
C	-0.254763	5.323679	3.018226
C	0.859464	4.308672	3.283774
C	1.230310	3.580893	1.985197
H	1.750509	4.799131	3.694233
H	0.070542	6.020596	2.232515
H	-0.464856	5.927004	3.909722
H	-1.995485	4.134345	3.459827
H	-2.260181	5.298720	2.177308
H	1.791638	4.281045	1.351666
H	1.922507	2.757899	2.195865
H	0.520466	3.583980	4.037722
H	5.177591	0.304368	-0.533838
C	4.940692	2.837355	-1.379296
H	5.518526	3.211041	-0.519377
H	5.645632	2.243628	-1.975044
C	2.106358	3.754332	-1.291099
C	4.437191	4.037645	-2.189405
H	4.086206	3.700798	-3.175263
H	5.261575	4.738643	-2.369373
C	3.282658	4.723870	-1.453951
H	1.664393	3.576192	-2.284526
H	1.307506	4.210684	-0.703063
H	3.628987	5.062070	-0.466260
H	2.951046	5.617951	-1.996287
Ni	-1.874192	-2.260856	0.131714
C	-3.185607	-4.770273	2.107795
H	-3.478578	-5.211118	3.067523
H	-3.313403	-5.523184	1.323518
H	-2.126340	-4.496050	2.157007
C	-4.038427	-3.549016	1.822369
H	-5.100096	-3.819731	1.761573
H	-3.912066	-2.789237	2.602436
O	-3.646404	-2.996517	0.541863
H	-4.229299	-2.243923	0.309848

TS1a

SCF energy in Ethanol: -2425.393285 a.u.

Free energy in Ethanol: -2424.634172 a.u.

P	-0.397612	-1.134320	-0.468767
N	0.124220	-1.830333	-1.900515
C	0.190559	-3.285848	-2.009329
H	-0.295064	-3.612783	-2.938685
H	1.232429	-3.635977	-2.013634
H	-0.328872	-3.747119	-1.165233
C	0.677935	-1.118347	-3.049452
H	0.683321	-0.044973	-2.867754

H	1.702102	-1.452479	-3.255466	H	-5.176775	0.863217	-3.472003
H	0.066967	-1.319166	-3.940914	C	-2.918908	2.160770	-2.804129
O	-0.799606	0.352819	-1.126092	H	-2.713762	3.149597	-2.377716
O	0.908843	-0.669130	0.483880	H	-1.951079	1.673629	-2.968954
C	-0.982286	1.412069	-0.240175	H	-3.393983	2.304812	-3.779813
C	0.153412	2.028545	0.299723	C	-4.106673	0.237755	1.782299
C	-2.288195	1.828377	0.063945	H	-3.051731	0.041902	2.001707
C	-0.013501	3.025368	1.296160	H	-4.389845	1.133749	2.350025
C	1.514883	1.574926	-0.131292	H	-4.687086	-0.602084	2.174800
C	-2.412046	2.885810	0.966644	C	-7.016312	-0.716883	-2.223021
C	-1.311907	3.466723	1.608221	H	-6.741629	-1.639267	-2.752291
C	1.876712	0.230397	0.064396	H	-7.745459	-0.987561	-1.452129
C	2.456379	2.463372	-0.705760	H	-7.517331	-0.066618	-2.949428
H	-3.409932	3.246411	1.206926	C	-1.578032	4.527582	2.666754
C	3.199677	-0.221755	-0.099923	C	-0.319242	5.266258	3.132187
C	3.780937	2.029610	-0.895234	C	0.806482	4.258580	3.376442
C	4.130142	0.719492	-0.550856	C	1.188500	3.565988	2.061878
C	3.614103	-1.627174	0.206142	H	1.690926	4.749785	3.799802
C	4.155760	-2.455841	-0.801535	H	-0.000133	5.986746	2.365453
C	3.508967	-2.125508	1.529236	H	-0.539079	5.844072	4.037914
C	4.527155	-3.769887	-0.484228	H	-2.045660	4.041959	3.536638
C	3.904682	-3.437153	1.799455	H	-2.323524	5.238886	2.287521
C	4.403255	-4.285407	0.805096	H	1.740993	4.287822	1.444754
H	4.931452	-4.402790	-1.272564	H	1.890908	2.747362	2.254876
H	3.824948	-3.805752	2.820587	H	0.475086	3.512105	4.112036
C	4.390261	-1.981513	-2.221661	H	5.166042	0.407393	-0.663172
H	5.411994	-1.598511	-2.349213	C	4.865048	2.960968	-1.419519
H	4.271434	-2.808583	-2.930496	H	5.456253	3.325475	-0.564996
H	3.713203	-1.176160	-2.512681	H	5.565491	2.393572	-2.045161
C	4.788220	-5.711714	1.122720	C	2.019487	3.825116	-1.231697
H	5.373277	-5.772948	2.047980	C	4.319484	4.168884	-2.189397
H	3.900509	-6.342812	1.262880	H	3.948244	3.847273	-3.172826
H	5.383200	-6.155064	0.317433	H	5.126601	4.887940	-2.375185
C	3.008200	-1.266735	2.668947	C	3.174067	4.818293	-1.407855
H	3.458398	-0.267730	2.649273	H	1.549788	3.660199	-2.214544
H	1.921936	-1.135473	2.619329	H	1.232359	4.255537	-0.609841
H	3.249825	-1.727711	3.631937	H	3.541849	5.142942	-0.423490
C	-3.497045	1.171808	-0.524554	H	2.810739	5.716578	-1.921772
C	-4.358273	0.413615	0.298735	Ni	-1.768772	-2.216510	0.674301
C	-3.799617	1.332362	-1.895845	C	-4.763947	-4.481231	1.414883
C	-5.491085	-0.183908	-0.270754	H	-5.226746	-5.435254	1.131799
C	-4.945283	0.726096	-2.417050	H	-5.085341	-4.229546	2.431277
C	-5.801900	-0.044942	-1.624470	H	-5.126314	-3.701390	0.736238
H	-6.147738	-0.771418	0.368135	C	-3.245212	-4.584058	1.345863

H	-2.891199	-5.391815	2.004850
H	-2.934686	-4.828848	0.321394
O	-2.672353	-3.350482	1.784765
H	-1.301194	-3.380565	1.516728

TS1b

SCF energy in Ethanol: -3068.623032 a.u.

Free energy in Ethanol: -3067.604390 a.u.

N	0.398810	-0.592652	-2.668711
C	-0.611406	-1.491191	-3.228975
H	-0.907533	-1.145742	-4.228310
H	-0.227918	-2.517351	-3.308241
H	-1.501072	-1.510513	-2.591705
C	1.579854	-0.427770	-3.513783
H	2.333415	0.170340	-3.005329
H	2.011098	-1.403266	-3.770045
H	1.299854	0.078660	-4.448043
O	1.307482	1.231886	-1.243472
O	0.940794	-0.981803	0.021062
C	1.852348	1.813681	-0.101819
C	2.752666	1.064439	0.666657
C	1.533082	3.147305	0.202953
C	3.196356	1.583053	1.909755
C	3.227987	-0.267079	0.173120
C	2.087877	3.668018	1.374668
C	2.863677	2.904582	2.254263
C	2.295750	-1.291964	-0.055383
C	4.603180	-0.517965	-0.059461
H	1.881006	4.705980	1.625421
C	2.688008	-2.617723	-0.316852
C	5.018528	-1.832289	-0.338688
C	4.063675	-2.850149	-0.417033
C	1.731199	-3.761109	-0.451676
C	1.673966	-4.512725	-1.647472
C	0.944968	-4.162075	0.655878
C	0.814122	-5.615764	-1.724972
C	0.114468	-5.280005	0.536355
C	0.024461	-6.018590	-0.648090
H	0.773387	-6.181884	-2.654159
H	-0.473770	-5.586452	1.398795
C	2.534457	-4.204649	-2.856379
H	3.452139	-4.808432	-2.857396
H	1.999275	-4.441519	-3.782739
H	2.844662	-3.158855	-2.893129
C	-0.903386	-7.206011	-0.760139
H	-0.997275	-7.732439	0.196010
H	-1.913928	-6.896155	-1.058879
H	-0.548776	-7.922291	-1.509151
C	1.008502	-3.439345	1.982708
H	2.043653	-3.261690	2.296572
H	0.514158	-2.463316	1.928458
H	0.513408	-4.024471	2.763788
C	0.670810	4.002913	-0.670488
C	-0.577248	4.463784	-0.195110
C	1.121739	4.401134	-1.948206
C	-1.354982	5.291127	-1.013142
C	0.311680	5.231858	-2.729818
C	-0.931353	5.687930	-2.284479
H	-2.318821	5.635389	-0.642536
H	0.668029	5.535056	-3.712730
C	2.466937	3.966325	-2.485471
H	3.264658	4.118493	-1.749531
H	2.466889	2.901610	-2.745358
H	2.725639	4.531543	-3.386589
C	-1.100363	4.077217	1.171283
H	-1.084274	2.991299	1.318608
H	-0.505731	4.517126	1.980066
H	-2.130667	4.419873	1.299492
C	-1.775103	6.609831	-3.134443
H	-2.844452	6.453659	-2.954977
H	-1.560288	7.664381	-2.913820
H	-1.584960	6.456920	-4.202272
C	3.293273	3.533577	3.571494
C	4.362071	2.729461	4.318682
C	3.988888	1.245001	4.311522
C	3.986908	0.707291	2.874744
H	4.689438	0.659466	4.918936
H	5.339679	2.860498	3.832862
H	4.464681	3.107473	5.342863
H	2.407128	3.629475	4.217123
H	3.639665	4.559025	3.387822
H	5.030217	0.617928	2.541781
H	3.582984	-0.311155	2.850546
H	2.994324	1.116838	4.761590
H	4.400253	-3.869545	-0.591496
C	6.486575	-2.194255	-0.513728
H	6.855420	-2.627173	0.429133
H	6.580692	-2.989921	-1.263302

C	5.605443	0.627862	-0.136994
C	7.373044	-1.000892	-0.885762
H	7.189258	-0.710481	-1.929950
H	8.429855	-1.285982	-0.817692
C	7.064301	0.186572	0.029825
H	5.493317	1.092860	-1.129411
H	5.361856	1.417727	0.575839
H	7.250840	-0.100901	1.074945
H	7.728934	1.031379	-0.188168
P	0.187707	-0.001702	-1.111655
Ni	-1.825476	0.295305	-0.669679
B	-4.055208	-0.364034	1.054018
O	-3.691777	0.264986	-0.296402
O	-5.218443	0.372905	1.471668
C	-4.777963	1.139016	-0.710803
C	-5.402645	1.543486	0.680576
C	-5.727089	0.292516	-1.572051
H	-6.140785	-0.539421	-0.996830
H	-6.551581	0.893605	-1.970821
H	-5.167930	-0.124276	-2.416896
C	-4.214069	2.295379	-1.535064
H	-5.008506	3.006330	-1.792293
H	-3.427412	2.835765	-1.002570
H	-3.793529	1.920128	-2.476604
C	-4.666920	2.720636	1.343816
H	-5.032733	2.820169	2.371134
H	-3.592351	2.534448	1.387771
H	-4.847021	3.668805	0.822557
C	-6.902455	1.852139	0.619692
H	-7.110824	2.699269	-0.045366
H	-7.474475	0.986570	0.277316
H	-7.258675	2.113650	1.621775
C	-4.315494	-1.955715	0.992111
C	-5.563608	-2.493680	1.351044
C	-3.331943	-2.863765	0.558815
C	-5.824201	-3.864648	1.277530
H	-6.341188	-1.814371	1.690574
C	-3.581610	-4.235378	0.473412
H	-2.345190	-2.492298	0.282186
C	-4.832627	-4.741918	0.834484
H	-6.801206	-4.248582	1.564322
H	-2.797033	-4.905045	0.130412
H	-5.031271	-5.809687	0.772613
O	-2.780895	-0.015932	1.853448
C	-2.486644	-0.677744	3.083952
H	-3.383912	-0.627171	3.714357
H	-2.269569	-1.737897	2.901552
C	-1.313772	0.010017	3.768309
H	-0.416348	-0.033896	3.140275
H	-1.543279	1.062672	3.965242
H	-1.088493	-0.481371	4.722339
H	-1.757756	0.068027	0.829342

IM3

SCF energy in Ethanol: -2657.543602 a.u.

Free energy in Ethanol: -2656.696299 a.u.

P	0.064031	-0.701122	-0.931883
N	0.587737	-0.457970	-2.508071
C	0.092822	0.547032	-3.444174
H	0.916598	1.175501	-3.804616
H	-0.369852	0.057478	-4.313575
H	-0.651883	1.180091	-2.965372
C	1.682469	-1.271672	-3.024990
H	1.958781	-2.035467	-2.294188
H	1.380812	-1.771110	-3.956505
H	2.569736	-0.655975	-3.226796
O	-1.449497	0.002541	-1.141980
O	0.744658	0.457026	0.092215
C	-2.159705	0.437665	-0.028958
C	-1.749023	1.617628	0.608976
C	-3.289114	-0.286148	0.392581
C	-2.374531	2.003084	1.822915
C	-0.626864	2.424504	0.032134
C	-3.953174	0.192290	1.524570
C	-3.498859	1.286465	2.267987
C	0.631723	1.820305	-0.124194
C	-0.791002	3.782999	-0.334403
H	-4.846538	-0.331662	1.857591
C	1.784131	2.560828	-0.449835
C	0.344718	4.541121	-0.671020
C	1.601685	3.927794	-0.680754
C	3.145512	1.946478	-0.539957
C	3.874126	1.991259	-1.750010
C	3.735474	1.346845	0.600732
C	5.142621	1.398190	-1.810529
C	5.005924	0.776749	0.494153
C	5.725949	0.781212	-0.704748
H	5.686943	1.425238	-2.753215

H	5.441092	0.306782	1.373539	H	-1.840302	2.291531	4.658027
C	3.357209	2.676375	-2.999230	H	2.476417	4.533677	-0.906213
H	3.682133	3.724901	-3.043837	C	0.256360	6.029160	-0.979311
H	3.746816	2.185685	-3.898145	H	0.550116	6.591224	-0.079055
H	2.266830	2.682443	-3.053066	H	0.995857	6.289886	-1.746878
C	7.099417	0.156312	-0.784119	C	-2.181453	4.387417	-0.489995
H	7.848438	0.766752	-0.262090	C	-1.142163	6.486858	-1.408382
H	7.110472	-0.834890	-0.316065	H	-1.352513	6.135500	-2.428556
H	7.430719	0.046103	-1.822116	H	-1.184081	7.582572	-1.435731
C	3.040149	1.322510	1.943359	C	-2.196974	5.920210	-0.453929
H	2.576429	2.287896	2.175964	H	-2.573031	4.059107	-1.466051
H	2.249115	0.565739	1.964610	H	-2.876688	3.979568	0.246427
H	3.752855	1.085955	2.739414	H	-1.991407	6.272569	0.567568
C	-3.801498	-1.504558	-0.309555	H	-3.197886	6.283274	-0.717730
C	-3.777966	-2.756229	0.344689	C	5.478054	-2.738058	2.928016
C	-4.365159	-1.402942	-1.600668	C	5.658765	-3.068660	1.583331
C	-4.302934	-3.877878	-0.307718	C	4.559181	-3.362020	0.777698
C	-4.879686	-2.549774	-2.213697	C	3.248680	-3.342785	1.291587
C	-4.860157	-3.798615	-1.586580	C	3.084148	-2.992258	2.646677
H	-4.275623	-4.840552	0.199952	C	4.181711	-2.699535	3.451929
H	-5.314689	-2.461451	-3.207696	H	6.332862	-2.509598	3.558870
C	-4.439260	-0.079590	-2.328278	H	6.660080	-3.107563	1.160869
H	-4.861413	0.707347	-1.692647	H	4.713270	-3.626738	-0.266134
H	-3.443853	0.256439	-2.639487	H	2.082797	-2.926297	3.063928
H	-5.063701	-0.163441	-3.223462	H	4.024798	-2.430506	4.493675
C	-3.187206	-2.922774	1.729406	C	2.122597	-3.699199	0.412917
H	-2.197160	-2.457886	1.804301	H	2.384968	-3.775325	-0.642188
H	-3.812933	-2.464529	2.504297	C	0.949138	-4.310478	0.861107
H	-3.084274	-3.984036	1.978147	H	0.838762	-4.446498	1.936353
C	-5.454374	-5.016441	-2.256310	C	-0.240468	-4.592015	0.096156
H	-4.997879	-5.940565	-1.885665	H	-1.101874	-4.893182	0.689081
H	-6.534306	-5.088668	-2.067937	C	-0.478520	-4.220330	-1.232245
H	-5.318198	-4.983836	-3.342979	H	0.313254	-4.183585	-1.979858
C	-4.225180	1.631010	3.560277	H	-1.480398	-4.347089	-1.631263
C	-3.822221	2.985600	4.151421	Ni	0.218037	-2.617304	-0.091846
C	-2.299033	3.129007	4.113409	**TS2**			
C	-1.805609	3.142661	2.660672	SCF energy in Ethanol: -3455.839763 a.u.			
H	-1.976366	4.048520	4.616539	Free energy in Ethanol: -3454.668762 a.u.			
H	-4.277445	3.800524	3.570436	P	-0.872198	-0.227434	-0.361644
H	-4.204342	3.074950	5.175475	N	-0.119931	0.275454	-1.759309
H	-4.012173	0.845251	4.301085	C	-0.625223	0.145542	-3.124762
H	-5.309017	1.591631	3.389030	H	-0.704320	1.130265	-3.600036
H	-2.073602	4.111998	2.218711	H	0.067207	-0.467501	-3.717104
H	-0.711057	3.099261	2.631119	H	-1.604536	-0.330348	-3.126500

C	1.167247	0.971349	-1.642862	C	0.088257	-5.826494	-0.065734
H	1.436949	1.089915	-0.591467	H	0.374083	-5.514116	2.039619
H	1.973526	0.414537	-2.132616	H	-0.490414	-5.923230	-2.135210
H	1.091762	1.974754	-2.079446	C	-2.524719	-4.178697	-2.308526
O	-1.973650	-1.271292	-1.049414	H	-3.600002	-4.239024	-2.104848
O	-1.901488	0.951433	0.232787	H	-2.319557	-3.162164	-2.662007
C	-3.073152	-1.644308	-0.272003	H	-2.295025	-4.871298	-3.124100
C	-4.114149	-0.721207	-0.117732	C	-1.482236	-3.688506	2.677673
C	-3.094963	-2.919133	0.313825	H	-1.647969	-2.605639	2.644582
C	-5.185434	-1.032181	0.758279	H	-2.373952	-4.128828	3.140625
C	-4.035872	0.600423	-0.817869	H	-0.638670	-3.884075	3.347377
C	-4.221419	-3.233453	1.078007	C	1.197761	-6.843399	-0.202003
C	-5.244926	-2.314417	1.334004	H	1.548280	-7.187910	0.776267
C	-2.950422	1.449804	-0.541624	H	0.868571	-7.720794	-0.770867
C	-5.033511	1.026515	-1.727211	H	2.061428	-6.422357	-0.733004
H	-4.285186	-4.224996	1.520896	C	-6.364183	-2.730623	2.278057
C	-2.907799	2.782599	-0.987478	C	-7.542237	-1.751653	2.309441
C	-5.007181	2.352285	-2.195789	C	-7.016726	-0.316463	2.386315
C	-3.976900	3.203934	-1.785595	C	-6.223820	0.023600	1.117937
C	-1.810296	3.735567	-0.631496	H	-7.839482	0.398762	2.503743
C	-1.010399	4.318822	-1.640273	H	-8.151017	-1.866637	1.401300
C	-1.610100	4.114159	0.718283	H	-8.195126	-1.982278	3.159480
C	-0.004471	5.224503	-1.279572	H	-5.948810	-2.818092	3.293444
C	-0.602863	5.031633	1.027192	H	-6.707532	-3.738278	2.009716
C	0.222997	5.590515	0.047031	H	-6.937915	0.151943	0.292986
H	0.613580	5.658044	-2.063825	H	-5.726108	0.993592	1.228540
H	-0.460889	5.317102	2.067188	H	-6.374381	-0.209102	3.271864
C	-1.208095	4.034443	-3.115710	H	-3.987291	4.237440	-2.123746
H	-1.880024	4.770433	-3.577801	C	-6.097716	2.906947	-3.101179
H	-0.254953	4.095815	-3.652191	H	-6.799153	3.490014	-2.484560
H	-1.645143	3.050668	-3.298015	H	-5.658785	3.621435	-3.808570
C	1.332181	6.547493	0.416359	C	-6.045315	0.038423	-2.293468
H	1.039439	7.200323	1.246538	C	-6.884024	1.826203	-3.851922
H	2.234649	6.006993	0.732826	H	-6.264422	1.405347	-4.656424
H	1.614566	7.181575	-0.430567	H	-7.764320	2.271524	-4.330791
C	-2.479315	3.581065	1.835123	C	-7.289985	0.705512	-2.890552
H	-3.542699	3.618852	1.571676	H	-5.537784	-0.528933	-3.089712
H	-2.235166	2.539383	2.068443	H	-6.328281	-0.708143	-1.548949
H	-2.333928	4.167557	2.747206	H	-7.912797	1.122734	-2.085804
C	-1.974606	-3.899832	0.168788	H	-7.899534	-0.047857	-3.404042
C	-1.214968	-4.269227	1.302158	C	0.279140	3.153561	4.902854
C	-1.706930	-4.508169	-1.080235	C	1.301655	3.381269	3.979779
C	-0.199383	-5.225710	1.160419	C	1.697810	2.368944	3.106266
C	-0.683696	-5.454353	-1.172176	C	1.086196	1.102866	3.148371

C	0.047635	0.891308	4.075597
C	-0.349207	1.904334	4.944093
H	-0.028903	3.941924	5.584488
H	1.799382	4.346541	3.943158
H	2.510354	2.544901	2.405349
H	-0.460492	-0.069311	4.100464
H	-1.153691	1.722919	5.652092
C	1.587292	0.037533	2.261167
H	2.305947	0.379809	1.515972
C	1.687360	-1.319108	2.671556
H	1.310161	-1.614909	3.647876
C	2.061217	-2.341651	1.772260
H	1.967212	-3.353822	2.164745
C	2.632436	-2.226132	0.454606
H	2.348559	-1.368625	-0.168248
H	2.633415	-3.156183	-0.114133
Ni	0.402736	-1.186666	1.102182
B	5.512812	-0.291629	-0.560852
O	6.705284	-0.906469	-1.107692
O	4.457170	-0.443374	-1.565468
C	6.352738	-1.636088	-2.282403
C	5.072490	-0.863790	-2.786860
C	6.051510	-3.098908	-1.899728
H	5.181173	-3.163119	-1.240626
H	5.871257	-3.728810	-2.779426
H	6.915291	-3.505308	-1.362108
C	7.544019	-1.606198	-3.246191
H	7.295435	-2.074288	-4.207016
H	7.878159	-0.582340	-3.430180
H	8.384293	-2.157880	-2.809504
C	5.429631	0.391497	-3.605843
H	4.523326	0.991885	-3.742757
H	6.161300	1.006661	-3.074621
H	5.829718	0.143753	-4.596320
C	4.079732	-1.721428	-3.578398
H	4.544579	-2.137620	-4.480798
H	3.693329	-2.546587	-2.974354
H	3.227587	-1.108755	-3.897548
C	5.769086	1.218238	-0.029472
C	4.730871	2.165093	0.028749
C	7.038473	1.647991	0.395951
C	4.935832	3.463513	0.503345
H	3.743975	1.883803	-0.334815
C	7.257930	2.941124	0.880504
H	7.874333	0.954689	0.328941
C	6.203880	3.855462	0.940858
H	4.111566	4.175849	0.517236
H	8.253920	3.239821	1.202233
H	6.371104	4.864654	1.310892
O	4.981484	-1.119100	0.695408
H	3.861699	-1.771848	0.568805
C	5.885349	-1.714063	1.623215
H	5.559087	-2.752611	1.789306
H	6.875796	-1.755439	1.159288
C	5.919078	-0.961698	2.950835
H	6.595094	-1.462836	3.655853
H	6.267060	0.065056	2.805272
H	4.920168	-0.923927	3.401026

IM4a

SCF energy in Ethanol: -2812.687805 a.u.

Free energy in Ethanol: -2811.766166 a.u.

P	-0.216192	-1.489441	-0.288224
N	0.294824	-2.777215	-1.244608
C	0.363938	-4.109007	-0.653387
H	-0.193001	-4.828163	-1.270476
H	1.405336	-4.451062	-0.567459
H	-0.080955	-4.099490	0.345997
C	0.743579	-2.716248	-2.631282
H	0.776753	-1.684940	-2.978619
H	1.741299	-3.159700	-2.735942
H	0.053157	-3.279397	-3.277032
O	-0.667618	-0.506687	-1.594923
O	1.127680	-0.611423	0.243548
C	-0.860992	0.842599	-1.337571
C	0.264619	1.656657	-1.155909
C	-2.169276	1.352765	-1.294714
C	0.086062	2.995408	-0.725430
C	1.628523	1.079305	-1.383250
C	-2.307539	2.704911	-0.973426
C	-1.217271	3.517914	-0.642046
C	2.042971	-0.016740	-0.606911
C	2.508692	1.610304	-2.357616
H	-3.307080	3.133786	-0.947604
C	3.370057	-0.488935	-0.632464
C	3.834530	1.143944	-2.409258
C	4.242713	0.139762	-1.525406
C	3.855996	-1.589692	0.258484

C	4.344172	-2.799421	-0.281126	H	0.036652	6.113244	-1.145669
C	3.881603	-1.399303	1.662210	H	-0.466584	6.750898	0.419863
C	4.782621	-3.810563	0.585953	H	-1.903327	4.871290	0.863924
C	4.338430	-2.429754	2.486138	H	-2.277513	5.385740	-0.773263
C	4.778849	-3.654037	1.971131	H	1.826538	4.186297	-1.203574
H	5.144406	-4.744193	0.157870	H	1.996001	3.207492	0.234290
H	4.358176	-2.268332	3.562518	H	0.617993	4.751097	1.541788
C	4.456975	-3.050827	-1.770891	H	5.279644	-0.188407	-1.549618
H	5.467144	-2.817977	-2.135037	C	4.857918	1.731283	-3.370939
H	4.272850	-4.106161	-2.001796	H	5.477530	2.458981	-2.823809
H	3.762675	-2.442269	-2.352415	H	5.546464	0.943134	-3.700812
C	5.229444	-4.766147	2.889747	C	1.999916	2.575235	-3.421834
H	5.834882	-4.381163	3.718563	C	4.230410	2.433617	-4.580094
H	4.371741	-5.288494	3.334529	H	3.815313	1.685978	-5.271022
H	5.825434	-5.512435	2.353847	H	5.000886	2.983981	-5.133839
C	3.464482	-0.087379	2.286528	C	3.110424	3.370138	-4.119215
H	3.968708	0.761558	1.809491	H	1.470765	1.976519	-4.180396
H	2.387268	0.077749	2.185601	H	1.244858	3.251248	-3.015900
H	3.714269	-0.071890	3.352517	H	3.523495	4.119439	-3.428064
C	-3.365563	0.503743	-1.590590	H	2.688410	3.922261	-4.967956
C	-4.309643	0.221182	-0.577104	Ni	-1.584326	-2.048117	1.282852
C	-3.578896	0.004110	-2.896927	C	-0.546255	4.949717	4.560876
C	-5.425856	-0.574320	-0.882350	C	0.672354	4.280048	4.689290
C	-4.711294	-0.773545	-3.158307	C	0.757899	2.916966	4.409070
C	-5.649538	-1.078030	-2.167512	C	-0.366481	2.175606	3.992365
H	-6.146205	-0.788322	-0.094467	C	-1.587519	2.872472	3.865306
H	-4.865053	-1.150042	-4.167887	C	-1.674702	4.233181	4.146459
C	-2.611657	0.298796	-4.020361	H	-0.618638	6.011283	4.781579
H	-2.363601	1.364825	-4.067623	H	1.559785	4.819426	5.011657
H	-1.671159	-0.245721	-3.880759	H	1.712024	2.405658	4.516321
H	-3.035358	0.003228	-4.985391	H	-2.479117	2.342344	3.543379
C	-4.154484	0.755377	0.830759	H	-2.631954	4.739816	4.046161
H	-3.118383	0.691343	1.174800	C	-0.214532	0.744366	3.723051
H	-4.451297	1.809756	0.895311	H	0.799992	0.361193	3.827879
H	-4.784793	0.195257	1.529351	C	-1.186002	-0.130649	3.374960
C	-6.882131	-1.892729	-2.486314	H	-2.213565	0.225258	3.295327
H	-7.316182	-2.335989	-1.583683	C	-1.004694	-1.554729	3.112058
H	-7.659720	-1.270235	-2.948941	H	-0.007154	-1.947647	3.316039
H	-6.658934	-2.702848	-3.189674	C	-2.121278	-2.449500	3.105599
C	-1.491527	4.932540	-0.154550	H	-3.106945	-2.068794	3.387195
C	-0.246072	5.823772	-0.122901	H	-1.961601	-3.494697	3.376178
C	0.910839	5.064104	0.531167	C	-3.450748	-5.141185	0.759108
C	1.286087	3.838436	-0.312091	H	-3.063804	-5.536387	-0.185997
H	1.790910	5.709630	0.641518	H	-2.627013	-5.080140	1.476662

H	-4.199812	-5.839445	1.149710
C	-4.074264	-3.773553	0.553383
H	-4.891224	-3.827141	-0.177090
H	-4.470638	-3.380497	1.497303
O	-3.067750	-2.874491	0.042301
H	-3.514362	-2.089307	-0.328213

IM4b

SCF energy in Ethanol: -2812.684178 a.u.

Free energy in Ethanol: -2811.761693 a.u.

P	-0.179594	-0.652072	-0.796352
N	0.185523	-0.594382	-2.435913
C	1.064695	-1.618659	-2.990274
H	0.579185	-2.118157	-3.840705
H	2.013585	-1.182309	-3.332247
H	1.285274	-2.373954	-2.230226
C	-0.281231	0.388419	-3.407126
H	-0.831632	1.186534	-2.910957
H	0.565492	0.824358	-3.950412
H	-0.946510	-0.089928	-4.141907
O	-1.658982	0.177623	-0.939298
O	0.705512	0.528958	0.020875
C	-2.206944	0.745401	0.200690
C	-1.620390	1.907606	0.722703
C	-3.354355	0.171331	0.776503
C	-2.063681	2.408828	1.972601
C	-0.522213	2.585144	-0.036795
C	-3.836751	0.762542	1.947143
C	-3.192309	1.830784	2.579449
C	0.661154	1.875976	-0.303956
C	-0.649137	3.922953	-0.484123
H	-4.738059	0.354381	2.399448
C	1.800645	2.503450	-0.844595
C	0.474318	4.567265	-1.031883
C	1.673488	3.860289	-1.160318
C	3.102196	1.801330	-1.074064
C	3.653215	1.717086	-2.373024
C	3.827302	1.268784	0.020268
C	4.878750	1.063218	-2.557046
C	5.051676	0.637022	-0.210434
C	5.594393	0.514526	-1.493561
H	5.284579	0.989517	-3.565010
H	5.594552	0.225232	0.637000
C	2.997037	2.330518	-3.594036
H	3.395002	3.334259	-3.797700
H	3.198042	1.724849	-4.485089
H	1.916463	2.435711	-3.484244
C	6.928055	-0.162409	-1.708994
H	7.760596	0.510398	-1.461343
H	7.029958	-1.048287	-1.073068
H	7.056938	-0.470106	-2.752511
C	3.326597	1.389157	1.441900
H	2.961793	2.400368	1.657006
H	2.500675	0.695043	1.628489
H	4.128550	1.158113	2.149551
C	-4.089245	-0.990569	0.183816
C	-4.186603	-2.209392	0.897517
C	-4.776500	-0.847633	-1.045508
C	-4.965597	-3.249811	0.371839
C	-5.545382	-1.913024	-1.528380
C	-5.665576	-3.119534	-0.831548
H	-5.036359	-4.181871	0.929573
H	-6.079022	-1.788258	-2.468653
C	-4.720986	0.439933	-1.835430
H	-4.952588	1.305794	-1.204867
H	-3.721310	0.604239	-2.252104
H	-5.437321	0.419172	-2.662617
C	-3.477614	-2.421016	2.218539
H	-2.450144	-2.045023	2.189327
H	-3.988702	-1.905842	3.040804
H	-3.442923	-3.485872	2.469392
C	-6.555311	-4.230435	-1.341193
H	-6.194663	-5.214478	-1.022698
H	-7.579036	-4.121639	-0.958524
H	-6.617741	-4.228439	-2.434825
C	-3.722921	2.300988	3.925665
C	-3.130910	3.636253	4.389310
C	-1.616212	3.632598	4.167420
C	-1.300424	3.528418	2.669775
H	-1.156196	4.540900	4.574939
H	-3.578653	4.463969	3.820668
H	-3.377294	3.806928	5.444186
H	-3.492171	1.532552	4.679244
H	-4.818697	2.358213	3.885354
H	-1.532896	4.495115	2.202127
H	-0.225567	3.380028	2.517255
H	-1.171134	2.783120	4.704559
H	2.545471	4.378954	-1.552167

C	0.440358	6.030248	-1.450933
H	0.891930	6.635769	-0.649553
H	1.080985	6.175243	-2.329846
C	-2.005341	4.618895	-0.496898
C	-0.972103	6.556958	-1.726629
H	-1.345749	6.144132	-2.674621
H	-0.947983	7.647319	-1.843478
C	-1.915391	6.146594	-0.592767
H	-2.557098	4.246791	-1.374979
H	-2.610966	4.326592	0.363308
H	-1.544310	6.559348	0.356816
H	-2.917989	6.563870	-0.747952
Ni	-0.283146	-2.615258	0.095776
C	7.467048	-2.584323	1.905409
C	6.842806	-1.855642	2.919807
C	5.451250	-1.799639	2.989944
C	4.636404	-2.465677	2.051491
C	5.287265	-3.188831	1.029631
C	6.676460	-3.250343	0.961956
H	8.551071	-2.634046	1.848673
H	7.440339	-1.332043	3.662222
H	4.975902	-1.237001	3.790681
H	4.697958	-3.703754	0.276503
H	7.148081	-3.822352	0.166133
C	3.180780	-2.388183	2.188966
H	2.826796	-1.718038	2.973245
C	2.254934	-3.079618	1.485984
H	2.584161	-3.784394	0.720881
C	0.812622	-3.019927	1.700668
H	0.498378	-2.377856	2.526884
C	-0.042581	-4.098941	1.308684
H	0.404273	-4.988501	0.856342
H	-0.938845	-4.307908	1.895034
O	-1.726224	-3.290308	-1.266129
H	-2.551926	-2.812536	-1.065100
C	-2.022862	-4.693944	-1.413448
H	-1.051354	-5.191370	-1.413604
H	-2.582231	-5.042907	-0.537241
C	-2.781111	-4.963970	-2.704949
H	-2.199254	-4.631633	-3.571076
H	-2.979239	-6.037397	-2.811028
H	-3.742172	-4.438079	-2.712525

TS3a

SCF energy in Ethanol: -3455.876459 a.u.

Free energy in Ethanol: -3454.696074 a.u.

P	0.260746	0.377469	-0.591654
N	0.881484	1.192578	-1.918498
C	2.150456	1.911744	-1.780785
H	2.779063	1.716991	-2.657362
H	1.988115	2.992610	-1.693555
H	2.696236	1.569519	-0.903026
C	0.166532	1.492325	-3.158558
H	-0.753688	0.915277	-3.218850
H	-0.078859	2.559679	-3.231036
H	0.805988	1.228733	-4.011653
O	-0.842531	-0.540024	-1.461589
O	-0.767368	1.385744	0.280460
C	-2.101815	-0.912554	-1.001679
C	-3.047078	0.075523	-0.684439
C	-2.425529	-2.281670	-0.963649
C	-4.265964	-0.305558	-0.063807
C	-2.790055	1.521236	-0.988867
C	-3.677070	-2.616974	-0.442215
C	-4.574332	-1.670109	0.060500
C	-1.710376	2.169610	-0.374572
C	-3.643500	2.264315	-1.842746
H	-3.955138	-3.667994	-0.414512
C	-1.570164	3.570803	-0.379174
C	-3.498402	3.662031	-1.901364
C	-2.507308	4.283115	-1.133423
C	-0.517915	4.289431	0.406409
C	0.436181	5.113442	-0.230704
C	-0.518286	4.199618	1.820575
C	1.403005	5.768580	0.544091
C	0.459427	4.877874	2.551784
C	1.443662	5.656174	1.933445
H	2.142347	6.388219	0.039838
H	0.444100	4.805840	3.637750
C	0.444295	5.358747	-1.725733
H	-0.167600	6.232561	-1.987889
H	1.460402	5.563320	-2.079363
H	0.047227	4.513339	-2.291080
C	2.516248	6.344855	2.745029
H	2.130005	6.689221	3.710988
H	3.353320	5.665598	2.956380
H	2.925968	7.211334	2.215216
C	-1.587559	3.431827	2.565460

H	-2.592497	3.731319	2.244471	H	-4.050329	1.189054	-3.636404
H	-1.501945	2.354081	2.395244	H	-5.044046	0.668295	-2.304120
H	-1.510391	3.610766	3.642542	H	-6.445163	2.703471	-2.478131
C	-1.566913	-3.372648	-1.526991	H	-6.317654	1.943392	-4.063350
C	-1.036626	-4.373633	-0.684602	Ni	1.762174	-0.415020	0.803520
C	-1.393534	-3.477180	-2.926026	C	-4.391360	-3.311524	5.012280
C	-0.346678	-5.451046	-1.251476	C	-4.615569	-1.945520	4.829620
C	-0.695824	-4.570686	-3.448731	C	-3.622226	-1.141100	4.271821
C	-0.163165	-5.570857	-2.630953	C	-2.377787	-1.672394	3.879868
H	0.060055	-6.216397	-0.592728	C	-2.166917	-3.051455	4.084712
H	-0.576630	-4.647470	-4.528003	C	-3.158862	-3.856672	4.637454
C	-1.966541	-2.448242	-3.874672	H	-5.161199	-3.942416	5.448114
H	-3.024382	-2.250756	-3.667040	H	-5.562979	-1.502974	5.127178
H	-1.436963	-1.492393	-3.789312	H	-3.802823	-0.076498	4.140757
H	-1.881539	-2.786960	-4.912062	H	-1.215086	-3.498174	3.814443
C	-1.193889	-4.308817	0.818481	H	-2.967673	-4.916878	4.783571
H	-1.037120	-3.294226	1.196333	C	-1.370310	-0.767680	3.318678
H	-2.196822	-4.610611	1.144223	H	-1.678560	0.275419	3.258546
H	-0.476703	-4.975877	1.309055	C	-0.114510	-1.072316	2.922080
C	0.608468	-6.730314	-3.218026	H	0.231296	-2.104796	2.986478
H	1.682859	-6.507707	-3.274808	C	0.889366	-0.098214	2.480260
H	0.498338	-7.634855	-2.609897	H	0.566586	0.941214	2.549898
H	0.272467	-6.962018	-4.234572	C	2.303037	-0.377208	2.797099
C	-5.845252	-2.160848	0.735526	H	2.828309	0.480728	3.229942
C	-6.903625	-1.068030	0.914243	H	2.449102	-1.272107	3.411704
C	-6.243782	0.192078	1.479117	B	4.747318	-0.675110	0.105815
C	-5.219074	0.751785	0.483626	O	3.336349	-0.956085	-0.373060
H	-6.991077	0.963569	1.701938	O	5.567847	-1.645419	-0.553505
H	-7.372587	-0.833750	-0.052482	C	3.397012	-2.026784	-1.367925
H	-7.702048	-1.426044	1.575359	C	4.765896	-2.727378	-1.022852
H	-5.579251	-2.560542	1.725242	C	3.402216	-1.365580	-2.753303
H	-6.254234	-3.006774	0.167707	H	4.273921	-0.716533	-2.875958
H	-5.768853	1.227474	-0.339782	H	3.405971	-2.114233	-3.553074
H	-4.639197	1.556260	0.950396	H	2.498581	-0.758738	-2.860025
H	-5.747635	-0.057050	2.426539	C	2.181899	-2.936765	-1.230008
H	-2.443421	5.368764	-1.142463	H	2.279481	-3.807066	-1.888480
C	-4.428322	4.535433	-2.732217	H	2.063286	-3.300393	-0.206311
H	-5.176845	4.985860	-2.061926	H	1.263768	-2.418160	-1.517421
H	-3.862476	5.376243	-3.152720	C	4.638975	-3.796571	0.081073
C	-4.624880	1.560865	-2.772916	H	5.647484	-4.073877	0.406294
C	-5.158278	3.774192	-3.844284	H	4.098569	-3.417616	0.950972
H	-4.457265	3.539477	-4.657772	H	4.137193	-4.700789	-0.282250
H	-5.943212	4.407177	-4.275458	C	5.471697	-3.352453	-2.231986
C	-5.743365	2.471559	-3.292542	H	4.854236	-4.129636	-2.698339

H	5.718810	-2.600240	-2.984792
H	6.407892	-3.816762	-1.903746
C	5.282223	0.837431	-0.102434
C	6.238699	1.119799	-1.094022
C	4.824651	1.927295	0.662029
C	6.706545	2.416437	-1.321520
H	6.625834	0.295641	-1.687413
C	5.278379	3.230576	0.441583
H	4.090652	1.760797	1.449533
C	6.224421	3.479804	-0.554977
H	7.450177	2.597964	-2.094844
H	4.894996	4.049061	1.047359
H	6.585598	4.490910	-0.728660
H	3.411536	-0.704401	1.955036
O	4.582906	-0.993279	1.619004
C	5.645106	-0.715960	2.540393
H	5.501287	0.279877	2.980075
H	6.575789	-0.690030	1.965661
C	5.712274	-1.787601	3.619823
H	5.877089	-2.773020	3.172756
H	6.538466	-1.575555	4.308884
H	4.786663	-1.825204	4.205141

TS3b

SCF energy in Ethanol: -3455.874509 a.u.

Free energy in Ethanol: -3454.695326 a.u.

