

Conformational Control Allows for [3,3]-Sigmatropic Rearrangements to Proceed with Torquoselectivity.

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1 Gaussian reference

See References section at the end of this document (cite 1)

2 Cartesian Coordinates

Geometries: M06-2X/Def2TZVPP

SCF energies: M06-2X/Def2TZVPP

1 CH3

SCF Energy: -311.961834649

Num. Imaginary Frequencies: 0

C	-2.558937	1.722721	-0.213787
C	-1.801911	0.781036	0.332446
C	-2.025562	-0.690820	0.171586
C	-0.828884	-1.400237	-0.482526
C	0.403867	-1.352534	0.382199
C	1.506979	-0.733335	0.067165
C	2.599124	-0.099556	-0.256616
H	0.344514	-1.857694	1.343518
H	-0.616705	-0.945375	-1.450454
H	-2.920183	-0.862029	-0.428967
H	-0.943096	1.071904	0.931021
H	-2.345997	2.774202	-0.072650
H	-1.098489	-2.443660	-0.659287
H	-2.200642	-1.143203	1.152575
C	2.869942	1.345168	0.062405
H	3.372299	-0.642971	-0.792309
H	-3.421089	1.469676	-0.820536
H	3.050641	1.911303	-0.852275
H	2.029457	1.793002	0.588575
H	3.761577	1.440193	0.683567

1 CHO

SCF Energy: -385.986347504

Num. Imaginary Frequencies: 0

C	-2.554872	2.025559	-0.225462
C	-2.020646	0.958655	0.352234
C	-2.491518	-0.446988	0.138522
C	-1.418468	-1.338709	-0.504966
C	-0.217064	-1.508951	0.388228
C	0.982577	-1.121420	0.086375
C	2.184584	-0.690379	-0.215960
H	-0.373217	-1.978088	1.356521
H	-1.109898	-0.917139	-1.461039
H	-3.376180	-0.445141	-0.499310
H	-1.173757	1.086249	1.020680
H	-2.170436	3.020467	-0.043743
H	-1.846297	-2.324293	-0.696305
H	-2.780438	-0.888094	1.096814
C	2.575179	0.678147	0.143647
H	2.910251	-1.311655	-0.727617
H	-3.399314	1.936296	-0.899427
O	3.660279	1.152522	-0.097951
H	1.798423	1.265739	0.661330

1 CN

SCF Energy: -364.904643696

Num. Imaginary Frequencies: 0

C	-2.395470	1.995300	-0.271490
C	-1.822176	0.955055	0.317097
C	-2.313479	-0.456036	0.210515
C	-1.282083	-1.391769	-0.439079
C	-0.044083	-1.530141	0.407676
C	1.133171	-1.121992	0.055513
C	2.319896	-0.709491	-0.317424
H	-0.154230	-1.980263	1.391091
H	-1.014350	-1.020715	-1.427619
H	-3.231730	-0.482374	-0.377186
H	-0.926616	1.109915	0.912594
H	-1.995611	2.995381	-0.169026
H	-1.725797	-2.381124	-0.560003
H	-2.552014	-0.839808	1.206595
C	2.751955	0.626325	-0.040879
H	3.013502	-1.353550	-0.843241
H	-3.288603	1.878214	-0.874700
N	3.112723	1.695831	0.172846

1 F

SCF Energy: -371.895974492

Num. Imaginary Frequencies: 0

C	-2.670428	1.626046	-0.207961
C	-1.866311	0.728197	0.343969
C	-1.990348	-0.752249	0.153860
C	-0.741997	-1.369683	-0.497318
C	0.466785	-1.256252	0.388573
C	1.548474	-0.593859	0.092951
C	2.638659	0.032621	-0.230237
F	2.817565	1.345694	0.057732
H	0.409489	-1.754277	1.354210
H	-0.545401	-0.890334	-1.455797
H	-2.860306	-0.971365	-0.466184
H	-1.045471	1.065898	0.970576
H	-2.532513	2.686683	-0.044676
H	-0.933453	-2.428564	-0.683197
H	-2.150565	-1.235126	1.122367
H	3.488433	-0.398968	-0.738295
H	-3.497300	1.325872	-0.841608

1 H

SCF Energy: -272.651084463

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-2.639801	1.203007	-0.181602
C	-1.630460	0.528714	0.351836
C	-1.365275	-0.927310	0.123725
C	0.008730	-1.184839	-0.514042
C	1.143316	-0.785726	0.393021
C	2.024747	0.131645	0.116447
C	2.902866	1.048832	-0.172788
H	1.211609	-1.296728	1.350116
H	0.085035	-0.644413	-1.457803
H	-2.143862	-1.345771	-0.515687
H	-0.924150	1.049522	0.992308
H	-2.780786	2.258590	0.009871
H	0.094133	-2.250646	-0.736099
H	-1.407419	-1.460173	1.078614
H	2.736745	2.086163	0.091015
H	3.825278	0.800802	-0.683488
H	-3.361323	0.716718	-0.828431

1 NH2

SCF Energy: -328.009257931

Num. Imaginary Frequencies: 0

C	2.612519	1.689813	0.218399
C	1.830519	0.768348	-0.327194
C	2.019922	-0.709022	-0.172178
C	0.810258	-1.391529	0.487240
C	-0.423136	-1.316702	-0.374781
C	-1.514962	-0.672115	-0.067592
C	-2.617146	-0.034888	0.234240
H	-0.361007	-1.830842	-1.333412
H	0.610936	-0.932251	1.455759
H	2.914240	-0.902964	0.421811
H	0.976154	1.082106	-0.920658
H	2.424260	2.746591	0.081808
H	1.057992	-2.441203	0.660994
H	2.178297	-1.162204	-1.155687
N	-2.939200	1.283097	-0.137016
H	-3.405404	-0.556005	0.766553
H	3.471364	1.414049	0.819928
H	-3.469217	1.767860	0.573003
H	-2.131055	1.829751	-0.399797