P	-0.161881	0.177788	-0.789079
N	-0.594016	-0.172316	-2.370869
C	-1.439068	-1.353531	-2.590337
H	-2.099543	-1.168269	-3.444428
H	-0.834943	-2.246331	-2.795258
H	-2.068469	-1.545426	-1.720423
C	0.098821	0.292296	-3.572767
H	0.765736	1.118549	-3.334188
H	0.681994	-0.512806	-4.034931
H	-0.645381	0.637507	-4.302915
O	0.593687	1.638955	-1.125430
O	1.137178	-0.780380	-0.330707
C	1.550617	2.172091	-0.266059
C	2.765783	1.489308	-0.104702
C	1.309578	3.416273	0.351268
C	3.666877	1.909780	0.907072
C	3.125950	0.355384	-1.017707
C	2.277678	3.856999	1.258343
C	3.410778	3.108471	1.594066
C	2.331067	-0.800941	-1.043948
C	4.267064	0.433971	-1.855265
H	2.131734	4.823901	1.733702
C	2.726048	-1.967678	-1.729021
C	4.674136	-0.713320	-2.558442
C	3.925018	-1.887849	-2.444664
C	1.959924	-3.254229	-1.709783
C	1.483473	-3.832760	-2.909815
C	1.785161	-3.952875	-0.490553
C	0.788407	-5.047760	-2.856966
C	1.094348	-5.168237	-0.490112
C	0.570107	-5.727780	-1.658781
H	0.413289	-5.474074	-3.786001
H	0.975548	-5.698781	0.452692
C	1.718239	-3.226044	-4.279298
H	2.575099	-3.699912	-4.777581
H	0.848555	-3.382594	-4.927015
H	1.929334	-2.156502	-4.237916
C	-0.212723	-7.019535	-1.627896
H	-0.028420	-7.623328	-2.523589
H	0.044823	-7.624304	-0.751773
H	-1.292919	-6.825169	-1.585910
C	2.371852	-3.443631	0.803998
H	3.429937	-3.180083	0.687481
H	1.852298	-2.548461	1.157200
H	2.299430	-4.201172	1.589639
C	0.154108	4.310487	0.021873
C	-0.743949	4.738240	1.026279
C	0.027289	4.838115	-1.287148
C	-1.762220	5.641825	0.696798
C	-1.000939	5.742630	-1.565688
C	-1.915690	6.153023	-0.591956
H	-2.452146	5.956320	1.477945
H	-1.080528	6.148390	-2.572669
C	0.999638	4.487337	-2.391491
H	2.038198	4.525651	-2.044648
H	0.823787	3.475386	-2.772333
H	0.896219	5.183209	-3.230023
C	-0.641816	4.285849	2.468342
H	-0.257068	3.268748	2.563079
H	0.027633	4.935319	3.047986
H	-1.623010	4.326751	2.953292
C	-3.038087	7.106566	-0.929491

H	-3.905820	6.571501	-1.338757	C	-0.670652	0.338351	2.375001
H	-3.381327	7.652244	-0.044126	H	-0.016212	1.209886	2.316058
H	-2.728342	7.840529	-1.681815	C	-2.089154	0.572478	2.707911
C	4.326229	3.627853	2.691894	H	-2.385339	1.617679	2.827638
C	5.694941	2.940067	2.721995	H	-2.435193	-0.017026	3.565577
C	5.509500	1.424907	2.609452	H	-3.190282	-0.080512	2.011028
C	4.883149	1.060089	1.256491	B	-4.559914	-0.685385	0.227899
H	6.465845	0.900183	2.721335	O	-3.474041	0.235733	-0.283853
H	6.312079	3.294275	1.883800	O	-5.792634	-0.051803	-0.137812
H	6.227412	3.206236	3.642855	C	-4.106860	1.337093	-1.008290
H	3.832315	3.475863	3.663897	C	-5.570769	1.328409	-0.421023
H	4.441719	4.714104	2.583722	C	-4.069362	0.988001	-2.502596
H	5.654717	1.166127	0.482006	H	-4.596202	0.050653	-2.702673
H	4.599075	0.001575	1.243101	H	-4.521543	1.781262	-3.107911
H	4.861958	1.080957	3.428788	H	-3.027126	0.876551	-2.812527
H	4.272802	-2.779427	-2.961134	C	-3.340537	2.633920	-0.766881
C	5.934319	-0.733832	-3.411475	H	-3.868040	3.476369	-1.230043
H	6.744556	-1.200295	-2.829645	H	-3.225292	2.852440	0.296352
H	5.777952	-1.385955	-4.279804	H	-2.343109	2.587857	-1.213977
C	4.973681	1.763267	-2.097713	C	-5.707490	2.154545	0.873865
C	6.391568	0.657449	-3.862003	H	-6.686835	1.944179	1.316233
H	5.713651	1.040247	-4.638090	H	-4.945679	1.883715	1.607904
H	7.388568	0.594721	-4.314656	H	-5.644470	3.231243	0.678686
C	6.388974	1.618451	-2.670499	C	-6.648010	1.786619	-1.411014
H	4.362744	2.332171	-2.816705	H	-6.475953	2.817073	-1.744842
H	4.992847	2.375726	-1.194060	H	-6.689712	1.134587	-2.286537
H	7.068374	1.236550	-1.894422	H	-7.626864	1.749979	-0.920815
H	6.767402	2.605597	-2.962664	C	-4.456284	-2.217754	-0.267793
Ni	-1.704865	0.203635	0.748433	C	-5.416555	-2.759303	-1.139646
C	3.320765	-4.063441	5.416553	C	-3.400396	-3.063938	0.119547
C	3.985950	-2.895465	5.041451	C	-5.328041	-4.073078	-1.607268
C	3.298906	-1.881404	4.375926	H	-6.248695	-2.131284	-1.447280
C	1.931362	-2.001170	4.062384	C	-3.296162	-4.377965	-0.343461
C	1.276393	-3.187386	4.453404	H	-2.637017	-2.687737	0.801388
C	1.960971	-4.200856	5.117683	C	-4.265030	-4.887835	-1.211054
H	3.851135	-4.856283	5.936910	H	-6.090214	-4.463360	-2.278602
H	5.042079	-2.771922	5.267685	H	-2.461010	-4.999435	-0.028452
H	3.826173	-0.974452	4.088457	H	-4.194657	-5.911711	-1.571636
H	0.219756	-3.317481	4.238103	O	-4.284872	-0.597912	1.762299
H	1.430070	-5.104004	5.408382	C	-4.880619	-1.466981	2.731578
C	1.262628	-0.894754	3.369147	H	-4.924907	-2.479290	2.316478
H	1.888208	-0.019877	3.188226	H	-4.206737	-1.489004	3.597745
C	-0.024097	-0.839225	2.963144	C	-6.267932	-0.985784	3.139102
H	-0.673962	-1.699438	3.129578	H	-6.926611	-0.943713	2.267294

H	-6.701012	-1.672165	3.877126
H	-6.220028	0.014723	3.582327

TS3a'

SCF energy in Ethanol: -2812.645876 a.u.

Free energy in Ethanol: -2811.726117 a.u.

P	-0.016958	-1.553787	-0.073371
N	0.603715	-2.880015	-0.889871
C	1.050919	-4.034781	-0.114425
H	0.631679	-4.956368	-0.538248
H	2.146889	-4.109712	-0.109168
H	0.707760	-3.948476	0.921160
C	0.884078	-2.969191	-2.321037
H	0.603052	-2.044644	-2.822095
H	1.948524	-3.164518	-2.497921
H	0.305520	-3.794306	-2.759367
O	-0.713204	-0.819863	-1.399915
O	1.206482	-0.459724	0.279617
C	-1.086424	0.520623	-1.277562
C	-0.077209	1.491488	-1.259150
C	-2.450246	0.846083	-1.220817
C	-0.420281	2.832543	-0.953244
C	1.339289	1.091825	-1.542506
C	-2.757683	2.193823	-1.018939
C	-1.778250	3.177135	-0.831722
C	1.968529	0.160001	-0.702430
C	2.060307	1.632137	-2.635671
H	-3.805955	2.482631	-0.981269
C	3.343691	-0.125496	-0.792503
C	3.434452	1.353921	-2.752684
C	4.048442	0.518421	-1.813989
C	4.047793	-1.044566	0.156909
C	4.666483	-2.227330	-0.302796
C	4.148597	-0.699225	1.527301
C	5.310925	-3.067134	0.617248
C	4.808748	-1.561281	2.405161
C	5.384947	-2.762148	1.975616
H	5.774053	-3.982583	0.252762
H	4.885285	-1.281418	3.454414
C	4.702825	-2.620837	-1.765410
H	5.627444	-2.272393	-2.245523
H	4.680110	-3.710693	-1.876059
H	3.873073	-2.196438	-2.333387
C	6.060701	-3.693627	2.955043
H	6.678273	-3.141735	3.673148
H	5.324175	-4.263884	3.536905
H	6.703836	-4.416419	2.442241
C	3.597972	0.607333	2.051165
H	3.955983	1.457875	1.458871
H	2.504468	0.625282	2.012510
H	3.906349	0.766706	3.089625
C	-3.535812	-0.164887	-1.423056
C	-4.388509	-0.528537	-0.360601
C	-3.746443	-0.713573	-2.708050
C	-5.426272	-1.436506	-0.598496
C	-4.799745	-1.611324	-2.902236
C	-5.649879	-1.991845	-1.859607
H	-6.071152	-1.721284	0.230243
H	-4.962496	-2.021090	-3.897658
C	-2.868156	-0.338523	-3.881306
H	-2.759006	0.747935	-3.977040
H	-1.859148	-0.754438	-3.773087
H	-3.287538	-0.721081	-4.817382
C	-4.211712	0.037253	1.030865
H	-3.160730	0.022086	1.338277
H	-4.549314	1.080003	1.096105
H	-4.783540	-0.546982	1.757838
C	-6.759706	-2.992687	-2.086334
H	-6.403328	-4.021686	-1.942152
H	-7.589123	-2.836949	-1.387951
H	-7.157175	-2.927577	-3.105408
C	-2.224267	4.584596	-0.468112
C	-1.121443	5.636325	-0.622577
C	0.169584	5.122308	0.019368
C	0.669169	3.871745	-0.716965
H	0.951830	5.891050	-0.001757
H	-0.944543	5.843608	-1.688128
H	-1.440567	6.580169	-0.164354
H	-2.558192	4.579832	0.580278
H	-3.104733	4.853781	-1.066239
H	1.103787	4.187036	-1.675871
H	1.492091	3.409720	-0.159733
H	-0.017170	4.886942	1.075194
H	5.118107	0.337832	-1.894501
C	4.290431	1.973759	-3.848235
H	4.834979	2.831598	-3.423838
H	5.060817	1.257710	-4.161042
C	1.342340	2.397091	-3.740609

C	3.484632	2.455043	-5.059682
H	3.138306	1.590783	-5.644035
H	4.126227	3.048899	-5.721966
C	2.271988	3.266565	-4.595355
H	0.861687	1.652506	-4.395019
H	0.521874	2.994302	-3.338646
H	2.614276	4.133399	-4.011483
H	1.715918	3.663396	-5.453412
Ni	-1.128044	-2.068989	1.692410
C	-1.160797	5.378987	4.133520
C	0.162553	4.958164	4.277668
C	0.495848	3.617078	4.091482
C	-0.479079	2.655622	3.758973
C	-1.808601	3.102583	3.607069
C	-2.142706	4.440868	3.795588
H	-1.425802	6.422497	4.280262
H	0.937774	5.674340	4.538282
H	1.528864	3.297877	4.211175
H	-2.587409	2.397109	3.333173
H	-3.176831	4.756012	3.678962
C	-0.072142	1.257789	3.598395
H	1.001977	1.081820	3.643735
C	-0.882092	0.187087	3.433554
H	-1.961997	0.337777	3.430249
C	-0.444560	-1.198028	3.277537
H	0.622077	-1.366166	3.433342
C	-1.372831	-2.287459	3.683876
H	-0.890469	-3.132016	4.182802
H	-2.261589	-1.949143	4.226285
C	-2.677296	-4.835281	-0.408125
H	-1.873060	-4.288191	-0.912509
H	-2.626387	-5.891620	-0.705351
H	-3.629030	-4.419252	-0.755209
C	-2.559776	-4.685258	1.107929
H	-3.367465	-5.262129	1.590467
H	-1.610283	-5.137180	1.448745
O	-2.667493	-3.334780	1.499780
H	-2.075682	-2.970632	2.705847

TS3b'

SCF energy in Ethanol: -2812.642370 a.u.

Free energy in Ethanol: -2811.722856 a.u.

P	-0.454606	-0.656554	-1.065137
N	-0.351026	-0.592697	-2.730779
C	0.202349	-1.739434	-3.455827
H	-0.411480	-1.933308	-4.344348
H	1.236159	-1.547511	-3.774070
H	0.169281	-2.636193	-2.833145
C	-0.652140	0.565847	-3.569665
H	-0.949282	1.416700	-2.958684
H	0.221261	0.846143	-4.169527
H	-1.475575	0.322014	-4.255498
O	-1.665041	0.490005	-0.913662
O	0.821709	0.156818	-0.344245
C	-1.861662	1.149233	0.295614
C	-0.909445	2.092353	0.705403
C	-3.031035	0.891280	1.032831
C	-1.013389	2.659077	2.001602
C	0.211107	2.472038	-0.214956
C	-3.155082	1.557251	2.254885
C	-2.157620	2.391104	2.772627
C	1.110372	1.483606	-0.644025
C	0.394072	3.807688	-0.652135
H	-4.057967	1.396837	2.839810
C	2.300903	1.794738	-1.327312
C	1.563674	4.139736	-1.359342
C	2.503631	3.142169	-1.639787
C	3.330173	0.764825	-1.673202
C	3.684022	0.505307	-3.015175
C	4.006612	0.081221	-0.632450
C	4.649875	-0.472508	-3.291719
C	4.969217	-0.877413	-0.955808
C	5.295235	-1.184463	-2.281468
H	4.906340	-0.673287	-4.330813
H	5.479403	-1.395493	-0.146290
C	3.096772	1.265121	-4.187235
H	3.771461	2.068490	-4.513938
H	2.953245	0.603175	-5.048819
H	2.140690	1.732498	-3.946911
C	6.310624	-2.256486	-2.603194
H	7.154397	-2.232092	-1.904110
H	5.866537	-3.258928	-2.536660
H	6.707729	-2.142305	-3.617485
C	3.740486	0.392066	0.822693
H	3.711165	1.473228	1.001609
H	2.780905	-0.023121	1.148010
H	4.518643	-0.038683	1.458422
C	-4.123006	-0.012853	0.552932

C	-4.461778	-1.175379	1.280593
C	-4.877753	0.333749	-0.592643
C	-5.519042	-1.978461	0.834541
C	-5.929098	-0.494240	-0.995434
C	-6.263219	-1.661836	-0.303202
H	-5.767428	-2.875530	1.399233
H	-6.508883	-0.212960	-1.872710
C	-4.598278	1.596934	-1.375966
H	-4.489686	2.465676	-0.716718
H	-3.670311	1.511068	-1.952094
H	-5.412356	1.804077	-2.077906
C	-3.736644	-1.580489	2.546943
H	-2.675894	-1.320776	2.515957
H	-4.160638	-1.087329	3.431700
H	-3.821818	-2.660065	2.710512
C	-7.379742	-2.560219	-0.782479
H	-7.010334	-3.303902	-1.501605
H	-7.836526	-3.110782	0.047030
H	-8.167540	-1.987948	-1.284593
C	-2.342721	2.955036	4.173891
C	-1.352383	4.070331	4.524301
C	0.057358	3.659552	4.091837
C	0.119712	3.507453	2.566486
H	0.800656	4.398008	4.415475
H	-1.633749	4.999329	4.007996
H	-1.392326	4.280770	5.599747
H	-2.223514	2.135844	4.899349
H	-3.376393	3.306317	4.289804
H	0.102478	4.511646	2.121048
H	1.079308	3.070857	2.267227
H	0.323353	2.708703	4.574883
H	3.425263	3.419136	-2.146811
C	1.866673	5.568094	-1.789298
H	2.573306	6.008458	-1.068667
H	2.392202	5.557009	-2.752374
C	-0.709840	4.844114	-0.477252
C	0.625121	6.462451	-1.868626
H	0.024546	6.190376	-2.748296
H	0.926786	7.508383	-2.002347
C	-0.224653	6.292896	-0.606237
H	-1.462300	4.657007	-1.259857
H	-1.240784	4.702341	0.466070
H	0.374182	6.565823	0.274957
H	-1.088654	6.968399	-0.622494
Ni	-0.793726	-2.624249	-0.270455
C	6.138746	-2.753236	3.617539
C	5.283775	-1.973701	4.398567
C	3.930134	-1.882280	4.078316
C	3.388030	-2.563716	2.970765
C	4.268739	-3.342677	2.191466
C	5.620172	-3.436903	2.512433
H	7.194502	-2.827725	3.863460
H	5.670684	-1.435380	5.260192
H	3.271806	-1.273339	4.694146
H	3.893839	-3.872315	1.320663
H	6.275339	-4.047119	1.895446
C	1.956334	-2.434678	2.689472
H	1.421594	-1.735729	3.334134
C	1.240541	-3.101265	1.755180
H	1.742611	-3.830127	1.117719
C	-0.196792	-2.957490	1.541805
H	-0.695469	-2.321773	2.274880
C	-0.974843	-4.126016	1.042658
H	-1.931102	-4.281254	1.548967
H	-0.400372	-5.054118	0.961804
C	-3.521939	-4.768579	-2.807677
H	-2.913367	-4.885333	-3.711456
H	-3.477503	-5.709729	-2.247314
H	-4.562878	-4.593513	-3.110235
C	-2.997992	-3.611879	-1.958429
H	-3.085229	-2.667737	-2.520557
H	-3.628823	-3.498880	-1.061440
O	-1.643356	-3.838377	-1.608602
H	-1.433552	-4.139857	-0.274187

IM5a

SCF energy in Ethanol: -3455.910521 a.u.

Free energy in Ethanol: -3454.723946 a.u.

P	0.002145	0.729310	-0.597692
N	0.416905	1.752706	-1.846714
C	1.523373	2.698149	-1.654995
H	2.091123	2.778395	-2.588612
H	1.148177	3.690898	-1.376215
H	2.211240	2.344252	-0.887967
C	-0.404450	2.037988	-3.023813
H	-1.238578	1.342637	-3.089718
H	-0.795897	3.061836	-2.991252
H	0.212950	1.934819	-3.925907

O	-1.032304	-0.244943	-1.475326	H	-3.282940	-2.035941	-3.473567
O	-1.051116	1.494412	0.452175	H	-1.928208	-0.943310	-3.758094
C	-2.063128	-0.970179	-0.875077	H	-2.386681	-2.116908	-5.000031
C	-3.103465	-0.274842	-0.240128	C	-0.121332	-4.369724	0.046952
C	-2.078842	-2.371858	-1.005589	H	-0.002644	-3.430918	0.594809
C	-4.035244	-0.997802	0.548465	H	-0.970909	-4.891938	0.502984
C	-3.255664	1.205806	-0.420449	H	0.768156	-4.980901	0.228207
C	-3.079752	-3.048334	-0.302915	C	1.042112	-5.667986	-4.678110
C	-4.008289	-2.402279	0.520109	H	1.957227	-6.058737	-4.220607
C	-2.244203	2.065655	0.025374	H	0.437556	-6.532083	-4.985700
C	-4.417699	1.759704	-1.014542	H	1.322237	-5.129642	-5.590396
H	-3.126243	-4.130680	-0.394887	C	-4.955121	-3.252261	1.352995
C	-2.413715	3.460259	0.102674	C	-6.131643	-2.466725	1.941786
C	-4.600075	3.154052	-0.979679	C	-5.628780	-1.148203	2.535096
C	-3.623867	3.961495	-0.386039	C	-5.035770	-0.261458	1.432049
C	-1.394717	4.376157	0.704869	H	-6.439450	-0.608914	3.039619
C	-0.796049	5.401372	-0.060590	H	-6.869783	-2.251310	1.155963
C	-1.071777	4.259989	2.079921	H	-6.643423	-3.072373	2.699135
C	0.154279	6.239165	0.539257	H	-4.381269	-3.705583	2.175499
C	-0.126620	5.125350	2.635821	H	-5.316746	-4.093005	0.746914
C	0.515034	6.112473	1.880121	H	-5.863662	0.128974	0.823999
H	0.620270	7.015561	-0.064941	H	-4.553931	0.619448	1.871186
H	0.108545	5.031289	3.694269	H	-4.865782	-1.358028	3.298241
C	-1.159290	5.670239	-1.507073	H	-3.799545	5.032914	-0.322566
H	-1.942107	6.437261	-1.582176	C	-5.858076	3.815995	-1.523819
H	-0.292332	6.045277	-2.061602	H	-6.527011	4.042916	-0.679216
H	-1.537292	4.782218	-2.017270	H	-5.599233	4.785724	-1.966970
C	1.568148	7.002995	2.496816	C	-5.397281	0.882288	-1.784982
H	1.320135	7.260076	3.532778	C	-6.619024	2.951992	-2.535254
H	2.547256	6.505611	2.513443	H	-6.071042	2.922402	-3.487783
H	1.685391	7.935101	1.934152	H	-7.597337	3.400159	-2.746489
C	-1.760176	3.255611	2.977552	C	-6.772157	1.527346	-1.996632
H	-2.847970	3.277007	2.843809	H	-4.949951	0.680852	-2.771459
H	-1.426387	2.233575	2.771475	H	-5.504749	-0.097723	-1.315910
H	-1.545388	3.470549	4.028922	H	-7.322030	1.555113	-1.044522
C	-1.193841	-3.151361	-1.930646	H	-7.363317	0.910566	-2.684311
C	-0.316807	-4.141310	-1.434558	Ni	1.730811	-0.055763	0.518925
C	-1.333741	-2.983695	-3.328696	C	-0.484233	-6.116033	4.752713
C	0.404132	-4.930641	-2.339322	C	-1.635475	-5.353772	4.547047
C	-0.592165	-3.794820	-4.192923	C	-1.543492	-4.090510	3.964783
C	0.281189	-4.779009	-3.721674	C	-0.302615	-3.548827	3.576303
H	1.081393	-5.686030	-1.945499	C	0.847290	-4.337537	3.784903
H	-0.709601	-3.658649	-5.266538	C	0.756501	-5.599226	4.366171
C	-2.284643	-1.966916	-3.920641	H	-0.551150	-7.102345	5.203736

H	-2.607123	-5.742737	4.841285	H	6.979401	4.839166	0.074159
H	-2.443825	-3.497929	3.816137	O	3.572158	-0.313338	1.210023
H	1.819426	-3.964018	3.476100	C	4.241535	-1.066784	2.224153
H	1.658982	-6.187164	4.513792	H	3.589914	-1.075407	3.100862
C	-0.265820	-2.206576	2.984612	H	4.365692	-2.102236	1.882152
H	-1.239658	-1.797971	2.710676	C	5.596001	-0.487316	2.623387
C	0.823433	-1.426909	2.793691	H	6.007647	-1.086505	3.445599
H	1.790527	-1.808861	3.112672	H	6.303226	-0.512651	1.791118
C	0.779783	-0.056797	2.239678	H	5.499340	0.548927	2.961516
H	-0.263219	0.219366	2.084116	H	1.341903	2.009733	2.661591
C	1.446553	1.016872	3.113480				
H	0.965872	1.055600	4.103447	**IM5b**			
H	2.513010	0.835541	3.270262	SCF energy in Ethanol: -3455.907681 a.u.			
B	4.293647	-0.010678	-0.115626	Free energy in Ethanol: -3454.723037 a.u.			
O	3.061484	0.007129	-1.023156	P	0.173802	0.316379	-0.660351
O	5.104482	-1.087451	-0.617664	N	-0.060549	0.185900	-2.309426
C	3.348182	-0.853036	-2.163828	C	-1.174486	-0.643665	-2.790470
C	4.378029	-1.878143	-1.558485	H	-1.564364	-0.209968	-3.717656
C	3.970130	0.042440	-3.248623	H	-0.853645	-1.672180	-2.984391
H	4.902228	0.499097	-2.908235	H	-1.989975	-0.652808	-2.069367
H	4.167421	-0.522122	-4.166548	C	0.947095	0.483707	-3.329022
H	3.267240	0.846215	-3.489212	H	1.710606	1.146252	-2.925780
C	2.066032	-1.476485	-2.700579	H	1.433665	-0.426723	-3.701008
H	2.296565	-2.186176	-3.502916	H	0.454898	0.984050	-4.172588
H	1.508832	-2.013089	-1.931657	O	1.316936	1.532501	-0.699306
H	1.412281	-0.704474	-3.116893	O	1.065451	-0.993774	-0.114297
C	3.695993	-3.050339	-0.828348	C	2.402520	1.629938	0.170041
H	4.460005	-3.605026	-0.272881	C	3.347909	0.594520	0.203206
H	2.945271	-2.699946	-0.113510	C	2.566476	2.807918	0.926503
H	3.208495	-3.741455	-1.524652	C	4.360041	0.608592	1.197383
C	5.375049	-2.442362	-2.577253	C	3.310013	-0.520276	-0.797395
H	4.863744	-2.990827	-3.377686	C	3.651567	2.835292	1.807029
H	5.980105	-1.650050	-3.024316	C	4.510021	1.749382	2.002224
H	6.055197	-3.137125	-2.072730	C	2.203547	-1.379082	-0.831354
C	5.081552	1.399852	-0.025147	C	4.396921	-0.751305	-1.677816
C	6.302399	1.588855	-0.696022	H	3.816874	3.740783	2.385359
C	4.581473	2.498948	0.697820	C	2.221706	-2.598124	-1.539010
C	6.983422	2.808639	-0.664879	C	4.415603	-1.933847	-2.436966
H	6.730121	0.750019	-1.239915	C	3.362791	-2.845986	-2.308463
C	5.247556	3.726718	0.732138	C	1.137959	-3.625963	-1.449905
H	3.657983	2.387786	1.263133	C	0.430784	-4.057195	-2.594163
C	6.454134	3.887137	0.046762	C	0.877895	-4.243252	-0.201665
H	7.929092	2.916944	-1.192255	C	-0.582760	-5.014677	-2.448613
H	4.830495	4.555761	1.300945	C	-0.136076	-5.198098	-0.105558

C	-0.897802	-5.582453	-1.214619	H	6.023599	-0.651742	0.621192
H	-1.136695	-5.325341	-3.332700	H	4.661912	-1.520046	1.287197
H	-0.333163	-5.655911	0.861179	H	5.239913	-0.808018	3.568304
C	0.746898	-3.576290	-3.996673	H	3.419415	-3.787343	-2.849807
H	1.484632	-4.231391	-4.479878	C	5.579454	-2.288877	-3.350822
H	-0.150852	-3.591920	-4.623882	H	6.221256	-3.017610	-2.832000
H	1.159551	-2.565830	-4.016651	H	5.201161	-2.806601	-4.241102
C	-2.023307	-6.580654	-1.074963	C	5.470293	0.309472	-1.890781
H	-2.272456	-7.042733	-2.036074	C	6.432343	-1.081931	-3.755965
H	-1.766308	-7.378802	-0.369461	H	5.886800	-0.467122	-4.485909
H	-2.935020	-6.099325	-0.696139	H	7.348962	-1.423122	-4.251860
C	1.728000	-3.945408	1.012555	C	6.757529	-0.232905	-2.524062
H	2.792019	-4.106543	0.797756	H	5.048504	1.075852	-2.560468
H	1.612194	-2.910180	1.344264	H	5.695465	0.835987	-0.961082
H	1.447151	-4.594546	1.846189	H	7.302883	-0.847144	-1.792749
C	1.698529	4.020856	0.801746	H	7.416247	0.603338	-2.787729
C	1.004770	4.523226	1.927353	Ni	-1.678454	0.618950	0.458585
C	1.656261	4.742577	-0.415588	C	-1.772786	-6.052903	4.539773
C	0.237393	5.687519	1.794557	C	-0.520003	-5.526401	4.860360
C	0.894851	5.911996	-0.492629	C	-0.139273	-4.276871	4.372082
C	0.161003	6.395372	0.594372	C	-0.998482	-3.515928	3.555903
H	-0.304982	6.055801	2.663448	C	-2.252796	-4.070271	3.231256
H	0.880702	6.464737	-1.430263	C	-2.635028	-5.316804	3.720849
C	2.445682	4.310298	-1.631002	H	-2.072309	-7.027098	4.916663
H	3.464540	4.006502	-1.366399	H	0.162547	-6.088530	5.492880
H	1.972696	3.457649	-2.130424	H	0.835794	-3.870823	4.632827
H	2.512782	5.127347	-2.356287	H	-2.925337	-3.526993	2.573729
C	1.092898	3.884651	3.298633	H	-3.608312	-5.721402	3.454339
H	1.234419	2.803046	3.251776	C	-0.560143	-2.197075	3.080272
H	1.935340	4.295217	3.871496	H	0.509944	-2.005495	3.159111
H	0.185760	4.086569	3.876841	C	-1.351373	-1.207844	2.615760
C	-0.693034	7.635433	0.469324	H	-2.425691	-1.375992	2.608980
H	-1.698627	7.389276	0.102189	C	-0.879710	0.125504	2.172085
H	-0.815066	8.138361	1.434546	H	0.215074	0.120557	2.126577
H	-0.258212	8.352897	-0.235429	C	-1.330129	1.283328	3.082588
C	5.563468	1.842744	3.095721	H	-1.084035	2.258662	2.649246
C	6.632597	0.748366	3.014488	H	-0.818289	1.216876	4.054870
C	5.964757	-0.606445	2.766916	H	-2.404256	1.271042	3.278050
C	5.256133	-0.606973	1.406100	B	-4.146897	1.016063	-0.410580
H	6.700312	-1.419266	2.793941	O	-2.810411	1.369473	-1.051293
H	7.330066	0.964418	2.192521	O	-4.938166	2.212682	-0.526108
H	7.224826	0.735853	3.937210	C	-2.928066	2.696132	-1.644422
H	5.059754	1.773840	4.071921	C	-4.111840	3.335854	-0.821774
H	6.026204	2.837926	3.069806	C	-3.289196	2.484545	-3.123208

H	-4.229904	1.936883	-3.224790	C	1.328847	2.502264	2.628708
H	-3.375737	3.437963	-3.655459	H	1.982058	1.648999	2.801675
H	-2.499804	1.899785	-3.604884	H	1.944133	3.387215	2.427698
C	-1.604242	3.444730	-1.538350	H	0.746666	2.690527	3.541600
H	-1.715815	4.468583	-1.913836	O	1.115031	-0.155739	1.654032
H	-1.241806	3.501369	-0.510026	O	1.643434	0.993922	-0.601739
H	-0.838695	2.947801	-2.140972	C	1.799599	-1.297979	1.236498
C	-3.646157	4.001906	0.487677	C	3.016579	-1.143180	0.557051
H	-4.530994	4.252127	1.082255	C	1.285701	-2.565004	1.566900
H	-3.023654	3.331276	1.083968	C	3.633292	-2.280526	-0.024578
H	-3.086060	4.925704	0.301593	C	3.650606	0.209477	0.434828
C	-4.949962	4.345569	-1.615642	C	1.986171	-3.669289	1.074514
H	-4.341513	5.190609	-1.960541	C	3.106197	-3.554980	0.244848
H	-5.425690	3.878090	-2.480876	C	2.965577	1.227007	-0.244085
H	-5.743307	4.741403	-0.972431	C	4.939110	0.477195	0.959495
C	-4.877693	-0.283332	-1.038644	H	1.624542	-4.662313	1.330308
C	-6.057799	-0.154401	-1.791167	C	3.579911	2.439991	-0.606264
C	-4.354109	-1.583021	-0.899146	C	5.565629	1.695201	0.638544
C	-6.678705	-1.256669	-2.384639	C	4.895468	2.621027	-0.168276
H	-6.493351	0.835135	-1.903938	C	2.902964	3.479238	-1.443986
C	-4.960305	-2.693245	-1.492240	C	2.687922	4.784473	-0.948985
H	-3.451323	-1.733839	-0.307280	C	2.526447	3.173168	-2.776070
C	-6.128701	-2.532123	-2.240653	C	2.049909	5.730851	-1.763061
H	-7.592945	-1.121444	-2.959052	C	1.905849	4.153331	-3.553253
H	-4.523477	-3.682262	-1.368218	C	1.640353	5.436257	-3.062527
H	-6.607667	-3.392474	-2.702644	H	1.876197	6.729166	-1.364997
O	-3.607563	0.731082	1.001394	H	1.625987	3.908213	-4.576026
C	-4.511363	0.248988	2.000330	C	3.149773	5.234681	0.422280
H	-5.096158	-0.577812	1.578602	H	4.128017	5.731605	0.366479
H	-3.918347	-0.151652	2.825325	H	2.449497	5.960972	0.849513
C	-5.440351	1.340432	2.527063	H	3.256718	4.404210	1.122115
H	-6.052419	1.756122	1.723684	C	0.928829	6.461103	-3.914724
H	-6.099128	0.919071	3.297103	H	1.312032	6.464464	-4.941804
H	-4.865240	2.158324	2.975203	H	-0.147108	6.249894	-3.974082
				H	1.043664	7.471066	-3.507492
TS4a				C	2.811168	1.823341	-3.396221
SCF energy in Ethanol: -3455.882079 a.u.				H	3.828631	1.483049	-3.172794
Free energy in Ethanol: -3454.700799 a.u.				H	2.121860	1.058388	-3.023833
P	0.421031	0.886552	0.538665	H	2.701267	1.869917	-4.484122
N	0.418724	2.239155	1.515580	C	0.096112	-2.780141	2.450460
C	-0.427869	3.377411	1.148769	C	-1.060177	-3.425903	1.950439
H	-0.939929	3.751820	2.043286	C	0.162028	-2.428425	3.817134
H	0.172890	4.188081	0.715093	C	-2.128140	-3.675846	2.818920
H	-1.196157	3.079002	0.433531	C	-0.931167	-2.703294	4.648287

C	-2.088865	-3.320903	4.170991	C	-0.994880	-3.689924	-3.361631
H	-3.014703	-4.169826	2.425230	C	-2.329242	-4.016918	-3.681404
H	-0.866582	-2.437735	5.701876	C	-2.654470	-5.260808	-4.215523
C	1.394385	-1.787622	4.416259	H	-1.923038	-7.192060	-4.856734
H	2.306566	-2.327451	4.137732	H	0.444029	-6.657125	-4.288470
H	1.514240	-0.753729	4.073287	H	1.024044	-4.446060	-3.348106
H	1.330035	-1.773246	5.508906	H	-3.117443	-3.293853	-3.495790
C	-1.176003	-3.858631	0.505422	H	-3.691661	-5.486163	-4.452808
H	-0.887084	-3.065801	-0.190459	C	-0.589006	-2.392068	-2.811918
H	-0.539378	-4.722991	0.283011	H	0.449564	-2.343548	-2.478469
H	-2.204744	-4.146272	0.268978	C	-1.339003	-1.272375	-2.695595
C	-3.264848	-3.596284	5.079556	H	-2.366648	-1.281568	-3.054606
H	-4.110544	-2.934551	4.850610	C	-0.837736	0.001406	-2.134341
H	-3.625235	-4.625809	4.967739	H	0.239163	-0.106370	-1.983617
H	-3.002061	-3.443930	6.131473	C	-1.071675	1.220885	-3.039962
C	3.695202	-4.823156	-0.354546	H	-0.541571	1.095669	-3.997335
C	5.074694	-4.621413	-0.989937	H	-2.128946	1.368642	-3.274543
C	5.067466	-3.351172	-1.843833	H	-0.695737	2.142688	-2.581139
C	4.825663	-2.120279	-0.960352	B	-3.692757	1.314486	0.704522
H	6.015270	-3.232406	-2.382448	O	-3.732289	2.579040	0.072388
H	5.840078	-4.527073	-0.206194	O	-4.882026	1.084412	1.418185
H	5.341648	-5.500231	-1.588922	C	-4.886556	3.295891	0.557257
H	3.001930	-5.198002	-1.122926	C	-5.817250	2.144519	1.136815
H	3.734864	-5.604571	0.415522	C	-5.494256	4.083319	-0.606447
H	5.740353	-1.929540	-0.381892	H	-5.755036	3.430171	-1.442136
H	4.680591	-1.229905	-1.582198	H	-6.395085	4.623086	-0.291007
H	4.277775	-3.427615	-2.604657	H	-4.768287	4.819902	-0.967634
H	5.409426	3.537209	-0.449945	C	-4.392426	4.281856	1.630238
C	6.978987	2.020648	1.100295	H	-5.204397	4.903038	2.024480
H	7.672513	1.832067	0.266150	H	-3.917815	3.758100	2.465427
H	7.056105	3.094040	1.314286	H	-3.644493	4.943361	1.180384
C	5.592142	-0.478844	1.950518	C	-6.528723	2.501181	2.446685
C	7.432944	1.200259	2.312480	H	-7.105505	1.636976	2.792643
H	6.920156	1.556417	3.217272	H	-5.821743	2.769612	3.235267
H	8.507094	1.345238	2.479579	H	-7.224734	3.336259	2.303860
C	7.105499	-0.279633	2.096593	C	-6.859421	1.619757	0.137454
H	5.120956	-0.308042	2.931546	H	-7.634674	2.367422	-0.065239
H	5.366209	-1.518078	1.703613	H	-6.402315	1.320781	-0.807164
H	7.618422	-0.638003	1.192163	H	-7.340937	0.735514	0.567807
H	7.475720	-0.887764	2.930876	C	-3.545106	-0.036666	-0.832198
Ni	-1.583728	0.389773	-0.339868	C	-3.858865	-1.350936	-0.415197
C	-1.663579	-6.221705	-4.441714	C	-4.218203	0.425908	-1.984762
C	-0.338484	-5.920593	-4.121695	C	-4.771863	-2.156322	-1.101920
C	-0.012635	-4.674519	-3.588595	H	-3.384862	-1.758434	0.475589

C	-5.129043	-0.364376	-2.685241
H	-4.042403	1.446030	-2.314849
C	-5.406492	-1.664029	-2.244099
H	-4.989080	-3.162325	-0.749858
H	-5.631070	0.027998	-3.567231
H	-6.121414	-2.282282	-2.782299
O	-2.465916	0.945628	1.384198
C	-2.506523	0.145436	2.588513
H	-1.597970	-0.458816	2.595858
H	-3.370074	-0.523189	2.551310
C	-2.569373	1.033884	3.821790
H	-1.718070	1.722537	3.845015
H	-3.495914	1.614896	3.834782
H	-2.535544	0.412540	4.724817

TS4b

SCF energy in Ethanol: -3455.881086 a.u.

Free energy in Ethanol: -3454.696683 a.u.

P	-0.506280	0.006402	-0.489084
N	-0.301576	0.543137	-2.056977
C	0.915582	1.282665	-2.402362
H	0.682065	2.332872	-2.620828
H	1.641415	1.243666	-1.588060
H	1.382990	0.831222	-3.285661
C	-1.267195	0.433638	-3.148062
H	-2.139081	-0.136221	-2.832733
H	-1.595991	1.425195	-3.484173
H	-0.799963	-0.079638	-4.000027
O	-1.593649	-1.225560	-0.841735
O	-1.495823	1.064267	0.365791
C	-2.596615	-1.630345	0.037542
C	-3.632309	-0.736914	0.343676
C	-2.591103	-2.949205	0.526385
C	-4.578958	-1.081486	1.342677
C	-3.729765	0.585559	-0.350747
C	-3.605705	-3.290864	1.424115
C	-4.562096	-2.379098	1.880249
C	-2.692139	1.514082	-0.186378
C	-4.868830	0.945049	-1.111507
H	-3.634335	-4.311311	1.799296
C	-2.841525	2.870234	-0.529049
C	-5.010515	2.279429	-1.531599
C	-4.030176	3.213829	-1.182663
C	-1.869271	3.945683	-0.155881
C	-1.264196	4.753758	-1.144302
C	-1.653554	4.245760	1.211757
C	-0.454362	5.827138	-0.752595
C	-0.841132	5.330355	1.553361
C	-0.230065	6.137877	0.589985
H	0.003209	6.444119	-1.524306
H	-0.690365	5.557499	2.606637
C	-1.479832	4.526926	-2.626399
H	-2.359333	5.069883	-2.997471
H	-0.618204	4.884986	-3.200126
H	-1.635767	3.472132	-2.862826
C	0.656695	7.293360	0.989533
H	0.350973	7.716751	1.952390
H	1.700571	6.969305	1.089061
H	0.631111	8.094496	0.242425
C	-2.316169	3.455288	2.318337
H	-3.396952	3.363763	2.156624
H	-1.910950	2.440092	2.387784
H	-2.160305	3.943865	3.284993
C	-1.617977	-4.003511	0.101966
C	-0.718196	-4.556899	1.040397
C	-1.674271	-4.530456	-1.207683
C	0.120729	-5.604705	0.643446
C	-0.821319	-5.583354	-1.557215
C	0.089653	-6.132134	-0.650555
H	0.814222	-6.023577	1.370361
H	-0.879767	-5.992027	-2.564390
C	-2.650018	-3.997261	-2.233045
H	-3.669700	-3.949570	-1.834001
H	-2.380147	-2.982838	-2.548949
H	-2.664005	-4.633868	-3.123353
C	-0.645475	-4.055610	2.467292
H	-0.664272	-2.962618	2.516569
H	-1.488419	-4.417783	3.068884
H	0.274186	-4.396402	2.951461
C	1.023483	-7.248036	-1.058722
H	0.626555	-7.810821	-1.910248
H	2.005913	-6.856254	-1.354436
H	1.192086	-7.951384	-0.235712
C	-5.532856	-2.826875	2.962433
C	-6.709574	-1.867815	3.168556
C	-6.197219	-0.426107	3.205214
C	-5.577408	-0.049013	1.853253
H	-7.007024	0.274349	3.442096

H	-7.431403	-1.975465	2.346164	C	5.268491	-0.260348	-1.748901
H	-7.241970	-2.123206	4.092534	C	5.585520	-1.805427	-1.549473
H	-4.980351	-2.918016	3.909966	C	6.349645	0.687704	-1.225350
H	-5.893871	-3.837417	2.730608	H	6.545074	0.528660	-0.162596
H	-6.392245	0.082509	1.127831	H	7.288889	0.556629	-1.776062
H	-5.085029	0.927523	1.922113	H	6.020626	1.724037	-1.353456
H	-5.447214	-0.325581	4.002367	C	4.928630	0.112967	-3.202300
H	-4.186916	4.257709	-1.444400	H	5.798150	0.031674	-3.864246
C	-6.234732	2.756257	-2.300165	H	4.128182	-0.518571	-3.599963
H	-6.913535	3.266527	-1.599393	H	4.578561	1.150286	-3.222798
H	-5.934367	3.517570	-3.030995	C	6.073285	-2.523418	-2.812820
C	-5.867623	-0.112458	-1.566077	H	6.214115	-3.587193	-2.593611
C	-7.001679	1.624209	-2.991892	H	5.355903	-2.442040	-3.633011
H	-6.433065	1.265560	-3.861627	H	7.034732	-2.118660	-3.150763
H	-7.959055	2.000329	-3.372159	C	6.568378	-2.100616	-0.406431
C	-7.215359	0.463974	-2.015910	H	7.581192	-1.759838	-0.649555
H	-5.416181	-0.648781	-2.415870	H	6.255042	-1.634864	0.528979
H	-6.015275	-0.872677	-0.795539	H	6.600202	-3.182939	-0.243250
H	-7.778562	0.822868	-1.142108	C	3.115952	-1.465534	1.256244
H	-7.817645	-0.328961	-2.475644	C	2.707678	-2.753662	1.670944
Ni	1.441401	-0.512359	0.508633	C	4.202100	-0.904160	1.963814
C	5.440999	5.550279	0.742622	C	3.316066	-3.426558	2.735557
C	4.304315	5.595657	-0.066980	H	1.896863	-3.255178	1.146929
C	3.262131	4.690284	0.132136	C	4.823427	-1.563197	3.024367
C	3.323359	3.706713	1.140320	H	4.587316	0.060642	1.645813
C	4.476280	3.684557	1.953153	C	4.373225	-2.827610	3.420987
C	5.516394	4.588357	1.755124	H	2.972024	-4.417404	3.025670
H	6.253932	6.255624	0.592142	H	5.661871	-1.099905	3.540730
H	4.228396	6.337657	-0.858553	H	4.853877	-3.344547	4.248429
H	2.380350	4.733805	-0.502672	O	2.057797	-1.438042	-1.185317
H	4.551314	2.960209	2.759130	C	1.567903	-2.700733	-1.693428
H	6.390982	4.547153	2.400136	H	0.525222	-2.782035	-1.385328
C	2.206968	2.768365	1.292508	H	0.253189	-0.899353	3.374551
H	1.305445	3.025253	0.735198	H	2.130194	-3.518495	-1.236448
C	2.216688	1.618822	2.008818	C	1.684575	-2.753316	-3.209692
H	3.124400	1.357208	2.547665	H	1.136457	-1.924809	-3.671436
C	1.120963	0.636288	2.090929	H	2.731612	-2.702122	-3.521159
H	0.167640	1.131127	1.896809	H	1.259849	-3.694924	-3.578410
C	1.033030	-0.129940	3.412288				
H	0.778641	0.550217	4.241256	**IM6a**			
H	1.974083	-0.626260	3.666229	SCF energy in Ethanol: -2889.880718 a.u.			
B	3.447763	-1.316298	-0.792645	Free energy in Ethanol: -2888.942110 a.u.			
O	4.070057	-0.064890	-0.969877	P	-0.009337	0.977095	0.977479
O	4.299277	-2.357308	-1.198326	N	0.468403	2.006860	2.208263

C	0.096863	3.419741	2.137782	C	-3.340297	-1.870917	1.427806
H	-0.327034	3.741441	3.097948	C	-2.000822	-2.191501	3.446243
H	0.968048	4.047689	1.906360	C	-4.441199	-1.570638	2.237360
H	-0.658415	3.571035	1.360494	C	-3.132068	-1.897593	4.215040
C	1.359207	1.674515	3.319328	C	-4.358966	-1.571524	3.632639
H	1.688596	0.639281	3.247765	H	-5.386932	-1.322144	1.760303
H	2.236989	2.331515	3.319742	H	-3.049713	-1.925682	5.300101
H	0.828905	1.808549	4.272171	C	-0.705028	-2.542791	4.143173
O	0.185237	-0.435003	1.842912	H	-0.251783	-3.448979	3.725266
O	1.199146	0.786828	-0.179734	H	0.032833	-1.737960	4.043257
C	0.211387	-1.636695	1.132635	H	-0.873379	-2.710523	5.211820
C	1.368598	-1.955128	0.412034	C	-3.514877	-1.874634	-0.075873
C	-0.904193	-2.485606	1.197297	H	-2.733134	-1.302405	-0.586442
C	1.358365	-3.098251	-0.427791	H	-3.483621	-2.890260	-0.488812
C	2.570378	-1.064210	0.510376	H	-4.479800	-1.437346	-0.347053
C	-0.838262	-3.654798	0.437182	C	-5.559267	-1.216324	4.479349
C	0.242898	-3.954705	-0.400046	H	-5.740089	-0.133366	4.475477
C	2.459614	0.281937	0.122552	H	-6.471455	-1.694713	4.104089
C	3.820814	-1.544534	0.972209	H	-5.420090	-1.523930	5.521122
H	-1.678785	-4.344094	0.474478	C	0.142453	-5.184353	-1.290282
C	3.580315	1.122067	-0.008569	C	1.470083	-5.583820	-1.941595
C	4.954132	-0.717525	0.866029	C	2.152938	-4.339110	-2.513881
C	4.816628	0.572643	0.343762	C	2.515062	-3.367624	-1.382929
C	3.483824	2.524844	-0.522153	H	3.059878	-4.605165	-3.070209
C	3.841056	3.621082	0.292012	H	2.130653	-6.051017	-1.197094
C	3.080595	2.758526	-1.860606	H	1.292154	-6.332779	-2.722552
C	3.729742	4.921754	-0.220481	H	-0.591473	-4.975935	-2.083143
C	2.996429	4.070266	-2.330928	H	-0.270537	-6.020086	-0.710528
C	3.300823	5.171831	-1.522970	H	3.370164	-3.787000	-0.834995
H	3.995949	5.760230	0.420964	H	2.870963	-2.417526	-1.797601
H	2.691058	4.236932	-3.362318	H	1.473034	-3.849539	-3.224931
C	4.382547	3.459453	1.697857	H	5.705262	1.189743	0.230536
H	5.481079	3.471503	1.701439	C	6.344028	-1.201401	1.254984
H	4.055374	4.286062	2.338599	H	6.881251	-1.490821	0.338362
H	4.075358	2.519243	2.158983	H	6.915499	-0.368629	1.683724
C	3.167250	6.580974	-2.051808	C	3.924388	-2.884210	1.691581
H	3.625723	6.682272	-3.042670	C	6.335847	-2.394783	2.216498
H	2.112965	6.869335	-2.155701	H	6.041985	-2.062160	3.222167
H	3.643349	7.306541	-1.384256	H	7.347288	-2.809737	2.303365
C	2.774931	1.619646	-2.807466	C	5.346186	-3.456215	1.728322
H	3.544190	0.840416	-2.761428	H	3.584926	-2.725639	2.727543
H	1.817529	1.145294	-2.567365	H	3.228204	-3.613627	1.273599
H	2.718796	1.980453	-3.839212	H	5.638835	-3.793194	0.723182
C	-2.100291	-2.168053	2.038153	H	5.369354	-4.340027	2.377395

Ni	-2.011404	1.626591	0.094368
C	-2.637351	-3.113756	-5.412252
C	-1.284577	-2.939330	-5.112459
C	-0.877264	-1.880738	-4.302285
C	-1.804437	-0.961952	-3.770012
C	-3.166215	-1.158682	-4.080826
C	-3.573574	-2.215599	-4.889905
H	-2.959674	-3.938254	-6.042401
H	-0.543632	-3.626213	-5.514400
H	0.179383	-1.747132	-4.081004
H	-3.913390	-0.481761	-3.676861
H	-4.630303	-2.343602	-5.111376
C	-1.315467	0.137436	-2.935358
H	-0.269157	0.063401	-2.639953
C	-2.014606	1.221903	-2.516309
H	-3.053538	1.335595	-2.824560
C	-1.486510	2.294042	-1.662565
H	-0.393856	2.245138	-1.593386
C	-1.939128	3.706660	-2.018639
H	-1.468924	4.028572	-2.961536
H	-3.023887	3.766708	-2.142303
C	-3.767786	2.302167	0.086527
C	-4.867698	1.687753	-0.546737
C	-4.060055	3.346419	0.990939
C	-6.184287	2.070892	-0.274645
H	-4.699273	0.886836	-1.263859
C	-5.374721	3.735519	1.270677
H	-3.249588	3.875912	1.491000
C	-6.442748	3.097480	0.637235
H	-7.010158	1.569823	-0.776446
H	-5.563313	4.541887	1.976978
H	-7.465791	3.401918	0.845473
H	-1.653499	4.429022	-1.246340

IM6b

SCF energy in Ethanol: -2889.879656 a.u.