1 NO2

SCF Energy: -477.169194872

Num. Imaginary Frequencies: 0

C	-3.806134	1.450154	-0.401657
C	-2.986804	0.649127	0.264473
C	-2.841195	-0.818952	0.005004
C	-1.423524	-1.201247	-0.447411
C	-0.405534	-0.944515	0.630054
C	0.600064	-0.137704	0.513947
C	1.598416	0.691071	0.393057
H	-0.528706	-1.466679	1.575989
H	-1.155705	-0.652470	-1.349090
H	-3.548089	-1.129059	-0.765049
H	-2.360516	1.064464	1.049196
H	-3.869278	2.507182	-0.179940
H	-1.400357	-2.266910	-0.681525
H	-3.079830	-1.379968	0.912941
H	1.602661	1.741161	0.634713
N	2.882746	0.218919	-0.114406
H	-4.444081	1.070558	-1.191655
O	3.764012	1.050911	-0.193074
O	3.010105	-0.944450	-0.425619

1 OH

SCF Energy: -347.878602144

Num. Imaginary Frequencies: 0

C	-2.659486	1.664641	-0.202497
C	-1.860510	0.753540	0.335500
C	-2.015446	-0.725127	0.155796
C	-0.783557	-1.370589	-0.499540
C	0.433906	-1.287358	0.381703
C	1.522432	-0.629585	0.095850
C	2.621247	-0.000326	-0.219017
H	0.366686	-1.807153	1.336225
H	-0.579699	-0.891630	-1.457194
H	-2.896901	-0.929865	-0.453314
H	-1.018347	1.077769	0.940503
H	-2.497089	2.723203	-0.048076
H	-1.004622	-2.422805	-0.691915
H	-2.176269	-1.197717	1.129602
O	2.830056	1.319730	0.093091
H	3.424834	-0.502855	-0.744472
H	-3.506539	1.378114	-0.815572
H	3.695986	1.583917	-0.227279

1 OMe

SCF Energy: -387.169948668

Num. Imaginary Frequencies: 0

2 *CARTESIAN COORDINATES*

C	3.463652	1.638940	0.225396
C	2.673433	0.732993	-0.333696
C	2.691836	-0.728687	-0.008081
C	1.346050	-1.227547	0.541279
C	0.245924	-1.130630	-0.481861
C	-0.841356	-0.424521	-0.349624
C	-1.901231	0.323401	-0.199999
H	0.398660	-1.694651	-1.400687
H	1.073597	-0.659887	1.430990
H	3.476660	-0.932170	0.721618
H	1.943279	1.050245	-1.073109
H	3.403090	2.685957	-0.040802
H	1.458154	-2.273848	0.834578
H	2.930003	-1.300941	-0.909899
H	-1.913141	1.357968	-0.531871
O	-3.044072	-0.121291	0.404112
H	4.201027	1.359152	0.969327
C	-4.197727	0.634926	0.070350
H	-5.017357	0.237045	0.661172
H	-4.052490	1.689468	0.314463
H	-4.432396	0.538738	-0.991262

1 tBut

SCF Energy: -429.890408811

Num. Imaginary Frequencies: 0

C	4.233088	1.542048	0.177917
C	3.413369	0.649753	-0.360645
C	3.314987	-0.782217	0.066063
C	1.906836	-1.156245	0.554895
C	0.879121	-1.078617	-0.543789
C	-0.148940	-0.276657	-0.542571
C	-1.178490	0.522249	-0.520243
H	1.028600	-1.734991	-1.398047
H	1.615185	-0.501500	1.376784
H	4.038217	-0.978829	0.858914
H	2.744508	0.957878	-1.159430
H	4.256945	2.568697	-0.163064
H	1.934505	-2.177703	0.940986
H	3.571037	-1.432483	-0.776150
H	-1.073739	1.517624	-0.948134
C	-2.544444	0.197230	0.055669
H	4.910878	1.271110	0.979578
C	-2.860913	1.224578	1.148208
C	-3.581983	0.318394	-1.065728
C	-2.580392	-1.208917	0.643415
H	-3.570309	-1.416834	1.052163
H	-2.358922	-1.956834	-0.119279
H	-1.847506	-1.315503	1.444835
H	-4.584479	0.141378	-0.671675
H	-3.561337	1.315623	-1.508669
H	-3.387332	-0.410514	-1.853510
H	-3.860112	1.049496	1.551331
H	-2.141823	1.154080	1.965395
H	-2.827742	2.239710	0.748829

3 CH3 Z

SCF Energy: -311.981423614

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-2.991537	-0.505790	-0.354550
C	-1.731688	-0.915182	-0.374691
C	-0.737170	-0.711893	0.735711
C	0.554512	-0.082412	0.258784
C	0.541397	1.347033	-0.071678
C	-0.502935	2.163054	0.065485
C	1.653771	-0.839538	0.138813
H	1.562182	-1.885251	0.419230
H	1.464326	1.767469	-0.451051
H	-1.462609	1.820728	0.428165
H	-3.392245	0.040279	0.492382
H	-1.358482	-1.455909	-1.240347
H	-0.499322	-1.685570	1.169430
H	-0.421908	3.210444	-0.191829
H	-3.663777	-0.700522	-1.179589
C	3.015591	-0.441884	-0.332908
H	-1.191797	-0.110157	1.525977
H	3.307265	-1.051789	-1.190263
H	3.090859	0.602562	-0.620547
H	3.753864	-0.632616	0.448651