Free energy in Ethanol: -2888.937895 a.u.

P	-0.090886	0.198909	-0.615080
N	-0.628058	-0.390516	-2.084678
C	-2.061775	-0.430948	-2.374416
H	-2.396617	-1.463854	-2.536637
H	-2.634839	-0.014548	-1.542751
H	-2.279562	0.152858	-3.279040
C	0.216267	-0.866700	-3.179724
H	1.261905	-0.890138	-2.877685
H	-0.091525	-1.874381	-3.484357
H	0.117238	-0.200312	-4.047952
O	1.369109	0.775799	-1.182117
O	0.451502	-1.030447	0.395149
C	2.416366	1.015222	-0.295184
C	3.101355	-0.082989	0.237257
C	2.770455	2.343343	-0.009700
C	4.093788	0.140933	1.226771
C	2.742149	-1.471112	-0.199375
C	3.828184	2.526603	0.882728
C	4.467908	1.462459	1.529457
C	1.433151	-1.937567	0.008449
C	3.696119	-2.343198	-0.780275
H	4.142638	3.543140	1.108541
C	1.090458	-3.295322	-0.120265
C	3.364326	-3.698290	-0.960250
C	2.095436	-4.150143	-0.583116
C	-0.247071	-3.843539	0.269577
C	-1.074121	-4.480322	-0.681659
C	-0.652690	-3.805790	1.626088
C	-2.290162	-5.040678	-0.269153
C	-1.872482	-4.382313	1.991253
C	-2.712874	-5.001803	1.061231
H	-2.917213	-5.531040	-1.012200
H	-2.170502	-4.354839	3.037431
C	-0.686575	-4.610045	-2.140179
H	-0.130702	-5.538412	-2.328494
H	-1.578255	-4.637980	-2.775955
H	-0.049969	-3.787586	-2.473092
C	-4.039582	-5.591232	1.479586
H	-4.026787	-5.897784	2.530925
H	-4.851181	-4.861261	1.361192
H	-4.298806	-6.466790	0.873801
C	0.215973	-3.191063	2.701134
H	1.248155	-3.555796	2.643145
H	0.253096	-2.099769	2.611817
H	-0.172725	-3.433616	3.695011
C	2.047267	3.508373	-0.607225
C	1.246521	4.332512	0.216746
C	2.166327	3.797670	-1.982852
C	0.555602	5.403282	-0.358271
C	1.465607	4.887310	-2.512707
C	0.645250	5.695363	-1.722560

H	-0.085831	6.011869	0.275138
H	1.563157	5.106348	-3.574494
C	3.040675	2.964335	-2.893282
H	4.042499	2.819886	-2.472352
H	2.612174	1.968478	-3.055419
H	3.151317	3.444852	-3.870695
C	1.110710	4.084026	1.704150
H	0.881364	3.034818	1.921601
H	2.032480	4.329786	2.245884
H	0.305063	4.694644	2.119310
C	-0.124221	6.854451	-2.312679
H	-0.026444	6.886514	-3.402746
H	-1.191131	6.782139	-2.069746
H	0.231698	7.815217	-1.918314
C	5.522247	1.788052	2.578010
C	6.336208	0.572834	3.033032
C	5.395863	-0.606550	3.292243
C	4.707311	-1.028595	1.987952
H	5.940864	-1.461782	3.709580
H	7.062101	0.293639	2.255994
H	6.913800	0.825289	3.930277
H	5.019523	2.225698	3.453777
H	6.185284	2.573759	2.192791
H	5.448694	-1.544170	1.362271
H	3.929594	-1.772834	2.193964
H	4.642621	-0.315412	4.037881
H	1.869045	-5.210293	-0.672248
C	4.368593	-4.708889	-1.496272
H	4.783268	-5.272643	-0.646236
H	3.848441	-5.448353	-2.117959
C	5.016633	-1.805212	-1.317889
C	5.525281	-4.074911	-2.276611
H	5.169339	-3.731451	-3.258272
H	6.301637	-4.825850	-2.466589
C	6.092318	-2.881911	-1.501709
H	4.808844	-1.349405	-2.299034
H	5.391766	-0.987791	-0.699183
H	6.452701	-3.222169	-0.519907
H	6.955901	-2.452119	-2.023615
Ni	-1.553364	1.606462	0.422132
C	-7.845719	-2.062216	-1.004681
C	-6.745271	-2.913979	-1.114280
C	-5.515500	-2.544360	-0.571179
C	-5.346705	-1.315389	0.099106
C	-6.469586	-0.466601	0.194898
C	-7.696942	-0.836214	-0.347413
H	-8.806282	-2.346271	-1.425994
H	-6.843316	-3.868733	-1.625450
H	-4.660370	-3.210002	-0.665267
H	-6.380566	0.491381	0.698767
H	-8.545588	-0.162483	-0.257745
C	-4.029277	-0.985728	0.649390
H	-3.265930	-1.750928	0.503022
C	-3.672399	0.145022	1.305144
H	-4.416222	0.920152	1.486036
C	-2.318617	0.443962	1.795618
H	-1.670203	-0.437316	1.726783
C	-2.249382	1.038012	3.199863
H	-2.481798	0.262962	3.947210
H	-2.967259	1.851621	3.333880
C	-2.641627	3.115216	0.708374
C	-2.579676	4.070757	1.741854
C	-3.398929	3.461400	-0.432637
C	-3.207858	5.314509	1.632436
H	-2.023860	3.849049	2.650130
C	-4.027654	4.707137	-0.553170
H	-3.510686	2.748930	-1.250360
C	-3.932613	5.639082	0.481319
H	-3.133561	6.032967	2.446830
H	-4.601712	4.940864	-1.447775
H	-4.428060	6.603663	0.398904
H	-1.249942	1.424266	3.430920

IM7a

SCF energy in Ethanol: -2889.911779 a.u.

Free energy in Ethanol: -2888.966753 a.u.

P	-0.237329	-1.004497	-0.389732
N	0.084364	-1.855848	-1.799700
C	0.168244	-3.313939	-1.712142
H	-0.687458	-3.787879	-2.206966
H	1.100230	-3.661845	-2.172349
H	0.170636	-3.634646	-0.667079
C	-0.085252	-1.349995	-3.160942
H	0.051472	-0.270570	-3.190160
H	0.664071	-1.814189	-3.813056
H	-1.085249	-1.595191	-3.546825
O	-0.735206	0.417067	-1.119877
O	1.242596	-0.554131	0.260620

C	-0.617147	1.636469	-0.455448	H	-2.829729	2.714072	-4.001372
C	0.666105	2.138444	-0.195743	C	-3.930003	1.512211	1.741990
C	-1.778756	2.367130	-0.145507	H	-3.175179	0.741598	1.934459
C	0.807832	3.278854	0.633492	H	-3.568132	2.439109	2.199820
C	1.864067	1.486881	-0.818106	H	-4.847639	1.218015	2.261260
C	-1.595889	3.548197	0.579557	C	-7.142914	1.153464	-2.113636
C	-0.342971	3.983542	1.025810	H	-7.316582	1.588683	-3.103549
C	2.162812	0.152108	-0.508906	H	-7.286479	0.068252	-2.201457
C	2.696899	2.194547	-1.720362	H	-7.919825	1.527723	-1.437305
H	-2.473584	4.146420	0.815017	C	-0.277247	5.206382	1.927768
C	3.355424	-0.464970	-0.927269	C	1.132710	5.789475	2.070581
C	3.892293	1.595553	-2.155937	C	2.135070	4.660222	2.320555
C	4.209667	0.304852	-1.722092	C	2.187002	3.714533	1.113605
C	3.744688	-1.858800	-0.545220	H	3.137995	5.060148	2.513336
C	3.874428	-2.863997	-1.527906	H	1.411078	6.327684	1.152977
C	4.061530	-2.157080	0.800181	H	1.151694	6.523390	2.885313
C	4.256798	-4.154792	-1.140167	H	-0.644552	4.924541	2.926720
C	4.446042	-3.456816	1.140259	H	-0.975684	5.969011	1.559136
C	4.536139	-4.477642	0.188473	H	2.728184	4.220597	0.302118
H	4.342378	-4.926224	-1.903510	H	2.780436	2.825851	1.355266
H	4.693888	-3.674375	2.177786	H	1.838636	4.097608	3.216143
C	3.643210	-2.590085	-2.999312	H	5.152147	-0.136147	-2.039085
H	4.537484	-2.165804	-3.474655	C	4.877851	2.323942	-3.058684
H	3.406063	-3.516379	-3.533565	H	5.692436	2.726030	-2.436292
H	2.830995	-1.877818	-3.161535	H	5.351002	1.605100	-3.739432
C	4.915778	-5.884279	0.590037	C	2.253525	3.526093	-2.315493
H	5.675959	-5.884841	1.379478	C	4.249469	3.476093	-3.849929
H	4.048831	-6.436473	0.977492	H	3.613648	3.074701	-4.651847
H	5.309789	-6.451786	-0.259741	H	5.035077	4.068438	-4.334519
C	4.035823	-1.086490	1.865890	C	3.399587	4.345882	-2.920327
H	4.615326	-0.206793	1.561197	H	1.524665	3.303167	-3.111009
H	3.017336	-0.745626	2.075942	H	1.704098	4.123490	-1.585690
H	4.462072	-1.462265	2.801729	H	4.034521	4.747733	-2.117249
C	-3.146188	2.006022	-0.640538	H	2.988067	5.208188	-3.458927
C	-4.179340	1.655226	0.257342	Ni	-1.613275	-1.913211	1.055138
C	-3.432710	2.109017	-2.020462	C	1.468970	1.443976	5.058252
C	-5.460793	1.397999	-0.238607	C	2.013964	0.163911	4.944219
C	-4.730059	1.841086	-2.472414	C	1.330156	-0.830417	4.245117
C	-5.758869	1.476785	-1.601399	C	0.086192	-0.576600	3.639264
H	-6.246087	1.119054	0.461261	C	-0.439123	0.724405	3.747625
H	-4.941049	1.928201	-3.536619	C	0.238709	1.716350	4.453030
C	-2.377903	2.521169	-3.023200	H	1.993969	2.218670	5.610700
H	-1.850827	3.428780	-2.707656	H	2.969988	-0.065821	5.407974
H	-1.622312	1.737676	-3.152771	H	1.753856	-1.829830	4.180501

H	-1.381599	0.967374	3.267339
H	-0.196889	2.709547	4.529637
C	-0.643704	-1.689861	2.998655
H	-0.056759	-2.602473	2.874655
C	-2.038514	-1.826008	3.079245
H	-2.620225	-0.976358	3.438274
C	-2.732541	-2.884538	2.457500
H	-2.205043	-3.838811	2.368658
C	-4.237363	-2.987420	2.510983
H	-4.563514	-3.524076	3.413866
H	-4.703021	-1.995487	2.524044
C	-2.753961	-2.618158	-0.342280
C	-2.930566	-4.005759	-0.527128
C	-3.439579	-1.778474	-1.241872
C	-3.734028	-4.526585	-1.547161
H	-2.433182	-4.710502	0.138961
C	-4.250291	-2.290040	-2.263149
H	-3.340354	-0.700334	-1.160994
C	-4.401653	-3.668057	-2.423479
H	-3.840567	-5.604950	-1.652957
H	-4.761139	-1.601366	-2.933639
H	-5.030593	-4.067648	-3.215675
H	-4.624566	-3.527616	1.642814

IM7b

SCF energy in Ethanol: -2889.912048 a.u.

Free energy in Ethanol: -2888.967889 a.u.

P	-0.272891	-0.793327	-0.559033
N	0.055741	-1.410339	-2.080585
C	0.128191	-2.863312	-2.235690
H	-0.698718	-3.231563	-2.854237
H	1.084728	-3.143680	-2.692249
H	0.062802	-3.355440	-1.262737
C	0.003362	-0.676229	-3.342031
H	0.114759	0.392863	-3.171427
H	0.817345	-1.011755	-3.995873
H	-0.952405	-0.859307	-3.854480
O	-0.779311	0.727916	-1.050414
O	1.195728	-0.425449	0.167283
C	-0.641234	1.842686	-0.227293
C	0.649979	2.305383	0.066469
C	-1.793380	2.515599	0.225949
C	0.817911	3.324490	1.037566
C	1.835137	1.729472	-0.646475
C	-1.584023	3.597155	1.086923
C	-0.318081	3.977653	1.544380
C	2.124006	0.364662	-0.504737
C	2.672520	2.538858	-1.453705
H	-2.452496	4.151272	1.434875
C	3.313309	-0.204259	-0.996166
C	3.862740	1.989353	-1.962895
C	4.171614	0.652902	-1.691312
C	3.693556	-1.635155	-0.781211
C	3.865064	-2.509837	-1.877307
C	3.954754	-2.101874	0.527984
C	4.232779	-3.840110	-1.639802
C	4.326244	-3.436259	0.715916
C	4.456578	-4.329079	-0.351690
H	4.351333	-4.509565	-2.490253
H	4.527349	-3.783679	1.727550
C	3.695785	-2.058473	-3.313399
H	4.624334	-1.628085	-3.711678
H	3.436055	-2.905548	-3.957514
H	2.922754	-1.293957	-3.417701
C	4.817395	-5.777789	-0.117633
H	5.469548	-5.892927	0.755247
H	3.921813	-6.387192	0.065252
H	5.331232	-6.208883	-0.983773
C	3.880091	-1.180668	1.722490
H	4.416498	-0.242555	1.536988
H	2.845381	-0.924011	1.970172
H	4.319701	-1.654570	2.604203
C	-3.184255	2.165317	-0.201171
C	-4.160983	1.797312	0.752580
C	-3.559247	2.289476	-1.561394
C	-5.459794	1.496855	0.322839
C	-4.872442	1.996321	-1.939505
C	-5.836370	1.576942	-1.018063
H	-6.198158	1.196703	1.064315
H	-5.150426	2.102017	-2.986600
C	-2.586545	2.763592	-2.618227
H	-2.016325	3.636626	-2.281508
H	-1.862574	1.981918	-2.871848
H	-3.118466	3.038822	-3.534496
C	-3.879444	1.749649	2.240751
H	-2.840386	1.499159	2.464497
H	-4.080152	2.720023	2.714611
H	-4.524494	1.015610	2.735093

C	-7.231052	1.205563	-1.463769
H	-7.278429	0.150388	-1.764482
H	-7.961789	1.348678	-0.660500
H	-7.550346	1.803489	-2.324645
C	-0.223661	5.076806	2.592082
C	1.195819	5.620289	2.785643
C	2.185658	4.455468	2.871245
C	2.209234	3.679427	1.548068
H	3.196261	4.812932	3.102502
H	1.469231	6.266568	1.939274
H	1.237278	6.243615	3.686882
H	-0.583364	4.677260	3.552658
H	-0.915361	5.888292	2.330598
H	2.744436	4.284305	0.803355
H	2.797389	2.761233	1.657325
H	1.890579	3.787002	3.692697
H	5.111947	0.249001	-2.059581
C	4.851912	2.817862	-2.769753
H	5.667268	3.139616	-2.103156
H	5.322913	2.185281	-3.532452
C	2.238334	3.938214	-1.875579
C	4.227448	4.059178	-3.415340
H	3.586025	3.759238	-4.256179
H	5.014618	4.700632	-3.829823
C	3.386871	4.817541	-2.384963
H	1.501654	3.822682	-2.686512
H	1.699645	4.445711	-1.072806
H	4.027762	5.119712	-1.543573
H	2.977567	5.739390	-2.815987
H	-3.891408	-4.216540	1.987707
Ni	-1.731115	-1.805362	0.707341
C	2.413298	-1.612367	5.060449
C	1.837954	-0.361682	4.826949
C	0.704527	-0.248431	4.022588
C	0.110249	-1.379275	3.432064
C	0.726622	-2.627270	3.647133
C	1.854612	-2.742467	4.456825
H	3.290117	-1.704977	5.695694
H	2.266237	0.528823	5.280628
H	0.254020	0.728455	3.861369
H	0.318042	-3.517895	3.177033
H	2.302092	-3.720783	4.614673
C	-1.162196	-1.228375	2.697558
H	-1.507690	-0.198315	2.609475
C	-2.141899	-2.242724	2.673495
H	-1.869333	-3.236172	3.032954
C	-3.340695	-2.122924	1.947001
H	-3.742180	-1.119830	1.788912
C	-4.362690	-3.230762	1.903824
H	-4.929856	-3.211639	0.969590
H	-5.076610	-3.130246	2.734315
C	-2.767141	-2.474134	-0.774760
C	-3.461451	-1.647156	-1.678257
C	-2.852081	-3.863100	-0.995825
C	-4.191758	-2.176854	-2.749111
H	-3.435483	-0.567384	-1.554735
C	-3.574900	-4.401186	-2.066291
H	-2.344580	-4.551583	-0.319423
C	-4.249939	-3.557467	-2.951547
H	-4.716425	-1.504522	-3.426062
H	-3.613616	-5.480339	-2.205221
H	-4.816340	-3.970536	-3.783041

TS5a

SCF energy in Ethanol: -2889.851387 a.u.

Free energy in Ethanol: -2888.912240 a.u

P	-0.476363	0.695395	-0.806605
N	-1.126872	1.434942	-2.164691
C	-0.793028	2.827083	-2.451684
H	-0.512411	2.931418	-3.508054
H	-1.643681	3.491125	-2.243517
H	0.057827	3.141796	-1.845135
C	-2.115684	0.862818	-3.075705
H	-2.396470	-0.139556	-2.758900
H	-3.015230	1.490059	-3.113157
H	-1.697190	0.806346	-4.090629
O	-0.734793	-0.874085	-1.352381
O	-1.587185	0.730533	0.472283
C	-0.806282	-1.931805	-0.456163
C	-1.937044	-2.048186	0.365783
C	0.226394	-2.885814	-0.447423
C	-1.953787	-3.040873	1.380083
C	-3.094427	-1.111690	0.192517
C	0.118546	-3.918345	0.486537
C	-0.916865	-3.988912	1.424957
C	-2.886284	0.267133	0.355740
C	-4.399570	-1.581183	-0.097296
H	0.890850	-4.684289	0.500044

C	-3.952255	1.181969	0.448401	C	-2.155366	-5.240394	3.280168
C	-5.479145	-0.681648	-0.033841	C	-2.684069	-3.862421	3.684200
C	-5.238335	0.660368	0.279750	C	-3.054307	-3.051937	2.435463
C	-3.744989	2.635552	0.739237	H	-3.562734	-3.951839	4.334406
C	-4.160538	3.622942	-0.181717	H	-2.910901	-5.753086	2.667560
C	-3.174192	3.037173	1.972578	H	-1.979302	-5.871859	4.159339
C	-3.953793	4.975688	0.120834	H	-0.040999	-4.840099	3.185621
C	-2.998242	4.398162	2.234267	H	-0.572017	-6.029098	2.013172
C	-3.367215	5.387486	1.317025	H	-3.979561	-3.472448	2.017965
H	-4.268392	5.726217	-0.602411	H	-3.299571	-2.020248	2.711658
H	-2.567090	4.694416	3.189015	H	-1.914195	-3.331485	4.261951
C	-4.855250	3.288080	-1.485804	H	-6.085948	1.335953	0.371117
H	-5.946014	3.254089	-1.360346	C	-6.917411	-1.134250	-0.243623
H	-4.645669	4.051607	-2.242842	H	-7.393443	-1.256145	0.741888
H	-4.553220	2.316564	-1.881946	H	-7.481659	-0.340859	-0.749815
C	-3.129350	6.850176	1.612976	C	-4.623833	-3.005253	-0.591400
H	-3.353135	7.089437	2.659006	C	-7.042195	-2.452682	-1.015213
H	-2.081294	7.127895	1.437071	H	-6.811354	-2.286772	-2.077132
H	-3.748685	7.493468	0.979035	H	-8.076490	-2.814832	-0.969165
C	-2.777647	2.034878	3.033606	C	-6.070960	-3.490162	-0.445245
H	-3.556338	1.278878	3.186073	H	-4.354985	-3.027434	-1.659546
H	-1.860464	1.503880	2.756601	H	-3.935315	-3.703232	-0.111181
H	-2.602614	2.537319	3.990395	H	-6.302282	-3.661390	0.616336
C	1.382872	-2.847226	-1.396479	H	-6.187790	-4.455200	-0.953355
C	2.691232	-2.633480	-0.910501	Ni	1.362789	1.432155	-0.017329
C	1.181957	-3.093207	-2.773015	C	8.528756	-0.640268	2.915898
C	3.765571	-2.651272	-1.807829	C	7.413297	-1.244928	3.497420
C	2.284726	-3.104457	-3.632557	C	6.131127	-0.795962	3.183844
C	3.585274	-2.878367	-3.174167	C	5.928097	0.270055	2.287357
H	4.770375	-2.484080	-1.423874	C	7.065038	0.859029	1.699470
H	2.121229	-3.302281	-4.690496	C	8.345612	0.412691	2.013771
C	-0.195058	-3.366885	-3.335013	H	9.529767	-0.988533	3.155639
H	-0.731332	-4.118555	-2.744476	H	7.540395	-2.067978	4.196041
H	-0.809799	-2.459514	-3.336919	H	5.266674	-1.269661	3.643971
H	-0.128286	-3.729796	-4.365721	H	6.943143	1.662255	0.978668
C	2.965763	-2.382912	0.556725	H	9.206905	0.882809	1.545818
H	2.286817	-1.627620	0.968296	C	4.555862	0.710883	2.003862
H	2.837047	-3.289534	1.160601	H	3.773795	0.044668	2.368362
H	3.991974	-2.033252	0.702881	C	4.180764	1.837311	1.368768
C	4.755411	-2.859379	-4.130373	H	4.938217	2.546212	1.035389
H	4.889130	-1.863723	-4.575110	C	2.776600	2.240685	1.103653
H	5.691834	-3.117945	-3.624388	H	2.102356	1.516393	1.656840
H	4.610509	-3.564211	-4.956816	C	2.460897	3.662426	1.579267
C	-0.855833	-5.079319	2.485276	H	2.584923	3.728329	2.668091

H	3.138457	4.391789	1.122949
C	2.810809	2.283000	-0.915397
C	3.681224	1.368873	-1.550544
C	2.704556	3.576544	-1.463900
C	4.350010	1.713770	-2.724788
H	3.824627	0.377934	-1.130773
C	3.388610	3.922415	-2.632900
H	2.072635	4.320757	-0.987211
C	4.210971	2.993434	-3.272323
H	4.990776	0.980302	-3.209301
H	3.276763	4.924339	-3.042044
H	4.746081	3.264900	-4.178569
H	1.431914	3.953497	1.341761

TS6a

SCF energy in Ethanol: -2889.877025 a.u.

Free energy in Ethanol: -2888.932464 a.u.

P	0.208523	0.988018	-0.563176
N	-0.099565	1.822656	-1.988937
C	-0.184355	3.278378	-1.932552
H	0.495615	3.730016	-2.665961
H	-1.209428	3.619647	-2.131717
H	0.105642	3.632486	-0.940851
C	-0.403107	1.255863	-3.299181
H	-0.439889	0.169726	-3.245984
H	-1.367919	1.626055	-3.668516
H	0.373242	1.546944	-4.021169
O	0.556311	-0.480025	-1.310029
O	-1.266966	0.620920	0.178357
C	0.465525	-1.664124	-0.588263
C	-0.800806	-2.110729	-0.183042
C	1.630220	-2.416261	-0.347283
C	-0.893145	-3.194686	0.725118
C	-2.034983	-1.454160	-0.724338
C	1.485130	-3.547478	0.460909
C	0.270481	-3.911229	1.052331
C	-2.265695	-0.096109	-0.458512
C	-2.975113	-2.180105	-1.497310
H	2.363948	-4.159395	0.651951
C	-3.485172	0.532021	-0.777207
C	-4.193139	-1.566767	-1.841846
C	-4.434591	-0.248128	-1.443393
C	-3.793201	1.949824	-0.408930
C	-4.051228	2.918429	-1.403074
C	-3.893796	2.315775	0.955946
C	-4.337602	4.236477	-1.019723
C	-4.192205	3.638427	1.290459
C	-4.402401	4.622778	0.318287
H	-4.521196	4.977554	-1.795990
H	-4.274091	3.905314	2.342790
C	-4.071056	2.590125	-2.881890
H	-5.085918	2.337245	-3.217997
H	-3.745140	3.450892	-3.476236
H	-3.435167	1.737807	-3.127751
C	-4.687710	6.053911	0.710953
H	-5.401226	6.107502	1.541591
H	-3.774290	6.567942	1.039143
H	-5.101704	6.624539	-0.126949
C	-3.732844	1.294977	2.058860
H	-4.356527	0.411315	1.878895
H	-2.698411	0.947721	2.142388
H	-4.025999	1.721636	3.023817
C	2.958734	-2.122267	-0.974185
C	4.084017	-1.822697	-0.175586
C	3.117932	-2.243663	-2.374577
C	5.332547	-1.644080	-0.783822
C	4.383198	-2.056351	-2.939440
C	5.507661	-1.760110	-2.164499
H	6.190678	-1.406636	-0.157313
H	4.493192	-2.154832	-4.017951
C	1.957759	-2.594016	-3.279119
H	1.400494	-3.459980	-2.904208
H	1.249042	-1.762046	-3.354871
H	2.310886	-2.828499	-4.288327
C	3.976410	-1.670439	1.326237
H	3.099710	-1.076489	1.601967
H	3.879280	-2.637034	1.835612
H	4.868077	-1.177610	1.728458
C	6.872198	-1.606178	-2.796397
H	6.805152	-1.158963	-3.794441
H	7.528661	-0.976505	-2.186141
H	7.370135	-2.578641	-2.911627
C	0.262322	-5.061937	2.046849
C	-1.141197	-5.579997	2.377065
C	-2.079292	-4.398033	2.635096
C	-2.229532	-3.552787	1.363587
H	-3.067570	-4.744538	2.961409
H	-1.528711	-6.175989	1.538063

H	-1.097003	-6.248234	3.245705
H	0.737809	-4.716867	2.977703
H	0.896709	-5.875190	1.670251
H	-2.854388	-4.108916	0.650418
H	-2.780860	-2.632227	1.584338
H	-1.673470	-3.777042	3.445569
H	-5.395318	0.202375	-1.683116
C	-5.284264	-2.308810	-2.600866
H	-6.044296	-2.649511	-1.880439
H	-5.802174	-1.611977	-3.271948
C	-2.631634	-3.555631	-2.056613
C	-4.770587	-3.522373	-3.383296
H	-4.207778	-3.186160	-4.265698
H	-5.617081	-4.113667	-3.753320
C	-3.855503	-4.368701	-2.494665
H	-1.983305	-3.401394	-2.933995
H	-2.025558	-4.128630	-1.352463
H	-4.416522	-4.705484	-1.610588
H	-3.525389	-5.272277	-3.021693
Ni	1.586802	1.738480	0.888446
C	-0.626494	-1.445853	5.392198
C	-1.336693	-0.275312	5.118442
C	-0.770341	0.720349	4.323851
C	0.515413	0.577846	3.768684
C	1.215150	-0.610645	4.054008
C	0.654879	-1.603133	4.854609
H	-1.059329	-2.219851	6.020351
H	-2.331770	-0.131050	5.532056
H	-1.327461	1.633596	4.130137
H	2.210038	-0.763033	3.648181
H	1.224509	-2.505955	5.062457
C	1.070802	1.680939	2.960971
H	0.415259	2.552578	2.902926
C	2.433566	1.874467	2.692125
H	3.142885	1.089656	2.955844
C	2.969043	2.998739	1.928738
H	2.357423	3.902392	1.994360
C	4.446023	3.293828	2.172018
H	4.584728	3.613915	3.213624
H	5.058340	2.400634	2.009903
C	3.018257	2.812133	-0.016475
C	2.845796	4.068466	-0.632147
C	3.964930	1.936881	-0.589172
C	3.542469	4.413624	-1.790730
H	2.161513	4.793048	-0.193069
C	4.640616	2.267027	-1.765191
H	4.163898	0.973311	-0.127193
C	4.436147	3.508964	-2.371947
H	3.388429	5.392385	-2.240609
H	5.333277	1.551010	-2.200883
H	4.977327	3.775838	-3.276029
H	4.815665	4.081318	1.509793

TS6b

SCF energy in Ethanol: -2889.879578 a.u.

Free energy in Ethanol: -2888.935382 a.u.

P	-0.302423	-0.528433	-0.765066
N	0.023536	-0.898106	-2.369391
C	-0.018678	-2.296588	-2.788545
H	-0.689377	-2.414855	-3.649297
H	0.983246	-2.654713	-3.060840
H	-0.398640	-2.922808	-1.978586
C	0.423167	0.028987	-3.422597
H	0.488403	1.043399	-3.034128
H	1.396977	-0.252512	-3.843376
H	-0.318121	0.009676	-4.234606
O	-0.630524	1.105497	-1.027105
O	1.155815	-0.393260	0.075901
C	-0.407747	2.065399	-0.050698
C	0.912444	2.376442	0.311860
C	-1.508162	2.751818	0.498186
C	1.145138	3.253486	1.403136
C	2.066801	1.761469	-0.419882
C	-1.229677	3.699461	1.486478
C	0.057696	3.929871	1.981090
C	2.205671	0.364928	-0.415584
C	3.042807	2.551891	-1.075424
H	-2.059787	4.261730	1.908281
C	3.378695	-0.274843	-0.860288
C	4.214969	1.933653	-1.546291
C	4.374820	0.553106	-1.387309
C	3.587320	-1.753602	-0.763497
C	3.841936	-2.524237	-1.921197
C	3.589411	-2.387878	0.503993
C	4.036003	-3.906296	-1.797536
C	3.796997	-3.767848	0.576812
C	4.007542	-4.551737	-0.561493
H	4.219398	-4.490427	-2.697946

H	3.796662	-4.241464	1.556631	H	2.184316	3.282899	4.107253
C	3.946846	-1.920933	-3.307518	H	5.305917	0.095237	-1.713332
H	4.983528	-1.647570	-3.547224	C	5.346976	2.729728	-2.180547
H	3.624756	-2.640943	-4.067822	H	6.134111	2.882693	-1.425751
H	3.348651	-1.014178	-3.414953	H	5.811616	2.135394	-2.977403
C	4.188250	-6.048267	-0.453114	C	2.783652	4.022846	-1.378136
H	4.790058	-6.317376	0.422576	C	4.911389	4.096582	-2.720093
H	3.222009	-6.560310	-0.348920	H	4.326018	3.964363	-3.641181
H	4.680781	-6.458821	-1.341073	H	5.793958	4.689930	-2.988642
C	3.406012	-1.614044	1.789348	C	4.055317	4.824481	-1.679883
H	3.984142	-0.682916	1.785323	H	2.127085	4.065716	-2.261810
H	2.355845	-1.349271	1.947717	H	2.213239	4.497232	-0.577039
H	3.726926	-2.212082	2.647097	H	4.639346	4.959748	-0.757747
C	-2.924668	2.539038	0.063564	H	3.782566	5.827299	-2.030841
C	-3.887399	2.067577	0.985625	Ni	-1.711337	-1.722367	0.290425
C	-3.333573	2.896137	-1.242527	H	-4.747136	-3.983618	0.718451
C	-5.220510	1.933427	0.577838	C	1.594697	-3.539148	4.796087
C	-4.677772	2.753522	-1.602388	C	1.139258	-2.236638	5.009398
C	-5.639011	2.266116	-0.712333	C	0.124077	-1.707808	4.212782
H	-5.951668	1.562540	1.294273	C	-0.465668	-2.461084	3.180628
H	-4.982625	3.041390	-2.606926	C	0.021772	-3.765024	2.965873
C	-2.359796	3.457834	-2.253509	C	1.029853	-4.297674	3.765984
H	-1.739077	4.249249	-1.818636	H	2.381475	-3.956604	5.418772
H	-1.681391	2.680657	-2.621709	H	1.569996	-1.631165	5.803204
H	-2.892909	3.877156	-3.112723	H	-0.232341	-0.696559	4.396990
C	-3.535539	1.719189	2.417615	H	-0.385199	-4.360864	2.153319
H	-2.526314	1.309322	2.506183	H	1.382515	-5.309319	3.579663
H	-3.578245	2.601280	3.069901	C	-1.571248	-1.877449	2.394678
H	-4.242474	0.987444	2.823031	H	-1.782899	-0.834283	2.629481
C	-7.076972	2.081933	-1.138657	C	-2.601711	-2.645049	1.820105
H	-7.249841	1.067106	-1.521756	H	-2.529219	-3.733233	1.861276
H	-7.766999	2.233625	-0.301361	C	-3.679917	-2.104980	0.999020
H	-7.351537	2.781536	-1.935591	H	-3.897549	-1.048238	1.171905
C	0.220825	4.885176	3.154467	C	-4.958685	-2.933639	0.944057
C	1.676289	5.272170	3.435539	H	-5.652517	-2.556370	0.187644
C	2.558240	4.022510	3.385098	H	-5.451582	-2.894227	1.925224
C	2.549101	3.425661	1.971766	C	-3.247285	-2.095585	-0.924388
H	3.589746	4.255516	3.675711	C	-3.880414	-1.084435	-1.675077
H	2.026193	5.993205	2.682858	C	-3.164418	-3.381849	-1.497481
H	1.748670	5.770983	4.409495	C	-4.362740	-1.338763	-2.959232
H	-0.197624	4.408865	4.054343	H	-3.982209	-0.087202	-1.256707
H	-0.390421	5.780646	2.981137	C	-3.634344	-3.633862	-2.788397
H	3.146912	4.078696	1.321363	H	-2.728753	-4.200147	-0.924743
H	3.061036	2.456999	1.965508	C	-4.237465	-2.612085	-3.526143

H	-4.834255	-0.536295	-3.522634
H	-3.542810	-4.631624	-3.212658
H	-4.619338	-2.808450	-4.524787

IM8a

SCF energy in Ethanol: -2889.920854 a.u.

Free energy in Ethanol: -2888.976885 a.u.

P	0.368135	0.432767	-0.726538
N	0.238150	1.067895	-2.279237
C	0.939170	2.307569	-2.599748
H	1.630990	2.151294	-3.437901
H	0.228411	3.101559	-2.867781
H	1.523436	2.641347	-1.738133
C	-0.462391	0.467203	-3.410034
H	-1.066001	-0.377718	-3.083670
H	-1.115932	1.206123	-3.889661
H	0.259041	0.113219	-4.161676
O	0.067948	-1.165012	-1.188605
O	-1.064406	0.734257	0.124289
C	-0.400589	-2.071773	-0.249309
C	-1.738526	-1.981917	0.158220
C	0.459799	-3.076200	0.224672
C	-2.200328	-2.816068	1.208110
C	-2.639060	-0.971835	-0.484722
C	-0.060557	-3.950535	1.181251
C	-1.349482	-3.817134	1.709116
C	-2.305577	0.389610	-0.385711
C	-3.824642	-1.345844	-1.163741
H	0.576670	-4.751532	1.550496
C	-3.209062	1.406288	-0.749798
C	-4.724938	-0.344632	-1.570024
C	-4.420097	0.996672	-1.314861
C	-2.936645	2.857212	-0.500587
C	-2.834346	3.776464	-1.565608
C	-2.848923	3.328470	0.832779
C	-2.589792	5.128210	-1.285374
C	-2.617671	4.686217	1.064377
C	-2.468446	5.604711	0.019026
H	-2.500655	5.826096	-2.116467
H	-2.565662	5.040142	2.092729
C	-3.013822	3.372629	-3.013993
H	-4.047907	3.537607	-3.346615
H	-2.370623	3.971975	-3.668218
H	-2.790548	2.317752	-3.179735
C	-2.181674	7.061762	0.299852
H	-2.770650	7.430550	1.147691
H	-1.124113	7.220191	0.550684
H	-2.409212	7.689732	-0.568041
C	-3.037230	2.400804	2.011318
H	-3.912447	1.754882	1.877572
H	-2.167021	1.751167	2.152699
H	-3.178637	2.973819	2.933373
C	1.862898	-3.246424	-0.267685
C	2.953766	-3.001578	0.596433
C	2.102164	-3.716423	-1.577505
C	4.255921	-3.216974	0.129838
C	3.420587	-3.923093	-1.999804
C	4.514048	-3.673802	-1.165759
H	5.091254	-3.024912	0.800988
H	3.595387	-4.297938	-3.006859
C	0.964077	-4.019334	-2.525983
H	0.208978	-4.661325	-2.058072
H	0.455229	-3.100593	-2.839704
H	1.331273	-4.525960	-3.424313
C	2.749821	-2.507137	2.012582
H	2.086657	-1.635365	2.046190
H	2.298270	-3.272368	2.655074
H	3.707389	-2.223448	2.461844
C	5.930616	-3.865767	-1.655925
H	5.978508	-4.602055	-2.465532
H	6.345971	-2.925645	-2.043675
H	6.592430	-4.203486	-0.850705
C	-1.762447	-4.742446	2.844550
C	-3.260150	-4.697788	3.164566
C	-3.734473	-3.242877	3.203722
C	-3.578932	-2.598810	1.820175
H	-4.782556	-3.178252	3.520343
H	-3.825778	-5.243005	2.395252
H	-3.453160	-5.204363	4.117955
H	-1.200406	-4.458317	3.747245
H	-1.449322	-5.768384	2.609933
H	-4.356577	-3.011413	1.162450
H	-3.782621	-1.523766	1.877709
H	-3.143459	-2.686339	3.944596
H	-5.146085	1.759618	-1.588070
C	-6.054976	-0.677168	-2.231792
H	-6.850600	-0.611443	-1.473169
H	-6.294042	0.089037	-2.980068

C	-4.068222	-2.796252	-1.562766
C	-6.096192	-2.072655	-2.864463
H	-5.497283	-2.082673	-3.786337
H	-7.124945	-2.321042	-3.152688
C	-5.533490	-3.109128	-1.887883
H	-3.461423	-2.997292	-2.460050
H	-3.688804	-3.483528	-0.804055
H	-6.130686	-3.101463	-0.964344
H	-5.609345	-4.120785	-2.305052
Ni	2.130035	0.944704	0.356032
C	0.098070	1.238457	5.525974
C	-0.322723	2.278968	4.695833
C	0.375572	2.573094	3.525474
C	1.515118	1.838927	3.146909
C	1.927253	0.795195	3.998748
C	1.228696	0.499426	5.167284
H	-0.442759	1.009051	6.440237
H	-1.197335	2.867817	4.961318
H	0.035548	3.383024	2.884135
H	2.807288	0.210044	3.749513
H	1.574076	-0.310345	5.805807
C	2.241461	2.224387	1.915906
H	1.921462	3.185776	1.507392
C	3.505583	1.740708	1.521856
H	3.982277	0.975820	2.139447
C	4.460019	2.501202	0.604414
H	4.076289	3.524792	0.487682
C	5.874982	2.601041	1.211089
H	5.839029	3.097498	2.187629
H	6.305160	1.601931	1.352491
C	4.500517	1.885973	-0.798573
C	4.935005	2.639775	-1.898109
C	4.067652	0.566728	-1.031852
C	4.951668	2.096704	-3.183794
H	5.260293	3.666761	-1.743576
C	4.078976	0.018214	-2.321757
H	3.808835	-0.088426	-0.187164
C	4.520795	0.783736	-3.400552
H	5.297919	2.700377	-4.019240
H	3.743311	-1.004280	-2.467689
H	4.531550	0.362948	-4.402623
H	6.552307	3.166506	0.560625

IM8b

SCF energy in Ethanol: -2889.916340 a.u.

Free energy in Ethanol: -2888.973396 a.u.