3 CH3 E

SCF Energy: -311.982557021

Num. Imaginary Frequencies: 0

C	-2.371469	-1.522085	-0.277114
C	-1.053973	-1.383038	-0.256116
C	-0.285425	-0.594375	0.768175
C	0.544888	0.495102	0.128474
C	1.831526	0.336791	-0.208155
C	-0.106644	1.774426	-0.179164
C	-1.383282	2.085179	0.037662
H	0.538836	2.518971	-0.635993
H	-2.084128	1.387039	0.475698
H	-2.998638	-1.055035	0.474000
H	-0.452290	-1.858956	-1.025882
H	0.366202	-1.270632	1.321817
H	-1.767310	3.059866	-0.230550
H	-2.867055	-2.106324	-1.041034
C	2.681936	-0.879171	-0.037491
H	2.326680	1.184424	-0.674048
H	-0.977288	-0.162908	1.492651
H	3.080444	-1.194915	-1.003841
H	3.543842	-0.658148	0.595781
H	2.145362	-1.720360	0.393768

3 CHO E

SCF Energy: -386.004581598

Num. Imaginary Frequencies: 0

C	-2.508118	-1.782684	-0.318476
C	-1.224119	-1.462613	-0.276004
C	-0.593357	-0.593035	0.779972
C	0.103552	0.598545	0.166897
C	1.418570	0.627001	-0.124957
C	-0.699534	1.776019	-0.177259
C	-2.012726	1.896455	0.002202
H	-0.150196	2.598110	-0.622943
H	-2.617165	1.108135	0.429447
H	-3.206734	-1.416354	0.424984
H	-0.547518	-1.842089	-1.036210
H	0.115537	-1.186362	1.354991
H	-2.526323	2.802458	-0.288258
H	-2.902983	-2.424438	-1.094489
C	2.362347	-0.461766	0.104702
H	1.846218	1.510861	-0.585268
H	-1.355205	-0.252878	1.480786
O	3.535850	-0.387545	-0.196150
H	1.977868	-1.384611	0.563698

3 CHO Z

SCF Energy: -386.003460098

Num. Imaginary Frequencies: 0

C	-3.238474	-0.838682	-0.431237
C	-1.937851	-1.079849	-0.372584
C	-1.044745	-0.691846	0.776665
C	0.168346	0.081061	0.314024
C	1.353899	-0.556795	0.245340
C	-0.006049	1.485683	-0.069099
C	-1.155070	2.152489	0.017191
H	0.859981	2.013676	-0.443306
H	-2.068733	1.696517	0.372001
H	-3.751514	-0.310447	0.364447
H	-1.450129	-1.610071	-1.185211
H	-0.699994	-1.599198	1.274928
H	-1.209357	3.191409	-0.277493
H	-3.834175	-1.163244	-1.273730
H	1.419938	-1.595872	0.547842
C	2.617493	0.017417	-0.209602
H	-1.612311	-0.113895	1.507065
O	3.646846	-0.624451	-0.248184
H	2.626238	1.069868	-0.525266

3 CN E

SCF Energy: -364.930169305

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-2.113301	-2.033366	-0.230363
C	-0.904242	-1.503030	-0.327531
C	-0.283772	-0.597250	0.704148
C	0.156505	0.708299	0.095223
C	1.433411	0.935345	-0.258047
C	-0.829070	1.758550	-0.165756
C	-2.126783	1.670090	0.112881
H	-0.442402	2.662342	-0.623498
H	-2.564542	0.787728	0.559414
H	-2.753037	-1.828819	0.620523
H	-0.283730	-1.723612	-1.191049
H	0.584157	-1.096336	1.138574
H	-2.795100	2.490242	-0.109517
H	-2.501940	-2.692432	-0.994862
C	2.469333	-0.025072	-0.062558
H	1.732941	1.866325	-0.720319
H	-0.992115	-0.414189	1.512113
N	3.314754	-0.790379	0.085805

3 CN Z

SCF Energy: -364.929623207

Num. Imaginary Frequencies: 0

C	-3.238994	-0.410477	-0.480750
C	-1.999990	-0.874405	-0.432658
C	-1.072160	-0.711747	0.742819
C	0.255884	-0.123919	0.337783
C	1.330541	-0.927927	0.261402
C	0.349337	1.299131	0.010936
C	-0.660370	2.160855	0.100442
H	1.319547	1.654035	-0.318056
H	-1.650649	1.862061	0.415867
H	-3.664023	0.150674	0.343699
H	-1.598419	-1.432412	-1.273153
H	-0.892030	-1.690708	1.190078
H	-0.517981	3.203264	-0.148626
H	-3.870108	-0.578306	-1.342972
H	1.266823	-1.978569	0.509097
C	2.619085	-0.465233	-0.142881
H	-1.543966	-0.086736	1.502353
N	3.664401	-0.111566	-0.465835

3 H

SCF Energy: -272.671808511

Num. Imaginary Frequencies: 0

C	0.382709	-0.747722	-0.671011
C	1.484017	-0.628470	0.347482
C	2.593185	0.077825	0.188007
C	-0.528943	2.038926	-0.090675
C	-1.306496	0.992382	0.174673
C	-0.973461	-0.412089	-0.095900
C	-1.861025	-1.367662	0.185222
H	-2.281694	1.158859	0.621841
H	0.454272	1.928494	-0.528377
H	2.771855	0.649527	-0.715880
H	1.331801	-1.188015	1.266280
H	0.351514	-1.777138	-1.034071
H	-0.858204	3.044974	0.130666
H	3.358659	0.108983	0.951862
H	-1.649994	-2.410949	-0.011010
H	-2.823709	-1.126954	0.618691
H	0.605590	-0.106921	-1.526792

3 NH2 E

SCF Energy: -328.039438731

Num. Imaginary Frequencies: 0

C	-2.404878	-1.438812	-0.297973
C	-1.082427	-1.365886	-0.250664
C	-0.300839	-0.590729	0.774431
C	0.566378	0.465681	0.136368
C	1.846555	0.222777	-0.210469
C	0.002342	1.770364	-0.173429
C	-1.253926	2.171986	0.040514
H	0.694311	2.473714	-0.629944
H	-2.002537	1.522312	0.474821
H	-3.021484	-0.933925	0.437320
H	-0.489978	-1.876626	-1.005107
H	0.319258	-1.282524	1.351689
H	-1.566747	3.171992	-0.225716
H	-2.914898	-2.002581	-1.067860
N	2.520690	-0.966602	-0.097242
H	2.423930	1.011757	-0.678737
H	-0.988916	-0.132528	1.487084
H	3.525349	-0.919691	-0.079613
H	2.137650	-1.677978	0.504095