P	0.247707	0.302854	-0.474272
N	0.306396	0.894801	-2.037381
C	1.040461	2.133017	-2.294443
H	1.763045	1.980107	-3.104856
H	0.351759	2.943930	-2.569152
H	1.589257	2.434638	-1.398892
C	-0.349190	0.333644	-3.215079
H	-0.932416	-0.544895	-2.945894
H	-1.013276	1.075279	-3.677093
H	0.409356	0.042815	-3.955076
O	-0.234780	-1.256698	-0.890078
O	-1.166681	0.822385	0.299945
C	-0.809480	-2.054640	0.092102
C	-2.130866	-1.791595	0.481087
C	-0.069066	-3.119490	0.633275
C	-2.685648	-2.503598	1.575302
C	-2.915799	-0.729870	-0.226105
C	-0.688679	-3.871917	1.633730
C	-1.955331	-3.563287	2.141597
C	-2.433044	0.588906	-0.208602
C	-4.138854	-1.010223	-0.882468
H	-0.147740	-4.717921	2.052502
C	-3.209042	1.676867	-0.651410
C	-4.923726	0.059746	-1.349054
C	-4.463721	1.370880	-1.187159
C	-2.749215	3.096979	-0.542325
C	-2.592806	3.894382	-1.698641
C	-2.516077	3.671711	0.731158
C	-2.164699	5.221600	-1.564524
C	-2.103475	5.004075	0.815308
C	-1.906245	5.795945	-0.319870
H	-2.036452	5.822366	-2.463481
H	-1.935433	5.436418	1.799994
C	-2.896431	3.385385	-3.093130
H	-3.947425	3.557001	-3.362549
H	-2.287425	3.910712	-3.836906
H	-2.716453	2.313086	-3.194381
C	-1.418199	7.221079	-0.199446
H	-1.843287	7.717460	0.680293
H	-0.325430	7.260859	-0.094973
H	-1.682667	7.812303	-1.082739
C	-2.728906	2.893670	2.010307

H	-3.668128	2.329364	1.988564	H	-3.972593	-2.762485	-2.081225
H	-1.919994	2.173579	2.174575	H	-4.236910	-3.126268	-0.399149
H	-2.758982	3.569290	2.870971	H	-6.623976	-2.485738	-0.575456
C	1.305937	-3.483026	0.166925	H	-6.229057	-3.631347	-1.855738
C	2.414232	-3.321296	1.026248	Ni	1.901477	0.675155	0.816079
C	1.490135	-4.062112	-1.108576	H	6.470378	1.612017	-0.132181
C	3.681389	-3.730163	0.591251	C	2.151619	4.077180	4.691775
C	2.772438	-4.460416	-1.499582	C	2.337558	2.748339	5.078018
C	3.885097	-4.299867	-0.667995	C	2.784044	1.804565	4.154961
H	4.530808	-3.602767	1.259967	C	3.058139	2.155874	2.816595
H	2.903686	-4.916009	-2.479547	C	2.869395	3.504563	2.447420
C	0.326774	-4.279023	-2.050007	C	2.422839	4.446577	3.370733
H	-0.498548	-4.806231	-1.557703	H	1.805446	4.816097	5.409298
H	-0.072073	-3.324869	-2.412954	H	2.137841	2.444747	6.102796
H	0.635187	-4.868648	-2.919269	H	2.932193	0.772950	4.467865
C	2.269738	-2.718286	2.407379	H	3.083942	3.819255	1.430171
H	1.704142	-1.779186	2.379428	H	2.290121	5.479339	3.057630
H	1.741559	-3.387439	3.097161	C	3.507454	1.106271	1.881733
H	3.253058	-2.507674	2.840060	H	3.842436	0.184987	2.366664
C	5.265865	-4.703460	-1.130812	C	3.784903	1.251400	0.508780
H	5.727930	-3.910274	-1.733924	H	3.750262	2.249725	0.065731
H	5.931802	-4.899826	-0.283801	C	4.711417	0.288660	-0.233052
H	5.233068	-5.604876	-1.753051	H	4.493205	-0.728691	0.114113
C	-2.475693	-4.372085	3.321394	C	6.188458	0.583827	0.122449
C	-3.958224	-4.134597	3.626083	H	6.863311	-0.093925	-0.413643
C	-4.257904	-2.634674	3.581731	H	6.348931	0.457553	1.198453
C	-4.029981	-2.092477	2.164970	C	4.474553	0.313621	-1.739434
H	-5.290538	-2.429620	3.888983	C	3.816256	-0.751164	-2.370006
H	-4.582865	-4.651025	2.883119	C	4.905023	1.387239	-2.534101
H	-4.210997	-4.561821	4.603909	C	3.600122	-0.749203	-3.750221
H	-1.885551	-4.109305	4.212572	H	3.467584	-1.589962	-1.773755
H	-2.284675	-5.438431	3.142546	C	4.690361	1.394746	-3.913933
H	-4.850840	-2.448058	1.527043	H	5.421356	2.227172	-2.075872
H	-4.106329	-0.999428	2.159172	C	4.037742	0.323815	-4.529541
H	-3.604865	-2.110658	4.293946	H	3.094510	-1.592332	-4.214603
H	-5.098668	2.190980	-1.515092	H	5.039462	2.235274	-4.508968
C	-6.289354	-0.160716	-1.984386	H	3.878054	0.324093	-5.604846
H	-7.064429	0.038900	-1.228048				
H	-6.449436	0.581423	-2.776653	**TS3c**			
C	-4.544995	-2.445187	-1.195031	SCF energy in Ethanol: -3455.868311 a.u.			
C	-6.491477	-1.577797	-2.532481	Free energy in Ethanol: -3454.690591 a.u.			
H	-5.905501	-1.708073	-3.453398	P	0.803358	0.283937	0.612964
H	-7.543984	-1.726450	-2.802980	N	1.277594	1.190889	1.940234
C	-6.038620	-2.612018	-1.498075	C	0.879331	2.603393	1.981835

H	0.692470	2.891519	3.022516	C	-0.211283	-3.699938	2.735382
H	1.659063	3.255828	1.569691	C	-2.636659	-4.321967	1.500477
H	-0.043307	2.759904	1.423462	C	-1.353028	-3.989202	3.489895
C	2.365620	0.851725	2.858544	C	-2.580473	-4.291287	2.895691
H	2.580124	-0.214703	2.817348	H	-3.575868	-4.576800	1.012358
H	3.283800	1.406464	2.625392	H	-1.275147	-3.987957	4.575614
H	2.057604	1.110325	3.879784	C	1.087251	-3.424279	3.460431
O	1.215132	-1.206683	1.250196	H	1.927813	-3.957586	3.002887
O	1.928370	0.438462	-0.628535	H	1.334720	-2.357135	3.443858
C	1.669471	-2.277988	0.487719	H	1.017533	-3.736201	4.507401
C	2.888937	-2.162004	-0.196903	C	-1.668004	-4.168675	-0.800293
C	0.932117	-3.478735	0.494752	H	-1.082129	-3.419455	-1.338901
C	3.282739	-3.192062	-1.090979	H	-1.334680	-5.150084	-1.161621
C	3.770223	-0.962332	-0.016090	H	-2.716378	-4.062149	-1.096679
C	1.423110	-4.517210	-0.300670	C	-3.809012	-4.563200	3.732309
C	2.541870	-4.384742	-1.128161	H	-4.392055	-3.646049	3.892708
C	3.288828	0.303299	-0.379441	H	-4.473403	-5.286827	3.247294
C	5.102589	-1.084636	0.451213	H	-3.543220	-4.955328	4.719885
H	0.890998	-5.465188	-0.291960	C	2.894936	-5.536445	-2.057411
C	4.137477	1.416107	-0.533816	C	4.282271	-5.410162	-2.694669
C	5.959174	0.027387	0.362466	C	4.486429	-3.980156	-3.200229
C	5.476013	1.224923	-0.176471	C	4.472357	-2.994977	-2.023942
C	3.681545	2.725600	-1.097739	H	5.434794	-3.885069	-3.742563
C	3.818284	3.923075	-0.360599	H	5.060126	-5.648161	-1.954919
C	3.178505	2.783304	-2.422736	H	4.386605	-6.137350	-3.508737
C	3.409616	5.134462	-0.936185	H	2.141141	-5.582589	-2.858076
C	2.794296	4.015094	-2.955986	H	2.805630	-6.484140	-1.510402
C	2.889739	5.205810	-2.227501	H	5.413897	-3.109977	-1.469953
H	3.508469	6.047859	-0.352628	H	4.474478	-1.963641	-2.394314
H	2.419885	4.047242	-3.977633	H	3.687455	-3.727130	-3.911456
C	4.420272	3.974304	1.029301	H	6.165577	2.056219	-0.302860
H	5.503083	4.154913	0.989375	C	7.422279	-0.047461	0.776073
H	3.981696	4.793432	1.609041	H	8.037475	-0.159676	-0.130185
H	4.274033	3.045632	1.584587	H	7.725365	0.906882	1.224754
C	2.444620	6.519651	-2.827127	C	5.573809	-2.359419	1.141191
H	2.806983	7.370511	-2.241075	C	7.732580	-1.207620	1.728040
H	2.811341	6.635865	-3.853883	H	7.331581	-0.987848	2.727631
H	1.349649	6.590148	-2.868027	H	8.817978	-1.317997	1.839411
C	3.088702	1.553746	-3.299424	C	7.099308	-2.499303	1.204171
H	4.016391	0.970323	-3.272427	H	5.182366	-2.340272	2.170816
H	2.279340	0.889088	-2.979383	H	5.127339	-3.244494	0.683042
H	2.900121	1.837546	-4.339582	H	7.495942	-2.718636	0.202103
C	-0.293000	-3.710534	1.323200	H	7.363269	-3.351581	1.841956
C	-1.518942	-4.049904	0.702860	Ni	-1.157955	0.597848	-0.234164

C	-7.456686	-3.848288	-2.803882
C	-7.265138	-2.999510	-3.895459
C	-6.256373	-2.037576	-3.866837
C	-5.407043	-1.900779	-2.753339
C	-5.626822	-2.753449	-1.653186
C	-6.633008	-3.716041	-1.681898
H	-8.244319	-4.596657	-2.821050
H	-7.903122	-3.084864	-4.771497
H	-6.112439	-1.382629	-4.723462
H	-5.019387	-2.644233	-0.759127
H	-6.785051	-4.358942	-0.818332
C	-4.343615	-0.886711	-2.782235
H	-4.446819	-0.130287	-3.562076
C	-3.259665	-0.833315	-1.984672
H	-3.112343	-1.610191	-1.235182
C	-2.205496	0.210862	-2.033925
H	-2.353455	0.923047	-2.855438
C	-0.799766	-0.208302	-1.888287
H	-0.063147	0.325369	-2.490318
H	-0.588330	-1.278456	-1.832645
B	-3.135301	2.706395	0.677101
O	-2.262773	1.553914	1.157992
O	-4.323093	2.629109	1.480726
C	-2.894799	0.971203	2.340301
C	-4.406927	1.367210	2.139445
C	-2.262640	1.639104	3.570739
H	-2.415962	2.721521	3.555783
H	-2.678205	1.237534	4.501414
H	-1.186844	1.441186	3.568379
C	-2.637360	-0.532409	2.389759
H	-3.181689	-0.980024	3.229875
H	-2.956356	-1.038579	1.475697
H	-1.574117	-0.741224	2.541011
C	-5.181287	0.373888	1.252103
H	-6.156571	0.811333	1.013861
H	-4.664620	0.179117	0.309376
H	-5.354007	-0.581876	1.760500
C	-5.180210	1.568349	3.448144
H	-5.207598	0.649866	4.047188
H	-4.743212	2.368400	4.050206
H	-6.212943	1.850101	3.216559
C	-2.440230	4.165706	0.734544
C	-2.854425	5.123304	1.676736
C	-1.388789	4.534900	-0.125014
C	-2.250008	6.380177	1.766381
H	-3.676132	4.871800	2.342439
C	-0.766011	5.782718	-0.037991
H	-1.047281	3.830030	-0.882277
C	-1.197538	6.712821	0.911182
H	-2.600217	7.100783	2.502777
H	0.055826	6.026328	-0.707483
H	-0.721106	7.688302	0.979751
O	-3.369750	2.301527	-0.792216
H	-2.714905	1.271813	-1.180506
C	-4.463865	2.830859	-1.553088
H	-5.023931	1.982362	-1.962936
H	-5.123917	3.354847	-0.855063
C	-3.991039	3.760188	-2.665007
H	-3.333387	3.234775	-3.367548
H	-4.851934	4.141509	-3.228039
H	-3.440750	4.609345	-2.249947

TS3d

SCF energy in Ethanol: -3455.863518 a.u.

Free energy in Ethanol: -3454.687199 a.u.

P	-0.722423	0.167509	0.836263
N	-0.777719	-0.030734	2.500119
C	0.377713	-0.670936	3.143366
H	0.504664	-0.251864	4.147838
H	0.242589	-1.756828	3.227583
H	1.292118	-0.470888	2.583765
C	-1.992420	-0.038480	3.316509
H	-2.802543	0.472007	2.799007
H	-2.313412	-1.059422	3.559598
H	-1.787620	0.489158	4.256793
O	-2.109118	1.097911	0.714164
O	-1.200294	-1.248689	0.066136
C	-2.859651	1.149048	-0.458051
C	-3.527087	-0.009787	-0.882793
C	-2.989230	2.375116	-1.139086
C	-4.139056	-0.025104	-2.162763
C	-3.591474	-1.224297	-0.005162
C	-3.697616	2.344866	-2.343614
C	-4.218613	1.170707	-2.896322
C	-2.403874	-1.878883	0.351291
C	-4.830171	-1.757695	0.430531
H	-3.831515	3.279678	-2.882743
C	-2.395755	-3.163084	0.928260

C	-4.847462	-3.019519	1.051243	C	-4.870494	-1.266820	-4.269935
C	-3.644765	-3.709045	1.239171	C	-4.673854	-1.326472	-2.749472
C	-1.144684	-3.951602	1.160256	H	-5.391042	-2.171922	-4.605185
C	-0.783341	-4.377808	2.457316	H	-6.613711	-0.002038	-4.116879
C	-0.348582	-4.347199	0.055200	H	-5.887710	0.002866	-5.723406
C	0.382775	-5.136717	2.630856	H	-4.031966	1.360819	-5.020964
C	0.797074	-5.113682	0.276905	H	-5.457387	2.139842	-4.362892
C	1.191388	-5.511514	1.559329	H	-5.638777	-1.580300	-2.289751
H	0.657919	-5.446881	3.637219	H	-3.998032	-2.147622	-2.485834
H	1.393456	-5.420792	-0.580450	H	-3.894301	-1.256840	-4.775050
C	-1.620773	-4.083627	3.685639	H	-3.676841	-4.708640	1.666529
H	-2.332565	-4.896138	3.885405	C	-6.145888	-3.691934	1.473635
H	-0.986082	-3.990469	4.573346	H	-6.418774	-4.437096	0.710338
H	-2.206593	-3.167905	3.584892	H	-5.980620	-4.259653	2.397871
C	2.448882	-6.323177	1.767341	C	-6.110553	-0.936289	0.336336
H	3.349009	-5.715222	1.607035	C	-7.314752	-2.716512	1.647805
H	2.501262	-6.726509	2.783727	H	-7.174842	-2.125984	2.564352
H	2.502990	-7.165022	1.066652	H	-8.250835	-3.274555	1.770309
C	-0.731376	-4.003395	-1.367381	C	-7.391889	-1.771620	0.445525
H	-1.786693	-4.225161	-1.564464	H	-6.095782	-0.209523	1.164008
H	-0.579845	-2.939808	-1.579864	H	-6.126317	-0.331970	-0.573116
H	-0.128025	-4.577524	-2.077516	H	-7.532276	-2.361276	-0.472233
C	-2.496070	3.689331	-0.616943	H	-8.258173	-1.103928	0.527050
C	-1.569287	4.458358	-1.355152	Ni	1.126095	0.786616	-0.095821
C	-3.049722	4.225734	0.571900	C	6.239146	-3.257514	-5.481874
C	-1.199244	5.724902	-0.883171	C	6.112507	-1.976955	-6.021886
C	-2.652128	5.494111	1.001108	C	5.303638	-1.029674	-5.395568
C	-1.726424	6.264352	0.289900	C	4.596965	-1.332538	-4.216900
H	-0.475985	6.303855	-1.454584	C	4.742096	-2.628567	-3.683013
H	-3.088705	5.896738	1.913521	C	5.549144	-3.575354	-4.307732
C	-4.089752	3.479080	1.377182	H	6.870594	-3.998296	-5.964819
H	-4.887412	3.081838	0.739381	H	6.645063	-1.712931	-6.932103
H	-3.648945	2.629130	1.909645	H	5.210567	-0.034116	-5.824333
H	-4.547922	4.139334	2.120242	H	4.225634	-2.895873	-2.765418
C	-0.961191	3.976900	-2.656137	H	5.645701	-4.567082	-3.872827
H	-0.806026	2.895730	-2.666223	C	3.755326	-0.293359	-3.606365
H	-1.601041	4.214684	-3.516099	H	3.831737	0.689051	-4.075760
H	0.004654	4.462461	-2.831797	C	2.907675	-0.430929	-2.571074
C	-1.334773	7.643881	0.767041	H	2.786542	-1.402676	-2.092535
H	-1.114690	7.650265	1.841075	C	2.050497	0.655386	-2.014079
H	-0.449881	8.013607	0.238948	H	2.198609	1.611591	-2.528692
H	-2.143662	8.367916	0.601429	C	0.633310	0.286940	-1.826161
C	-4.839468	1.235947	-4.283482	H	-0.120821	0.951590	-2.253073
C	-5.653476	-0.008441	-4.652266	H	0.373628	-0.763089	-1.966602

B	3.754821	1.322912	1.329697
O	2.258391	1.608657	1.346598
O	4.367946	2.557207	1.741042
C	2.059927	2.914709	1.975418
C	3.429937	3.629111	1.681148
C	1.825126	2.674806	3.474165
H	2.677109	2.167875	3.934491
H	1.646795	3.617089	4.003817
H	0.939219	2.045633	3.597125
C	0.847536	3.619302	1.376319
H	0.780066	4.644182	1.759487
H	0.896339	3.672512	0.286659
H	-0.079592	3.108241	1.649794
C	3.476764	4.283071	0.285202
H	4.507575	4.590438	0.079481
H	3.169719	3.584863	-0.498346
H	2.839697	5.172855	0.226532
C	3.833931	4.671607	2.729784
H	3.098986	5.482989	2.796525
H	3.948587	4.218172	3.717046
H	4.797546	5.110950	2.450249
C	4.197412	0.057874	2.231908
C	4.912181	0.235217	3.429094
C	3.868100	-1.263841	1.878606
C	5.271726	-0.844525	4.240608
H	5.198102	1.243712	3.717488
C	4.210090	-2.351149	2.685948
H	3.337827	-1.448089	0.945015
C	4.915481	-2.143891	3.874126
H	5.831161	-0.672738	5.158043
H	3.928810	-3.358969	2.387651
H	5.190086	-2.987375	4.503622
H	2.944294	0.908597	-0.861407
O	3.999270	1.008551	-0.162831
C	5.266548	1.309807	-0.775795
H	5.690448	2.168074	-0.246797
H	5.057544	1.610009	-1.807134
C	6.221168	0.123492	-0.744855
H	5.798896	-0.732573	-1.279464
H	7.165716	0.398061	-1.231185
H	6.436766	-0.177543	0.284176

TS3e

SCF energy in Ethanol: -3455.869895 a.u.

Free energy in Ethanol: -3454.692269 a.u.

P	-0.135694	0.242528	-0.552796
N	0.227608	0.912412	-2.042940
C	1.474462	1.663817	-2.209965
H	1.964414	1.359987	-3.142268
H	1.283278	2.743552	-2.243938
H	2.166449	1.454377	-1.396137
C	-0.674707	1.014809	-3.189576
H	-1.597872	0.469746	-3.005994
H	-0.918496	2.062734	-3.403835
H	-0.183483	0.590424	-4.075672
O	-1.299352	-0.823326	-1.135907
O	-1.091383	1.295562	0.349896
C	-2.417477	-1.243124	-0.424077
C	-3.364482	-0.298283	0.003601
C	-2.623521	-2.625101	-0.241332
C	-4.389310	-0.702316	0.898395
C	-3.321005	1.117086	-0.489084
C	-3.710375	-2.994306	0.554918
C	-4.549380	-2.068332	1.182619
C	-2.208804	1.915002	-0.194328
C	-4.400473	1.681494	-1.215134
H	-3.898558	-4.054899	0.702897
C	-2.204519	3.308583	-0.392685
C	-4.403468	3.065959	-1.463469
C	-3.337297	3.849245	-1.007487
C	-1.084890	4.191375	0.063209
C	-0.334361	4.953768	-0.858254
C	-0.812856	4.315665	1.448093
C	0.708298	5.764458	-0.389128
C	0.229807	5.144178	1.870110
C	1.017816	5.866018	0.966716
H	1.290191	6.335182	-1.110656
H	0.425556	5.235525	2.936768
C	-0.630683	4.970165	-2.343548
H	-1.321697	5.784887	-2.599746
H	0.284964	5.135125	-2.921316
H	-1.093351	4.043199	-2.687044
C	2.168514	6.719905	1.446407
H	1.941687	7.196514	2.406694
H	3.076446	6.118680	1.590561
H	2.411110	7.507653	0.725390
C	-1.658582	3.615011	2.488552
H	-2.727014	3.801894	2.327643

H	-1.514402	2.529839	2.466139	H	-5.714681	-0.047536	-1.169508
H	-1.401925	3.965012	3.493158	H	-7.305226	1.842524	-1.282962
C	-1.829269	-3.698133	-0.921263	H	-7.429080	0.889295	-2.760340
C	-1.127917	-4.662084	-0.164448	Ni	1.627354	-0.203840	0.696712
C	-1.888817	-3.830445	-2.329599	B	4.490994	-0.438245	-0.394183
C	-0.492556	-5.721289	-0.824368	O	3.039288	-0.846137	-0.597802
C	-1.236214	-4.902980	-2.944223	O	5.257445	-1.563456	-0.849689
C	-0.528677	-5.861078	-2.212432	C	3.022664	-2.130427	-1.299080
H	0.047935	-6.455978	-0.230102	C	4.436585	-2.723721	-0.941796
H	-1.295964	-4.999703	-4.026869	C	2.857256	-1.826997	-2.795479
C	-2.668930	-2.862827	-3.191628	H	3.691478	-1.230137	-3.173743
H	-3.667944	-2.670849	-2.784251	H	2.785515	-2.747337	-3.385344
H	-2.159437	-1.895688	-3.266563	H	1.932482	-1.259913	-2.941081
H	-2.786531	-3.257934	-4.205647	C	1.855510	-2.982081	-0.813889
C	-1.037718	-4.588953	1.343481	H	1.919118	-3.991040	-1.235755
H	-0.938293	-3.562509	1.703050	H	1.842706	-3.071640	0.276040
H	-1.928577	-5.009033	1.828242	H	0.899657	-2.562085	-1.135531
H	-0.176373	-5.159573	1.704755	C	4.455759	-3.477301	0.403574
C	0.187074	-6.997649	-2.905409	H	5.500191	-3.668760	0.672588
H	1.175899	-6.685284	-3.267837	H	4.006948	-2.885279	1.204445
H	0.341246	-7.845566	-2.229630	H	3.936660	-4.440903	0.344067
H	-0.375573	-7.355224	-3.775154	C	5.020758	-3.636465	-2.026338
C	-5.599913	-2.581651	2.154891	H	4.378537	-4.506890	-2.207317
C	-6.667327	-1.542513	2.513128	H	5.158663	-3.099052	-2.967521
C	-5.999384	-0.198543	2.814057	H	6.001491	-4.001320	-1.702626
C	-5.290171	0.333785	1.561733	C	4.951300	0.936998	-1.115322
H	-6.735238	0.538805	3.156928	C	5.666614	0.894405	-2.325964
H	-7.367000	-1.418809	1.674061	C	4.663804	2.213433	-0.597703
H	-7.257633	-1.892014	3.368654	C	6.056603	2.055729	-2.997094
H	-5.092362	-2.900749	3.078369	H	5.934069	-0.076496	-2.734790
H	-6.064818	-3.487464	1.744404	C	5.045074	3.384286	-1.259782
H	-6.059187	0.676476	0.855534	H	4.141269	2.300948	0.352331
H	-4.701599	1.224733	1.808301	C	5.741527	3.309346	-2.467637
H	-5.274758	-0.325553	3.631178	H	6.612188	1.983802	-3.929979
H	-3.376848	4.925567	-1.159381	H	4.804101	4.354127	-0.828862
C	-5.563869	3.756598	-2.166020	H	6.044452	4.216919	-2.985007
H	-6.200714	4.232629	-1.404320	O	4.526223	-0.294301	1.144566
H	-5.180682	4.575709	-2.787437	H	3.382580	0.036448	1.614560
C	-5.482841	0.796542	-1.822042	C	5.751202	0.089331	1.789447
C	-6.427428	2.808021	-3.004741	H	6.560793	-0.088867	1.075305
H	-5.885420	2.517088	-3.915824	H	5.722200	1.161603	2.010853
H	-7.339423	3.323267	-3.329465	C	5.979250	-0.728182	3.053751
C	-6.763445	1.552980	-2.195259	H	6.028384	-1.796289	2.819332
H	-5.065073	0.346614	-2.736876	H	6.924544	-0.432834	3.524813

H	5.178115	-0.572573	3.785294
C	-0.816891	-3.026647	4.649022
C	-1.598878	-1.954480	4.211197
C	-1.027966	-0.926900	3.462944
C	0.342281	-0.934090	3.134300
C	1.109125	-2.037483	3.561933
C	0.538352	-3.064682	4.312640
H	-1.257900	-3.823078	5.242376
H	-2.656083	-1.912842	4.461685
H	-1.642597	-0.092594	3.135495
H	2.167229	-2.085429	3.319845
H	1.157237	-3.896195	4.640647
C	0.928940	0.222585	2.412562
H	0.265811	1.085173	2.389679
C	2.368408	0.527934	2.537212
H	2.866428	-0.049034	3.324593
C	2.698550	1.980591	2.619395
H	2.129913	2.631920	1.954622
C	3.600434	2.528899	3.442910
H	4.184411	1.929979	4.138953
H	3.779572	3.600565	3.455761

TS3f

SCF energy in Ethanol: -3455.872357 a.u.

Free energy in Ethanol: -3454.691413 a.u.

P	-0.151043	0.078431	-0.655598
N	0.042124	0.763644	-2.175061
C	0.904158	1.952522	-2.252227
H	1.350752	2.003305	-3.250722
H	0.343099	2.875222	-2.065863
H	1.717304	1.883373	-1.528962
C	-0.894160	0.623031	-3.291536
H	-1.445758	-0.311572	-3.205404
H	-1.612378	1.451257	-3.338709
H	-0.320595	0.608817	-4.226857
O	-1.037712	-1.252784	-1.151585
O	-1.290160	0.963690	0.206574
C	-2.020802	-1.855658	-0.373070
C	-3.159148	-1.112241	-0.027704
C	-1.886931	-3.215404	-0.022004
C	-4.088700	-1.651746	0.898019
C	-3.410192	0.236613	-0.631086
C	-2.895161	-3.749279	0.786773
C	-3.951840	-2.990815	1.299282
C	-2.513116	1.286068	-0.381800
C	-4.566463	0.478204	-1.413794
H	-2.836699	-4.802236	1.049432
C	-2.826055	2.625871	-0.690192
C	-4.878493	1.800524	-1.772956
C	-4.035916	2.836863	-1.360404
C	-1.992370	3.806642	-0.298836
C	-1.520004	4.721320	-1.269309
C	-1.771585	4.080435	1.073219
C	-0.795533	5.846495	-0.855523
C	-1.053198	5.222855	1.436771
C	-0.544030	6.116088	0.489663
H	-0.426194	6.535352	-1.613069
H	-0.901829	5.427520	2.494909
C	-1.790381	4.573916	-2.753964
H	-2.712149	5.095061	-3.045788
H	-0.976000	5.015862	-3.337845
H	-1.903373	3.532895	-3.061849
C	0.251972	7.330142	0.909228
H	-0.096501	7.725204	1.869997
H	1.317202	7.089081	1.025943
H	0.181185	8.132100	0.166549
C	-2.341028	3.199852	2.159974
H	-3.401889	2.984055	1.984808
H	-1.817652	2.241549	2.221794
H	-2.251945	3.685977	3.135328
C	-0.777263	-4.103427	-0.490814
C	0.026841	-4.801191	0.444328
C	-0.584593	-4.338715	-1.874184
C	1.037665	-5.650962	-0.021885
C	0.428009	-5.209491	-2.288871
C	1.265674	-5.863354	-1.382595
H	1.656303	-6.171939	0.706851
H	0.557208	-5.388681	-3.354763
C	-1.468045	-3.714177	-2.931577
H	-2.509961	-3.644030	-2.602783
H	-1.137964	-2.699154	-3.178636
H	-1.441081	-4.306801	-3.851743
C	-0.174550	-4.716581	1.944959
H	-0.587011	-3.757944	2.265630
H	-0.866027	-5.494812	2.294925
H	0.772391	-4.868722	2.471456
C	2.382075	-6.763956	-1.856999
H	2.582295	-7.567371	-1.139802

H	2.144850	-7.222306	-2.823239	H	2.298842	-3.183947	1.457733
H	3.317449	-6.202421	-1.984359	C	3.750429	-3.112621	2.965499
C	-4.903400	-3.646527	2.289016	H	4.267590	-2.543969	3.735994
C	-6.179608	-2.837889	2.542951	H	4.056734	-4.147214	2.837595
C	-5.823278	-1.363445	2.747090	B	4.391735	0.620488	-0.280551
C	-5.203738	-0.783639	1.468969	O	3.185360	-0.140031	-0.802642
H	-6.709497	-0.778130	3.020171	O	5.510028	0.076068	-0.995336
H	-6.860713	-2.930613	1.684840	C	3.626716	-1.026689	-1.879287
H	-6.710173	-3.242090	3.413240	C	5.171296	-1.176568	-1.585679
H	-4.374635	-3.782733	3.244717	C	3.349624	-0.314145	-3.210462
H	-5.149939	-4.657680	1.939703	H	3.871374	0.645763	-3.258143
H	-6.003272	-0.655456	0.726361	H	3.664540	-0.927456	-4.061613
H	-4.815426	0.223142	1.659252	H	2.275537	-0.135271	-3.301106
H	-5.114030	-1.271964	3.582216	C	2.844603	-2.337141	-1.831401
H	-4.320702	3.860832	-1.589559	H	3.220025	-3.029573	-2.594779
C	-6.139891	2.151964	-2.548398	H	2.925635	-2.829085	-0.860288
H	-6.893450	2.528888	-1.839549	H	1.784445	-2.164088	-2.039928
H	-5.929976	2.985538	-3.230196	C	5.498254	-2.320500	-0.606779
C	-5.399906	-0.676362	-1.957800	H	6.552770	-2.238159	-0.322558
C	-6.736153	0.968764	-3.318387	H	4.902936	-2.267815	0.306467
H	-6.111715	0.740641	-4.193956	H	5.347474	-3.304168	-1.067450
H	-7.730009	1.233852	-3.698733	C	6.033458	-1.350368	-2.842670
C	-6.805022	-0.264179	-2.413683	H	5.761621	-2.256926	-3.397171
H	-4.860478	-1.092678	-2.823511	H	5.948299	-0.490375	-3.511008
H	-5.459327	-1.495811	-1.238416	H	7.084002	-1.439588	-2.546052
H	-7.430559	-0.038516	-1.537594	C	4.290891	2.229469	-0.403060
H	-7.281726	-1.104308	-2.933153	C	5.103720	2.936009	-1.306500
Ni	1.638904	-0.347680	0.513928	C	3.374683	2.986622	0.350777
C	-1.006786	1.604869	5.149701	C	5.003369	4.321274	-1.460250
C	-1.663673	0.483339	4.639817	H	5.831078	2.379541	-1.891904
C	-1.065931	-0.289922	3.644437	C	3.257294	4.370707	0.202188
C	0.206829	0.028521	3.136854	H	2.730666	2.483621	1.072246
C	0.841422	1.179543	3.642738	C	4.075200	5.044393	-0.707833
C	0.245706	1.953509	4.637030	H	5.650370	4.837777	-2.166423
H	-1.465945	2.202861	5.932412	H	2.526959	4.918517	0.793137
H	-2.641229	0.202497	5.024631	H	3.991992	6.122360	-0.826930
H	-1.582026	-1.168518	3.264382	O	4.355750	0.193356	1.207182
H	1.817419	1.466524	3.259711	H	3.269913	-0.396147	1.534756
H	0.763652	2.831561	5.014974	C	5.197547	0.762004	2.213544
C	0.866271	-0.892150	2.173028	H	5.327775	1.828144	1.998191
H	0.256290	-1.776013	1.976006	H	4.660668	0.678704	3.167635
C	2.320258	-1.157394	2.305025	C	6.544170	0.052557	2.291707
H	2.748139	-0.651235	3.178742	H	7.072977	0.137148	1.338461
C	2.786618	-2.567770	2.212559	H	7.160817	0.501660	3.080236

H	6.409039	-1.010530	2.517811

TS3g

SCF energy in Ethanol: -3455.870354 a.u.

Free energy in Ethanol: -3454.690318 a.u.

P	-0.349567	-0.024660	-0.522319
N	-0.088942	0.348231	-2.132848
C	1.180822	0.970163	-2.517407
H	1.569624	0.488238	-3.421736
H	1.053780	2.042541	-2.710362
H	1.926979	0.842103	-1.734427
C	-1.089361	0.333402	-3.199069
H	-2.014733	-0.120025	-2.850563
H	-1.305001	1.348625	-3.555002
H	-0.705425	-0.251322	-4.045879
O	-1.646619	-1.058507	-0.794672
O	-1.104100	1.258463	0.258822
C	-2.726317	-1.222852	0.067490
C	-3.538773	-0.121260	0.377302
C	-3.035405	-2.517427	0.530922
C	-4.508776	-0.243013	1.406271
C	-3.408922	1.173324	-0.367936
C	-4.076872	-2.617734	1.456735
C	-4.769475	-1.509389	1.953815
C	-2.207953	1.891143	-0.300905
C	-4.495059	1.710533	-1.103996
H	-4.346000	-3.607433	1.818183
C	-2.099418	3.221758	-0.747362
C	-4.399326	3.024764	-1.595487
C	-3.232472	3.760544	-1.364652
C	-0.878980	4.065995	-0.549674
C	-0.186824	4.610968	-1.656108
C	-0.459147	4.399271	0.760352
C	0.930159	5.424753	-1.433194
C	0.656010	5.225581	0.933563
C	1.374849	5.740911	-0.148633
H	1.461206	5.828245	-2.293624
H	0.963660	5.480493	1.945569
C	-0.622642	4.386983	-3.089821
H	-1.338810	5.154117	-3.413790
H	0.235327	4.444555	-3.767951
H	-1.109201	3.420248	-3.232881
C	2.596532	6.605642	0.060531
H	3.521373	6.021420	-0.040504
H	2.647549	7.414650	-0.677021
H	2.601694	7.057287	1.058240
C	-1.214639	3.927883	1.983130
H	-2.286662	4.143160	1.900072
H	-1.112302	2.847595	2.129792
H	-0.839452	4.424882	2.882982
C	-2.399511	-3.777858	0.029774
C	-1.724197	-4.646049	0.915913
C	-2.593570	-4.175042	-1.315346
C	-1.245321	-5.873565	0.441879
C	-2.098264	-5.410066	-1.743048
C	-1.416999	-6.276505	-0.883121
H	-0.722313	-6.531745	1.133523
H	-2.262687	-5.709194	-2.776703
C	-3.354647	-3.315623	-2.300086
H	-4.287260	-2.934143	-1.869686
H	-2.763228	-2.447022	-2.610828
H	-3.605035	-3.887858	-3.198943
C	-1.504171	-4.301220	2.373698
H	-1.354859	-3.229157	2.520509
H	-2.360460	-4.594972	2.995350
H	-0.628506	-4.830588	2.764721
C	-0.869619	-7.595169	-1.378924
H	0.117637	-7.468470	-1.843708
H	-0.753646	-8.314241	-0.561041
H	-1.525263	-8.043163	-2.133949
C	-5.775273	-1.723161	3.074290
C	-6.702735	-0.525496	3.304573
C	-5.882657	0.767023	3.305930
C	-5.238086	0.988779	1.931113
H	-6.509555	1.630995	3.557452
H	-7.457427	-0.475294	2.506585
H	-7.247168	-0.650479	4.248171
H	-5.223476	-1.926032	4.004996
H	-6.358767	-2.630632	2.871211
H	-6.026493	1.292170	1.228526
H	-4.541186	1.833697	1.971403
H	-5.104546	0.704051	4.079831
H	-3.192011	4.794007	-1.700928
C	-5.552639	3.700079	-2.323580
H	-6.073454	4.362919	-1.615260
H	-5.156247	4.356092	-3.108651
C	-5.701537	0.849862	-1.459846
C	-6.568304	2.715542	-2.912732

H	-6.139708	2.219732	-3.795277	H	5.601007	0.556557	1.747856
H	-7.457505	3.258253	-3.255537	C	6.196642	-1.457009	2.297800
C	-6.938749	1.657938	-1.869332	H	6.273981	-2.443999	1.832839
H	-5.408985	0.206456	-2.304960	H	7.191603	-1.155651	2.647908
H	-5.947799	0.161065	-0.649321	H	5.539788	-1.532973	3.171592
H	-7.369207	2.153166	-0.986645	C	4.607156	3.412898	3.774016
H	-7.707960	0.978670	-2.256382	C	4.690330	2.211550	4.479145
Ni	1.451874	-0.516264	0.638812	C	3.970270	1.094466	4.050796
B	4.159318	-1.187535	-0.662649	C	3.154062	1.149459	2.909885
O	2.663394	-1.461830	-0.679098	C	3.075434	2.366799	2.213058
O	4.765678	-2.446135	-1.002750	C	3.791838	3.484589	2.641686
C	2.455379	-2.807820	-1.208986	H	5.168307	4.283376	4.103061
C	3.824826	-3.507305	-0.875213	H	5.314491	2.140612	5.366497
C	2.199284	-2.672544	-2.717400	H	4.037452	0.164923	4.611583
H	3.056556	-2.228113	-3.229412	H	2.445729	2.441122	1.329901
H	1.980470	-3.644258	-3.173673	H	3.714685	4.413931	2.083649
H	1.332185	-2.022639	-2.870251	C	2.375627	-0.069087	2.481806
C	1.249045	-3.458459	-0.541941	H	2.614309	-0.927877	3.120271
H	1.180211	-4.514086	-0.826364	C	0.912345	0.126010	2.336158
H	1.311330	-3.408031	0.548619	H	0.570712	1.161375	2.321600
H	0.317475	-2.981015	-0.854521	C	0.006260	-0.785023	3.053412
C	3.873591	-4.074868	0.557524	H	0.386739	-1.790790	3.240637
H	4.905002	-4.370903	0.776493	C	-1.218071	-0.466558	3.503261
H	3.576394	-3.326645	1.296561	H	-1.641352	0.522285	3.346417
H	3.234669	-4.958061	0.671975	H	-1.836471	-1.185234	4.032831
C	4.217193	-4.614530	-1.860237				
H	3.477741	-5.424556	-1.871020	**TS3h**			
H	4.326408	-4.224720	-2.875099	SCF energy in Ethanol: -3455.869624 a.u.			
H	5.180705	-5.040391	-1.560329	Free energy in Ethanol: -3454.686867 a.u.			
C	4.667146	0.010562	-1.629443	P	0.444715	-0.237455	-0.538790
C	5.245200	-0.280955	-2.878214	N	0.525773	-1.115965	-1.967516
C	4.546146	1.371910	-1.293715	C	-0.144679	-2.423311	-1.977654
C	5.657291	0.724139	-3.756587	H	-0.452066	-2.657560	-3.002290
H	5.386933	-1.323290	-3.151662	H	0.510834	-3.221832	-1.612059
C	4.951288	2.388546	-2.163225	H	-1.042698	-2.395772	-1.361985
H	4.139145	1.649022	-0.323260	C	1.564358	-0.969374	-2.989327
C	5.505867	2.067038	-3.403898	H	1.981742	0.035831	-2.964283
H	6.103215	0.460602	-4.713565	H	2.380276	-1.691620	-2.856886
H	4.841562	3.430477	-1.868970	H	1.109503	-1.138203	-3.973619
H	5.826714	2.853651	-4.083151	O	1.162789	1.153352	-1.127989
O	4.362391	-0.807207	0.817686	O	1.608914	-0.821620	0.521816
H	3.291843	-0.475517	1.414989	C	1.992510	1.980405	-0.376968
C	5.666860	-0.438378	1.298539	C	3.195353	1.464456	0.127267
H	6.328622	-0.370815	0.430283	C	1.639575	3.334955	-0.215018

C	3.966677	2.250469	1.022308	H	0.083654	5.556038	1.797762
C	3.677022	0.098344	-0.258572	H	-1.456013	4.702053	1.900521
C	2.495216	4.112460	0.570440	C	-2.941134	5.974242	-2.704288
C	3.610070	3.592353	1.234214	H	-3.321446	6.795927	-2.087596
C	2.916228	-1.027867	0.088126	H	-2.690082	6.378603	-3.690912
C	4.920198	-0.078946	-0.915937	H	-3.767855	5.264709	-2.844861
H	2.262040	5.167317	0.691820	C	4.378827	4.501117	2.181883
C	3.445526	-2.333142	0.032752	C	5.735371	3.934192	2.611913
C	5.444581	-1.377041	-1.039376	C	5.577577	2.459830	2.991048
C	4.727047	-2.456653	-0.514162	C	5.148445	1.640139	1.767250
C	2.753936	-3.546470	0.574006	H	6.514066	2.053139	3.391405
C	2.476490	-4.659967	-0.250534	H	6.458094	4.021644	1.787967
C	2.475102	-3.628744	1.961919	H	6.136034	4.518862	3.448543
C	1.877590	-5.796916	0.310096	H	3.765303	4.667595	3.080420
C	1.889624	-4.787466	2.475975	H	4.501476	5.488753	1.718443
C	1.570021	-5.883141	1.666797	H	6.013460	1.546979	1.096315
H	1.656261	-6.642023	-0.339082	H	4.896650	0.616543	2.066293
H	1.692790	-4.842271	3.545146	H	4.825329	2.366603	3.787064
C	2.835436	-4.714138	-1.722429	H	5.173440	-3.447452	-0.552971
H	3.827882	-5.160490	-1.872447	C	6.803025	-1.642297	-1.672498
H	2.119715	-5.336482	-2.270098	H	7.542859	-1.787075	-0.869969
H	2.856664	-3.727897	-2.189627	H	6.771348	-2.591036	-2.222747
C	0.918626	-7.115965	2.249830	C	5.626818	1.097596	-1.578922
H	-0.154965	-6.959988	2.420851	C	7.283738	-0.509823	-2.586135
H	1.021006	-7.977096	1.581352	H	6.702534	-0.511210	-3.519213
H	1.361264	-7.382887	3.216483	H	8.331504	-0.674536	-2.864871
C	2.853490	-2.517568	2.914418	C	7.107290	0.838852	-1.883578
H	3.902260	-2.222868	2.786689	H	5.104646	1.303396	-2.526877
H	2.243767	-1.622650	2.759004	H	5.514063	2.009020	-0.988032
H	2.720851	-2.841189	3.952040	H	7.686108	0.839673	-0.948336
C	0.447889	3.977041	-0.852699	H	7.502212	1.655973	-2.499355
C	-0.535141	4.606208	-0.052174	Ni	-1.505566	-0.074570	0.448433
C	0.345408	4.055287	-2.262512	C	-5.296908	3.536089	3.052609
C	-1.616381	5.244450	-0.672775	C	-5.251341	2.402834	3.865486
C	-0.746653	4.714528	-2.835058	C	-4.334074	1.383801	3.600316
C	-1.749446	5.304119	-2.061070	C	-3.440274	1.469089	2.520800
H	-2.368627	5.721153	-0.046444	C	-3.500210	2.615021	1.711466
H	-0.808190	4.777166	-3.920028	C	-4.414093	3.635886	1.974664
C	1.405025	3.482607	-3.177600	H	-6.011280	4.329701	3.254001
H	2.415359	3.689666	-2.808419	H	-5.928262	2.309281	4.711052
H	1.310062	2.394737	-3.265866	H	-4.304651	0.509400	4.246991
H	1.317008	3.908967	-4.181987	H	-2.824685	2.710545	0.865925
C	-0.455427	4.660617	1.460367	H	-4.442239	4.508062	1.325973
H	0.065896	3.799274	1.883708	C	-2.465050	0.350617	2.265305

H	-2.592345	-0.442772	3.012712	H	-4.658344	-1.652401	2.790558
C	-1.022573	0.685204	2.124502	C	-6.491974	-1.326785	1.677933
H	-0.811119	1.743468	1.946927	H	-6.870024	-1.477655	0.663135
C	-0.072811	0.071083	3.067025	H	-7.127974	-1.882541	2.378419
H	-0.258058	-0.972359	3.327347	H	-6.555860	-0.260989	1.920335
C	0.954530	0.710978	3.644222				
H	1.179428	1.751140	3.418200	**IM1-Z**			
H	1.608922	0.214584	4.355094	SCF energy in Ethanol: -3044.786104 a.u.			
B	-3.952655	-1.588944	-0.579008	Free energy in Ethanol: -3043.783717 a.u.			
O	-2.842712	-0.634223	-0.989909	P	0.067058	0.324484	0.515090
O	-5.045337	-1.283848	-1.457616	N	0.424566	0.580170	2.133199
C	-3.285016	0.097132	-2.178868	C	-0.245571	1.688852	2.811039
C	-4.855003	-0.012201	-2.073498	H	-0.579845	1.363952	3.802541
C	-2.727198	-0.629529	-3.411066	H	0.419450	2.555915	2.919616
H	-3.075847	-1.665160	-3.450856	H	-1.128080	1.997452	2.244080
H	-3.025557	-0.123870	-4.335816	C	1.500209	-0.041637	2.903420
H	-1.635521	-0.627869	-3.360786	H	1.913978	-0.885777	2.354731
C	-2.749454	1.526629	-2.150491	H	2.307837	0.670555	3.118986
H	-3.141704	2.091066	-3.005089	H	1.092915	-0.406959	3.854640
H	-3.035754	2.055442	-1.239818	O	0.783462	-1.194647	0.399337
H	-1.657905	1.537212	-2.226171	O	1.147394	1.219795	-0.441108
C	-5.481859	1.088865	-1.197939	C	1.317205	-1.655441	-0.798185
H	-6.530889	0.831189	-1.018462	C	2.492470	-1.068760	-1.292621
H	-4.988760	1.170560	-0.227857	C	0.702343	-2.741231	-1.446528
H	-5.452221	2.067899	-1.690727	C	2.974322	-1.448931	-2.572797
C	-5.574063	-0.031887	-3.428082	C	3.200294	-0.008007	-0.506640
H	-5.389825	0.888427	-3.995890	C	1.270904	-3.163260	-2.650247
H	-5.266179	-0.887217	-4.034041	C	2.359704	-2.518979	-3.245182
H	-6.653328	-0.112986	-3.259928	C	2.512870	1.179972	-0.214561
C	-3.553007	-3.156303	-0.599900	C	4.552003	-0.141548	-0.106983
C	-4.076662	-4.018443	-1.578971	H	0.825512	-4.016609	-3.157443
C	-2.651132	-3.718212	0.322947	C	3.174622	2.330307	0.258212
C	-3.712197	-5.365728	-1.646138	C	5.224960	0.981623	0.406271
H	-4.789565	-3.615419	-2.293592	C	4.539883	2.195478	0.529006
C	-2.271443	-5.061297	0.263764	C	2.486899	3.648834	0.428596
H	-2.230258	-3.090312	1.108848	C	2.441304	4.290060	1.686823
C	-2.802837	-5.891712	-0.725897	C	1.923078	4.299228	-0.698146
H	-4.139005	-6.006574	-2.415051	C	1.786050	5.523619	1.806071
H	-1.559110	-5.455806	0.984289	C	1.288322	5.532326	-0.531351
H	-2.514303	-6.939235	-0.775879	C	1.192219	6.158250	0.715909
O	-4.193148	-1.117034	0.872776	H	1.746297	6.000401	2.783982
H	-3.228400	-0.429693	1.329381	H	0.864935	6.023597	-1.405603
C	-5.053005	-1.816629	1.780524	C	3.101288	3.719616	2.925826
H	-4.986879	-2.888964	1.568317	H	4.141171	4.061265	3.017155

H	2.577546	4.049593	3.829449	H	7.282710	1.384958	-0.042136
H	3.125689	2.628107	2.921871	H	6.879183	1.572828	1.652810
C	0.465994	7.474268	0.871392	C	5.236738	-1.502421	-0.119820
H	0.690410	8.156502	0.043257	C	7.226351	-0.481361	1.033498
H	-0.622756	7.330345	0.882623	H	6.846845	-0.851634	1.996511
H	0.739674	7.975274	1.805831	H	8.320366	-0.464715	1.109613
C	2.027322	3.715981	-2.089897	C	6.767531	-1.423065	-0.083363
H	3.050549	3.392499	-2.313598	H	4.894983	-2.050386	0.772643
H	1.377902	2.842614	-2.207813	H	4.903140	-2.104375	-0.968018
H	1.735910	4.457836	-2.840140	H	7.146142	-1.055341	-1.048339
C	-0.486088	-3.473361	-0.906679	H	7.184160	-2.427934	0.057160
C	-1.725388	-3.400484	-1.580811	Ni	-1.982149	0.587780	-0.150266
C	-0.350308	-4.318678	0.215510	C	-8.425134	2.906763	-1.201282
C	-2.805423	-4.154838	-1.109266	C	-8.474379	1.627487	-1.760747
C	-1.454808	-5.063282	0.645865	C	-7.329050	1.061783	-2.316771
C	-2.694797	-4.991354	0.004789	C	-6.097583	1.746718	-2.317854
H	-3.758535	-4.088261	-1.630648	C	-6.074385	3.045836	-1.773074
H	-1.337213	-5.729266	1.498947	C	-7.220888	3.613844	-1.218272
C	0.965105	-4.447649	0.949483	H	-9.317510	3.352167	-0.769752
H	1.803545	-4.582216	0.257322	H	-9.407871	1.070261	-1.766293
H	1.173622	-3.549679	1.542750	H	-7.376554	0.065623	-2.751176
H	0.947818	-5.303128	1.632433	H	-5.159810	3.628011	-1.819214
C	-1.912131	-2.527603	-2.803884	H	-7.175511	4.620338	-0.809501
H	-1.507080	-1.522185	-2.646232	C	-4.924453	1.099040	-2.930652
H	-1.404037	-2.940839	-3.683681	H	-5.163671	0.445358	-3.769496
H	-2.973882	-2.430321	-3.051733	C	-3.618689	1.175732	-2.581320
C	-3.882491	-5.777244	0.510155	H	-2.919231	0.618607	-3.205879
H	-4.487024	-5.179766	1.205628	C	-3.000925	1.869089	-1.453432
H	-4.541003	-6.081707	-0.310806	H	-3.657850	2.442139	-0.804551
H	-3.567924	-6.679627	1.045450	C	-1.619707	2.116109	-1.385273
C	2.809259	-2.985723	-4.621710	H	-0.972073	1.807676	-2.205155
C	4.159050	-2.407438	-5.058252	H	-1.234869	2.946492	-0.797449
C	4.199393	-0.909428	-4.748011	C	-0.355759	-3.390632	5.576530
C	4.112913	-0.679590	-3.233415	C	-0.659995	-2.182860	6.208471
H	5.118165	-0.451375	-5.133804	C	-1.481695	-1.252487	5.575571
H	4.975870	-2.911065	-4.521548	C	-2.012665	-1.486218	4.288857
H	4.318286	-2.596248	-6.126675	C	-1.708352	-2.718630	3.676653
H	2.044784	-2.692177	-5.357205	C	-0.891398	-3.651724	4.313032
H	2.834782	-4.083155	-4.642023	H	0.279054	-4.123651	6.067103
H	5.075241	-0.968299	-2.789014	H	-0.264666	-1.968296	7.198256
H	3.999867	0.388848	-3.018348	H	-1.723135	-0.319434	6.080671
H	3.359959	-0.409888	-5.252247	H	-2.133531	-2.968140	2.712042
H	5.086402	3.070663	0.872859	H	-0.679978	-4.595892	3.818351
C	6.700632	0.935525	0.777570	C	-2.871183	-0.446746	3.706632

H	-3.269224	0.240419	4.453731
C	-3.228359	-0.171419	2.428507
H	-3.904509	0.677558	2.313710
C	-2.886365	-0.807632	1.155131
H	-2.241679	-1.679287	1.153365
C	-3.659251	-0.530072	0.022206
H	-4.550585	0.087943	0.099917
H	-3.633677	-1.195277	-0.835642

IM9a

SCF energy in Ethanol: -2812.675764 a.u.

Free energy in Ethanol: -2811.750213 a.u.

P	-0.413957	-1.317531	-0.133234
N	-0.084955	-2.711170	-1.039004
C	0.162193	-3.952976	-0.307681
H	-0.332258	-4.791951	-0.816577
H	1.237469	-4.172158	-0.239475
H	-0.241403	-3.877658	0.707114
C	0.390625	-2.748789	-2.418895
H	0.285130	-1.770026	-2.884265
H	1.441510	-3.057338	-2.465789
H	-0.202816	-3.475258	-2.992536
O	-0.781829	-0.351328	-1.477848
O	1.063221	-0.594758	0.299961
C	-0.938084	1.001350	-1.201570
C	0.210284	1.771422	-0.971609
C	-2.231643	1.550391	-1.174010
C	0.061968	3.099748	-0.497191
C	1.556550	1.171825	-1.249342
C	-2.333478	2.896831	-0.818751
C	-1.225798	3.661807	-0.433083
C	1.951238	-0.004674	-0.582524
C	2.420273	1.748346	-2.213719
H	-3.318145	3.358994	-0.805795
C	3.235727	-0.563161	-0.756876
C	3.724055	1.240375	-2.356186
C	4.105801	0.122501	-1.611132
C	3.684634	-1.846581	-0.125215
C	4.071113	-2.938624	-0.939337
C	3.786583	-1.974286	1.281696
C	4.471274	-4.139296	-0.335459
C	4.203767	-3.186109	1.837636
C	4.533902	-4.292390	1.049131
H	4.752323	-4.974763	-0.974608
H	4.282169	-3.262541	2.920718
C	4.121224	-2.874711	-2.454030
H	5.117759	-2.571790	-2.802876
H	3.921236	-3.861098	-2.887233
H	3.410598	-2.160929	-2.874340
C	4.945171	-5.602782	1.679234
H	5.634254	-5.445658	2.517233
H	4.076600	-6.145140	2.076319
H	5.438399	-6.259053	0.954529
C	3.496479	-0.815631	2.203842
H	3.925736	0.115699	1.818084
H	2.419763	-0.656890	2.309110
H	3.912993	-0.996368	3.199765
C	-3.441293	0.740439	-1.520487
C	-4.435334	0.481444	-0.547762
C	-3.611311	0.244301	-2.834481
C	-5.544743	-0.305578	-0.895732
C	-4.741701	-0.520818	-3.139594
C	-5.719812	-0.815696	-2.185814
H	-6.298583	-0.508547	-0.136952
H	-4.861578	-0.894361	-4.154952
C	-2.604807	0.532470	-3.925143
H	-2.328542	1.592303	-3.947335
H	-1.682011	-0.037917	-3.771908
H	-3.009593	0.264699	-4.906342
C	-4.353967	1.039035	0.857189
H	-3.337288	1.017408	1.257849
H	-4.688788	2.083952	0.888583
H	-5.001343	0.472173	1.534466
C	-6.947659	-1.619075	-2.548983
H	-7.363643	-2.134582	-1.676607
H	-7.739524	-0.972966	-2.951402
H	-6.724960	-2.370296	-3.314739
C	-1.468890	5.072041	0.084018
C	-0.193867	5.912877	0.204200
C	0.907699	5.083702	0.869068
C	1.275021	3.886425	-0.016488
H	1.803390	5.691096	1.047135
H	0.141095	6.231980	-0.793621
H	-0.403222	6.825741	0.774934
H	-1.938408	5.000068	1.076620
H	-2.204094	5.573750	-0.559240
H	1.852591	4.257176	-0.874781
H	1.946083	3.211705	0.525530

H	0.564296	4.730370	1.850125
H	5.116723	-0.260961	-1.728575
C	4.743704	1.882438	-3.285743
H	5.390562	2.547560	-2.692405
H	5.406171	1.109133	-3.694315
C	1.914672	2.805054	-3.189715
C	4.111192	2.698828	-4.417749
H	3.659833	2.022664	-5.157784
H	4.884786	3.272827	-4.942430
C	3.029018	3.623127	-3.853476
H	1.355446	2.275421	-3.977806
H	1.185550	3.466943	-2.720839
H	3.479727	4.305364	-3.117913
H	2.600220	4.250702	-4.644459
Ni	-1.696987	-1.737784	1.528799
C	2.155708	3.373419	4.410995
C	1.012773	3.855688	5.054209
C	-0.213025	3.222163	4.865654
C	-0.335354	2.081806	4.043817
C	0.822063	1.623744	3.384737
C	2.048942	2.261154	3.572061
H	3.114960	3.864288	4.552949
H	1.076597	4.726392	5.702395
H	-1.098342	3.601847	5.371436
H	0.747321	0.793477	2.691536
H	2.927359	1.891056	3.051051
C	-1.657226	1.466732	3.900273
H	-2.478356	2.146994	4.127750
C	-2.025145	0.195727	3.596362
H	-3.103973	0.032079	3.582164
C	-1.266700	-1.034924	3.363566
H	-0.197390	-1.025250	3.562950
C	-1.986170	-2.263480	3.381618
H	-3.040122	-2.268190	3.666412
H	-1.456469	-3.193110	3.596134
C	-3.488801	-4.949998	0.731943
H	-2.565027	-4.942162	1.319093
H	-4.334782	-4.933297	1.426577
H	-3.526901	-5.881811	0.156016
C	-3.540633	-3.755726	-0.204000
H	-2.712810	-3.778056	-0.923595
H	-4.484676	-3.746291	-0.763859
O	-3.461544	-2.548420	0.579550
H	-3.761984	-1.803738	0.025791

IM9b

SCF energy in Ethanol: -2812.678274 a.u.

Free energy in Ethanol: -2811.753964 a.u.

P	-0.404612	-1.308092	-0.381019
N	-0.161953	-2.526037	-1.515210
C	-0.162218	-3.912038	-1.060902
H	-0.844155	-4.513067	-1.678538
H	0.844956	-4.349203	-1.119849
H	-0.504325	-3.966520	-0.023173
C	0.161269	-2.358411	-2.926975
H	0.259696	-1.302197	-3.173812
H	1.098319	-2.871461	-3.173879
H	-0.637458	-2.788311	-3.549785
O	-0.904791	-0.144523	-1.508922
O	1.082602	-0.629214	0.044914
C	-0.982614	1.164252	-1.052811
C	0.209619	1.875879	-0.865454
C	-2.244065	1.738710	-0.816829
C	0.165439	3.137314	-0.220195
C	1.496334	1.278915	-1.347673
C	-2.255250	3.032287	-0.290326
C	-1.085009	3.717073	0.058849
C	1.917228	0.039429	-0.833746
C	2.283060	1.927621	-2.331229
H	-3.214693	3.514179	-0.115311
C	3.177606	-0.507418	-1.148575
C	3.548919	1.403970	-2.649202
C	3.976993	0.225831	-2.030708
C	3.673979	-1.800740	-0.581241
C	3.975781	-2.891276	-1.427884
C	3.904093	-1.923118	0.810488
C	4.425852	-4.093458	-0.864639
C	4.367682	-3.136455	1.324709
C	4.617632	-4.244101	0.508505
H	4.642136	-4.930877	-1.526260
H	4.546841	-3.214402	2.395678
C	3.881028	-2.815658	-2.938587
H	4.849309	-2.543805	-3.380957
H	3.603802	-3.789012	-3.358965
H	3.158674	-2.071950	-3.278968
C	5.077802	-5.557091	1.098408
H	5.803459	-5.401939	1.905181
H	4.236866	-6.118984	1.527009

H	5.545321	-6.195443	0.341130
C	3.696228	-0.760337	1.751620
H	4.090064	0.172443	1.333047
H	2.633682	-0.602907	1.962629
H	4.204877	-0.945543	2.703478
C	-3.520100	1.024678	-1.135380
C	-4.433852	0.691147	-0.108612
C	-3.843198	0.715797	-2.478783
C	-5.625300	0.027754	-0.441207
C	-5.050049	0.069555	-2.764144
C	-5.958482	-0.285660	-1.762395
H	-6.321102	-0.226148	0.356864
H	-5.290152	-0.154945	-3.801765
C	-2.923140	1.086685	-3.619503
H	-2.578066	2.123095	-3.536223
H	-2.031611	0.450093	-3.630633
H	-3.433455	0.973207	-4.581223
C	-4.183634	1.048502	1.341204
H	-3.141531	0.888153	1.629481
H	-4.416909	2.102455	1.538491
H	-4.817047	0.447191	2.001150
C	-7.277392	-0.941066	-2.103541
H	-7.689198	-1.487409	-1.248166
H	-8.024834	-0.193185	-2.400675
H	-7.175774	-1.642823	-2.939013
C	-1.217240	5.056956	0.767572
C	0.094150	5.845912	0.842714
C	1.231593	4.914782	1.269910
C	1.453511	3.828799	0.209061
H	2.163263	5.475037	1.415696
H	0.328243	6.279906	-0.140293
H	-0.015868	6.684414	1.541029
H	-1.577180	4.874349	1.791478
H	-1.998975	5.652471	0.277521
H	1.944301	4.290331	-0.659307
H	2.157097	3.075603	0.580463
H	0.986309	4.450842	2.234989
H	4.967173	-0.157639	-2.266922
C	4.488875	2.101168	-3.622752
H	5.225762	2.680959	-3.045024
H	5.068206	1.350496	-4.175071
C	1.723272	3.094578	-3.136825
C	3.774871	3.047071	-4.594358
H	3.220493	2.463438	-5.343167
H	4.512221	3.646854	-5.141894
C	2.797206	3.942058	-3.828724
H	1.061963	2.670866	-3.909652
H	1.076639	3.726402	-2.525594
H	3.349831	4.528002	-3.079679
H	2.317347	4.662927	-4.502116
Ni	-1.724707	-1.794167	1.253028
C	1.207547	3.307421	5.273883
C	2.353334	2.562695	4.981968
C	2.248035	1.211248	4.659849
C	0.998583	0.560637	4.600901
C	-0.141723	1.322189	4.929352
C	-0.038036	2.674328	5.253785
H	1.286247	4.359924	5.533635
H	3.332529	3.034704	5.010715
H	3.147341	0.641085	4.440350
H	-1.112342	0.839807	4.965513
H	-0.935518	3.232735	5.509738
C	0.957153	-0.873533	4.268128
H	1.857320	-1.419097	4.550728
C	-0.014334	-1.589716	3.650781
H	0.163588	-2.662749	3.564182
C	-1.273568	-1.123946	3.070368
H	-1.410075	-0.044075	3.059766
C	-2.451348	-1.936772	3.039735
H	-2.409575	-2.947110	3.455907
H	-3.427775	-1.459112	3.142974
O	-3.224558	-2.645195	0.036676
H	-3.680637	-1.865006	-0.331421
C	-4.213815	-3.525013	0.609446
H	-3.640551	-4.296143	1.128068
H	-4.798655	-2.980740	1.360678
C	-5.104858	-4.131980	-0.464650
H	-5.828518	-4.820366	-0.011939
H	-5.664723	-3.355389	-0.998034
H	-4.507223	-4.687365	-1.194948

TS7a

SCF energy in Ethanol: -3455.868554 a.u.

Free energy in Ethanol: -3454.687042 a.u.

P	0.219717	0.147926	-0.524718
N	0.878271	0.788637	-1.922270
C	2.112677	1.571415	-1.828142
H	2.835880	1.226716	-2.575692

H	1.910009	2.637874	-1.985661	C	-0.112635	-5.796006	-0.944084
H	2.573888	1.447783	-0.850429	C	-0.467895	-4.902946	-3.131606
C	0.264648	0.811558	-3.249020	C	0.103614	-5.887126	-2.318036
H	-0.727434	0.366145	-3.226797	H	0.311389	-6.554680	-0.288461
H	0.182061	1.842178	-3.612631	H	-0.336331	-4.964230	-4.210550
H	0.889552	0.249969	-3.957553	C	-1.847132	-2.861278	-3.565459
O	-0.840287	-0.890337	-1.306795	H	-2.906052	-2.693693	-3.338544
O	-0.843800	1.252612	0.170747	H	-1.348100	-1.887907	-3.517282
C	-2.057776	-1.308287	-0.778763	H	-1.774942	-3.224668	-4.595428
C	-3.048582	-0.354346	-0.495348	C	-1.064877	-4.770202	1.127616
C	-2.299774	-2.689984	-0.645478	H	-1.209999	-3.766533	1.530330
C	-4.207965	-0.754816	0.217955	H	-1.945802	-5.362991	1.409469
C	-2.918396	1.053408	-0.999843	H	-0.202537	-5.224989	1.628174
C	-3.502874	-3.053189	-0.034348	C	0.927080	-7.005129	-2.914626
C	-4.421604	-2.122139	0.460499	H	1.135726	-7.786391	-2.176502
C	-1.844764	1.856777	-0.584660	H	0.413978	-7.472384	-3.763779
C	-3.869819	1.585897	-1.906308	H	1.891942	-6.636911	-3.287728
H	-3.724327	-4.112458	0.072064	C	-5.621400	-2.628913	1.244686
C	-1.763689	3.229318	-0.893764	C	-6.744871	-1.596593	1.376047
C	-3.822311	2.957589	-2.214162	C	-6.151938	-0.251524	1.802046
C	-2.804039	3.747055	-1.673548	C	-5.204240	0.284084	0.720603
C	-0.650947	4.132621	-0.454916	H	-6.942698	0.486223	1.985875
C	0.132541	4.818728	-1.415394	H	-7.264981	-1.482357	0.413770
C	-0.414297	4.376913	0.918959	H	-7.490526	-1.946653	2.100137
C	1.156945	5.671208	-0.985703	H	-5.282955	-2.909675	2.253646
C	0.611428	5.247503	1.299567	H	-5.993607	-3.553293	0.783882
C	1.423779	5.894121	0.365505	H	-5.811110	0.657541	-0.115493
H	1.759789	6.179868	-1.736016	H	-4.657848	1.153763	1.100727
H	0.771361	5.431864	2.360448	H	-5.607200	-0.374656	2.746621
C	-0.096766	4.708567	-2.909990	H	-2.793933	4.810373	-1.900503
H	-0.752089	5.512678	-3.271363	C	-4.868926	3.622342	-3.097475
H	0.850122	4.803230	-3.452480	H	-5.613677	4.111614	-2.450479
H	-0.566157	3.766223	-3.196632	H	-4.401253	4.428809	-3.675828
C	2.555578	6.794385	0.802190	C	-4.846752	0.677932	-2.645766
H	2.335779	7.280368	1.759106	C	-5.594010	2.645864	-4.028982
H	3.486129	6.225660	0.934088	H	-4.918608	2.329170	-4.836369
H	2.755808	7.576332	0.061731	H	-6.445046	3.147012	-4.505954
C	-1.259371	3.751164	2.002426	C	-6.051730	1.415259	-3.242035
H	-2.303789	3.644488	1.692157	H	-4.287461	0.202912	-3.467755
H	-0.893046	2.752175	2.258541	H	-5.181367	-0.147754	-2.015597
H	-1.232677	4.358543	2.912996	H	-6.732532	1.729685	-2.437489
C	-1.411525	-3.759705	-1.204907	H	-6.618011	0.729205	-3.883615
C	-0.862775	-4.758856	-0.372247	Ni	1.661198	-0.442516	1.028795
C	-1.220984	-3.850288	-2.607561	C	-4.214109	1.048989	5.095726

C	-4.096891	-0.245635	5.608150	H	6.613904	-0.142152	-1.604018
C	-3.181452	-1.136364	5.051785	C	5.440760	3.353613	-0.442444
C	-2.347328	-0.758986	3.979338	H	4.226277	2.305933	0.982758
C	-2.504084	0.536657	3.453091	C	6.370100	3.247970	-1.479715
C	-3.419174	1.429489	4.011596	H	7.521926	1.887029	-2.693484
H	-4.924949	1.748347	5.527667	H	5.115803	4.334343	-0.100379
H	-4.717539	-0.560967	6.443146	H	6.772157	4.142182	-1.950571
H	-3.088976	-2.139279	5.462902	O	4.442319	-0.158827	1.913539
H	-1.934442	0.829004	2.579555	C	5.447516	-0.341166	2.920044
H	-3.518072	2.426470	3.590259	H	5.061751	-1.059946	3.654931
C	-1.373391	-1.740943	3.484401	H	6.315419	-0.798450	2.437078
H	-1.662132	-2.773588	3.680479	C	5.812675	0.975754	3.593470
C	-0.144384	-1.575842	2.937107	H	6.579143	0.806703	4.359775
H	0.399636	-2.503578	2.751350	H	6.203252	1.687294	2.860122
C	0.647482	-0.367549	2.663792	H	4.939720	1.426186	4.079677
H	0.151042	0.584991	2.835367	H	3.247078	-0.335676	2.218704
C	2.075552	-0.427050	3.039032				
H	2.368476	-1.338999	3.570913	**TS7b**			
H	2.407469	0.463664	3.581876	SCF energy in Ethanol: -3455.868586 a.u.			
B	4.723334	-0.437206	0.417825	Free energy in Ethanol: -3454.689922 a.u.			
O	3.343736	-0.886362	-0.059935	P	0.196259	0.271990	-0.707671
O	5.574102	-1.574337	0.201227	N	0.780070	1.035988	-2.083413
C	3.508872	-2.169135	-0.743973	C	1.906148	1.962455	-1.909692
C	4.803470	-2.744536	-0.060960	H	2.521162	1.952287	-2.816310
C	3.697595	-1.869210	-2.238537	H	1.564372	2.988183	-1.725493
H	4.583985	-1.254474	-2.413604	H	2.539914	1.646291	-1.081094
H	3.786786	-2.790968	-2.823822	C	0.041930	1.218199	-3.333799
H	2.821940	-1.321554	-2.600576	H	-0.747812	0.474086	-3.420810
C	2.271725	-3.042203	-0.555614	H	-0.406173	2.217280	-3.404694
H	2.454707	-4.048568	-0.948901	H	0.737802	1.093438	-4.173447
H	1.995402	-3.141391	0.498151	O	-0.842597	-0.771420	-1.507289
H	1.414215	-2.637663	-1.098721	O	-0.879244	1.285052	0.092758
C	4.508952	-3.473950	1.265055	C	-2.016781	-1.248814	-0.930029
H	5.459301	-3.664022	1.774953	C	-3.042910	-0.338780	-0.637647
H	3.884314	-2.869315	1.928442	C	-2.174088	-2.634119	-0.732165
H	4.011096	-4.436570	1.103046	C	-4.173648	-0.778254	0.097266
C	5.630444	-3.668227	-0.962103	C	-2.951107	1.087519	-1.089777
H	5.054801	-4.549357	-1.270368	C	-3.351209	-3.042426	-0.098053
H	5.977603	-3.144559	-1.855946	C	-4.319188	-2.148681	0.369876
H	6.512908	-4.015361	-0.413966	C	-1.919931	1.900945	-0.598455
C	5.319296	0.911233	-0.250032	C	-3.912549	1.643503	-1.969521
C	6.266200	0.837824	-1.287091	H	-3.506574	-4.107811	0.055330
C	4.934246	2.200350	0.162784	C	-1.928513	3.300877	-0.758910
C	6.786678	1.982078	-1.896990	C	-3.915243	3.032771	-2.185075

C	-2.963364	3.827980	-1.538236	C	-5.201333	0.225382	0.607049
C	-0.941508	4.214239	-0.101062	H	-6.915093	0.373549	1.914233
C	-0.116854	5.075007	-0.860244	H	-7.193263	-1.625962	0.374566
C	-0.892414	4.281161	1.313469	H	-7.358671	-2.077903	2.070861
C	0.783789	5.921125	-0.198986	H	-5.114539	-2.957527	2.181089
C	0.012657	5.149551	1.927643	H	-5.829774	-3.636370	0.728269
C	0.876291	5.967160	1.191503	H	-5.843781	0.558827	-0.219661
H	1.426497	6.566317	-0.795328	H	-4.683433	1.125324	0.957383
H	0.035251	5.197025	3.014912	H	-5.524677	-0.425431	2.650057
C	-0.183671	5.165038	-2.371573	H	-3.012618	4.907167	-1.663676
H	-0.875037	5.957236	-2.689798	C	-4.961389	3.710842	-3.058587
H	0.798352	5.412300	-2.788755	H	-5.730256	4.153139	-2.406126
H	-0.529013	4.238693	-2.833777	H	-4.502932	4.553555	-3.591147
C	1.876795	6.864176	1.882302	C	-4.854313	0.745149	-2.762498
H	1.472518	7.272985	2.815267	C	-5.643058	2.760445	-4.048564
H	2.791725	6.314284	2.141636	H	-4.947142	2.505468	-4.860373
H	2.172052	7.703562	1.243801	H	-6.502047	3.259510	-4.513259
C	-1.832714	3.472541	2.178020	C	-6.074541	1.477842	-3.332489
H	-2.867791	3.550927	1.825331	H	-4.277140	0.323327	-3.600713
H	-1.566902	2.410786	2.182094	H	-5.169282	-0.117078	-2.170923
H	-1.802526	3.830362	3.212602	H	-6.771278	1.731164	-2.520039
C	-1.211491	-3.672351	-1.219788	H	-6.615479	0.811519	-4.015371
C	-0.589786	-4.563465	-0.318172	Ni	1.643778	-0.605072	0.660590
C	-1.013104	-3.847903	-2.612447	C	-3.927485	-2.367111	5.145609
C	0.238141	-5.579133	-0.817137	C	-4.112466	-0.982277	5.188680
C	-0.188178	-4.880532	-3.062687	C	-3.090266	-0.126715	4.782231
C	0.456798	-5.756110	-2.182185	C	-1.858245	-0.623649	4.311807
H	0.718181	-6.254278	-0.110536	C	-1.682448	-2.021569	4.297980
H	-0.053844	-5.012091	-4.134982	C	-2.705059	-2.878995	4.703507
C	-1.704905	-2.971829	-3.633048	H	-4.718092	-3.037362	5.472431
H	-2.775025	-2.870062	-3.419909	H	-5.050568	-0.568127	5.549833
H	-1.280846	-1.961734	-3.646161	H	-3.240281	0.949665	4.826882
H	-1.598393	-3.393216	-4.637655	H	-0.725121	-2.437239	4.004377
C	-0.798569	-4.497766	1.180635	H	-2.538050	-3.953217	4.691656
H	-1.119086	-3.511106	1.518082	C	-0.805804	0.336741	3.941164
H	-1.567851	-5.211568	1.505623	H	-0.898895	1.300830	4.440921
H	0.123987	-4.762182	1.709882	C	0.242027	0.198988	3.098241
C	1.366144	-6.846658	-2.699138	H	0.930336	1.044011	3.055101
H	1.557639	-7.605561	-1.933408	C	0.590523	-0.946388	2.232964
H	0.934295	-7.348813	-3.572710	H	-0.241190	-1.612163	2.007410
H	2.338706	-6.441844	-3.010093	C	1.911352	-1.579980	2.427942
C	-5.484501	-2.696332	1.178394	H	2.380477	-1.327944	3.386287
C	-6.645303	-1.707659	1.324571	H	1.940567	-2.660715	2.262454
C	-6.099126	-0.333167	1.718999	B	4.668684	-0.335487	0.255170

O	3.367484	-0.693243	-0.446701
O	5.629896	-1.285462	-0.230871
C	3.683619	-1.675021	-1.485357
C	4.978804	-2.358273	-0.910557
C	3.948470	-0.902073	-2.786453
H	4.778220	-0.199549	-2.673505
H	4.174479	-1.583777	-3.613724
H	3.049556	-0.338164	-3.049426
C	2.509375	-2.624845	-1.695192
H	2.787575	-3.416212	-2.401103
H	2.185744	-3.101843	-0.767724
H	1.653109	-2.094864	-2.121137
C	4.667667	-3.491449	0.087074
H	5.597753	-3.778957	0.588892
H	3.953968	-3.172484	0.850751
H	4.262398	-4.377705	-0.414240
C	5.936740	-2.890639	-1.982231
H	5.459133	-3.658635	-2.602635
H	6.293542	-2.086284	-2.629438
H	6.809026	-3.342094	-1.497291
C	5.150507	1.197652	0.087654
C	6.244729	1.523672	-0.732284
C	4.494096	2.267108	0.725148
C	6.658172	2.845263	-0.920445
H	6.785844	0.716467	-1.219541
C	4.890545	3.593768	0.538707
H	3.656304	2.057036	1.388434
C	5.977493	3.887825	-0.288357
H	7.513072	3.062057	-1.557783
H	4.353892	4.396717	1.040104
H	6.294049	4.918306	-0.433022
O	4.283350	-0.580024	1.740654
C	5.265175	-0.943466	2.722638
H	4.859982	-1.789790	3.292369
H	6.152061	-1.297234	2.189024
C	5.593368	0.220094	3.649466
H	6.340153	-0.089667	4.390950
H	5.993653	1.064970	3.082143
H	4.699102	0.559086	4.184611
H	3.133598	-1.016259	1.871182

IM10a

SCF energy in Ethanol: -3455.908753 a.u.

Free energy in Ethanol: -3454.719189 a.u.

P	0.174735	0.385062	-0.677617
N	0.651056	1.162024	-2.075005
C	1.738696	2.143976	-2.015619
H	2.410602	1.994392	-2.867931
H	1.345204	3.166951	-2.044498
H	2.330375	2.016422	-1.110103
C	-0.076621	1.158631	-3.344338
H	-0.856123	0.399701	-3.336338
H	-0.534347	2.135798	-3.543282
H	0.625649	0.935169	-4.158206
O	-0.745972	-0.798232	-1.404492
O	-0.985389	1.292062	0.118820
C	-1.881624	-1.362182	-0.818737
C	-2.989657	-0.545392	-0.550602
C	-1.915050	-2.751602	-0.605254
C	-4.077794	-1.074857	0.190613
C	-3.037970	0.870756	-1.038235
C	-3.048438	-3.255499	0.038076
C	-4.094480	-2.446465	0.492267
C	-2.087337	1.789844	-0.575510
C	-4.054500	1.316470	-1.919526
H	-3.107054	-4.328918	0.202906
C	-2.227755	3.177940	-0.758906
C	-4.193479	2.695791	-2.155532
C	-3.316302	3.590717	-1.533594
C	-1.317085	4.186627	-0.132364
C	-0.571905	5.088439	-0.923865
C	-1.258908	4.293152	1.279615
C	0.261321	6.024374	-0.296118
C	-0.421644	5.248899	1.859752
C	0.363369	6.115469	1.091541
H	0.842935	6.703653	-0.916742
H	-0.388813	5.324930	2.944911
C	-0.657874	5.121965	-2.436335
H	-1.433622	5.822309	-2.774414
H	0.288328	5.461233	-2.871171
H	-0.903027	4.147910	-2.864335
C	1.294308	7.108962	1.746413
H	0.854682	7.531186	2.657140
H	2.241284	6.634031	2.036062
H	1.536974	7.936437	1.071536
C	-2.122273	3.433985	2.177112
H	-3.173860	3.463816	1.867964
H	-1.809545	2.384859	2.160193

H	-2.065887	3.784832	3.212398	H	-6.910735	1.115638	-2.427473
C	-0.889979	-3.717989	-1.115731	H	-6.689847	0.195103	-3.914218
C	-0.109816	-4.481949	-0.221300	Ni	1.847659	-0.107304	0.644923
C	-0.803865	-3.967692	-2.504940	C	-3.840882	-1.333570	5.079350
C	0.743362	-5.468671	-0.731477	C	-3.204420	-2.577914	5.078082
C	0.059143	-4.965420	-2.968245	C	-1.871223	-2.679419	4.687068
C	0.845480	-5.727913	-2.099755	C	-1.135937	-1.550050	4.272916
H	1.341217	-6.052602	-0.034451	C	-1.793351	-0.304187	4.287807
H	0.109493	-5.158302	-4.038436	C	-3.126452	-0.199808	4.683612
C	-1.643835	-3.200721	-3.501953	H	-4.874463	-1.245733	5.403615
H	-2.704038	-3.199393	-3.223766	H	-3.742343	-3.466806	5.398373
H	-1.326804	-2.153301	-3.568663	H	-1.378092	-3.648750	4.704781
H	-1.556125	-3.639737	-4.500747	H	-1.245234	0.594225	4.029186
C	-0.169263	-4.265888	1.274473	H	-3.604001	0.776744	4.701376
H	-0.047451	-3.212308	1.544156	C	0.285991	-1.725927	3.936791
H	-1.126161	-4.590525	1.700736	H	0.734335	-2.597587	4.415874
H	0.623632	-4.831327	1.774457	C	1.112654	-0.989973	3.156444
C	1.789368	-6.783241	-2.628390	H	2.144821	-1.329485	3.155461
H	1.999541	-7.547948	-1.873144	C	0.797356	0.170252	2.273891
H	1.377802	-7.283190	-3.512344	H	-0.274179	0.186510	2.068249
H	2.752344	-6.345206	-2.924189	C	1.205461	1.556335	2.804717
C	-5.204622	-3.086084	1.310109	H	0.726754	1.761040	3.775504
C	-6.454049	-2.208972	1.438267	H	0.889953	2.342894	2.111538
C	-6.041031	-0.780175	1.800338	B	4.454309	-0.159127	0.162970
C	-5.200180	-0.163984	0.674355	O	3.275966	-0.339784	-0.788643
H	-6.920674	-0.150247	1.981409	O	5.327930	-1.269678	-0.116838
H	-7.008693	-2.201222	0.488662	C	3.625904	-1.397147	-1.729178
H	-7.128181	-2.628509	2.194800	C	4.654738	-2.253968	-0.899344
H	-4.812585	-3.292953	2.316948	C	4.273478	-0.711762	-2.943241
H	-5.458420	-4.062682	0.877625	H	5.171213	-0.158351	-2.657065
H	-5.872216	0.082407	-0.159266	H	4.538435	-1.439891	-3.717615
H	-4.774896	0.791804	1.000979	H	3.560080	-0.003326	-3.376384
H	-5.459117	-0.796275	2.730992	C	2.379410	-2.150400	-2.174140
H	-3.469659	4.657785	-1.676942	H	2.655344	-2.988087	-2.824315
C	-5.311857	3.255808	-3.023001	H	1.812623	-2.552549	-1.332930
H	-6.109695	3.631848	-2.364002	H	1.719190	-1.490483	-2.744356
H	-4.944905	4.130494	-3.574454	C	3.968246	-3.278227	0.023856
C	-4.910476	0.319800	-2.691582	H	4.720823	-3.697828	0.700025
C	-5.914309	2.229133	-3.988462	H	3.192608	-2.810269	0.635509
H	-5.210928	2.031839	-4.809887	H	3.515198	-4.099190	-0.542536
H	-6.825559	2.635975	-4.443089	C	5.700559	-2.977227	-1.756430
C	-6.206163	0.920663	-3.249143	H	5.230376	-3.682137	-2.453021
H	-4.304836	-0.047530	-3.535440	H	6.306064	-2.269130	-2.327127
H	-5.126256	-0.565102	-2.089401	H	6.373967	-3.544382	-1.104732

C	5.214332	1.267968	0.056990
C	6.506800	1.351947	-0.489803
C	4.622127	2.478545	0.463965
C	7.168422	2.573416	-0.641101
H	6.998824	0.431870	-0.794337
C	5.269287	3.707886	0.315341
H	3.633453	2.461402	0.920997
C	6.548766	3.759506	-0.242649
H	8.169342	2.600083	-1.067120
H	4.778998	4.623560	0.640096
H	7.059231	4.712894	-0.358632
O	3.658059	-0.277888	1.470773
C	4.343035	-0.091389	2.713910
H	5.017881	0.766931	2.613845
H	3.601536	0.160233	3.475995
C	5.123936	-1.333470	3.135070
H	5.631241	-1.143897	4.089582
H	4.455390	-2.192327	3.265561
H	5.869582	-1.594524	2.380636
H	2.283001	1.656575	2.956593

IM10b

SCF energy in Ethanol: -3455.903510 a.u.

Free energy in Ethanol: -3454.717596 a.u.

P	0.193997	0.044571	-0.763893
N	0.646306	0.605671	-2.272168
C	1.675825	1.650674	-2.355965
H	2.270989	1.488347	-3.261390
H	1.229319	2.649955	-2.396833
H	2.355047	1.595313	-1.507461
C	-0.138108	0.448874	-3.498929
H	-0.827738	-0.387929	-3.407628
H	-0.712158	1.353747	-3.735276
H	0.550221	0.248725	-4.329785
O	-0.731892	-1.236612	-1.290310
O	-0.951367	1.063458	-0.092831
C	-1.891638	-1.688043	-0.662932
C	-2.983566	-0.817387	-0.532729
C	-1.961942	-3.035878	-0.258308
C	-4.098331	-1.216171	0.249541
C	-2.994103	0.517271	-1.215137
C	-3.131948	-3.426234	0.399406
C	-4.167482	-2.540321	0.712553
C	-2.034711	1.479382	-0.871729
C	-3.988946	0.840857	-2.172253
H	-3.226611	-4.466333	0.701369
C	-2.144010	2.826695	-1.269292
C	-4.094317	2.169419	-2.619193
C	-3.209704	3.131709	-2.121958
C	-1.236380	3.914243	-0.786530
C	-0.488371	4.701436	-1.691334
C	-1.195960	4.221580	0.596082
C	0.341986	5.714234	-1.192492
C	-0.362221	5.248826	1.043847
C	0.433653	5.996554	0.170090
H	0.928349	6.301580	-1.896742
H	-0.343715	5.479101	2.107449
C	-0.569235	4.539343	-3.196571
H	-1.351605	5.182119	-3.622407
H	0.374747	4.833010	-3.667897
H	-0.799658	3.516491	-3.500902
C	1.360382	7.071139	0.689028
H	0.905500	7.628275	1.516014
H	2.296242	6.639287	1.068763
H	1.625965	7.786330	-0.096515
C	-2.074088	3.502586	1.593570
H	-3.107808	3.427986	1.236646
H	-1.717436	2.487511	1.789576
H	-2.086563	4.036028	2.548904
C	-0.903064	-4.056118	-0.539533
C	-0.279044	-4.751897	0.522688
C	-0.594638	-4.412891	-1.874071
C	0.672368	-5.736964	0.231454
C	0.348714	-5.416522	-2.114896
C	1.008048	-6.082528	-1.078750
H	1.154787	-6.256103	1.057723
H	0.567885	-5.690203	-3.145365
C	-1.280605	-3.767729	-3.057592
H	-2.352262	-3.626903	-2.881124
H	-0.855300	-2.781302	-3.274139
H	-1.162566	-4.384943	-3.953941
C	-0.627459	-4.509256	1.976893
H	-0.921542	-3.475506	2.169970
H	-1.462667	-5.146474	2.297061
H	0.222919	-4.749740	2.622759
C	2.054797	-7.133970	-1.365207
H	2.062570	-7.913061	-0.595136
H	1.884685	-7.615767	-2.334106

H	3.061810	-6.695963	-1.391806	C	1.254372	-1.575776	2.921440
C	-5.325347	-3.045706	1.559667	H	0.621017	-1.823990	3.786503
C	-6.539940	-2.112249	1.557299	H	1.283938	-2.459117	2.274279
C	-6.077286	-0.669101	1.770173	B	4.463491	-0.006227	0.241235
C	-5.192256	-0.214410	0.602505	O	3.364213	-0.424325	-0.732080
H	-6.934095	0.009490	1.860145	O	5.479383	-1.016077	0.100930
H	-7.070266	-2.188711	0.597125	C	3.854951	-1.554059	-1.512717
H	-7.248397	-2.420419	2.335534	C	4.964371	-2.163280	-0.571077
H	-4.974053	-3.164586	2.596220	C	4.438021	-0.968175	-2.807836
H	-5.608281	-4.052054	1.224284	H	5.255934	-0.275206	-2.593864
H	-5.835522	-0.035081	-0.269573	H	4.806619	-1.755897	-3.473847
H	-4.733324	0.753256	0.834042	H	3.653441	-0.417912	-3.336184
H	-5.515626	-0.597828	2.711282	C	2.712107	-2.507875	-1.848665
H	-3.340363	4.166912	-2.427781	H	3.097942	-3.388628	-2.375245
C	-5.185294	2.613275	-3.583324	H	2.183941	-2.854871	-0.957837
H	-5.982245	3.105764	-3.004852	H	1.987005	-2.017829	-2.505343
H	-4.787881	3.383070	-4.256678	C	4.398039	-3.161503	0.456755
C	-4.857707	-0.244114	-2.797939	H	5.180093	-3.385571	1.189759
C	-5.800025	1.463782	-4.388983	H	3.544930	-2.744765	0.996820
H	-5.091565	1.126471	-5.158846	H	4.088582	-4.102120	-0.013543
H	-6.695549	1.815275	-4.915339	C	6.124095	-2.830480	-1.321051
C	-6.131833	0.291634	-3.461715	H	5.778333	-3.673353	-1.932086
H	-4.251288	-0.750015	-3.566169	H	6.643905	-2.117818	-1.965522
H	-5.103799	-1.020719	-2.071300	H	6.848645	-3.214836	-0.595075
H	-6.842226	0.625543	-2.691461	C	5.034873	1.491310	0.022957
H	-6.623782	-0.517319	-4.015226	C	6.340383	1.701089	-0.454106
Ni	1.855812	-0.262266	0.606953	C	4.255341	2.639518	0.259393
C	-3.912230	0.249191	5.488035	C	6.841476	2.983017	-0.695183
C	-3.391392	1.527415	5.700192	H	6.971135	0.833871	-0.631833
C	-2.163171	1.880711	5.147360	C	4.740058	3.926860	0.015540
C	-1.414303	0.981459	4.358603	H	3.244442	2.527397	0.650724
C	-1.958349	-0.303898	4.158997	C	6.039793	4.102979	-0.465072
C	-3.185533	-0.661007	4.716548	H	7.858212	3.108992	-1.061811
H	-4.864695	-0.037209	5.925913	H	4.105212	4.790761	0.202448
H	-3.938771	2.247981	6.302544	H	6.424640	5.102669	-0.653573
H	-1.763010	2.875961	5.327616	O	3.620715	-0.110386	1.521731
H	-1.414863	-1.039939	3.581793	C	4.177111	0.310301	2.771393
H	-3.569765	-1.665496	4.555959	H	4.660172	1.284718	2.629417
C	-0.118390	1.452143	3.843250	H	3.351964	0.448722	3.474415
H	0.170676	2.414677	4.266991	C	5.177505	-0.698678	3.329383
C	0.762183	0.923797	2.962962	H	5.578029	-0.330991	4.282636
H	1.661123	1.521606	2.821579	H	4.698490	-1.667960	3.507553
C	0.698733	-0.346679	2.171486	H	6.004091	-0.852645	2.631873
H	-0.339760	-0.552430	1.892680	H	2.262975	-1.409976	3.302110

TS8a

SCF energy in Ethanol: -3455.879954 a.u.