3 NH2 Z

SCF Energy: -328.036952597

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-2.983978	-0.475462	-0.336076
C	-1.731685	-0.906333	-0.380764
C	-0.714976	-0.734367	0.715418
C	0.566646	-0.088481	0.244713
C	1.676756	-0.843249	0.117264
C	0.573755	1.336212	-0.057783
C	-0.458741	2.173794	0.071393
H	1.511863	1.759373	-0.403530
H	-1.431919	1.839430	0.404954
H	-3.362084	0.063139	0.526072
H	-1.379909	-1.436816	-1.261845
H	-0.474540	-1.721284	1.118906
H	-0.351155	3.224263	-0.161297
H	-3.671877	-0.642975	-1.154268
H	1.626484	-1.892786	0.384196
N	2.937578	-0.436745	-0.262051
H	-1.160841	-0.157781	1.530981
H	3.546044	-1.163541	-0.599405
H	3.018225	0.413518	-0.795393

3 NO2 E

SCF Energy: -477.190513027

Num. Imaginary Frequencies: 0

C	-2.506306	-1.924702	-0.365625
C	-1.254420	-1.508372	-0.252916
C	-0.781244	-0.528873	0.789220
C	-0.194883	0.700023	0.145816
C	1.085836	0.862372	-0.215341
C	-1.074601	1.837648	-0.150250
C	-2.390973	1.856193	0.039153
H	-0.591906	2.708043	-0.579431
H	-2.937425	1.017817	0.447739
H	-3.283737	-1.571726	0.302078
H	-0.491676	-1.875374	-0.930840
H	-0.031548	-1.004501	1.417159
H	-2.967569	2.730513	-0.228625
H	-2.794295	-2.638687	-1.125486
N	2.131412	-0.115883	-0.041993
H	1.476857	1.773145	-0.637978
H	-1.613458	-0.235375	1.425543
O	3.272751	0.300444	-0.125804
O	1.854052	-1.282745	0.158734

3 NO2 Z

SCF Energy: -477.188399184

Num. Imaginary Frequencies: 0

C	-3.563200	-0.717018	-0.434640
C	-2.274788	-1.018545	-0.401263
C	-1.359720	-0.719184	0.755979
C	-0.111064	0.020070	0.323864
C	1.017771	-0.702423	0.320137
C	-0.235852	1.414510	-0.105811
C	-1.345304	2.132731	0.057065
H	0.620967	1.866795	-0.578253
H	-2.236007	1.743412	0.529741
H	-4.043633	-0.198340	0.387125
H	-1.818135	-1.537743	-1.238421
H	-1.062715	-1.657499	1.225845
H	-1.384619	3.157415	-0.285956
H	-4.181048	-0.980896	-1.282225
H	1.053078	-1.747297	0.579765
N	2.331949	-0.239141	-0.068476
H	-1.889950	-0.136905	1.510237
O	3.152916	-1.110340	-0.292075
O	2.578504	0.948365	-0.140490

3 OH E

SCF Energy: -347.909419332

Num. Imaginary Frequencies: 0

C	-2.499942	-1.311618	-0.247247
C	-1.175921	-1.284356	-0.291383
C	-0.292248	-0.628385	0.733752
C	0.602774	0.417570	0.118526
C	1.872238	0.143543	-0.200509
C	0.089098	1.750914	-0.175736
C	-1.151501	2.180294	0.056225
H	0.801841	2.437084	-0.624716
H	-1.909885	1.541157	0.489026
H	-3.045081	-0.841603	0.563723
H	-0.656795	-1.759264	-1.119389
H	0.333563	-1.389982	1.201981
H	-1.442260	3.191667	-0.191379
H	-3.082472	-1.803355	-1.014983
O	2.421823	-1.077257	0.013514
H	2.519350	0.887593	-0.650694
H	-0.907711	-0.182537	1.517362
H	3.347878	-1.070486	-0.240813

3 OH Z

SCF Energy: -347.908052970

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C -2.983256 -0.444719 -0.313217
C -1.734427 -0.881375 -0.382250
C -0.708551 -0.741549 0.709670
C 0.573577 -0.101348 0.237901
C 1.668923 -0.856865 0.099646
C 0.612460 1.325558 -0.071445
C -0.404234 2.175577 0.074971
H 1.560328 1.702022 -0.439169
H -1.375175 1.855592 0.429400
H -3.348711 0.076129 0.564987
H -1.394398 -1.393997 -1.278101
H -0.475090 -1.737206 1.095290
H -0.288279 3.223859 -0.164069
H -3.680706 -0.590260 -1.127385
H 1.661733 -1.914360 0.337246
O 2.851867 -0.356424 -0.341449
H -1.136339 -0.171253 1.538181
H 3.514760 -1.050800 -0.356448

3 OMe E

SCF Energy: -387.200987633

Num. Imaginary Frequencies: 0

C -2.673221 -1.734029 -0.286061
C -1.379160 -1.449228 -0.283101
C -0.681003 -0.620379 0.759799
C 0.013691 0.573183 0.155228
C 1.323335 0.547140 -0.122327
C -0.737739 1.777753 -0.178015
C -2.045922 1.959531 0.005023
H -0.155841 2.584972 -0.614043
H -2.680784 1.188843 0.421997
H -3.330606 -1.370450 0.495882
H -0.745462 -1.823141 -1.082645
H 0.065307 -1.237611 1.262686
H -2.518593 2.892551 -0.268414
H -3.118444 -2.339076 -1.064691
O 2.093130 -0.533729 0.116565
H 1.828636 1.400781 -0.565371
H -1.401387 -0.295091 1.512720
C 3.480959 -0.350487 -0.128560
H 3.965275 -1.298897 0.081318
H 3.652905 -0.074950 -1.169974
H 3.888308 0.420994 0.526100