Free energy in Ethanol: -3454.696040 a.u.

P	-0.095406	0.495880	-0.659273
N	0.116248	1.450983	-2.012392
C	1.114856	2.522355	-1.985350
H	1.752041	2.450380	-2.874644
H	0.630831	3.506814	-1.970408
H	1.764590	2.432259	-1.113597
C	-0.653950	1.382890	-3.252352
H	-1.342955	0.541106	-3.229653
H	-1.226113	2.304951	-3.415286
H	0.033798	1.251804	-4.099263
O	-0.769567	-0.820873	-1.446622
O	-1.416216	1.024503	0.233480
C	-1.764433	-1.626140	-0.894861
C	-3.036420	-1.082501	-0.658163
C	-1.485219	-2.985940	-0.678117
C	-4.025394	-1.879605	-0.020665
C	-3.341913	0.338526	-1.023708
C	-2.511987	-3.762941	-0.138258
C	-3.754242	-3.236220	0.227319
C	-2.594520	1.366281	-0.427989
C	-4.402887	0.679820	-1.898361
H	-2.322519	-4.822012	0.022722
C	-2.999183	2.712724	-0.468625
C	-4.804774	2.024450	-1.989379
C	-4.133332	2.994173	-1.237150
C	-2.310119	3.799372	0.295955
C	-1.739350	4.905786	-0.371161
C	-2.295893	3.760419	1.712582
C	-1.122075	5.915535	0.378854
C	-1.682413	4.798796	2.417046
C	-1.073514	5.880002	1.771959
H	-0.672796	6.756126	-0.147157
H	-1.683484	4.762210	3.504783
C	-1.793885	5.074380	-1.875750
H	-2.697517	5.616730	-2.185621
H	-0.936530	5.655949	-2.231488
H	-1.803454	4.118103	-2.402632
C	-0.379728	6.964862	2.562042
H	-0.959549	7.249473	3.447756
H	0.604261	6.629693	2.915751
H	-0.222686	7.863953	1.956963
C	-2.960190	2.646015	2.490050
H	-3.959336	2.421197	2.099597
H	-2.379000	1.718580	2.450148
H	-3.064505	2.922304	3.543746
C	-0.193218	-3.648917	-1.045271
C	0.716079	-4.049973	-0.040872
C	0.063530	-3.972847	-2.394826
C	1.864171	-4.759844	-0.411411
C	1.224998	-4.684442	-2.718207
C	2.141176	-5.086015	-1.742604
H	2.556994	-5.074378	0.367008
H	1.409608	-4.941987	-3.759563
C	-0.898485	-3.578198	-3.493426
H	-1.918258	-3.919027	-3.280201
H	-0.943125	-2.488894	-3.611417
H	-0.591491	-4.006950	-4.452608
C	0.486786	-3.719697	1.417284
H	0.548095	-2.640788	1.602057
H	-0.499561	-4.039921	1.766926
H	1.241900	-4.199933	2.046929
C	3.399843	-5.836981	-2.111775
H	3.631955	-6.615509	-1.376316
H	3.308522	-6.314325	-3.093126
H	4.267257	-5.164645	-2.153433
C	-4.755590	-4.154759	0.910011
C	-6.178221	-3.589461	0.943299
C	-6.135989	-2.134481	1.415355
C	-5.352890	-1.267709	0.418872
H	-7.147348	-1.726294	1.530289
H	-6.625656	-3.635749	-0.060048
H	-6.808612	-4.200025	1.600717
H	-4.419368	-4.330393	1.943060
H	-4.739904	-5.136184	0.418765
H	-5.994562	-1.097005	-0.455019
H	-5.169812	-0.274695	0.845205
H	-5.665775	-2.091099	2.407237
H	-4.489857	4.021083	-1.269855
C	-5.997556	2.452567	-2.832450
H	-6.862263	2.592182	-2.165352
H	-5.800956	3.437943	-3.273279
C	-5.021776	-0.363464	-2.820730
C	-6.376157	1.445705	-3.924865
H	-5.641169	1.487415	-4.741266

H	-7.346452	1.715334	-4.358992
C	-6.407143	0.026934	-3.349163
H	-4.344456	-0.482426	-3.681667
H	-5.051845	-1.345583	-2.344223
H	-7.145535	-0.021419	-2.535496
H	-6.727259	-0.695754	-4.109553
Ni	1.830565	0.235029	0.486198
C	-3.117429	-2.046558	4.890512
C	-2.162457	-2.103271	5.908492
C	-0.859820	-1.675812	5.667280
C	-0.460784	-1.168032	4.411464
C	-1.434741	-1.140512	3.392729
C	-2.739937	-1.567969	3.634271
H	-4.137052	-2.377267	5.071986
H	-2.432514	-2.481011	6.891798
H	-0.125141	-1.720950	6.468378
H	-1.173937	-0.802651	2.397734
H	-3.461046	-1.533265	2.823550
C	0.930042	-0.718624	4.276184
H	1.561652	-1.076996	5.090097
C	1.554535	0.100037	3.392719
H	2.601305	0.277155	3.628252
C	1.068284	0.855929	2.216061
H	-0.014319	0.773489	2.124439
C	1.422908	2.352209	2.311505
H	2.499786	2.514800	2.415278
H	0.936971	2.809580	3.186698
H	1.081279	2.908856	1.431616
B	4.044242	0.364771	-0.770628
O	5.187670	-0.299887	-1.244514
O	4.254029	1.762122	-0.758669
C	6.254892	0.653208	-1.420597
C	5.487415	2.044890	-1.452153
C	6.988064	0.302341	-2.720380
H	7.443396	-0.688836	-2.623171
H	6.312601	0.278546	-3.578871
H	7.788343	1.022541	-2.927363
C	7.237355	0.505688	-0.248819
H	8.105389	1.163960	-0.367768
H	6.762179	0.717517	0.710039
H	7.594086	-0.529155	-0.220794
C	6.203023	3.186362	-0.724936
H	5.580632	4.087172	-0.758985
H	6.386690	2.944141	0.324140
H	7.162317	3.420093	-1.201857
C	5.115191	2.507306	-2.871770
H	5.997108	2.783813	-3.460322
H	4.564136	1.732704	-3.413477
H	4.467411	3.386956	-2.794644
C	3.726916	-0.139468	1.205879
C	3.842381	-1.528089	1.446567
C	4.497006	0.701795	2.038771
C	4.652078	-2.045759	2.461024
H	3.288375	-2.229968	0.825365
C	5.318372	0.202083	3.048920
H	4.468578	1.774089	1.864886
C	5.389973	-1.178650	3.268330
H	4.709467	-3.120129	2.621911
H	5.902693	0.881064	3.666699
H	6.025227	-1.573690	4.057786
O	2.773310	-0.124077	-1.265535
C	2.720206	-1.369295	-2.002313
H	3.479753	-2.051662	-1.613359
H	1.736192	-1.798695	-1.815974
C	2.925335	-1.130512	-3.490737
H	2.822411	-2.080420	-4.028873
H	2.176630	-0.432263	-3.880481
H	3.922978	-0.728687	-3.687749

TS8b

SCF energy in Ethanol: -3455.866219 a.u.

Free energy in Ethanol: -3454.681431 a.u.

P	0.127822	0.122648	-0.760788
N	-0.064710	-0.177429	-2.390723
C	-0.902836	-1.302255	-2.812076
H	-1.600904	-0.968330	-3.588858
H	-0.286230	-2.118963	-3.208232
H	-1.498884	-1.679881	-1.979766
C	0.601197	0.521824	-3.487238
H	1.291184	1.271403	-3.105014
H	1.157284	-0.184844	-4.113386
H	-0.146789	1.021347	-4.119380
O	0.657752	1.709719	-0.922074
O	1.521073	-0.627492	-0.204472
C	1.478469	2.305105	0.033567
C	2.785212	1.823028	0.190869
C	1.003926	3.414731	0.756599
C	3.574079	2.295155	1.269334

C	3.335750	0.821411	-0.777516	H	-2.087666	3.171289	3.252614
C	1.854711	3.929684	1.738870	C	-4.036005	6.189357	-0.256728
C	3.096049	3.363356	2.047602	H	-4.490798	6.555704	0.669845
C	2.728538	-0.438078	-0.878141	H	-3.894858	7.044424	-0.926964
C	4.465181	1.116629	-1.580672	H	-4.765096	5.520193	-0.733319
H	1.519634	4.796318	2.304125	C	3.873217	3.917145	3.232334
C	3.311603	-1.495931	-1.601905	C	5.331001	3.447937	3.284157
C	5.045071	0.086555	-2.342083	C	5.397156	1.942107	3.019047
C	4.485756	-1.194755	-2.299498	C	4.905401	1.630728	1.599516
C	2.781163	-2.895521	-1.590478	H	6.419571	1.565023	3.141583
C	2.343699	-3.530492	-2.772142	H	5.923482	3.976813	2.523773
C	2.802522	-3.625310	-0.376710	H	5.768839	3.698819	4.257667
C	1.857956	-4.843957	-2.702501	H	3.367677	3.603519	4.158355
C	2.321045	-4.935226	-0.357368	H	3.820170	5.013671	3.221298
C	1.821958	-5.558884	-1.506320	H	5.678134	1.955434	0.888741
H	1.506481	-5.319537	-3.616810	H	4.813484	0.548018	1.458333
H	2.339941	-5.482467	0.582635	H	4.774313	1.414775	3.755346
C	2.422003	-2.878738	-4.137469	H	4.972980	-1.996211	-2.850399
H	3.325210	-3.200449	-4.674231	C	6.302542	0.306304	-3.171338
H	1.566290	-3.164877	-4.759350	H	7.164596	-0.086642	-2.610241
H	2.458715	-1.790035	-4.079603	H	6.246125	-0.294000	-4.088110
C	1.262102	-6.961042	-1.445976	C	4.975579	2.546134	-1.717446
H	1.870135	-7.608481	-0.803521	C	6.566094	1.777302	-3.510661
H	0.244033	-6.964001	-1.034084	H	5.854027	2.117316	-4.276083
H	1.215005	-7.418258	-2.440062	H	7.569179	1.886809	-3.940319
C	3.390190	-3.034890	0.883599	C	6.407775	2.640797	-2.256344
H	4.387947	-2.618349	0.698010	H	4.304260	3.071730	-2.415136
H	2.766143	-2.229319	1.281027	H	4.887585	3.089268	-0.774427
H	3.476642	-3.793795	1.665088	H	7.118497	2.301607	-1.488639
C	-0.307791	4.083501	0.487496	H	6.650063	3.688953	-2.469976
C	-1.306073	4.137182	1.485367	C	2.932155	-4.228315	4.896034
C	-0.515856	4.756551	-0.740746	C	2.220352	-5.302300	4.357051
C	-2.499369	4.823699	1.223343	C	1.116712	-5.068415	3.539178
C	-1.718481	5.437111	-0.952843	C	0.684043	-3.762225	3.224538
C	-2.730829	5.476403	0.011586	C	1.418314	-2.694139	3.780763
H	-3.264557	4.853081	1.997208	C	2.520943	-2.926223	4.601540
H	-1.863349	5.961728	-1.895592	H	3.790837	-4.403111	5.538860
C	0.543823	4.786283	-1.819857	H	2.521311	-6.323608	4.577512
H	1.522545	5.069805	-1.416278	H	0.565834	-5.913170	3.131079
H	0.661688	3.804078	-2.291011	H	1.129823	-1.673634	3.568806
H	0.278680	5.504702	-2.601952	H	3.063519	-2.079424	5.015160
C	-1.126224	3.502182	2.847832	C	-0.500158	-3.633534	2.361076
H	-0.459064	2.638769	2.815457	H	-0.926009	-4.604532	2.103360
H	-0.698310	4.214731	3.566031	C	-1.162185	-2.567116	1.854896

H	-2.043179	-2.842006	1.276756	C	-3.262136	2.065552	-2.954508
C	-0.891235	-1.089294	1.965657	H	-2.453319	1.633903	-3.553690
H	0.186613	-0.922197	1.855000	H	-4.206045	1.592371	-3.238509
C	-1.309116	-0.490998	3.324330	H	-3.327372	3.135736	-3.186227
H	-0.731125	-0.938134	4.145920				
H	-1.131329	0.589374	3.348476	**IM11a**			
H	-2.362672	-0.659922	3.547820	SCF energy in Ethanol: -2889.879409 a.u.			
Ni	-1.759882	-0.216842	0.428422	Free energy in Ethanol: -2888.938979 a.u.			
B	-3.983669	-0.311290	-0.753037	P	0.249405	0.502026	-1.176121
O	-3.966220	-1.684239	-1.092090	N	-0.077281	1.073277	-2.715276
O	-5.242594	0.248455	-1.035529	C	0.602336	2.265549	-3.217934
C	-5.164080	-1.981289	-1.840207	H	1.099294	2.037975	-4.170738
C	-6.147393	-0.799505	-1.437963	H	-0.108327	3.086861	-3.381130
C	-5.647700	-3.378572	-1.445457	H	1.362576	2.597789	-2.506944
H	-5.821764	-3.454388	-0.369835	C	-0.964911	0.439725	-3.690764
H	-6.575919	-3.638614	-1.968053	H	-1.526754	-0.371194	-3.231043
H	-4.887531	-4.118805	-1.717748	H	-1.667823	1.177693	-4.094449
C	-4.786680	-1.977735	-3.331481	H	-0.377777	0.029774	-4.524437
H	-5.636051	-2.241986	-3.971321	O	0.007374	-1.107513	-1.546090
H	-4.407586	-1.000232	-3.644436	O	-1.033292	0.747548	-0.123253
H	-3.993117	-2.714367	-3.495170	C	-0.246404	-2.025220	-0.529713
C	-7.002668	-0.262406	-2.590924	C	-1.513060	-2.024351	0.067090
H	-7.607932	0.576844	-2.232232	C	0.761328	-2.938912	-0.182001
H	-6.390862	0.097082	-3.421735	C	-1.750324	-2.885485	1.171130
H	-7.685214	-1.032727	-2.969243	C	-2.568622	-1.082922	-0.431565
C	-7.069727	-1.129278	-0.254246	C	0.457341	-3.839234	0.839884
H	-7.821532	-1.878106	-0.527995	C	-0.755549	-3.810206	1.539193
H	-6.509499	-1.491357	0.609152	C	-2.321981	0.300362	-0.404401
H	-7.590749	-0.215017	0.048492	C	-3.822467	-1.542460	-0.906967
C	-3.646581	-0.247613	1.266090	H	1.208715	-4.572721	1.123615
C	-3.927333	1.028039	1.809214	C	-3.333217	1.252564	-0.622106
C	-4.254642	-1.344143	1.915960	C	-4.843391	-0.607936	-1.160661
C	-4.742992	1.201405	2.930658	C	-4.592497	0.755267	-0.969311
H	-3.501975	1.915303	1.345166	C	-3.100224	2.721994	-0.455743
C	-5.074941	-1.189551	3.032699	C	-3.224542	3.606444	-1.547926
H	-4.098781	-2.342774	1.516966	C	-2.797217	3.240870	0.828033
C	-5.316585	0.089030	3.548262	C	-2.992413	4.975195	-1.352296
H	-4.935253	2.199235	3.319709	C	-2.586896	4.613119	0.976520
H	-5.528465	-2.059273	3.503390	C	-2.663658	5.500004	-0.103421
H	-5.954420	0.214655	4.420117	H	-3.077933	5.646608	-2.205111
O	-2.832652	0.483387	-1.139797	H	-2.360926	5.001694	1.967801
C	-2.993949	1.882253	-1.467839	C	-3.632333	3.146801	-2.932390
H	-2.067424	2.380369	-1.178869	H	-4.714410	3.259547	-3.085481
H	-3.813379	2.302808	-0.879402	H	-3.139612	3.749610	-3.703655

H	-3.395367	2.096227	-3.108813	H	-6.654275	-0.298594	-2.283909
C	-2.393399	6.974739	0.084738	C	-4.028292	-3.008634	-1.268719
H	-2.910423	7.367642	0.968154	C	-6.292829	-2.440403	-2.203543
H	-1.322006	7.167335	0.228126	H	-5.860988	-2.419765	-3.214199
H	-2.719485	7.556385	-0.783750	H	-7.336131	-2.760663	-2.311453
C	-2.729019	2.353375	2.050831	C	-5.501631	-3.425978	-1.339121
H	-3.578432	1.662140	2.094805	H	-3.574551	-3.167069	-2.260105
H	-1.816610	1.747553	2.064389	H	-3.473763	-3.665100	-0.595615
H	-2.736018	2.955991	2.964297	H	-5.932110	-3.451819	-0.327380
C	2.095183	-2.941706	-0.860119	H	-5.575771	-4.444005	-1.740373
C	3.248800	-2.534927	-0.150629	Ni	2.252336	1.230041	-0.353938
C	2.208544	-3.351117	-2.205947	C	-0.229606	-0.288126	5.301073
C	4.479720	-2.508047	-0.813856	C	0.595707	0.584540	6.015116
C	3.463591	-3.320781	-2.824086	C	1.494482	1.405496	5.339192
C	4.609634	-2.889372	-2.152324	C	1.591099	1.395231	3.931848
H	5.356205	-2.158478	-0.272923	C	0.762861	0.494997	3.231649
H	3.544028	-3.639565	-3.861774	C	-0.134010	-0.331280	3.908481
C	1.007929	-3.830632	-2.991301	H	-0.930362	-0.933390	5.824855
H	0.427611	-4.573333	-2.431760	H	0.541107	0.623073	7.100305
H	0.328894	-3.003214	-3.228666	H	2.134734	2.080202	5.903474
H	1.320705	-4.288024	-3.935545	H	0.837585	0.420439	2.153511
C	3.194452	-2.130150	1.306871	H	-0.750687	-1.020498	3.338060
H	2.343645	-1.478076	1.525441	C	2.561545	2.294138	3.297770
H	3.102568	-3.002871	1.966463	H	3.338900	2.640068	3.979809
H	4.105094	-1.594716	1.588555	C	2.625788	2.790782	2.036894
C	5.953701	-2.831300	-2.840652	H	3.478794	3.441437	1.841953
H	6.671378	-3.522212	-2.379581	C	1.712446	2.648471	0.891112
H	5.873111	-3.094089	-3.900556	H	0.725992	2.283988	1.196076
H	6.385156	-1.825324	-2.771901	C	1.570811	3.960771	0.109779
C	-0.929823	-4.765922	2.710683	H	2.534325	4.297847	-0.288841
C	-2.371184	-4.859281	3.219692	H	1.185041	4.754937	0.767750
C	-2.958399	-3.452692	3.353132	H	0.864664	3.872746	-0.721563
C	-3.041401	-2.779123	1.976728	C	4.104033	1.519752	-0.345678
H	-3.957731	-3.481709	3.803758	C	5.031193	1.200995	0.664682
H	-2.982248	-5.443477	2.516669	C	4.617922	1.748736	-1.640974
H	-2.395084	-5.391242	4.178210	C	6.394986	1.072148	0.390727
H	-0.283877	-4.428190	3.535146	H	4.680791	1.053770	1.684219
H	-0.555841	-5.758001	2.426248	C	5.984912	1.624393	-1.922674
H	-3.872113	-3.238574	1.424364	H	3.949379	2.027802	-2.455835
H	-3.312076	-1.722725	2.086636	C	6.877003	1.281519	-0.905993
H	-2.325002	-2.858351	4.026832	H	7.086558	0.812974	1.190354
H	-5.402429	1.464699	-1.124370	H	6.350128	1.807602	-2.931419
C	-6.240042	-1.038108	-1.587186	H	7.940341	1.193338	-1.116338
H	-6.896597	-1.015541	-0.703551	**IM11b**			

SCF energy in Ethanol: -2889.862564 a.u.

Free energy in Ethanol: -2888.923867 a.u.

P	-0.433019	-0.198307	-0.873875
N	-0.390536	-0.596268	-2.505370
C	-0.780065	-1.950666	-2.907564
H	-1.512504	-1.903428	-3.722919
H	0.092552	-2.528375	-3.238488
H	-1.241131	-2.481697	-2.068452
C	0.144038	0.217693	-3.595587
H	0.479151	1.182676	-3.220696
H	0.986230	-0.289451	-4.082339
H	-0.639006	0.383099	-4.347918
O	-0.291106	1.454382	-1.090669
O	1.027017	-0.535629	-0.117913
C	0.159541	2.259407	-0.046028
C	1.512429	2.191511	0.312852
C	-0.738066	3.149097	0.567734
C	1.959742	2.899122	1.457599
C	2.457287	1.356602	-0.496253
C	-0.230128	3.920508	1.615986
C	1.075407	3.783372	2.099610
C	2.228252	-0.023267	-0.606084
C	3.587067	1.921819	-1.138094
H	-0.891978	4.639357	2.093596
C	3.174249	-0.901330	-1.165957
C	4.538285	1.066464	-1.722795
C	4.332684	-0.316554	-1.686256
C	2.994437	-2.386303	-1.179729
C	2.953202	-3.102468	-2.396691
C	2.922887	-3.093009	0.045695
C	2.781231	-4.492905	-2.367477
C	2.762907	-4.480639	0.024070
C	2.673107	-5.201561	-1.170851
H	2.738119	-5.034082	-3.311266
H	2.709660	-5.012210	0.971956
C	3.123701	-2.437836	-3.747950
H	4.177103	-2.433419	-4.059573
H	2.567455	-2.979816	-4.520738
H	2.791490	-1.397699	-3.747328
C	2.457770	-6.697314	-1.161862
H	3.032198	-7.180346	-0.363095
H	1.401259	-6.946637	-0.994389
H	2.753733	-7.151448	-2.113485
C	3.051379	-2.390889	1.378186
H	3.862611	-1.654052	1.366554
H	2.130086	-1.861435	1.642632
H	3.253391	-3.109779	2.176137
C	-2.162595	3.306333	0.138327
C	-3.208244	2.960046	1.022621
C	-2.470695	3.864943	-1.122696
C	-4.535016	3.151088	0.618287
C	-3.810168	4.042526	-1.481628
C	-4.860096	3.683475	-0.631868
H	-5.335201	2.878303	1.303732
H	-4.038256	4.480505	-2.451668
C	-1.385713	4.302217	-2.081188
H	-0.630087	4.919851	-1.582221
H	-0.864282	3.439907	-2.511590
H	-1.808822	4.884906	-2.905606
C	-2.937548	2.398685	2.402964
H	-2.201848	1.587963	2.377128
H	-2.545255	3.161506	3.086165
H	-3.857585	2.006389	2.845468
C	-6.299740	3.849951	-1.059719
H	-6.964527	3.964741	-0.196903
H	-6.427919	4.725236	-1.706207
H	-6.648508	2.975587	-1.625698
C	1.475836	4.581002	3.331771
C	2.983212	4.576882	3.604298
C	3.528510	3.154537	3.455969
C	3.362674	2.671556	2.008955
H	4.587502	3.106508	3.736675
H	3.496319	5.238435	2.891642
H	3.182387	4.975444	4.606223
H	0.957177	4.158444	4.205769
H	1.104104	5.609396	3.234454
H	4.104674	3.191199	1.387393
H	3.610688	1.606830	1.933245
H	2.988663	2.484033	4.139431
H	5.096350	-0.969662	-2.102442
C	5.817839	1.596686	-2.354125
H	6.640646	1.472991	-1.632978
H	6.084578	0.975599	-3.218466
C	3.713347	3.430799	-1.309564
C	5.737970	3.072003	-2.761120
H	5.107063	3.178664	-3.654967
H	6.735546	3.438380	-3.032010
C	5.139435	3.899994	-1.620732

H	3.059590	3.721216	-2.147408
H	3.317044	3.962744	-0.442530
H	5.770057	3.797017	-0.725576
H	5.126531	4.966319	-1.877100
C	1.646604	-3.006741	5.075454
C	1.558237	-4.223471	4.395247
C	0.529066	-4.440889	3.481985
C	-0.445752	-3.456811	3.211819
C	-0.348654	-2.244047	3.926081
C	0.684163	-2.022913	4.835578
H	2.444653	-2.832863	5.792253
H	2.287918	-5.007749	4.582080
H	0.465420	-5.394900	2.963254
H	-1.107045	-1.481013	3.798340
H	0.726627	-1.079204	5.373975
C	-1.527954	-3.806369	2.281072
H	-1.579839	-4.878555	2.087671
C	-2.486437	-3.065968	1.668825
H	-3.234022	-3.648681	1.130376
C	-2.733881	-1.608204	1.620381
H	-1.910805	-1.020903	2.046090
C	-4.069162	-1.205426	2.253784
H	-4.012373	-1.297829	3.350094
H	-4.339497	-0.172872	2.015689
H	-4.883308	-1.848828	1.908463
Ni	-2.473370	-1.104168	-0.231238
C	-4.176372	-1.601393	-0.788985
C	-5.138188	-0.594037	-1.010935
C	-4.458633	-2.889576	-1.283849
C	-6.315052	-0.858518	-1.719209
H	-4.972443	0.410460	-0.625448
C	-5.634867	-3.157486	-1.991953
H	-3.752918	-3.702854	-1.119140
C	-6.567340	-2.141156	-2.212279
H	-7.039947	-0.062581	-1.880593
H	-5.824513	-4.160936	-2.368348
H	-7.485600	-2.348649	-2.756606

IM12a

SCF energy in Ethanol: -2889.909515 a.u.

Free energy in Ethanol: -2888.964811 a.u.

P	-0.125703	-0.547938	-0.578503
N	0.324814	-0.819925	-2.165703
C	0.683544	-2.178575	-2.570784
H	-0.033910	-2.567202	-3.303510
H	1.691396	-2.187625	-3.003222
H	0.678381	-2.846968	-1.707894
C	0.206171	0.124203	-3.273996
H	0.087985	1.140753	-2.903999
H	1.107426	0.080517	-3.897345
H	-0.661273	-0.130296	-3.900086
O	-0.979649	0.869934	-0.848933
O	1.209053	0.045210	0.259514
C	-1.086008	1.870347	0.112802
C	0.066931	2.577895	0.484248
C	-2.355489	2.199736	0.625353
C	0.005017	3.484301	1.573263
C	1.349972	2.374990	-0.261740
C	-2.393376	3.185836	1.615110
C	-1.244996	3.790233	2.136571
C	1.942034	1.103946	-0.268926
C	1.985635	3.442103	-0.943627
H	-3.362987	3.474988	2.013808
C	3.239784	0.884595	-0.765307
C	3.274475	3.240899	-1.469185
C	3.883813	1.989848	-1.330259
C	3.942676	-0.432592	-0.677148
C	4.351141	-1.114485	-1.843521
C	4.265228	-0.971975	0.592136
C	5.017229	-2.341761	-1.721176
C	4.940743	-2.190983	0.664628
C	5.314397	-2.902957	-0.480293
H	5.312400	-2.868369	-2.627141
H	5.175576	-2.599920	1.644694
C	4.126718	-0.561761	-3.236047
H	4.960039	0.080560	-3.551554
H	4.057822	-1.373758	-3.968167
H	3.219517	0.042251	-3.302555
C	6.020178	-4.233912	-0.364700
H	6.949642	-4.147142	0.212120
H	5.391267	-4.971100	0.150339
H	6.274575	-4.640086	-1.349113
C	3.924770	-0.241416	1.871506
H	4.229590	0.810793	1.826672
H	2.847850	-0.264180	2.067368
H	4.428661	-0.705435	2.724626
C	-3.633135	1.592877	0.137770
C	-4.458580	0.859327	1.019132

C	-4.068954	1.825787	-1.188168
C	-5.666409	0.331647	0.547285
C	-5.290396	1.292466	-1.610037
C	-6.098345	0.525667	-0.765527
H	-6.287041	-0.246125	1.229876
H	-5.620096	1.484138	-2.629560
C	-3.259632	2.657953	-2.157589
H	-2.905047	3.586920	-1.697093
H	-2.376640	2.111685	-2.507307
H	-3.859731	2.921952	-3.034167
C	-4.101103	0.643598	2.474936
H	-4.447879	1.475474	3.102513
H	-4.577290	-0.265075	2.857980
H	-3.022105	0.561200	2.628478
C	-7.382990	-0.092119	-1.265292
H	-8.109702	-0.220639	-0.455781
H	-7.847350	0.521656	-2.045046
H	-7.197077	-1.084344	-1.697646
C	-1.396560	4.742546	3.313279
C	-0.138674	5.568315	3.602567
C	1.093130	4.660567	3.559360
C	1.280891	4.088053	2.148243
H	1.996720	5.207511	3.854358
H	-0.029348	6.363570	2.851286
H	-0.232934	6.063375	4.576481
H	-1.646014	4.153913	4.209404
H	-2.258790	5.399649	3.140120
H	1.648011	4.893164	1.496980
H	2.071027	3.328724	2.148499
H	0.967318	3.842199	4.282449
H	4.897685	1.858134	-1.701220
C	4.052028	4.360542	-2.146255
H	4.772434	4.774462	-1.423502
H	4.655700	3.944972	-2.962761
C	1.245253	4.745955	-1.218066
C	3.165440	5.498162	-2.663321
H	2.615189	5.166139	-3.555168
H	3.788631	6.345915	-2.972851
C	2.166085	5.916907	-1.581590
H	0.561330	4.563479	-2.062141
H	0.597872	5.017466	-0.381825
H	2.714937	6.251266	-0.688946
H	1.560635	6.767998	-1.916478
Ni	-1.230569	-2.103488	0.484802
C	2.980474	-4.784508	2.826710
C	2.835403	-3.680229	3.670602
C	1.773655	-2.795850	3.492203
C	0.812949	-2.990987	2.479988
C	0.991057	-4.096590	1.625529
C	2.058178	-4.979667	1.798283
H	3.803306	-5.480380	2.967534
H	3.547506	-3.509965	4.474471
H	1.665946	-1.945548	4.161577
H	0.306083	-4.259206	0.800058
H	2.165873	-5.824370	1.122411
C	-0.326731	-2.036284	2.413853
H	-0.095362	-1.072486	2.864048
C	-1.702426	-2.368953	2.422774
H	-2.383210	-1.590941	2.767246
C	-2.266682	-3.433112	1.694267
H	-1.665104	-4.328202	1.537114
C	-3.757802	-3.657443	1.638393
H	-4.307056	-2.712680	1.711089
H	-4.089141	-4.309035	2.460134
H	-4.042816	-4.136501	0.697151
C	-2.212950	-2.716798	-1.061582
C	-2.078011	-4.035807	-1.542320
C	-3.101752	-1.882499	-1.767236
C	-2.772488	-4.493534	-2.667340
H	-1.417141	-4.736942	-1.031189
C	-3.805675	-2.332678	-2.890425
H	-3.253167	-0.856188	-1.444106
C	-3.642759	-3.640849	-3.350201
H	-2.636417	-5.519265	-3.006241
H	-4.481980	-1.653095	-3.406426
H	-4.187659	-3.992584	-4.223281

IM12b

SCF energy in Ethanol: -2889.910700 a.u.

Free energy in Ethanol: -2888.965247 a.u.

P	-0.088097	-0.917870	-0.576866
N	0.457515	-1.588130	-2.009723
C	0.500808	-3.043798	-2.135802
H	-0.215474	-3.389380	-2.890569
H	1.511000	-3.367429	-2.413344
H	0.241438	-3.516225	-1.185739
C	0.730466	-0.874258	-3.254596
H	0.781324	0.198482	-3.080732

H	1.687488	-1.208098	-3.674821	H	-4.602462	2.319668	-3.672197
H	-0.060855	-1.076777	-3.990268	C	-2.024391	2.755169	-3.074114
O	-0.483029	0.589082	-1.185370	H	-1.442439	3.606973	-2.704141
O	1.263399	-0.531821	0.362533	H	-1.324205	1.925442	-3.225672
C	-0.370940	1.761727	-0.440373	H	-2.438191	3.025599	-4.050739
C	0.902965	2.203586	-0.050412	C	-3.758561	1.692827	1.619306
C	-1.529830	2.514063	-0.173568	H	-2.873547	1.092823	1.849192
C	1.014913	3.310286	0.831745	H	-3.630282	2.650883	2.137809
C	2.136756	1.505548	-0.536788	H	-4.627820	1.196614	2.061991
C	-1.366077	3.659501	0.608874	C	-6.877497	1.613331	-2.331896
C	-0.138498	4.043161	1.157034	H	-7.070631	0.542255	-2.479439
C	2.329450	0.157700	-0.202550	H	-7.651755	1.989786	-1.653756
C	3.133197	2.181880	-1.282859	H	-7.006887	2.106240	-3.301400
H	-2.244075	4.267702	0.813919	C	-0.109187	5.234095	2.102906
C	3.558708	-0.497463	-0.398398	C	1.301739	5.756882	2.389897
C	4.363046	1.539397	-1.514791	C	2.236218	4.580721	2.682155
C	4.562809	0.242382	-1.030473	C	2.361055	3.679799	1.445990
C	3.818845	-1.898343	0.059469	H	3.232073	4.931962	2.978242
C	4.139132	-2.912406	-0.870094	H	1.680539	6.313621	1.520809
C	3.805346	-2.205425	1.441732	H	1.276116	6.460935	3.230229
C	4.381199	-4.213390	-0.410043	H	-0.577179	4.936210	3.053718
C	4.062433	-3.515435	1.854548	H	-0.742799	6.034247	1.698731
C	4.338160	-4.541592	0.945071	H	2.985402	4.200045	0.706918
H	4.614606	-4.989484	-1.136924	H	2.908565	2.764719	1.698438
H	4.058231	-3.737661	2.920175	H	1.840761	4.003209	3.530203
C	4.262061	-2.645202	-2.355943	H	5.533706	-0.225927	-1.175546
H	5.272695	-2.306945	-2.620834	C	5.511342	2.233608	-2.233593
H	4.071589	-3.558035	-2.930465	H	6.229390	2.593021	-1.480141
H	3.570311	-1.870929	-2.695097	H	6.059194	1.502042	-2.840744
C	4.574178	-5.957400	1.417681	C	2.845037	3.532513	-1.927240
H	5.147280	-5.978376	2.351624	C	5.069738	3.419969	-3.097515
H	3.625835	-6.476900	1.610585	H	4.565572	3.054601	-4.003371
H	5.121177	-6.543390	0.671585	H	5.948427	3.985412	-3.430676
C	3.562542	-1.143109	2.490605	C	4.106701	4.314189	-2.311792
H	4.162761	-0.245796	2.301331	H	2.260960	3.341732	-2.841587
H	2.513385	-0.830452	2.513271	H	2.193977	4.140593	-1.295771
H	3.820456	-1.518006	3.486107	H	4.608720	4.683340	-1.405445
C	-2.885836	2.209959	-0.731396	H	3.826293	5.197093	-2.899019
C	-3.955028	1.873753	0.130174	H	-2.909423	-5.265121	1.186214
C	-3.127479	2.370165	-2.113928	Ni	-1.536376	-2.111276	0.537580
C	-5.233217	1.694967	-0.409366	C	-0.688618	-2.068690	2.488433
C	-4.423916	2.185600	-2.606893	C	-1.451038	-3.231286	2.221731
C	-5.492068	1.843698	-1.774230	H	-0.907832	-4.163664	2.053086
H	-6.049052	1.426531	0.259234	C	-2.794318	-3.192604	1.800481

H	-3.403575	-2.334477	2.084322
C	-3.571636	-4.443339	1.481467
H	-4.282011	-4.276219	0.667334
H	-4.140768	-4.776792	2.361452
C	-2.649111	-2.465089	-1.011613
C	-3.435578	-1.476809	-1.634021
C	-2.703598	-3.754403	-1.580866
C	-4.228847	-1.757922	-2.753537
H	-3.434535	-0.461554	-1.250421
C	-3.486790	-4.044612	-2.702921
H	-2.126841	-4.566690	-1.139204
C	-4.257213	-3.042771	-3.297164
H	-4.816654	-0.960481	-3.203415
H	-3.497849	-5.055101	-3.108545
H	-4.870496	-3.261801	-4.168396
C	-1.146680	-0.900353	3.288093
C	-0.408277	0.299204	3.269710
C	-2.246552	-0.972646	4.165241
C	-0.756899	1.375729	4.083515
H	0.442133	0.383605	2.600885
C	-2.598728	0.107014	4.974589
H	-2.809274	-1.897537	4.240297
C	-1.857182	1.289751	4.939621
H	-0.165808	2.287169	4.044865
H	-3.448076	0.015910	5.647402
H	-2.128072	2.128120	5.575931
H	0.390369	-2.207712	2.496261

TS9a

SCF energy in Ethanol: -2889.875475 a.u.

Free energy in Ethanol: -2888.931704 a.u.

P	0.273989	0.419312	-0.687693
N	-0.093225	0.804588	-2.282077
C	-0.098252	2.213217	-2.667185
H	0.520962	2.364472	-3.560353
H	-1.119164	2.561883	-2.872453
H	0.315870	2.823992	-1.862587
C	-0.554339	-0.102488	-3.328136
H	-0.558860	-1.128953	-2.966941
H	-1.566399	0.159824	-3.663013
H	0.119274	-0.036541	-4.194409
O	0.537854	-1.219822	-0.970518
O	-1.166087	0.335901	0.197066
C	0.321569	-2.175013	0.012053
C	-0.995035	-2.447520	0.414361
C	1.418408	-2.893139	0.525168
C	-1.220757	-3.327023	1.504956
C	-2.151936	-1.792976	-0.277797
C	1.140538	-3.846211	1.508312
C	-0.137515	-4.044662	2.039343
C	-2.252096	-0.392204	-0.262773
C	-3.168056	-2.554342	-0.906232
H	1.965438	-4.438129	1.898287
C	-3.423575	0.277928	-0.666382
C	-4.338391	-1.904427	-1.336428
C	-4.457147	-0.521734	-1.164469
C	-3.601665	1.759618	-0.556579
C	-3.882352	2.539304	-1.701391
C	-3.554631	2.388188	0.713469
C	-4.052124	3.923961	-1.564600
C	-3.741124	3.769252	0.800406
C	-3.977710	4.561736	-0.327472
H	-4.252107	4.515840	-2.456278
H	-3.695165	4.239141	1.780538
C	-4.038816	1.946293	-3.087373
H	-5.085770	1.686723	-3.295546
H	-3.732599	2.667533	-3.853038
H	-3.454894	1.033617	-3.220039
C	-4.149146	6.057786	-0.200046
H	-4.940249	6.311995	0.516399
H	-3.228016	6.535030	0.158774
H	-4.407968	6.514984	-1.160710
C	-3.339527	1.603335	1.987820
H	-3.939279	0.686094	2.002643
H	-2.290270	1.312958	2.101577
H	-3.615182	2.205410	2.858934
C	2.829880	-2.699621	0.067031
C	3.812713	-2.259290	0.983965
C	3.212668	-3.034580	-1.251572
C	5.140663	-2.135058	0.558454
C	4.552791	-2.899847	-1.630666
C	5.533992	-2.444326	-0.746407
H	5.888551	-1.791679	1.271424
H	4.837819	-3.170983	-2.645642
C	2.216193	-3.565949	-2.256673
H	1.588474	-4.353132	-1.824118
H	1.545827	-2.772601	-2.604188
H	2.730159	-3.981792	-3.129162

C	3.479734	-1.929452	2.424623	H	-0.216070	6.008406	1.574006
H	3.381420	-2.833152	3.038922	C	1.642996	1.768707	2.452821
H	4.273880	-1.322936	2.872575	H	1.424757	0.932781	3.116130
H	2.535916	-1.382612	2.510465	C	2.960759	1.747185	1.945480
C	6.968475	-2.272131	-1.190021	H	3.545586	0.864052	2.203362
H	7.668650	-2.467339	-0.370219	C	3.562765	2.611987	0.939674
H	7.216514	-2.947805	-2.015705	H	3.182364	3.632246	0.919046
H	7.156484	-1.247701	-1.539138	C	5.087733	2.580669	0.905044
C	-0.293391	-5.010289	3.205146	H	5.460114	1.553618	0.833458
C	-1.750866	-5.350806	3.532328	H	5.477729	3.018146	1.834055
C	-2.591342	-4.071899	3.525120	H	5.484294	3.146669	0.057719
C	-2.610100	-3.460063	2.118244	C	3.194832	2.133619	-0.925504
H	-3.619584	-4.273751	3.848790	C	3.037881	3.296365	-1.706453
H	-2.150660	-6.050992	2.784815	C	3.919426	1.063738	-1.494798
H	-1.807027	-5.858023	4.503010	C	3.535766	3.373331	-3.008022
H	0.173038	-4.561907	4.095685	H	2.523002	4.160602	-1.288413
H	0.279305	-5.924023	2.998478	C	4.394416	1.128762	-2.805770
H	-3.250405	-4.086261	1.482126	H	4.106209	0.164486	-0.912531
H	-3.090223	-2.475348	2.138484	C	4.208269	2.284397	-3.570054
H	-2.168276	-3.353277	4.241416	H	3.399765	4.286287	-3.584156
H	-5.386221	-0.038039	-1.457209	H	4.919517	0.274140	-3.226724
C	-5.509454	-2.667502	-1.939217	H	4.596609	2.342504	-4.583635
H	-6.273836	-2.811272	-1.159613				
H	-5.987013	-2.054294	-2.713793	**TS9b**			
C	-2.955242	-4.029245	-1.226399	SCF energy in Ethanol: -2889.875839 a.u.			
C	-5.122701	-4.037745	-2.506397	Free energy in Ethanol: -2888.931648 a.u.			
H	-4.561305	-3.908449	-3.442662	P	0.062683	0.913274	-0.596174
H	-6.026488	-4.607327	-2.755095	N	-0.454242	1.636698	-2.022218
C	-4.254274	-4.796869	-1.499354	C	-0.459545	3.094332	-2.107205
H	-2.324380	-4.081351	-2.128131	H	0.158648	3.431963	-2.949141
H	-2.375464	-4.524637	-0.445036	H	-1.482078	3.473062	-2.236651
H	-4.814785	-4.928785	-0.562197	H	-0.050036	3.527578	-1.191836
H	-4.015670	-5.801900	-1.868367	C	-0.952622	0.970035	-3.220527
Ni	1.834698	1.419132	0.370858	H	-0.955961	-0.109394	-3.084364
C	-0.948465	5.093844	3.384504	H	-1.972429	1.300649	-3.456782
C	-0.893099	3.956685	4.194093	H	-0.308437	1.214036	-4.077609
C	-0.059907	2.893356	3.854078	O	0.308282	-0.615933	-1.258966
C	0.750677	2.925234	2.700430	O	-1.293661	0.595304	0.372430
C	0.658232	4.071521	1.883661	C	0.193363	-1.776567	-0.505962
C	-0.172074	5.138590	2.225018	C	-1.071273	-2.158664	-0.030943
H	-1.590404	5.929473	3.650376	C	1.332411	-2.579280	-0.307021
H	-1.494760	3.899747	5.098007	C	-1.174473	-3.251136	0.868493
H	-0.016486	2.019768	4.500613	C	-2.299547	-1.410746	-0.453354
H	1.216896	4.123253	0.955940	C	1.167958	-3.713878	0.491433

C	-0.037100	-4.035400	1.123380	H	6.833307	-0.899018	-2.963844
C	-2.410214	-0.049279	-0.133720	H	7.375375	-2.357734	-2.132918
C	-3.364897	-2.051444	-1.132734	H	6.636126	-2.473713	-3.739964
H	2.027566	-4.362479	0.643583	C	-0.059882	-5.216891	2.081237
C	-3.618242	0.659671	-0.280294	C	-1.472372	-5.670646	2.462065
C	-4.575146	-1.357374	-1.310593	C	-2.327185	-4.449173	2.808384
C	-4.687571	-0.043629	-0.843667	C	-2.491689	-3.548814	1.576506
C	-3.790480	2.081627	0.155011	H	-3.316174	-4.749730	3.175020
C	-4.148999	3.082806	-0.776019	H	-1.933892	-6.209786	1.622316
C	-3.657206	2.428243	1.522483	H	-1.426101	-6.373395	3.302715
C	-4.309520	4.404100	-0.337826	H	0.479965	-4.934038	2.997981
C	-3.836936	3.757327	1.913659	H	0.509022	-6.048920	1.646101
C	-4.148852	4.767851	0.998704	H	-3.192087	-4.039068	0.886634
H	-4.573716	5.167422	-1.067862	H	-2.972162	-2.604864	1.857805
H	-3.740374	4.008128	2.968616	H	-1.845559	-3.888318	3.622401
C	-4.401339	2.790348	-2.241112	H	-5.642127	0.467444	-0.947100
H	-5.459603	2.561556	-2.426483	C	-5.791155	-2.009758	-1.952904
H	-4.152236	3.660724	-2.858045	H	-6.480583	-2.328474	-1.155590
H	-3.825437	1.935387	-2.599921	H	-6.340791	-1.262932	-2.539634
C	-4.299066	6.203373	1.446372	C	-3.172819	-3.422578	-1.770079
H	-4.818463	6.271100	2.409223	C	-5.450809	-3.225029	-2.822449
H	-3.320674	6.685814	1.574464	H	-4.981695	-2.893564	-3.759777
H	-4.861783	6.794609	0.716228	H	-6.370555	-3.754684	-3.099123
C	-3.360160	1.393061	2.583608	C	-4.486298	-4.151744	-2.077133
H	-3.956531	0.485010	2.441004	H	-2.628904	-3.270598	-2.715964
H	-2.306608	1.095616	2.563085	H	-2.518210	-4.052022	-1.163859
H	-3.578918	1.789176	3.580451	H	-4.954797	-4.488155	-1.140595
C	2.663689	-2.330313	-0.946216	H	-4.276327	-5.052868	-2.666265
C	3.803702	-2.090047	-0.145731	H	4.174076	4.674320	0.969893
C	2.811696	-2.457093	-2.346059	Ni	1.515369	1.985998	0.536828
C	5.057763	-1.977985	-0.758184	C	1.252915	2.174923	2.599331
C	4.084762	-2.336840	-2.913705	C	2.201596	3.062292	2.044621
C	5.223432	-2.097407	-2.140440	H	1.918409	4.113973	1.959283
H	5.929292	-1.792624	-0.132459	C	3.396831	2.667052	1.303202
H	4.188762	-2.447761	-3.991555	H	3.765039	1.665501	1.532781
C	1.632774	-2.751148	-3.246067	C	4.534255	3.680518	1.253755
H	1.033310	-3.586789	-2.867154	H	5.311143	3.383384	0.543884
H	0.967346	-1.884008	-3.320803	H	4.983679	3.760275	2.253459
H	1.969774	-3.005856	-4.255929	C	3.051058	2.516075	-0.640955
C	3.712369	-1.946817	1.358123	C	3.824447	1.552818	-1.316892
H	2.848121	-1.351412	1.664946	C	2.852871	3.758155	-1.278920
H	3.617818	-2.917916	1.859610	C	4.329019	1.801178	-2.594290
H	4.613419	-1.467002	1.753495	H	4.018957	0.590886	-0.852044
C	6.586878	-1.953337	-2.777455	C	3.348750	4.005855	-2.560356

H	2.306383	4.547272	-0.763715
C	4.089443	3.025513	-3.225846
H	4.902004	1.028269	-3.100839
H	3.169284	4.969133	-3.033615
H	4.487345	3.218592	-4.218902
C	1.572544	0.903592	3.307419
C	0.631064	-0.141024	3.375555
C	2.780089	0.741054	4.012614
C	0.885824	-1.294308	4.115790
H	-0.298946	-0.047297	2.823189
C	3.038808	-0.416799	4.747252
H	3.506529	1.548838	4.009879
C	2.092377	-1.441672	4.805625
H	0.139708	-2.084533	4.148095
H	3.977337	-0.510148	5.288670
H	2.289612	-2.340061	5.384698
H	0.313245	2.630657	2.910298

IM13a

SCF energy in Ethanol: -2889.920037 a.u.

Free energy in Ethanol: -2888.973966 a.u.

P	0.316334	0.070916	-0.632439
N	0.329531	0.667809	-2.205316
C	1.318999	1.680131	-2.562217
H	1.826592	1.397549	-3.493887
H	0.849918	2.664916	-2.697486
H	2.074132	1.762494	-1.776182
C	-0.640591	0.381369	-3.256738
H	-1.398946	-0.311585	-2.896554
H	-1.130619	1.301232	-3.598531
H	-0.132182	-0.073126	-4.119928
O	-0.510503	-1.354235	-1.017079
O	-0.901088	0.843886	0.257245
C	-1.175516	-2.049648	-0.018527
C	-2.379336	-1.527096	0.475255
C	-0.653409	-3.275209	0.432762
C	-3.000592	-2.150038	1.587922
C	-2.969575	-0.300946	-0.150462
C	-1.359010	-3.923533	1.449014
C	-2.488699	-3.370450	2.061689
C	-2.222694	0.889908	-0.153625
C	-4.267991	-0.307164	-0.717257
H	-0.992554	-4.886292	1.798897
C	-2.792383	2.126382	-0.517927
C	-4.848873	0.913183	-1.105891
C	-4.119714	2.097103	-0.956937
C	-2.053403	3.424537	-0.428365
C	-1.856313	4.224824	-1.575752
C	-1.593544	3.893782	0.828275
C	-1.161245	5.436812	-1.457265
C	-0.920207	5.114215	0.898328
C	-0.677306	5.897555	-0.234760
H	-0.999882	6.035546	-2.352344
H	-0.565454	5.458703	1.867188
C	-2.388487	3.855187	-2.945835
H	-3.359118	4.333165	-3.137554
H	-1.706359	4.198837	-3.731675
H	-2.537502	2.780576	-3.062685
C	0.081090	7.199425	-0.124055
H	-0.423648	7.902672	0.550774
H	1.087775	7.033431	0.279164
H	0.184230	7.687975	-1.098580
C	-1.833135	3.122918	2.106908
H	-2.855628	2.731876	2.158173
H	-1.152567	2.268621	2.185471
H	-1.671594	3.766211	2.977700
C	0.590224	-3.888529	-0.128990
C	1.727867	-4.057273	0.693891
C	0.619971	-4.357127	-1.461471
C	2.871252	-4.666329	0.163398
C	1.784325	-4.962095	-1.948143
C	2.925375	-5.120705	-1.157202
H	3.743624	-4.789468	0.802972
H	1.793617	-5.329554	-2.972885
C	-0.585086	-4.243232	-2.367654
H	-1.496783	-4.594946	-1.871563
H	-0.760296	-3.202781	-2.662926
H	-0.443272	-4.835162	-3.277564
C	1.747203	-3.597536	2.137096
H	1.173396	-4.267236	2.789263
H	2.773403	-3.572934	2.518192
H	1.317006	-2.596724	2.247882
C	4.184367	-5.742378	-1.715994
H	4.718546	-6.321788	-0.954745
H	3.963434	-6.409134	-2.556448
H	4.877380	-4.972891	-2.082320
C	-3.093750	-4.101767	3.251090
C	-4.460644	-3.558049	3.679683

C	-4.420324	-2.028172	3.705226
C	-4.175410	-1.482119	2.292505
H	-5.357208	-1.615581	4.098859
H	-5.235320	-3.888093	2.972620
H	-4.733306	-3.965110	4.660807
H	-2.399033	-4.021156	4.101104
H	-3.160150	-5.173724	3.022706
H	-5.096802	-1.616552	1.709584
H	-4.006228	-0.400042	2.327690
H	-3.618633	-1.695951	4.380021
H	-4.595335	3.039283	-1.219981
C	-6.271957	0.995163	-1.640034
H	-6.935578	1.320502	-0.823600
H	-6.332975	1.781111	-2.403356
C	-4.981017	-1.619492	-1.022019
C	-6.796030	-0.332662	-2.198027
H	-6.312587	-0.548867	-3.161469
H	-7.872625	-0.256532	-2.393702
C	-6.494295	-1.469194	-1.217467
H	-4.548018	-2.020073	-1.952561
H	-4.766977	-2.373403	-0.261901
H	-6.975776	-1.254335	-0.252188
H	-6.914115	-2.417048	-1.576110
Ni	2.145896	-0.076579	0.438694
C	2.958922	5.199695	2.127945
C	2.270685	4.537292	3.147509
C	2.139830	3.150097	3.119148
C	2.695370	2.377966	2.079769
C	3.363570	3.067253	1.048018
C	3.496243	4.455472	1.075382
H	3.072597	6.280414	2.152363
H	1.841268	5.101392	3.972103
H	1.611763	2.644189	3.924284
H	3.765581	2.514373	0.205220
H	4.019945	4.958261	0.265787
C	2.572632	0.902621	2.155622
H	1.849965	0.580836	2.906501
C	3.550801	-0.066290	1.822523
H	3.457748	-1.015965	2.355381
C	4.905146	0.151337	1.154907
H	5.225896	1.189063	1.312859
C	5.986249	-0.766466	1.758592
H	5.713582	-1.822004	1.636449
H	6.102824	-0.567397	2.830356
H	6.955728	-0.612921	1.270711
C	4.778504	-0.066037	-0.354626
C	5.516489	0.695665	-1.270833
C	3.884524	-1.032994	-0.862275
C	5.385703	0.491507	-2.646609
H	6.201572	1.455883	-0.900708
C	3.757210	-1.242643	-2.242504
H	3.364735	-1.714839	-0.178432
C	4.505202	-0.477536	-3.137441
H	5.973760	1.090757	-3.337508
H	3.072626	-2.005721	-2.601615
H	4.407061	-0.634452	-4.208401

IM13b

SCF energy in Ethanol: -2889.916948 a.u.

Free energy in Ethanol: -2888.972593 a.u.

P	0.178934	0.693146	-0.777455
N	-0.161382	1.493149	-2.219945
C	0.442424	2.799638	-2.460596
H	1.025813	2.788490	-3.391663
H	-0.326335	3.581731	-2.534480
H	1.116912	3.058956	-1.638082
C	-1.003055	1.015404	-3.311338
H	-1.507461	0.092027	-3.032278
H	-1.757713	1.768268	-3.571837
H	-0.392964	0.823427	-4.206951
O	-0.145242	-0.853087	-1.389255
O	-1.150107	0.828234	0.272782
C	-0.449454	-1.892977	-0.525076
C	-1.709557	-1.909712	0.091600
C	0.485878	-2.926931	-0.338130
C	-1.980630	-2.883773	1.086902
C	-2.734537	-0.882891	-0.283086
C	0.138114	-3.932845	0.565933
C	-1.045191	-3.908515	1.311775
C	-2.438011	0.476097	-0.087473
C	-3.998467	-1.245061	-0.811178
H	0.833800	-4.755503	0.715471
C	-3.419128	1.480062	-0.202800
C	-4.986481	-0.254609	-0.959465
C	-4.690672	1.067876	-0.611785
C	-3.145702	2.917161	0.115572
C	-3.279184	3.915863	-0.873872
C	-2.798307	3.295946	1.436277

C	-3.010604	5.251487	-0.543352	H	-0.556789	-4.795068	3.199916
C	-2.550560	4.640592	1.721033	H	-0.966216	-5.959515	1.956360
C	-2.634950	5.636910	0.742627	H	-4.113752	-3.148072	1.358782
H	-3.104782	6.010024	-1.318759	H	-3.454498	-1.743590	2.160822
H	-2.291501	4.918725	2.741217	H	-2.471865	-3.134403	3.932829
C	-3.733818	3.616138	-2.287385	H	-5.476044	1.816631	-0.688160
H	-4.822714	3.723272	-2.386522	C	-6.391559	-0.584856	-1.443070
H	-3.280341	4.317077	-2.997008	H	-7.058318	-0.650794	-0.569064
H	-3.486560	2.599680	-2.598692	H	-6.775838	0.246035	-2.048101
C	-2.324850	7.078539	1.073235	C	-4.249464	-2.655100	-1.332841
H	-2.772934	7.376491	2.028442	C	-6.477683	-1.899556	-2.225819
H	-1.242702	7.243980	1.161043	H	-6.025577	-1.771754	-3.219717
H	-2.698573	7.756672	0.298875	H	-7.528382	-2.169506	-2.387895
C	-2.719473	2.286776	2.559510	C	-5.735009	-3.007368	-1.473990
H	-3.572839	1.599479	2.545410	H	-3.778435	-2.726061	-2.326244
H	-1.812223	1.678256	2.483331	H	-3.736284	-3.400495	-0.722177
H	-2.706284	2.791257	3.530957	H	-6.184799	-3.136634	-0.478642
C	1.785911	-2.999299	-1.076120	H	-5.836340	-3.968176	-1.993429
C	3.010084	-2.920928	-0.372320	H	5.383550	3.998726	1.527341
C	1.797843	-3.218970	-2.471893	Ni	1.927487	1.378293	0.198081
C	4.211919	-3.039321	-1.080130	C	1.991711	1.887942	2.151685
C	3.024288	-3.335674	-3.136174	C	3.042180	2.495189	1.439161
C	4.244623	-3.241339	-2.462457	H	2.869783	3.522815	1.106258
H	5.149948	-2.970601	-0.531905	C	4.474613	2.032292	1.199694
H	3.023011	-3.515172	-4.209901	H	4.606803	1.025404	1.612589
C	0.516630	-3.357751	-3.263153	C	5.528533	2.954849	1.829116
H	-0.175596	-4.062939	-2.789163	H	6.545017	2.656142	1.545195
H	-0.005890	-2.397849	-3.342506	H	5.454745	2.923442	2.921762
H	0.724026	-3.715473	-4.276807	C	4.545468	1.909414	-0.324610
C	3.063334	-2.715384	1.127011	C	3.934506	0.786200	-0.927063
H	2.341789	-1.968529	1.470575	C	5.050438	2.915627	-1.159739
H	2.841431	-3.640841	1.673091	C	3.845689	0.675855	-2.323499
H	4.062218	-2.390949	1.436151	H	3.641891	-0.067316	-0.313041
C	5.558317	-3.331875	-3.204044	C	4.958524	2.804238	-2.549433
H	5.977400	-2.333934	-3.391244	H	5.524662	3.791773	-0.727555
H	6.305925	-3.892187	-2.631061	C	4.349928	1.690745	-3.136611
H	5.437515	-3.823879	-4.175045	H	3.396831	-0.212998	-2.757310
C	-1.253487	-4.983348	2.368743	H	5.367917	3.592033	-3.177355
C	-2.680442	-5.033795	2.924630	H	4.284684	1.610091	-4.218469
C	-3.165701	-3.613902	3.227103	C	2.063395	0.728680	3.080454
C	-3.245729	-2.794866	1.932514	C	0.930268	-0.089461	3.262774
H	-4.149317	-3.627666	3.712030	C	3.202389	0.447819	3.857187
H	-3.354350	-5.497090	2.189639	C	0.942802	-1.149538	4.166238
H	-2.709985	-5.663288	3.822223	H	0.042070	0.106170	2.668715

C	3.217595	-0.619451	4.757804
H	4.071234	1.094129	3.785121
C	2.090315	-1.426382	4.915990
H	0.054117	-1.765522	4.281333
H	4.110876	-0.809554	5.348133
H	2.101153	-2.253633	5.620858
H	1.101826	2.504021	2.287133

IM11

SCF energy in Ethanol: -3455.893614 a.u.

Free energy in Ethanol: -3454.708223 a.u.

P	-0.211263	0.377209	-0.364760
N	0.060032	1.155776	-1.808270
C	1.201476	2.067708	-1.935858
H	1.821752	1.781005	-2.790159
H	0.855346	3.099659	-2.067053
H	1.831485	2.021689	-1.047357
C	-0.739765	1.039338	-3.027102
H	-1.628903	0.437120	-2.855114
H	-1.048208	2.034030	-3.370257
H	-0.140369	0.572620	-3.820177
O	-1.095504	-0.902277	-1.004519
O	-1.411530	1.171734	0.514866
C	-2.166894	-1.546207	-0.393087
C	-3.300437	-0.807099	-0.013990
C	-2.134376	-2.951938	-0.268957
C	-4.287884	-1.420766	0.800047
C	-3.499915	0.602365	-0.483861
C	-3.188129	-3.538548	0.437951
C	-4.216596	-2.803310	1.035696
C	-2.585843	1.588352	-0.100326
C	-4.614462	0.968877	-1.280623
H	-3.197341	-4.621282	0.534464
C	-2.830072	2.961242	-0.280531
C	-4.860019	2.334188	-1.516067
C	-3.996978	3.294029	-0.973893
C	-1.932928	4.020980	0.278064
C	-1.249788	4.920408	-0.567425
C	-1.814250	4.162470	1.682971
C	-0.415605	5.894366	-0.000723
C	-0.977907	5.153201	2.202942
C	-0.253340	6.022395	1.378264
H	0.117780	6.573628	-0.663065
H	-0.901922	5.260243	3.283598
C	-1.410462	4.907661	-2.073081
H	-2.228427	5.569352	-2.389024
H	-0.500917	5.267990	-2.564976
H	-1.640991	3.912728	-2.459004
C	0.672345	7.061496	1.967176
H	0.237656	7.526288	2.859543
H	1.629814	6.616867	2.269754
H	0.894298	7.854645	1.245898
C	-2.620226	3.306543	2.636155
H	-3.689497	3.341666	2.395393
H	-2.320233	2.254069	2.601107
H	-2.495776	3.654897	3.666163
C	-1.130630	-3.843601	-0.934739
C	-0.346660	-4.744787	-0.178842
C	-1.066799	-3.890157	-2.348451
C	0.506983	-5.633907	-0.842496
C	-0.203357	-4.799663	-2.966337
C	0.602754	-5.675468	-2.234768
H	1.112321	-6.316314	-0.248403
H	-0.167734	-4.829301	-4.053633
C	-1.934777	-3.011784	-3.221950
H	-2.978228	-3.009858	-2.886714
H	-1.588361	-1.972837	-3.212916
H	-1.913920	-3.361311	-4.258928
C	-0.400545	-4.799879	1.333023
H	-0.537390	-3.813800	1.782205
H	-1.225226	-5.433274	1.686209
H	0.524683	-5.225328	1.734568
C	1.557279	-6.621760	-2.924903
H	2.555803	-6.175176	-3.022707
H	1.673930	-7.555287	-2.363438
H	1.213487	-6.872856	-3.934092
C	-5.220620	-3.533455	1.914424
C	-6.478186	-2.713830	2.221636
C	-6.081393	-1.287291	2.609618
C	-5.399380	-0.586288	1.427436
H	-6.957054	-0.705774	2.921842
H	-7.130185	-2.681000	1.337028
H	-7.052666	-3.196808	3.020953
H	-4.729287	-3.795070	2.864310
H	-5.486740	-4.489498	1.445242
H	-6.167877	-0.352229	0.677987
H	-4.993796	0.381889	1.742409
H	-5.399016	-1.320308	3.470881

H	-4.228258	4.347018	-1.118202
C	-6.072994	2.809389	-2.303548
H	-6.846136	3.138211	-1.591904
H	-5.804990	3.700521	-2.884751
C	-5.465096	-0.091293	-1.970247
C	-6.670626	1.734275	-3.217299
H	-6.010909	1.569482	-4.080870
H	-7.633629	2.076391	-3.614823
C	-6.829695	0.421985	-2.445223
H	-4.899756	-0.446547	-2.846384
H	-5.589565	-0.971514	-1.336157
H	-7.488301	0.586761	-1.579939
H	-7.311295	-0.342285	-3.066972
Ni	1.654528	0.416461	0.955269
C	0.509950	-2.843926	5.094525
C	-0.572553	-2.491904	4.283748
C	-0.508169	-1.352488	3.486315
C	0.637118	-0.528833	3.477010
C	1.711075	-0.890149	4.312996
C	1.647395	-2.034714	5.107167
H	0.462086	-3.732244	5.718329
H	-1.470932	-3.103344	4.276295
H	-1.358434	-1.080511	2.865226
H	2.587497	-0.256654	4.375894
H	2.488136	-2.286863	5.747969
C	0.584003	0.701608	2.652893
H	-0.432350	1.034823	2.482501
C	1.548959	1.747830	2.555743
H	1.158521	2.731425	2.292280
C	2.918227	1.569368	2.459721
H	3.402771	0.654131	2.783853
C	3.832553	2.732172	2.206247
H	4.622372	2.428538	1.519068
H	3.290333	3.596400	1.806283
B	4.597238	0.102818	-0.618024
O	3.151268	-0.372527	-0.126173
O	5.151044	-1.138913	-1.139467
C	3.035455	-1.802690	-0.425049
C	4.536807	-2.254606	-0.526649
C	2.303494	-1.965917	-1.763563
H	2.867187	-1.493535	-2.571271
H	2.146966	-3.021258	-2.006571
H	1.317141	-1.499940	-1.718363
C	2.271769	-2.515269	0.690776
H	2.314812	-3.599439	0.540161
H	2.688788	-2.289033	1.675043
H	1.212617	-2.238909	0.687198
C	5.173626	-2.536510	0.851991
H	6.255286	-2.640645	0.714216
H	5.002288	-1.707777	1.541541
H	4.797530	-3.465564	1.297369
C	4.761980	-3.478100	-1.426186
H	4.207291	-4.354062	-1.067488
H	4.468320	-3.272470	-2.458197
H	5.828267	-3.729518	-1.426962
C	4.543219	1.218745	-1.807884
C	4.555131	0.835250	-3.162073
C	4.521475	2.602546	-1.555306
C	4.509794	1.767748	-4.202304
H	4.626129	-0.223365	-3.397348
C	4.474980	3.550194	-2.582951
H	4.547177	2.952284	-0.526659
C	4.461415	3.134943	-3.916182
H	4.523601	1.429970	-5.237122
H	4.460637	4.612266	-2.343914
H	4.430609	3.866140	-4.721171
O	5.268332	0.587437	0.592607
H	4.308564	3.038231	3.150008
C	6.667775	0.775390	0.497594
H	7.124748	-0.055041	-0.058519
H	6.899804	1.697917	-0.062105
C	7.280334	0.856116	1.892969
H	8.365228	1.007898	1.830769
H	6.854557	1.688370	2.465991
H	7.093764	-0.068810	2.450767

IM12

SCF energy in Ethanol: -3455.899472 a.u.

Free energy in Ethanol: -3454.715924 a.u.

P	-0.305997	0.247472	-0.574088
N	-0.108571	0.936850	-2.076079
C	1.028185	1.829347	-2.325578
H	1.542917	1.524579	-3.242971
H	0.689175	2.866331	-2.431507
H	1.752617	1.783701	-1.513346
C	-1.044596	0.847577	-3.198065
H	-1.914210	0.250117	-2.934046
H	-1.378175	1.849101	-3.495090

H	-0.542224	0.383708	-4.057451	C	-2.638741	-3.180142	-2.984443
O	-1.346766	-0.965097	-1.062394	H	-3.607276	-3.113194	-2.476190
O	-1.303794	1.186604	0.393148	H	-2.266120	-2.157048	-3.107250
C	-2.328447	-1.530981	-0.251461	H	-2.808782	-3.594447	-3.983149
C	-3.349430	-0.715190	0.259898	C	-0.343963	-4.664160	1.346537
C	-2.326310	-2.925611	-0.053047	H	-0.348190	-3.630523	1.699056
C	-4.221103	-1.238951	1.249057	H	-1.110634	-5.202619	1.919351
C	-3.547746	0.680321	-0.250945	H	0.623760	-5.101645	1.610592
C	-3.274521	-3.424875	0.844522	C	0.736665	-6.912996	-3.024104
C	-4.167103	-2.610283	1.549120	H	1.686260	-6.500677	-3.391324
C	-2.539345	1.633240	-0.065979	H	0.980056	-7.779391	-2.399656
C	-4.752344	1.068670	-0.890610	H	0.179755	-7.269333	-3.897599
H	-3.306542	-4.499248	1.008099	C	-5.048057	-3.244839	2.614504
C	-2.745405	3.006651	-0.284401	C	-6.210562	-2.352989	3.061959
C	-4.966031	2.431445	-1.167353	C	-5.705043	-0.928339	3.302091
C	-3.986516	3.367226	-0.816447	C	-5.185054	-0.321195	1.992409
C	-1.739149	4.051356	0.083428	H	-6.500033	-0.291338	3.707859
C	-1.158806	4.883873	-0.898067	H	-6.990542	-2.335581	2.287372
C	-1.420573	4.259754	1.447570	H	-6.671825	-2.767107	3.966383
C	-0.233446	5.860683	-0.507849	H	-4.423216	-3.477819	3.490322
C	-0.503371	5.256974	1.790561	H	-5.420088	-4.211177	2.250130
C	0.116818	6.060313	0.827482	H	-6.049404	-0.084736	1.356663
H	0.220060	6.485763	-1.274743	H	-4.694463	0.639125	2.188174
H	-0.276311	5.418463	2.842670	H	-4.901376	-0.947941	4.051890
C	-1.524864	4.793654	-2.364817	H	-4.187741	4.423031	-0.983309
H	-2.367249	5.456361	-2.605406	C	-6.260631	2.934207	-1.790570
H	-0.684697	5.104100	-2.994804	H	-6.897164	3.345585	-0.991944
H	-1.822609	3.784904	-2.658363	H	-6.041225	3.775577	-2.459590
C	1.138665	7.100875	1.222537	C	-5.750307	0.025144	-1.379717
H	0.899499	7.550054	2.192883	C	-7.045386	1.849019	-2.535021
H	2.141192	6.660310	1.308240	H	-6.537815	1.601364	-3.478007
H	1.200037	7.905073	0.481772	H	-8.040813	2.224838	-2.800299
C	-2.080446	3.460007	2.550021	C	-7.145795	0.590610	-1.669489
H	-3.168206	3.419427	2.421678	H	-5.347491	-0.405039	-2.310451
H	-1.718326	2.426104	2.574322	H	-5.818406	-0.813854	-0.684155
H	-1.871815	3.906849	3.527039	H	-7.651639	0.838162	-0.724780
C	-1.472127	-3.891020	-0.817050	H	-7.755436	-0.176359	-2.162174
C	-0.581862	-4.756581	-0.143926	Ni	1.522320	-0.160449	0.497344
C	-1.658111	-4.035556	-2.213008	C	2.271905	-3.336028	4.321196
C	0.111201	-5.728972	-0.874031	C	0.913283	-3.004733	4.374794
C	-0.941711	-5.020027	-2.900032	C	0.439747	-1.888854	3.691918
C	-0.047643	-5.877076	-2.252775	C	1.312557	-1.050691	2.965366
H	0.799918	-6.385005	-0.344884	C	2.682451	-1.395425	2.922329
H	-1.098579	-5.127766	-3.971724	C	3.145582	-2.535144	3.586471

H	2.642763	-4.208876	4.852093
H	0.224119	-3.620683	4.947020
H	-0.618425	-1.639975	3.730776
H	3.394408	-0.787825	2.366846
H	4.202115	-2.784579	3.535696
C	0.755346	0.124920	2.246794
H	-0.332414	0.152518	2.299912
C	1.338577	1.475820	2.387041
H	0.757783	2.265400	1.911273
C	2.463413	1.829853	3.045597
H	3.047672	1.069350	3.556811
C	2.965228	3.236787	3.163449
H	3.983321	3.325797	2.760913
H	2.320837	3.943518	2.630009
B	4.468843	0.131607	-0.534488
O	3.071826	-0.605141	-0.597128
O	5.311851	-0.771000	-1.305600
C	3.206710	-1.789570	-1.437201
C	4.752877	-2.070904	-1.361888
C	2.743092	-1.414510	-2.852426
H	3.366624	-0.619671	-3.269281
H	2.774057	-2.278677	-3.525109
H	1.708551	-1.058263	-2.810393
C	2.335250	-2.915498	-0.888569
H	2.519333	-3.845988	-1.437685
H	2.532274	-3.098117	0.170874
H	1.273088	-2.679912	-1.007211
C	5.152781	-2.869950	-0.103950
H	6.245171	-2.858451	-0.025660
H	4.746132	-2.407937	0.797638
H	4.824774	-3.915246	-0.153761
C	5.315042	-2.782365	-2.599461
H	4.846420	-3.762658	-2.752365
H	5.177665	-2.181204	-3.501713
H	6.390682	-2.939633	-2.465036
C	4.440977	1.609478	-1.219667
C	4.870807	1.816419	-2.542989
C	3.996806	2.745558	-0.518589
C	4.835687	3.077111	-3.145173
H	5.256129	0.965714	-3.099500
C	3.951497	4.013159	-1.107508
H	3.680096	2.628022	0.514458
C	4.367972	4.182949	-2.429819
H	5.179593	3.200837	-4.170560
H	3.596960	4.868438	-0.534690
H	4.341055	5.166763	-2.893635
O	4.758599	0.184326	0.906429
H	3.019223	3.544915	4.217282
C	6.058145	0.614479	1.259939
H	6.810381	0.049232	0.689540
H	6.198477	1.677634	1.002978
C	6.293579	0.414962	2.753190
H	7.301014	0.746186	3.033772
H	5.570079	0.987932	3.345134
H	6.192655	-0.642262	3.025803

TS10

SCF energy in Ethanol: -3455.888418 a.u.

Free energy in Ethanol: -3454.705164 a.u.

P	-0.257657	0.289988	-0.441288
N	-0.044935	0.966421	-1.943446
C	1.051368	1.914180	-2.162583
H	1.630691	1.619857	-3.043131
H	0.659348	2.927603	-2.308145
H	1.735904	1.925606	-1.315915
C	-0.909263	0.780758	-3.110090
H	-1.811473	0.232937	-2.847537
H	-1.195205	1.756973	-3.517466
H	-0.369557	0.226939	-3.890195
O	-1.212089	-0.988806	-0.946443
O	-1.319425	1.197312	0.471671
C	-2.179416	-1.614945	-0.161819
C	-3.224246	-0.847452	0.376593
C	-2.151241	-3.018912	-0.019901
C	-4.057246	-1.415321	1.372726
C	-3.518626	0.521506	-0.158565
C	-3.068061	-3.563016	0.886333
C	-3.954513	-2.789699	1.643574
C	-2.575902	1.547085	-0.020440
C	-4.750988	0.792761	-0.806780
H	-3.082836	-4.642629	1.010272
C	-2.871716	2.888946	-0.319188
C	-5.058460	2.121977	-1.147714
C	-4.138930	3.134275	-0.857774
C	-1.955748	4.040981	-0.045894
C	-1.488226	4.856635	-1.100027
C	-1.650361	4.390807	1.291122
C	-0.693532	5.971241	-0.803863

C	-0.873698	5.525730	1.538612	H	-5.131419	-4.444825	2.351350
C	-0.370854	6.324436	0.506418	H	-5.925287	-0.333442	1.523766
H	-0.326708	6.584274	-1.625156	H	-4.584666	0.432929	2.341620
H	-0.663053	5.798341	2.570819	H	-4.697257	-1.185857	4.187665
C	-1.842369	4.603467	-2.550899	H	-4.407925	4.163865	-1.082102
H	-2.732398	5.173976	-2.849511	C	-6.386210	2.506698	-1.784206
H	-1.026308	4.919232	-3.209771	H	-7.048834	2.904399	-0.999983
H	-2.059768	3.552236	-2.748654	H	-6.227742	3.333391	-2.487782
C	0.503521	7.520786	0.802201	C	-5.676877	-0.338104	-1.241117
H	0.219798	8.001473	1.744969	C	-7.092753	1.338596	-2.479620
H	1.558760	7.229386	0.891918	H	-6.566831	1.085504	-3.411061
H	0.441017	8.270418	0.006203	H	-8.111432	1.631991	-2.760124
C	-2.176058	3.590319	2.460757	C	-7.106873	0.116523	-1.558248
H	-3.250209	3.392926	2.366653	H	-5.242901	-0.787440	-2.148532
H	-1.666361	2.623991	2.535043	H	-5.692813	-1.143166	-0.504093
H	-2.011957	4.127813	3.399987	H	-7.632350	0.370500	-0.626058
C	-1.323828	-3.946125	-0.858741	H	-7.659725	-0.712886	-2.015558
C	-0.469870	-4.902642	-0.264180	Ni	1.528842	-0.153616	0.697046
C	-1.507514	-3.969381	-2.264577	C	2.960072	-3.118652	4.005463
C	0.207049	-5.820971	-1.075806	C	1.564638	-3.217169	3.896506
C	-0.808788	-4.904451	-3.032916	C	0.829669	-2.161318	3.375362
C	0.063203	-5.835904	-2.462983	C	1.463933	-0.960282	2.977558
H	0.869605	-6.543431	-0.602696	C	2.867706	-0.872983	3.101279
H	-0.964091	-4.914282	-4.110175	C	3.604412	-1.953287	3.598432
C	-2.477024	-3.046234	-2.968749	H	3.533083	-3.947518	4.412518
H	-3.435924	-2.985827	-2.442017	H	1.057348	-4.121055	4.223603
H	-2.081487	-2.027997	-3.040675	H	-0.252632	-2.234302	3.297439
H	-2.672154	-3.400116	-3.985897	H	3.382929	0.035055	2.808366
C	-0.253011	-4.984786	1.230617	H	4.684348	-1.869026	3.676833
H	-0.307897	-4.005101	1.707312	C	0.684506	0.164054	2.397938
H	-0.999748	-5.628048	1.715358	H	-0.388752	-0.034125	2.458497
H	0.730819	-5.410296	1.452070	C	1.014737	1.522325	2.952494
C	0.831342	-6.813104	-3.321695	H	0.645873	1.688321	3.970747
H	1.758242	-6.363678	-3.702706	C	1.732148	2.494871	2.380455
H	1.112441	-7.708519	-2.757239	H	2.111784	2.354690	1.369246
H	0.245402	-7.130007	-4.191684	C	2.092080	3.796328	3.037582
C	-4.787336	-3.469500	2.719211	H	1.730067	4.648862	2.449779
C	-5.971965	-2.625928	3.202155	H	1.669147	3.869099	4.046113
C	-5.514856	-1.186480	3.452887	B	4.451971	0.227496	-0.497652
C	-5.041726	-0.543090	2.142640	O	3.063787	-0.555252	-0.453595
H	-6.325435	-0.585263	3.881670	O	5.286016	-0.715916	-1.224538
H	-6.767192	-2.626841	2.443017	C	3.218436	-1.816725	-1.166449
H	-6.400001	-3.068524	4.109440	C	4.777026	-2.033951	-1.139006
H	-4.135561	-3.688780	3.578896	C	2.669468	-1.618995	-2.587772

H	3.238579	-0.856917	-3.125556
H	2.697835	-2.551795	-3.161534
H	1.626051	-1.292014	-2.528907
C	2.424705	-2.913024	-0.459208
H	2.613983	-3.885528	-0.928190
H	2.686382	-2.985963	0.599347
H	1.349113	-2.727174	-0.542706
C	5.265242	-2.700401	0.163909
H	6.359378	-2.652211	0.181976
H	4.888263	-2.167966	1.039075
H	4.969360	-3.754510	0.228929
C	5.313017	-2.832854	-2.334248
H	4.883546	-3.841725	-2.373841
H	5.106544	-2.324541	-3.279376
H	6.399841	-2.931824	-2.240372
C	4.397297	1.645450	-1.304445
C	4.636179	1.715277	-2.689241
C	4.152913	2.867100	-0.651123
C	4.591509	2.922543	-3.391115
H	4.886900	0.798849	-3.217334
C	4.103074	4.084958	-1.337272
H	4.020575	2.860977	0.428244
C	4.313655	4.115575	-2.717193
H	4.784672	2.937491	-4.462330
H	3.910669	5.009135	-0.795245
H	4.281190	5.058637	-3.258574
O	4.778949	0.422217	0.919618
H	3.182328	3.904201	3.118967
C	6.100840	0.831790	1.205982
H	6.812398	0.040694	0.923355
H	6.371062	1.721953	0.615421
C	6.244429	1.150389	2.690288
H	7.267052	1.473953	2.920113
H	5.556604	1.952372	2.984326
H	6.020490	0.270760	3.305770

IM13

SCF energy in Ethanol: -3455.897579 a.u.

Free energy in Ethanol: -3454.716286 a.u.

P	-0.264651	0.260100	-0.533909
N	-0.071543	0.934677	-2.045296
C	1.062710	1.827329	-2.306806
H	1.614241	1.482206	-3.188356
H	0.714053	2.852151	-2.481177
H	1.759785	1.835739	-1.468869
C	-0.969728	0.770668	-3.189003
H	-1.846438	0.187140	-2.916542
H	-1.297251	1.750957	-3.555595
H	-0.441371	0.258356	-4.004448
O	-1.203007	-1.035129	-1.031596
O	-1.362177	1.146062	0.385093
C	-2.172117	-1.658554	-0.249380
C	-3.260587	-0.904431	0.212938
C	-2.095915	-3.049176	-0.033885
C	-4.133317	-1.464063	1.179801
C	-3.533314	0.459810	-0.342673
C	-3.040616	-3.591019	0.843557
C	-4.002346	-2.823573	1.508203
C	-2.609669	1.490335	-0.130932
C	-4.728924	0.734730	-1.053514
H	-3.015378	-4.663327	1.020238
C	-2.920638	2.838225	-0.383694
C	-5.031655	2.067809	-1.383127
C	-4.153099	3.085201	-0.996093
C	-2.067939	3.990911	0.047887
C	-1.491363	4.869037	-0.892772
C	-1.944109	4.274320	1.430494
C	-0.769702	5.982105	-0.439825
C	-1.231970	5.406010	1.835085
C	-0.625216	6.270854	0.916597
H	-0.318635	6.645705	-1.175264
H	-1.156440	5.623658	2.898972
C	-1.655075	4.682574	-2.386156
H	-2.518226	5.246679	-2.764925
H	-0.773666	5.049362	-2.922925
H	-1.815313	3.637415	-2.656913
C	0.165466	7.470544	1.384422
H	-0.320838	7.965034	2.233140
H	1.172019	7.180770	1.714155
H	0.283651	8.208932	0.584764
C	-2.600427	3.403403	2.479933
H	-3.668050	3.261281	2.274728
H	-2.146572	2.406509	2.522909
H	-2.505051	3.855914	3.471834
C	-1.178233	-3.980094	-0.766036
C	-0.288530	-4.820574	-0.060374
C	-1.307854	-4.129712	-2.168383
C	0.457218	-5.773372	-0.764090

C	-0.537563	-5.091847	-2.827976	C	0.235713	-1.536952	3.647017
C	0.354814	-5.924656	-2.147675	C	1.273946	-0.810809	3.026935
H	1.143781	-6.410489	-0.209496	C	2.594771	-1.295543	3.153118
H	-0.651284	-5.202994	-3.904744	C	2.854328	-2.462267	3.874575
C	-2.286636	-3.308049	-2.978114	H	2.027981	-4.051890	5.078469
H	-3.275504	-3.273802	-2.506952	H	-0.308767	-3.215671	4.874479
H	-1.944626	-2.273232	-3.089181	H	-0.786241	-1.174749	3.560894
H	-2.404938	-3.729648	-3.981252	H	3.419019	-0.764811	2.682484
C	-0.102601	-4.721318	1.437415	H	3.876950	-2.820941	3.956992
H	-0.169454	-3.690766	1.792568	C	0.956951	0.429769	2.277281
H	-0.858391	-5.300254	1.984783	H	-0.089122	0.720009	2.358008
H	0.876808	-5.112606	1.729777	C	1.890091	1.568755	2.380573
C	1.195349	-6.937940	-2.889323	H	2.936630	1.357603	2.587417
H	2.140686	-6.496082	-3.232342	C	1.503652	2.856426	2.236303
H	1.449345	-7.792175	-2.252503	H	0.459581	3.069940	2.011637
H	0.675992	-7.317699	-3.776048	C	2.399016	4.045726	2.391884
C	-4.876102	-3.493588	2.557472	H	2.044839	4.691493	3.208089
C	-6.113852	-2.674949	2.938931	H	3.432359	3.757091	2.607486
C	-5.716852	-1.213892	3.164560	B	4.576843	0.250550	-0.408107
C	-5.187328	-0.599712	1.862047	O	3.196514	-0.510141	-0.475174
H	-6.568814	-0.625079	3.524985	O	5.473137	-0.702693	-1.045348
H	-6.861512	-2.728021	2.134637	C	3.385333	-1.757977	-1.204636
H	-6.581517	-3.100737	3.834644	C	4.929099	-2.010009	-1.032127
H	-4.270327	-3.660309	3.461400	C	2.977873	-1.508945	-2.665181
H	-5.166014	-4.492300	2.206164	H	3.608496	-0.745765	-3.127224
H	-6.039295	-0.439274	1.186558	H	3.040879	-2.427617	-3.258784
H	-4.773474	0.396935	2.053344	H	1.938935	-1.162737	-2.693192
H	-4.943691	-1.163051	3.944349	C	2.501386	-2.846894	-0.605948
H	-4.428488	4.118695	-1.194449	H	2.719942	-3.815361	-1.069693
C	-6.319949	2.451291	-2.096898	H	2.649438	-2.941435	0.472613
H	-7.031477	2.839503	-1.351706	H	1.444167	-2.635685	-0.792847
H	-6.123087	3.284775	-2.782636	C	5.276015	-2.705931	0.300756
C	-5.617840	-0.397469	-1.555182	H	6.363410	-2.674921	0.427933
C	-6.976295	1.286230	-2.845003	H	4.824273	-2.181964	1.145575
H	-6.396737	1.049164	-3.748477	H	4.959754	-3.755801	0.317668
H	-7.979815	1.575663	-3.179068	C	5.557407	-2.805094	-2.183956
C	-7.032208	0.051001	-1.942737	H	5.106432	-3.800415	-2.282977
H	-5.131360	-0.830152	-2.443743	H	5.455944	-2.276145	-3.134829
H	-5.664545	-1.213440	-0.830968	H	6.627124	-2.936577	-1.988633
H	-7.609596	0.287678	-1.037078	C	4.572440	1.655431	-1.234412
H	-7.553096	-0.775116	-2.441569	C	5.009116	1.723240	-2.569982
Ni	1.603098	0.008206	0.512281	C	4.148141	2.863099	-0.652969
C	1.817393	-3.155781	4.500833	C	4.991941	2.916071	-3.297409
C	0.504747	-2.685092	4.386218	H	5.391183	0.817717	-3.034396

C	4.126111	4.066501	-1.365388
H	3.836811	2.855687	0.387481
C	4.541971	4.095838	-2.698265
H	5.339548	2.929962	-4.328853
H	3.794762	4.982940	-0.879582
H	4.531299	5.028518	-3.258256
O	4.775921	0.441533	1.040054
H	2.392196	4.662793	1.483125
C	6.055178	0.898058	1.435173
H	6.832798	0.225039	1.043881
H	6.258912	1.895861	1.013054
C	6.146861	0.959326	2.955997
H	7.139737	1.303957	3.270162
H	5.402048	1.651032	3.368681
H	5.972285	-0.028687	3.398061

IM14

SCF energy in Ethanol: -3455.897942 a.u.