3 OMe Z

SCF Energy: -387.199526820

Num. Imaginary Frequencies: 0

C -3.354832 -0.866045 -0.364248
C -2.048201 -1.084311 -0.381324
C -1.100105 -0.741647 0.735991
C 0.072004 0.092637 0.281784
C 1.282904 -0.473956 0.197797
C -0.117161 1.496933 -0.070367
C -1.266175 2.167650 0.018567
H 0.767379 2.017491 -0.419528
H -2.182269 1.698238 0.351980
H -3.834498 -0.392366 0.485245
H -1.594398 -1.555220 -1.249232
H -0.716248 -1.671974 1.162181
H -1.318269 3.214258 -0.248607
H -3.988129 -1.150853 -1.193878
H 1.442551 -1.513376 0.470391
O 2.378165 0.191296 -0.228580
H -1.647205 -0.228675 1.531117
C 3.587790 -0.551340 -0.176977
H 4.371064 0.095645 -0.559365
H 3.820042 -0.837948 0.849684
H 3.517323 -1.445118 -0.798690

3 tBut E

SCF Energy: -429.904706786

Num. Imaginary Frequencies: 0

2 *CARTESIAN COORDINATES*

C	-3.080495	-1.810169	-0.199920
C	-1.828555	-1.387755	-0.297679
C	-1.130865	-0.519871	0.715323
C	-0.528936	0.718223	0.091226
C	0.766904	0.873606	-0.215768
C	-1.441758	1.829148	-0.219057
C	-2.752934	1.863911	0.010282
H	-0.972791	2.693518	-0.679661
H	-3.287016	1.034482	0.453907
H	-3.704394	-1.534606	0.642997
H	-1.232456	-1.675906	-1.159041
H	-0.352417	-1.101602	1.204608
H	-3.335195	2.736548	-0.252465
H	-3.523541	-2.444604	-0.956000
C	1.949768	-0.059994	-0.028366
H	1.028025	1.830771	-0.662131
H	-1.840219	-0.232371	1.493762
C	3.150713	0.563659	-0.750177
C	2.301818	-0.188793	1.461126
C	1.707957	-1.448445	-0.635994
H	3.186435	-0.818081	1.578925
H	2.520914	0.790642	1.888386
H	1.491175	-0.634023	2.036495
H	4.035390	-0.062456	-0.627542
H	2.949433	0.666899	-1.817960
H	3.373209	1.553494	-0.348102
H	2.630571	-2.030321	-0.589582
H	0.938782	-2.009800	-0.109639
H	1.412383	-1.363701	-1.682928

3 tBut Z

SCF Energy: -429.902922477
Num. Imaginary Frequencies: 0

C	3.949469	-0.801067	0.399386
C	2.654713	-1.071065	0.321995
C	1.757658	-0.694748	-0.825630
C	0.505019	0.031154	-0.375768
C	-0.660673	-0.632045	-0.365690
C	0.650900	1.429989	0.047064
C	1.780658	2.135346	0.006585
H	-0.236170	1.925988	0.414394
H	2.716377	1.716351	-0.337254
H	4.458008	-0.251702	-0.385214
H	2.173303	-1.619847	1.127140
H	1.453411	-1.608582	-1.339861
H	1.796110	3.167791	0.328533
H	4.544567	-1.118518	1.245297
H	-0.616844	-1.660542	-0.716420
C	-2.052273	-0.188874	0.057910
H	2.317680	-0.093563	-1.545197
C	-2.998628	-1.377354	-0.153540
C	-2.096849	0.186295	1.546102
C	-2.562661	0.974788	-0.804014
H	-4.015335	-1.110835	0.138249
H	-3.011397	-1.680174	-1.202025
H	-2.683920	-2.234096	0.444905
H	-3.591070	1.214299	-0.526010
H	-1.964062	1.875730	-0.685450
H	-2.551535	0.700012	-1.859737
H	-3.122515	0.424962	1.834750
H	-1.756991	-0.649482	2.159474
H	-1.473606	1.047691	1.778021

4 BH2

SCF Energy: -411.413851683
Num. Imaginary Frequencies: 0

C	0.147468	1.058009	-0.808290
C	1.328773	1.292280	0.135171
C	2.196039	0.058001	0.182084
C	1.471516	-1.205225	-0.205533
O	0.108025	-1.173238	0.218996
C	-0.626250	-0.141844	-0.321105
C	3.481674	0.058748	0.502653
C	-1.930969	-0.210269	-0.339327
C	-3.246968	-0.204016	-0.291929
H	1.912517	-2.080302	0.264416
H	4.005336	0.980727	0.721966
H	1.505810	-1.345065	-1.290777
B	-3.969558	0.311161	0.966660
H	-3.793164	-0.576426	-1.155881
H	4.050896	-0.861292	0.550942
H	-0.512202	1.920808	-0.853034
H	0.516389	0.873891	-1.820387
H	0.942162	1.499829	1.136348
H	1.910071	2.159418	-0.174559
H	-5.157482	0.308001	1.033616
H	-3.324443	0.716405	1.879749

4 CH3

SCF Energy: -425.291646775

Num. Imaginary Frequencies: 0

C	-0.278144	1.189066	0.509420
C	-1.633486	1.258738	-0.196823
C	-2.374342	-0.041449	-0.002851
C	-1.472078	-1.204646	0.319584
O	-0.222567	-1.099445	-0.359559
C	0.509560	0.028965	-0.045752
C	-3.691210	-0.171785	-0.074657
C	1.793195	0.059130	-0.294567
C	3.068379	0.137309	-0.555902
H	-1.910083	-2.148680	0.005613
H	-4.331845	0.683558	-0.249385
H	-1.292620	-1.254359	1.398844
H	3.380916	0.465609	-1.545202
C	4.170418	-0.196999	0.410179
H	-4.169487	-1.136232	0.044011
H	0.293328	2.104307	0.378807
H	-0.434573	1.052172	1.582772
H	-1.464696	1.420953	-1.264718
H	-2.225568	2.096718	0.168381
H	4.812844	0.670779	0.567544
H	3.769376	-0.516144	1.369383
H	4.799198	-0.993100	0.008636

4 CHO

SCF Energy: -499.314342879

Num. Imaginary Frequencies: 0

C	-0.675825	0.920719	1.013329
C	-1.761902	1.318629	0.011814
C	-2.651735	0.133842	-0.280534
C	-2.041482	-1.191904	0.088503
O	-0.635517	-1.216755	-0.180722
C	0.090356	-0.248015	0.451783
C	-3.872047	0.223549	-0.788468
C	1.394469	-0.336298	0.505621
C	2.704304	-0.342973	0.517100
H	-2.467754	-2.005963	-0.490795
H	-4.325085	1.185103	-0.994759
H	-2.202669	-1.403530	1.149741
C	3.457453	0.247636	-0.604196
H	3.283985	-0.772612	1.328210
H	-4.457432	-0.660526	-1.007928
H	0.009126	1.739260	1.216571
H	-1.133511	0.629697	1.961885
H	-1.282583	1.648714	-0.913066
H	-2.347090	2.155683	0.389469
O	4.663514	0.273844	-0.659236
H	2.837498	0.676347	-1.409378

4 CN

SCF Energy: -478.233433559

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-0.510077	1.142323	0.598012
C	-1.890413	1.271988	-0.049595
C	-2.626258	-0.044841	0.031418
C	-1.738286	-1.222809	0.328452
O	-0.478514	-1.114945	-0.346132
C	0.229957	0.015087	-0.071318
C	-3.935959	-0.178190	-0.116529
C	1.482775	0.107361	-0.434527
C	2.721082	0.269293	-0.822212
H	-2.176922	-2.155029	-0.015247
H	-4.573823	0.682757	-0.272230
H	-1.556328	-1.303036	1.404043
H	2.983994	0.649712	-1.803395
C	3.822849	-0.058348	0.039725
H	-4.410877	-1.150510	-0.080325
H	0.067535	2.058351	0.511128
H	-0.615849	0.917755	1.661974
H	-1.762154	1.551795	-1.097853
H	-2.464727	2.064242	0.428105
N	4.714749	-0.315379	0.716043

4 F

SCF Energy: -485.230981998

Num. Imaginary Frequencies: 0

C	-0.231453	1.148653	0.617853
C	-1.550476	1.286401	-0.146052
C	-2.331893	-0.003968	-0.067195
C	-1.517180	-1.180070	0.397404
O	-0.196414	-1.159412	-0.156817
C	0.527366	-0.031142	0.075983
C	-3.621368	-0.115613	-0.350145
C	1.807088	-0.004297	-0.214212
C	3.044114	0.108347	-0.574958
H	-1.954833	-2.122986	0.082609
H	-4.211818	0.748262	-0.628645
H	-1.440770	-1.183030	1.488691
H	3.410777	0.407117	-1.547807
F	4.072743	-0.156558	0.274131
H	-4.127383	-1.071765	-0.305695
H	0.383045	2.040014	0.531735
H	-0.433409	0.987716	1.679878
H	-1.329496	1.512973	-1.191695
H	-2.136684	2.116148	0.246214

4 H

SCF Energy: -385.979987528

Num. Imaginary Frequencies: 0

C	-1.043011	1.267517	-0.250398
C	-1.848698	0.002968	-0.077419
C	-1.026694	-1.179842	0.364283
O	0.276554	-1.155509	-0.216785
C	1.024778	-0.041874	0.099474
C	0.252799	1.169189	0.556749
C	-3.158092	-0.081815	-0.262855
C	2.322204	-0.065254	-0.062947
C	3.611684	-0.039924	-0.242444
H	-1.478461	-2.118597	0.054548
H	-3.746185	0.789148	-0.523727
H	-0.933671	-1.189279	1.455298
H	4.046896	0.229617	-1.199086
H	4.301384	-0.291194	0.556294
H	-3.682782	-1.022967	-0.154343
H	0.871161	2.055081	0.438366
H	0.014592	1.076518	1.619626
H	-0.789774	1.391639	-1.306548
H	-1.625415	2.138310	0.047191

4 NH2

SCF Energy: -441.343168351

Num. Imaginary Frequencies: 0

C	-0.269907	1.060094	0.799520
C	-1.453391	1.295012	-0.141139
C	-2.317344	0.058750	-0.191641
C	-1.604239	-1.189569	0.257599
O	-0.237276	-1.189372	-0.148652
C	0.520360	-0.134285	0.324303
C	-3.589228	0.047010	-0.563986
C	1.825237	-0.198833	0.281856
C	3.135437	-0.185130	0.276840
H	-2.049816	-2.081266	-0.176151
H	-4.105702	0.961009	-0.829595
H	-1.656449	-1.279672	1.347788
N	3.957684	0.303037	-0.740465
H	3.683871	-0.532174	1.147899
H	-4.154473	-0.875637	-0.609706
H	0.387066	1.924278	0.844071
H	-0.640196	0.878208	1.812292
H	-1.068155	1.506087	-1.142282
H	-2.037558	2.160560	0.168812
H	4.847111	-0.167518	-0.810720
H	3.507169	0.381554	-1.640043