Free energy in Ethanol: -3454.713875 a.u.

P	-0.110774	0.313155	-0.355104
N	0.279721	1.059867	-1.790435
C	1.478658	1.899172	-1.856874
H	2.109194	1.593399	-2.697212
H	1.208426	2.954705	-1.972576
H	2.071883	1.789700	-0.949777
C	-0.504605	1.047442	-3.024161
H	-1.372981	0.400160	-2.924693
H	-0.845522	2.058886	-3.278600
H	0.121587	0.677498	-3.846646
O	-1.090161	-0.871634	-1.018692
O	-1.239608	1.232915	0.492831
C	-2.275827	-1.364582	-0.482395
C	-3.335212	-0.489288	-0.191765
C	-2.416192	-2.760433	-0.344836
C	-4.453823	-0.975764	0.535237
C	-3.318241	0.939387	-0.646533
C	-3.586132	-3.212685	0.270036
C	-4.568742	-2.354624	0.773139
C	-2.320188	1.799496	-0.174972
C	-4.319042	1.455533	-1.508170
H	-3.725267	-4.285837	0.375195
C	-2.385876	3.196011	-0.332689
C	-4.384975	2.844998	-1.718309
C	-3.455449	3.681964	-1.090149
C	-1.404521	4.130141	0.303287
C	-0.582095	4.969081	-0.479233
C	-1.337941	4.217492	1.716358
C	0.334628	5.817443	0.157731
C	-0.415783	5.084176	2.306825
C	0.446096	5.883237	1.546056
H	0.975602	6.447111	-0.456366
H	-0.378415	5.147402	3.392930
C	-0.671540	5.024394	-1.990020
H	-1.415010	5.764268	-2.316087
H	0.287888	5.322408	-2.425324
H	-0.964806	4.067194	-2.425958
C	1.456565	6.787293	2.213269
H	1.005001	7.355432	3.035085
H	2.287225	6.210442	2.641028
H	1.884892	7.502208	1.503524
C	-2.279530	3.434327	2.604984
H	-3.320360	3.541515	2.278337
H	-2.050478	2.363503	2.600527
H	-2.212644	3.783890	3.639932
C	-1.456245	-3.771173	-0.894610
C	-0.825009	-4.699702	-0.037454
C	-1.284691	-3.890884	-2.294172
C	-0.025016	-5.706947	-0.589740
C	-0.474528	-4.912295	-2.799624
C	0.170974	-5.830189	-1.966627
H	0.460239	-6.414056	0.080910
H	-0.355964	-4.999887	-3.877978
C	-1.981422	-2.967850	-3.268726
H	-3.043925	-2.849131	-3.027657
H	-1.532812	-1.968539	-3.260777
H	-1.907520	-3.357839	-4.288703
C	-0.980801	-4.641810	1.466649
H	-1.005935	-3.616104	1.842012
H	-1.908014	-5.125377	1.800803
H	-0.151786	-5.161026	1.957791
C	1.066114	-6.906499	-2.535693
H	2.107306	-6.563175	-2.602607
H	1.061222	-7.805372	-1.909497
H	0.754927	-7.194513	-3.545715
C	-5.721078	-2.954016	1.564445
C	-6.891055	-1.987873	1.776608
C	-6.356802	-0.616819	2.198094
C	-5.504406	-0.011213	1.074990

H	-7.177311	0.068363	2.442732	O	5.261391	-1.464848	-0.882819
H	-7.465096	-1.881866	0.844994	C	3.047841	-2.090539	-0.472402
H	-7.579335	-2.393278	2.527838	C	4.533476	-2.602097	-0.458169
H	-5.340403	-3.270534	2.547699	C	2.440576	-2.099152	-1.882316
H	-6.062862	-3.872398	1.069742	H	3.095941	-1.586436	-2.589852
H	-6.179498	0.307159	0.268774	H	2.260385	-3.119933	-2.235233
H	-5.013471	0.904429	1.423658	H	1.477712	-1.581649	-1.873666
H	-5.753148	-0.725877	3.110785	C	2.141189	-2.856838	0.491413
H	-3.550435	4.757898	-1.217660	H	2.140645	-3.924510	0.245924
C	-5.475813	3.479437	-2.569893	H	2.470223	-2.745360	1.527738
H	-6.250842	3.884392	-1.900776	H	1.102879	-2.519498	0.413079
H	-5.064695	4.343935	-3.105931	C	4.997218	-3.041980	0.947501
C	-5.234114	0.520784	-2.290713	H	6.079834	-3.203745	0.919895
C	-6.133393	2.504594	-3.552291	H	4.790683	-2.266554	1.689042
H	-5.442091	2.284119	-4.377949	H	4.523231	-3.978976	1.263003
H	-7.021547	2.967984	-3.998412	C	4.809800	-3.743092	-1.446245
C	-6.495400	1.201430	-2.835396	H	4.193221	-4.624654	-1.230083
H	-4.653115	0.130980	-3.141765	H	4.627349	-3.429807	-2.476947
H	-5.499422	-0.359087	-1.700886	H	5.861740	-4.038873	-1.368573
H	-7.188321	1.420090	-2.009659	C	4.760301	0.944956	-1.468865
H	-7.018078	0.514664	-3.511996	C	4.913765	0.642477	-2.834681
Ni	1.636230	0.030927	0.987718	C	4.710549	2.311517	-1.137924
C	-1.344172	-2.822621	4.715261	C	4.981308	1.635576	-3.816322
C	-2.071182	-1.797157	4.104735	H	5.007658	-0.400870	-3.124254
C	-1.411628	-0.781514	3.416325	C	4.771172	3.318544	-2.106118
C	-0.006102	-0.755691	3.319857	H	4.632200	2.597651	-0.091679
C	0.708152	-1.811511	3.920944	C	4.901479	2.983156	-3.455982
C	0.048448	-2.826416	4.613074	H	5.107158	1.359733	-4.861833
H	-1.856466	-3.610364	5.260847	H	4.729753	4.364651	-1.807336
H	-3.156084	-1.783328	4.171167	H	4.957004	3.761172	-4.214346
H	-1.986354	0.012267	2.948617	O	5.233835	0.177796	0.950631
H	1.791792	-1.839806	3.860124	H	4.687378	1.883449	2.033421
H	0.626811	-3.621573	5.076346	C	6.617727	0.009516	1.205180
C	0.661843	0.388382	2.649710	H	6.730294	-0.256235	2.267825
H	-0.000100	1.235280	2.485861	H	7.006325	-0.831873	0.618639
C	2.027398	0.741118	3.005237	C	7.454858	1.258320	0.913414
H	2.623749	0.073103	3.623886	H	8.507582	1.074886	1.166913
C	2.625286	1.873858	2.526693	H	7.397528	1.532639	-0.144110
H	2.017102	2.570522	1.948265	H	7.110912	2.116117	1.504229
C	4.030877	2.276724	2.822523				
H	4.128701	3.366781	2.868209	**IM15**			
H	4.377834	1.844619	3.767682	SCF energy in Ethanol: -3455.910521 a.u.			
B	4.687676	-0.240124	-0.348373	Free energy in Ethanol: -3454.723946 a.u.			
O	3.186475	-0.704571	-0.034896	P	0.002145	0.729310	-0.597692

N	0.416905	1.752706	-1.846714	C	-1.193841	-3.151361	-1.930646
C	1.523373	2.698149	-1.654995	C	-0.316807	-4.141310	-1.434558
H	2.091123	2.778395	-2.588612	C	-1.333741	-2.983695	-3.328696
H	1.148177	3.690898	-1.376215	C	0.404132	-4.930641	-2.339322
H	2.211240	2.344252	-0.887967	C	-0.592165	-3.794820	-4.192923
C	-0.404450	2.037988	-3.023813	C	0.281189	-4.779009	-3.721674
H	-1.238578	1.342637	-3.089718	H	1.081393	-5.686030	-1.945499
H	-0.795897	3.061836	-2.991252	H	-0.709601	-3.658649	-5.266538
H	0.212950	1.934819	-3.925907	C	-2.284643	-1.966916	-3.920641
O	-1.032304	-0.244943	-1.475326	H	-3.282940	-2.035941	-3.473567
O	-1.051116	1.494412	0.452175	H	-1.928208	-0.943310	-3.758094
C	-2.063128	-0.970179	-0.875077	H	-2.386681	-2.116908	-5.000031
C	-3.103465	-0.274842	-0.240128	C	-0.121332	-4.369724	0.046952
C	-2.078842	-2.371858	-1.005589	H	-0.002644	-3.430918	0.594809
C	-4.035244	-0.997802	0.548465	H	-0.970909	-4.891938	0.502984
C	-3.255664	1.205806	-0.420449	H	0.768156	-4.980901	0.228207
C	-3.079752	-3.048334	-0.302915	C	1.042112	-5.667986	-4.678110
C	-4.008289	-2.402279	0.520109	H	1.957227	-6.058737	-4.220607
C	-2.244203	2.065655	0.025374	H	0.437556	-6.532083	-4.985700
C	-4.417699	1.759704	-1.014542	H	1.322237	-5.129642	-5.590396
H	-3.126243	-4.130680	-0.394887	C	-4.955121	-3.252261	1.352995
C	-2.413715	3.460259	0.102674	C	-6.131643	-2.466725	1.941786
C	-4.600075	3.154052	-0.979679	C	-5.628780	-1.148203	2.535096
C	-3.623867	3.961495	-0.386039	C	-5.035770	-0.261458	1.432049
C	-1.394717	4.376157	0.704869	H	-6.439450	-0.608914	3.039619
C	-0.796049	5.401372	-0.060590	H	-6.869783	-2.251310	1.155963
C	-1.071777	4.259989	2.079921	H	-6.643423	-3.072373	2.699135
C	0.154279	6.239165	0.539257	H	-4.381269	-3.705583	2.175499
C	-0.126620	5.125350	2.635821	H	-5.316746	-4.093005	0.746914
C	0.515034	6.112473	1.880121	H	-5.863662	0.128974	0.823999
H	0.620270	7.015561	-0.064941	H	-4.553931	0.619448	1.871186
H	0.108545	5.031289	3.694269	H	-4.865782	-1.358028	3.298241
C	-1.159290	5.670239	-1.507073	H	-3.799545	5.032914	-0.322566
H	-1.942107	6.437261	-1.582176	C	-5.858076	3.815995	-1.523819
H	-0.292332	6.045277	-2.061602	H	-6.527011	4.042916	-0.679216
H	-1.537292	4.782218	-2.017270	H	-5.599233	4.785724	-1.966970
C	1.568148	7.002995	2.496816	C	-5.397281	0.882288	-1.784982
H	1.320135	7.260076	3.532778	C	-6.619024	2.951992	-2.535254
H	2.547256	6.505611	2.513443	H	-6.071042	2.922402	-3.487783
H	1.685391	7.935101	1.934152	H	-7.597337	3.400159	-2.746489
C	-1.760176	3.255611	2.977552	C	-6.772157	1.527346	-1.996632
H	-2.847970	3.277007	2.843809	H	-4.949951	0.680852	-2.771459
H	-1.426387	2.233575	2.771475	H	-5.504749	-0.097723	-1.315910
H	-1.545388	3.470549	4.028922	H	-7.322030	1.555113	-1.044522

H	-7.363317	0.910566	-2.684311
Ni	1.730811	-0.055763	0.518925
C	-0.484233	-6.116033	4.752713
C	-1.635475	-5.353772	4.547047
C	-1.543492	-4.090510	3.964783
C	-0.302615	-3.548827	3.576303
C	0.847290	-4.337537	3.784903
C	0.756501	-5.599226	4.366171
H	-0.551150	-7.102345	5.203736
H	-2.607123	-5.742737	4.841285
H	-2.443825	-3.497929	3.816137
H	1.819426	-3.964018	3.476100
H	1.658982	-6.187164	4.513792
C	-0.265820	-2.206576	2.984612
H	-1.239658	-1.797971	2.710676
C	0.823433	-1.426909	2.793691
H	1.790527	-1.808861	3.112672
C	0.779783	-0.056797	2.239678
H	-0.263219	0.219366	2.084116
C	1.446553	1.016872	3.113480
H	0.965872	1.055600	4.103447
H	2.513010	0.835541	3.270262
B	4.293647	-0.010678	-0.115626
O	3.061484	0.007129	-1.023156
O	5.104482	-1.087451	-0.617664
C	3.348182	-0.853036	-2.163828
C	4.378029	-1.878143	-1.558485
C	3.970130	0.042440	-3.248623
H	4.902228	0.499097	-2.908235
H	4.167421	-0.522122	-4.166548
H	3.267240	0.846215	-3.489212
C	2.066032	-1.476485	-2.700579
H	2.296565	-2.186176	-3.502916
H	1.508832	-2.013089	-1.931657
H	1.412281	-0.704474	-3.116893
C	3.695993	-3.050339	-0.828348
H	4.460005	-3.605026	-0.272881
H	2.945271	-2.699946	-0.113510
H	3.208495	-3.741455	-1.524652
C	5.375049	-2.442362	-2.577253
H	4.863744	-2.990827	-3.377686
H	5.980105	-1.650050	-3.024316
H	6.055197	-3.137125	-2.072730
C	5.081552	1.399852	-0.025147
C	6.302399	1.588855	-0.696022
C	4.581473	2.498948	0.697820
C	6.983422	2.808639	-0.664879
H	6.730121	0.750019	-1.239915
C	5.247556	3.726718	0.732138
H	3.657983	2.387786	1.263133
C	6.454134	3.887137	0.046762
H	7.929092	2.916944	-1.192255
H	4.830495	4.555761	1.300945
H	6.979401	4.839166	0.074159
O	3.572158	-0.313338	1.210023
C	4.241535	-1.066784	2.224153
H	3.589914	-1.075407	3.100862
H	4.365692	-2.102236	1.882152
C	5.596001	-0.487316	2.623387
H	6.007647	-1.086505	3.445599
H	6.303226	-0.512651	1.791118
H	5.499340	0.548927	2.961516
H	1.341903	2.009733	2.661591

TS11

SCF energy in Ethanol: -3455.882079 a.u.

Free energy in Ethanol: -3454.700799 a.u.

P	0.421031	0.886552	0.538665
N	0.418724	2.239155	1.515580
C	-0.427869	3.377411	1.148769
H	-0.939929	3.751820	2.043286
H	0.172890	4.188081	0.715093
H	-1.196157	3.079002	0.433531
C	1.328847	2.502264	2.628708
H	1.982058	1.648999	2.801675
H	1.944133	3.387215	2.427698
H	0.746666	2.690527	3.541600
O	1.115031	-0.155739	1.654032
O	1.643434	0.993922	-0.601739
C	1.799599	-1.297979	1.236498
C	3.016579	-1.143180	0.557051
C	1.285701	-2.565004	1.566900
C	3.633292	-2.280526	-0.024578
C	3.650606	0.209477	0.434828
C	1.986171	-3.669289	1.074514
C	3.106197	-3.554980	0.244848
C	2.965577	1.227007	-0.244085
C	4.939110	0.477195	0.959495

H	1.624542	-4.662313	1.330308	C	3.695202	-4.823156	-0.354546
C	3.579911	2.439991	-0.606264	C	5.074694	-4.621413	-0.989937
C	5.565629	1.695201	0.638544	C	5.067466	-3.351172	-1.843833
C	4.895468	2.621027	-0.168276	C	4.825663	-2.120279	-0.960352
C	2.902964	3.479238	-1.443986	H	6.015270	-3.232406	-2.382448
C	2.687922	4.784473	-0.948985	H	5.840078	-4.527073	-0.206194
C	2.526447	3.173168	-2.776070	H	5.341648	-5.500231	-1.588922
C	2.049909	5.730851	-1.763061	H	3.001930	-5.198002	-1.122926
C	1.905849	4.153331	-3.553253	H	3.734864	-5.604571	0.415522
C	1.640353	5.436257	-3.062527	H	5.740353	-1.929540	-0.381892
H	1.876197	6.729166	-1.364997	H	4.680591	-1.229905	-1.582198
H	1.625987	3.908213	-4.576026	H	4.277775	-3.427615	-2.604657
C	3.149773	5.234681	0.422280	H	5.409426	3.537209	-0.449945
H	4.128017	5.731605	0.366479	C	6.978987	2.020648	1.100295
H	2.449497	5.960972	0.849513	H	7.672513	1.832067	0.266150
H	3.256718	4.404210	1.122115	H	7.056105	3.094040	1.314286
C	0.928829	6.461103	-3.914724	C	5.592142	-0.478844	1.950518
H	1.312032	6.464464	-4.941804	C	7.432944	1.200259	2.312480
H	-0.147108	6.249894	-3.974082	H	6.920156	1.556417	3.217272
H	1.043664	7.471066	-3.507492	H	8.507094	1.345238	2.479579
C	2.811168	1.823341	-3.396221	C	7.105499	-0.279633	2.096593
H	3.828631	1.483049	-3.172794	H	5.120956	-0.308042	2.931546
H	2.121860	1.058388	-3.023833	H	5.366209	-1.518078	1.703613
H	2.701267	1.869917	-4.484122	H	7.618422	-0.638003	1.192163
C	0.096112	-2.780141	2.450460	H	7.475720	-0.887764	2.930876
C	-1.060177	-3.425903	1.950439	Ni	-1.583728	0.389773	-0.339868
C	0.162028	-2.428425	3.817134	C	-1.663579	-6.221705	-4.441714
C	-2.128140	-3.675846	2.818920	C	-0.338484	-5.920593	-4.121695
C	-0.931167	-2.703294	4.648287	C	-0.012635	-4.674519	-3.588595
C	-2.088865	-3.320903	4.170991	C	-0.994880	-3.689924	-3.361631
H	-3.014703	-4.169826	2.425230	C	-2.329242	-4.016918	-3.681404
H	-0.866582	-2.437735	5.701876	C	-2.654470	-5.260808	-4.215523
C	1.394385	-1.787622	4.416259	H	-1.923038	-7.192060	-4.856734
H	2.306566	-2.327451	4.137732	H	0.444029	-6.657125	-4.288470
H	1.514240	-0.753729	4.073287	H	1.024044	-4.446060	-3.348106
H	1.330035	-1.773246	5.508906	H	-3.117443	-3.293853	-3.495790
C	-1.176003	-3.858631	0.505422	H	-3.691661	-5.486163	-4.452808
H	-0.887084	-3.065801	-0.190459	C	-0.589006	-2.392068	-2.811918
H	-0.539378	-4.722991	0.283011	H	0.449564	-2.343548	-2.478469
H	-2.204744	-4.146272	0.268978	C	-1.339003	-1.272375	-2.695595
C	-3.264848	-3.596284	5.079556	H	-2.366648	-1.281568	-3.054606
H	-4.110544	-2.934551	4.850610	C	-0.837736	0.001406	-2.134341
H	-3.625235	-4.625809	4.967739	H	0.239163	-0.106370	-1.983617
H	-3.002061	-3.443930	6.131473	C	-1.071675	1.220885	-3.039962

H	-0.541571	1.095669	-3.997335
H	-2.128946	1.368642	-3.274543
H	-0.695737	2.142688	-2.581139
B	-3.692757	1.314486	0.704522
O	-3.732289	2.579040	0.072388
O	-4.882026	1.084412	1.418185
C	-4.886556	3.295891	0.557257
C	-5.817250	2.144519	1.136815
C	-5.494256	4.083319	-0.606447
H	-5.755036	3.430171	-1.442136
H	-6.395085	4.623086	-0.291007
H	-4.768287	4.819902	-0.967634
C	-4.392426	4.281856	1.630238
H	-5.204397	4.903038	2.024480
H	-3.917815	3.758100	2.465427
H	-3.644493	4.943361	1.180384
C	-6.528723	2.501181	2.446685
H	-7.105505	1.636976	2.792643
H	-5.821743	2.769612	3.235267
H	-7.224734	3.336259	2.303860
C	-6.859421	1.619757	0.137454
H	-7.634674	2.367422	-0.065239
H	-6.402315	1.320781	-0.807164
H	-7.340937	0.735514	0.567807
C	-3.545106	-0.036666	-0.832198
C	-3.858865	-1.350936	-0.415197
C	-4.218203	0.425908	-1.984762
C	-4.771863	-2.156322	-1.101920
H	-3.384862	-1.758434	0.475589
C	-5.129043	-0.364376	-2.685241
H	-4.042403	1.446030	-2.314849
C	-5.406492	-1.664029	-2.244099
H	-4.989080	-3.162325	-0.749858
H	-5.631070	0.027998	-3.567231
H	-6.121414	-2.282282	-2.782299
O	-2.465916	0.945628	1.384198
C	-2.506523	0.145436	2.588513
H	-1.597970	-0.458816	2.595858
H	-3.370074	-0.523189	2.551310
C	-2.569373	1.033884	3.821790
H	-1.718070	1.722537	3.845015
H	-3.495914	1.614896	3.834782
H	-2.535544	0.412540	4.724817

IM16

SCF energy in Ethanol: -2889.880718 a.u.

Free energy in Ethanol: -2888.942110 a.u.

P	-0.009337	0.977095	0.977479
N	0.468403	2.006860	2.208263
C	0.096863	3.419741	2.137782
H	-0.327034	3.741441	3.097948
H	0.968048	4.047689	1.906360
H	-0.658415	3.571035	1.360494
C	1.359207	1.674515	3.319328
H	1.688596	0.639281	3.247765
H	2.236989	2.331515	3.319742
H	0.828905	1.808549	4.272171
O	0.185237	-0.435003	1.842912
O	1.199146	0.786828	-0.179734
C	0.211387	-1.636695	1.132635
C	1.368598	-1.955128	0.412034
C	-0.904193	-2.485606	1.197297
C	1.358365	-3.098251	-0.427791
C	2.570378	-1.064210	0.510376
C	-0.838262	-3.654798	0.437182
C	0.242898	-3.954705	-0.400046
C	2.459614	0.281937	0.122552
C	3.820814	-1.544534	0.972209
H	-1.678785	-4.344094	0.474478
C	3.580315	1.122067	-0.008569
C	4.954132	-0.717525	0.866029
C	4.816628	0.572643	0.343762
C	3.483824	2.524844	-0.522153
C	3.841056	3.621082	0.292012
C	3.080595	2.758526	-1.860606
C	3.729742	4.921754	-0.220481
C	2.996429	4.070266	-2.330928
C	3.300823	5.171831	-1.522970
H	3.995949	5.760230	0.420964
H	2.691058	4.236932	-3.362318
C	4.382547	3.459453	1.697857
H	5.481079	3.471503	1.701439
H	4.055374	4.286062	2.338599
H	4.075358	2.519243	2.158983
C	3.167250	6.580974	-2.051808
H	3.625723	6.682272	-3.042670
H	2.112965	6.869335	-2.155701
H	3.643349	7.306541	-1.384256

C	2.774931	1.619646	-2.807466
H	3.544190	0.840416	-2.761428
H	1.817529	1.145294	-2.567365
H	2.718796	1.980453	-3.839212
C	-2.100291	-2.168053	2.038153
C	-3.340297	-1.870917	1.427806
C	-2.000822	-2.191501	3.446243
C	-4.441199	-1.570638	2.237360
C	-3.132068	-1.897593	4.215040
C	-4.358966	-1.571524	3.632639
H	-5.386932	-1.322144	1.760303
H	-3.049713	-1.925682	5.300101
C	-0.705028	-2.542791	4.143173
H	-0.251783	-3.448979	3.725266
H	0.032833	-1.737960	4.043257
H	-0.873379	-2.710523	5.211820
C	-3.514877	-1.874634	-0.075873
H	-2.733134	-1.302405	-0.586442
H	-3.483621	-2.890260	-0.488812
H	-4.479800	-1.437346	-0.347053
C	-5.559267	-1.216324	4.479349
H	-5.740089	-0.133366	4.475477
H	-6.471455	-1.694713	4.104089
H	-5.420090	-1.523930	5.521122
C	0.142453	-5.184353	-1.290282
C	1.470083	-5.583820	-1.941595
C	2.152938	-4.339110	-2.513881
C	2.515062	-3.367624	-1.382929
H	3.059878	-4.605165	-3.070209
H	2.130653	-6.051017	-1.197094
H	1.292154	-6.332779	-2.722552
H	-0.591473	-4.975935	-2.083143
H	-0.270537	-6.020086	-0.710528
H	3.370164	-3.787000	-0.834995
H	2.870963	-2.417526	-1.797601
H	1.473034	-3.849539	-3.224931
H	5.705262	1.189743	0.230536
C	6.344028	-1.201401	1.254984
H	6.881251	-1.490821	0.338362
H	6.915499	-0.368629	1.683724
C	3.924388	-2.884210	1.691581
C	6.335847	-2.394783	2.216498
H	6.041985	-2.062160	3.222167
H	7.347288	-2.809737	2.303365
C	5.346186	-3.456215	1.728322
H	3.584926	-2.725639	2.727543
H	3.228204	-3.613627	1.273599
H	5.638835	-3.793194	0.723182
H	5.369354	-4.340027	2.377395
Ni	-2.011404	1.626591	0.094368
C	-2.637351	-3.113756	-5.412252
C	-1.284577	-2.939330	-5.112459
C	-0.877264	-1.880738	-4.302285
C	-1.804437	-0.961952	-3.770012
C	-3.166215	-1.158682	-4.080826
C	-3.573574	-2.215599	-4.889905
H	-2.959674	-3.938254	-6.042401
H	-0.543632	-3.626213	-5.514400
H	0.179383	-1.747132	-4.081004
H	-3.913390	-0.481761	-3.676861
H	-4.630303	-2.343602	-5.111376
C	-1.315467	0.137436	-2.935358
H	-0.269157	0.063401	-2.639953
C	-2.014606	1.221903	-2.516309
H	-3.053538	1.335595	-2.824560
C	-1.486510	2.294042	-1.662565
H	-0.393856	2.245138	-1.593386
C	-1.939128	3.706660	-2.018639
H	-1.468924	4.028572	-2.961536
H	-3.023887	3.766708	-2.142303
C	-3.767786	2.302167	0.086527
C	-4.867698	1.687753	-0.546737
C	-4.060055	3.346419	0.990939
C	-6.184287	2.070892	-0.274645
H	-4.699273	0.886836	-1.263859
C	-5.374721	3.735519	1.270677
H	-3.249588	3.875912	1.491000
C	-6.442748	3.097480	0.637235
H	-7.010158	1.569823	-0.776446
H	-5.563313	4.541887	1.976978
H	-7.465791	3.401918	0.845473
H	-1.653499	4.429022	-1.246340

IM17

SCF energy in Ethanol: -2889.911779 a.u.

Free energy in Ethanol: -2888.966753 a.u.

P	-0.237329	-1.004497	-0.389732
N	0.084364	-1.855848	-1.799700

C	0.168244	-3.313939	-1.712142	C	-4.179340	1.655226	0.257342
H	-0.687458	-3.787879	-2.206966	C	-3.432710	2.109017	-2.020462
H	1.100230	-3.661845	-2.172349	C	-5.460793	1.397999	-0.238607
H	0.170636	-3.634646	-0.667079	C	-4.730059	1.841086	-2.472414
C	-0.085252	-1.349995	-3.160942	C	-5.758869	1.476785	-1.601399
H	0.051472	-0.270570	-3.190160	H	-6.246087	1.119054	0.461261
H	0.664071	-1.814189	-3.813056	H	-4.941049	1.928201	-3.536619
H	-1.085249	-1.595191	-3.546825	C	-2.377903	2.521169	-3.023200
O	-0.735206	0.417067	-1.119877	H	-1.850827	3.428780	-2.707656
O	1.242596	-0.554131	0.260620	H	-1.622312	1.737676	-3.152771
C	-0.617147	1.636469	-0.455448	H	-2.829729	2.714072	-4.001372
C	0.666105	2.138444	-0.195743	C	-3.930003	1.512211	1.741990
C	-1.778756	2.367130	-0.145507	H	-3.175179	0.741598	1.934459
C	0.807832	3.278854	0.633492	H	-3.568132	2.439109	2.199820
C	1.864067	1.486881	-0.818106	H	-4.847639	1.218015	2.261260
C	-1.595889	3.548197	0.579557	C	-7.142914	1.153464	-2.113636
C	-0.342971	3.983542	1.025810	H	-7.316582	1.588683	-3.103549
C	2.162812	0.152108	-0.508906	H	-7.286479	0.068252	-2.201457
C	2.696899	2.194547	-1.720362	H	-7.919825	1.527723	-1.437305
H	-2.473584	4.146420	0.815017	C	-0.277247	5.206382	1.927768
C	3.355424	-0.464970	-0.927269	C	1.132710	5.789475	2.070581
C	3.892293	1.595553	-2.155937	C	2.135070	4.660222	2.320555
C	4.209667	0.304852	-1.722092	C	2.187002	3.714533	1.113605
C	3.744688	-1.858800	-0.545220	H	3.137995	5.060148	2.513336
C	3.874428	-2.863997	-1.527906	H	1.411078	6.327684	1.152977
C	4.061530	-2.157080	0.800181	H	1.151694	6.523390	2.885313
C	4.256798	-4.154792	-1.140167	H	-0.644552	4.924541	2.926720
C	4.446042	-3.456816	1.140259	H	-0.975684	5.969011	1.559136
C	4.536139	-4.477642	0.188473	H	2.728184	4.220597	0.302118
H	4.342378	-4.926224	-1.903510	H	2.780436	2.825851	1.355266
H	4.693888	-3.674375	2.177786	H	1.838636	4.097608	3.216143
C	3.643210	-2.590085	-2.999312	H	5.152147	-0.136147	-2.039085
H	4.537484	-2.165804	-3.474655	C	4.877851	2.323942	-3.058684
H	3.406063	-3.516379	-3.533565	H	5.692436	2.726030	-2.436292
H	2.830995	-1.877818	-3.161535	H	5.351002	1.605100	-3.739432
C	4.915778	-5.884279	0.590037	C	2.253525	3.526093	-2.315493
H	5.675959	-5.884841	1.379478	C	4.249469	3.476093	-3.849929
H	4.048831	-6.436473	0.977492	H	3.613648	3.074701	-4.651847
H	5.309789	-6.451786	-0.259741	H	5.035077	4.068438	-4.334519
C	4.035823	-1.086490	1.865890	C	3.399587	4.345882	-2.920327
H	4.615326	-0.206793	1.561197	H	1.524665	3.303167	-3.111009
H	3.017336	-0.745626	2.075942	H	1.704098	4.123490	-1.585690
H	4.462072	-1.462265	2.801729	H	4.034521	4.747733	-2.117249
C	-3.146188	2.006022	-0.640538	H	2.988067	5.208188	-3.458927

Ni	-1.613275	-1.913211	1.055138
C	1.468970	1.443976	5.058252
C	2.013964	0.163911	4.944219
C	1.330156	-0.830417	4.245117
C	0.086192	-0.576600	3.639264
C	-0.439123	0.724405	3.747625
C	0.238709	1.716350	4.453030
H	1.993969	2.218670	5.610700
H	2.969988	-0.065821	5.407974
H	1.753856	-1.829830	4.180501
H	-1.381599	0.967374	3.267339
H	-0.196889	2.709547	4.529637
C	-0.643704	-1.689861	2.998655
H	-0.056759	-2.602473	2.874655
C	-2.038514	-1.826008	3.079245
H	-2.620225	-0.976358	3.438274
C	-2.732541	-2.884538	2.457500
H	-2.205043	-3.838811	2.368658
C	-4.237363	-2.987420	2.510983
H	-4.563514	-3.524076	3.413866
H	-4.703021	-1.995487	2.524044
C	-2.753961	-2.618158	-0.342280
C	-2.930566	-4.005759	-0.527128
C	-3.439579	-1.778474	-1.241872
C	-3.734028	-4.526585	-1.547161
H	-2.433182	-4.710502	0.138961
C	-4.250291	-2.290040	-2.263149
H	-3.340354	-0.700334	-1.160994
C	-4.401653	-3.668057	-2.423479
H	-3.840567	-5.604950	-1.652957
H	-4.761139	-1.601366	-2.933639
H	-5.030593	-4.067648	-3.215675
H	-4.624566	-3.527616	1.642814

TS1c

SCF energy in Ethanol: -2812.627563 a.u.

Free energy in Ethanol: -2811.712928 a.u.

P	0.233399	-1.341068	-0.737002
N	1.107986	-2.200472	-1.884033
C	1.251820	-3.644475	-1.737401
H	0.856237	-4.161558	-2.623317
H	2.306574	-3.925607	-1.610561
H	0.692191	-3.990540	-0.863310
C	1.663746	-1.664644	-3.123794
H	1.651587	-0.576145	-3.112180
H	2.698031	-2.006507	-3.250670
H	1.079610	-2.011339	-3.989109
O	-0.228281	-0.104771	-1.773965
O	1.298844	-0.460550	0.251292
C	-0.682667	1.092001	-1.230332
C	0.259101	1.970303	-0.678430
C	-2.052255	1.397356	-1.292335
C	-0.195294	3.116738	0.021999
C	1.719066	1.655985	-0.801426
C	-2.453939	2.584039	-0.675472
C	-1.568840	3.417587	0.018034
C	2.204895	0.462421	-0.243102
C	2.625090	2.531684	-1.449647
H	-3.507309	2.852634	-0.711731
C	3.582532	0.199487	-0.122426
C	4.005523	2.271982	-1.369214
C	4.453061	1.141995	-0.675662
C	4.106837	-1.001449	0.601286
C	4.835685	-2.001048	-0.075245
C	3.911526	-1.113452	2.000284
C	5.303589	-3.112772	0.640541
C	4.401834	-2.233705	2.673760
C	5.091203	-3.256194	2.010704
H	5.854778	-3.884001	0.105070
H	4.250692	-2.305979	3.749446
C	5.169350	-1.908485	-1.549387
H	6.141462	-1.421424	-1.706461
H	5.238105	-2.906490	-1.996495
H	4.431278	-1.328592	-2.106357
C	5.585669	-4.470606	2.762075
H	6.105739	-4.186830	3.684828
H	4.754886	-5.127386	3.052273
H	6.277290	-5.063313	2.154492
C	3.223230	-0.020867	2.788514
H	3.691708	0.954746	2.611537
H	2.168829	0.075294	2.508277
H	3.272122	-0.228797	3.862129
C	-3.046549	0.537158	-2.007421
C	-4.064938	-0.126609	-1.290577
C	-3.003903	0.438157	-3.417197
C	-5.007347	-0.886921	-1.994616
C	-3.970005	-0.325782	-4.077413

C	-4.978421	-1.003591	-3.385351	C	-2.132053	0.646902	4.025530
H	-5.782909	-1.403662	-1.432764	C	-3.511876	0.362546	4.082226
H	-3.936269	-0.388192	-5.163854	C	-4.406518	1.273461	4.635945
C	-1.949980	1.157639	-4.229416	H	-4.655330	3.201599	5.579132
H	-1.876821	2.215838	-3.952850	H	-2.223119	3.736117	5.496983
H	-0.958778	0.715446	-4.075916	H	-0.632645	2.118544	4.512749
H	-2.180419	1.102524	-5.298315	H	-3.887556	-0.572014	3.676774
C	-4.176814	-0.038946	0.215735	H	-5.466210	1.033274	4.664980
H	-3.197344	-0.080704	0.700142	C	-1.145332	-0.268118	3.451551
H	-4.655403	0.896281	0.534808	H	-0.136226	0.135471	3.369541
H	-4.772238	-0.871584	0.600144	C	-1.347888	-1.538817	3.029399
C	-5.990311	-1.852950	-4.120097	H	-2.332556	-1.997194	3.103766
H	-5.620540	-2.877006	-4.266893	C	-0.299534	-2.366441	2.455311
H	-6.931963	-1.925186	-3.565068	H	0.694117	-1.930393	2.392729
H	-6.212227	-1.444714	-5.112558	C	-0.484234	-3.681433	2.093169
C	-2.143517	4.600718	0.782877	H	-1.414897	-4.198426	2.310335
C	-1.085734	5.603899	1.253777	H	0.363405	-4.296252	1.802540
C	0.095415	4.851071	1.871444	C	-3.113869	-4.674976	-1.675233
C	0.781513	3.981297	0.810284	H	-3.830808	-3.977964	-2.123064
H	0.826132	5.546806	2.301965	H	-2.119374	-4.440848	-2.074498
H	-0.729535	6.204737	0.404504	H	-3.375614	-5.694922	-1.985111
H	-1.529143	6.303564	1.972620	C	-3.133271	-4.550182	-0.150948
H	-2.679369	4.214204	1.662864	H	-4.127583	-4.846960	0.217697
H	-2.901471	5.100340	0.165409	H	-2.408170	-5.261739	0.282812
H	1.334717	4.644920	0.130836	O	-2.913731	-3.235715	0.323104
H	1.539307	3.340657	1.275224	H	-2.156564	-2.488593	-0.642468
H	-0.269364	4.219853	2.694025				
H	5.523985	0.974465	-0.581261	**TS1d**			
C	5.038826	3.213746	-1.970922	SCF energy in Ethanol: -2812.626006 a.u.			
H	5.450283	3.843410	-1.166564	Free energy in Ethanol: -2811.712475 a.u.			
H	5.885981	2.631426	-2.354789	P	0.121844	-0.486450	-0.495474
C	2.114719	3.666674	-2.329520	N	0.808204	-0.101012	-1.978446
C	4.476631	4.124456	-3.067930	C	2.146137	-0.592994	-2.295068
H	4.296133	3.540191	-3.981469	H	2.106302	-1.336182	-3.105082
H	5.212766	4.895652	-3.325543	H	2.794849	0.234048	-2.612708
C	3.159974	4.753904	-2.604871	H	2.595853	-1.064441	-1.418183
H	1.809424	3.223624	-3.290784	C	0.087448	0.441927	-3.127925
H	1.204242	4.107137	-1.918507	H	-0.844046	0.911139	-2.815838
H	3.337664	5.341237	-1.692087	H	0.709157	1.192014	-3.631763
H	2.774117	5.451167	-3.358615	H	-0.147211	-0.351775	-3.852706
Ni	-1.107296	-2.490836	0.413011	O	-1.447279	-0.648576	-1.061417
C	-3.952695	2.493399	5.148461	O	-0.079896	0.935812	0.415395
C	-2.589787	2.793104	5.099751	C	-2.515143	-0.555217	-0.176403
C	-1.693748	1.881208	4.544068	C	-2.875627	0.712459	0.297392

C	-3.220388	-1.718984	0.171112	H	-1.531534	-2.886817	1.997769
C	-3.869349	0.815362	1.304594	H	-2.915534	-3.872149	2.475256
C	-2.171864	1.925952	-0.228740	H	-1.333928	-4.628366	2.196933
C	-4.261132	-1.566916	1.089395	C	-2.144988	-6.981902	-2.106111
C	-4.570352	-0.340899	1.690615	H	-2.042057	-6.942297	-3.195881
C	-0.782913	2.034573	-0.049399	H	-1.232101	-7.428584	-1.696152
C	-2.866656	2.978317	-0.875017	H	-2.970621	-7.671052	-1.881327
H	-4.835476	-2.447998	1.367514	C	-5.638061	-0.319458	2.775201
C	-0.092708	3.239143	-0.278853	C	-6.091393	1.090106	3.168458
C	-2.184382	4.174639	-1.162748	C	-4.869056	1.996155	3.334978
C	-0.833874	4.294815	-0.816509	C	-4.136620	2.147128	1.995586
C	1.344950	3.431941	0.093453	H	-5.159537	2.986565	3.705926
C	2.323648	3.700361	-0.887109	H	-6.746706	1.505674	2.389413
C	1.716862	3.424205	1.459970	H	-6.683354	1.048128	4.090688
C	3.648656	3.929396	-0.491227	H	-5.238847	-0.824706	3.667870
C	3.049793	3.661073	1.808800	H	-6.495977	-0.923339	2.451626
C	4.036806	3.912816	0.850075	H	-4.740109	2.798464	1.348062
H	4.393414	4.139143	-1.257688	H	-3.187975	2.676406	2.140684
H	3.322176	3.662655	2.862470	H	-4.193025	1.561699	4.085104
C	1.989591	3.777207	-2.361469	H	-0.330387	5.243613	-0.990000
H	1.696023	4.793929	-2.655278	C	-2.885421	5.371503	-1.789821
H	2.859154	3.506546	-2.970284	H	-3.120343	6.096809	-0.995199
H	1.161375	3.117733	-2.627829	H	-2.193656	5.887298	-2.467737
C	5.474841	4.145119	1.253672	C	-4.295255	2.778895	-1.366587
H	5.542649	4.585173	2.254390	C	-4.181562	5.009858	-2.523455
H	6.041849	3.204861	1.273125	H	-3.945457	4.497229	-3.466816
H	5.984003	4.816516	0.553363	H	-4.727753	5.923542	-2.787627
C	0.698806	3.204045	2.557332	C	-5.039372	4.088682	-1.651830
H	-0.163148	3.871774	2.443742	H	-4.242977	2.197124	-2.300592
H	0.313608	2.178375	2.549351	H	-4.866894	2.155858	-0.675942
H	1.143868	3.389857	3.539827	H	-5.276928	4.597850	-0.706298
C	-2.912829	-3.059390	-0.419077	H	-5.996100	3.867787	-2.140599
C	-2.357725	-4.079144	0.383827	Ni	1.055932	-1.959492	0.684052
C	-3.213912	-3.318828	-1.773959	C	8.470168	-0.713137	-0.805482
C	-2.105116	-5.331513	-0.186964	C	7.744211	0.445412	-1.086938
C	-2.953398	-4.588220	-2.299215	C	6.464453	0.613307	-0.560810
C	-2.398182	-5.609994	-1.524000	C	5.874816	-0.370434	0.257747
H	-1.656805	-6.105356	0.432719	C	6.624683	-1.532152	0.533562
H	-3.191884	-4.782566	-3.343524	C	7.902021	-1.699604	0.007798
C	-3.815569	-2.256258	-2.666661	H	9.468839	-0.847598	-1.211933
H	-4.687789	-1.781734	-2.202185	H	8.174376	1.219534	-1.717157
H	-3.091793	-1.460725	-2.879916	H	5.898867	1.514053	-0.787888
H	-4.133319	-2.686242	-3.622051	H	6.206913	-2.307280	1.169321
C	-2.019029	-3.854563	1.841497	H	8.461290	-2.603416	0.235490

C	4.525728	-0.137005	0.775353
H	4.109932	0.846007	0.552916
C	3.752913	-0.996310	1.480624
H	4.113404	-1.995534	1.722100
C	2.421659	-0.658827	1.956923
H	2.084282	0.358813	1.776524
C	1.642108	-1.503964	2.706761
H	2.009480	-2.471838	3.037589
H	0.719296	-1.151543	3.160064
C	2.293007	-6.009769	0.401614
H	2.198011	-6.304222	1.452820
H	1.408868	-6.372288	-0.134258
H	3.182266	-6.498287	-0.017210
C	2.397696	-4.491264	0.281801
H	3.314874	-4.144202	0.790450
H	2.506129	-4.211605	-0.779650
O	1.250055	-3.893346	0.857289
H	0.593191	-3.111481	-0.138738