4 NO2

SCF Energy: -590.500455666

Num. Imaginary Frequencies: 0

C	-0.973429	0.259274	1.399922
C	-1.992419	1.135272	0.666258
C	-2.880363	0.281384	-0.209114
C	-2.373337	-1.118845	-0.417102
O	-0.948351	-1.142382	-0.597671
C	-0.226198	-0.555835	0.381687
C	-4.021460	0.693347	-0.740854
C	1.080900	-0.661329	0.390736
C	2.373908	-0.719276	0.446778
H	-2.787162	-1.570488	-1.313445
H	-4.408589	1.684414	-0.540333
H	-2.625129	-1.751013	0.438614
N	3.199043	0.276341	-0.267046
H	2.993256	-1.435421	0.965114
H	-4.606241	0.050923	-1.386892
H	-0.271206	0.850736	1.980194
H	-1.484830	-0.419375	2.086667
H	-1.454667	1.855982	0.046457
H	-2.586347	1.703268	1.380615
O	4.401058	0.130609	-0.176260
O	2.661294	1.163353	-0.888261

4 OH

SCF Energy: -461.213088283

Num. Imaginary Frequencies: 0

C	-0.267050	1.071403	0.807031
C	-1.451812	1.300152	-0.133829
C	-2.303669	0.055295	-0.198852
C	-1.602995	-1.181750	0.295920
O	-0.226542	-1.197276	-0.086044
C	0.519457	-0.123725	0.334857
C	-3.559215	0.028137	-0.621766
C	1.825066	-0.165273	0.251875
C	3.128169	-0.166903	0.229889
H	-2.040623	-2.084040	-0.122758
H	-4.070985	0.934249	-0.921267
H	-1.671935	-1.243189	1.386658
O	3.854076	0.225858	-0.863409
H	3.716483	-0.487087	1.084097
H	-4.115546	-0.899296	-0.676057
H	0.389460	1.935794	0.847379
H	-0.633207	0.888611	1.820924
H	-1.068065	1.527404	-1.131619
H	-2.044596	2.156038	0.186147
H	4.791030	0.138849	-0.668625

4 OMe

SCF Energy: -500.504318667

Num. Imaginary Frequencies: 0

C	-0.830408	1.061020	0.843106
C	-1.971045	1.304138	-0.147345
C	-2.828178	0.066178	-0.257067
C	-2.156087	-1.179917	0.254482
O	-0.764690	-1.199912	-0.068638
C	-0.031353	-0.136088	0.397095
C	-4.066406	0.051666	-0.728823
C	1.276186	-0.186793	0.374974
C	2.580200	-0.193704	0.411530
H	-2.580519	-2.075441	-0.191443
H	-4.559933	0.963910	-1.040056
H	-2.271849	-1.251680	1.340604
O	3.357110	0.209552	-0.634356
H	3.130288	-0.526125	1.289064
H	-4.626525	-0.871281	-0.812766
H	-0.170911	1.920780	0.918521
H	-1.241786	0.873682	1.838667
H	-1.542191	1.534125	-1.125969
H	-2.570954	2.162684	0.151475
C	4.753077	0.063047	-0.417365
H	5.249502	0.431707	-1.309775
H	5.075459	0.648479	0.445430
H	5.014137	-0.985250	-0.263311

4 tBut

SCF Energy: -543.220731036

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	1.423377	1.025428	-0.951905
C	2.450676	1.285499	0.151661
C	3.356988	0.087267	0.293839
C	2.756236	-1.187827	-0.239335
O	1.348654	-1.235930	-0.014958
C	0.634809	-0.211599	-0.604421
C	4.578569	0.128039	0.806068
C	-0.657692	-0.329985	-0.766051
C	-1.955343	-0.379956	-0.879076
H	3.172504	-2.062252	0.254337
H	5.020802	1.061424	1.131299
H	2.953266	-1.276595	-1.312907
C	-2.956293	0.029926	0.185608
H	-2.398015	-0.745204	-1.805828
H	5.175784	-0.769312	0.911117
H	0.739314	1.861700	-1.071723
H	1.939890	0.885340	-1.905276
H	1.918436	1.448404	1.092933
H	3.030620	2.184413	-0.052603
C	-3.849633	1.129901	-0.398635
C	-3.817476	-1.190934	0.527473
C	-2.257399	0.540670	1.439928
H	-2.996869	0.829360	2.188391
H	-1.614385	-0.229544	1.868538
H	-1.637558	1.409903	1.213759
H	-4.585780	-0.917567	1.253044
H	-4.313640	-1.579282	-0.363685
H	-3.207284	-1.987733	0.954787
H	-4.616823	1.414336	0.323795
H	-3.262525	2.015809	-0.644636
H	-4.347872	0.785674	-1.306603

6 BH2 E

SCF Energy: -411.467140959
 Num. Imaginary Frequencies: 0

C	-0.647607	1.324824	0.113763
C	0.796066	1.756667	0.189907
C	1.686218	0.769315	-0.568658
C	1.580986	-0.626844	-0.000779
C	0.292481	-0.937363	0.734232
C	-0.873116	-0.171414	0.178161
C	2.545654	-1.527738	-0.126663
C	-2.040075	-0.674488	-0.257387
O	-1.562032	2.105872	-0.003384
H	2.432911	-2.533277	0.258323
H	3.478162	-1.283830	-0.620307
H	1.366659	0.750067	-1.614859
H	2.721914	1.104105	-0.563242
H	0.417759	-0.619405	1.776907
B	-2.421360	-2.169392	-0.279832
H	-2.755098	0.069500	-0.598746
H	1.079061	1.779312	1.247232
H	0.877350	2.769873	-0.196500
H	0.100750	-2.005989	0.752044
H	-3.545213	-2.487796	-0.502239
H	-1.614837	-3.020337	-0.087843

6 BH2 Z

SCF Energy: -411.512686802

Num. Imaginary Frequencies: 0

C	-0.805645	-1.315742	0.394555
C	0.573719	-0.757716	0.150273
C	0.781482	0.649453	-0.047318
C	-0.318225	1.648959	-0.073790
C	-1.594225	1.082822	0.564368
C	-1.869690	-0.304400	0.047828
C	1.786850	-1.359145	0.069095
B	2.889028	-0.259214	-0.196293
O	1.984038	0.998874	-0.230334
C	-2.941967	-0.605289	-0.672721
H	-3.101966	-1.606207	-1.053479
H	-3.694222	0.140381	-0.897592
H	-1.456974	1.042771	1.648494
H	-2.432231	1.745802	0.360112
H	-0.948378	-2.238251	-0.166636
H	1.900571	-2.431883	0.178021
H	-0.500370	1.883240	-1.127530
H	0.016255	2.569775	0.403264
H	-0.897613	-1.567421	1.456271
H	3.687610	-0.120576	0.700062
H	3.436078	-0.346210	-1.270590

6 CHO E

SCF Energy: -499.367254020

Num. Imaginary Frequencies: 0

C	0.390962	1.544755	0.117789
C	1.881367	1.319098	0.120710
C	2.222392	0.031355	-0.634168
C	1.558983	-1.176916	-0.013934
C	0.319931	-0.890264	0.810952
C	-0.440136	0.290155	0.275807
C	2.020647	-2.409719	-0.168510
C	-1.725154	0.344585	-0.083302
O	-0.115533	2.632599	-0.015903
H	1.507651	-3.263024	0.256353
H	2.928658	-2.600394	-0.726767
H	1.875249	0.134106	-1.666448
H	3.300612	-0.110322	-0.678713
H	0.643819	-0.623247	1.824130
C	-2.662878	-0.785174	-0.037190
H	-2.131881	1.281329	-0.446664
H	2.203916	1.239509	1.163712
H	2.365259	2.192081	-0.310417
H	-0.291635	-1.782036	0.906575
O	-3.825120	-0.672157	-0.351916
H	-2.273109	-1.758783	0.291866

6 CHO Z

SCF Energy: -499.366435623

Num. Imaginary Frequencies: 0

C	-0.219734	1.223414	0.281625
C	1.167558	1.702735	-0.076848
C	1.942284	0.642779	-0.860145
C	2.070287	-0.642654	-0.078904
C	0.930784	-0.930064	0.882832
C	-0.341072	-0.268736	0.431954
C	3.097302	-1.470166	-0.210121
C	-1.457731	-0.944998	0.149126
O	-1.146078	1.976522	0.470723
H	3.145207	-2.402836	0.337508
H	3.921678	-1.236952	-0.872151
H	1.401738	0.436657	-1.789046
H	2.925093	1.014869	-1.142708
H	1.198121	-0.513814	1.860927
H	-1.483173	-2.021307	0.283489
C	-2.699511	-0.360044	-0.388051
H	1.678251	1.925710	0.865883
H	1.074003	2.639316	-0.622695
H	0.787692	-2.000391	1.014734
O	-3.719863	-1.005671	-0.469031
H	-2.662083	0.678340	-0.738288

6 CN E

SCF Energy: -478.292319942

Num. Imaginary Frequencies: 0

C	0.508282	1.540900	0.089557
C	1.932763	1.085336	0.257914
C	2.153855	-0.229020	-0.497960
C	1.241854	-1.331232	-0.006498
C	-0.015499	-0.878402	0.708765
C	-0.515163	0.433917	0.188430
C	1.514605	-2.616589	-0.179428
C	-1.762843	0.705467	-0.194182
O	0.187306	2.684228	-0.125389
H	0.830456	-3.388850	0.147960
H	2.434026	-2.933286	-0.655643
H	1.956987	-0.054084	-1.559429
H	3.194475	-0.538296	-0.419798
H	0.230909	-0.729124	1.767075
C	-2.805518	-0.269997	-0.156103
H	-2.025349	1.694064	-0.547866
H	2.109657	0.935767	1.327750
H	2.596220	1.875236	-0.084863
H	-0.787142	-1.644681	0.668538
N	-3.650386	-1.047551	-0.129083

6 CN Z

SCF Energy: -478.290242381

Num. Imaginary Frequencies: 0

C	-0.446542	1.050946	0.283353
C	0.890980	1.737325	0.175767
C	1.849353	0.912722	-0.687662
C	2.079720	-0.466540	-0.114563
C	0.971249	-0.998066	0.772844
C	-0.369299	-0.450562	0.380667
C	3.173646	-1.173927	-0.358205
C	-1.414341	-1.233228	0.109088
O	-1.500744	1.638355	0.288138
H	3.299035	-2.174526	0.035303
H	3.977537	-0.769953	-0.960619
H	1.414279	0.811944	-1.686343
H	2.796486	1.434774	-0.809319
H	1.169240	-0.665901	1.798953
H	-1.320187	-2.310612	0.162873
C	-2.711476	-0.771872	-0.281857
H	1.291096	1.838386	1.189852
H	0.734032	2.738103	-0.219247
H	0.963610	-2.085806	0.785311
N	-3.779845	-0.509148	-0.611210

6 F E

SCF Energy: -485.291783365

Num. Imaginary Frequencies: 0

C	-0.606265	1.338234	0.101334
C	0.829854	1.756731	0.295746
C	1.759022	0.813498	-0.475887
C	1.627805	-0.620999	-0.014158
C	0.327484	-0.972180	0.679206
C	-0.817340	-0.134869	0.180624
C	2.587966	-1.517916	-0.192962
C	-1.987946	-0.609885	-0.217397
O	-1.499573	2.127539	-0.120220
H	2.461920	-2.548524	0.113845
H	3.530282	-1.246297	-0.652363
H	1.499152	0.867988	-1.537017
H	2.792684	1.144128	-0.389531
H	0.448034	-0.772858	1.749733
F	-2.261500	-1.914976	-0.200260
H	-2.806255	-0.007615	-0.585206
H	1.052107	1.703554	1.366339
H	0.939723	2.791291	-0.020114
H	0.108961	-2.032884	0.579374

6 F Z

SCF Energy: -485.288144348

Num. Imaginary Frequencies: 0

C	-0.793056	0.990663	0.201936
C	0.515671	1.747289	0.228315
C	1.582231	1.010376	-0.586770
C	1.845247	-0.378040	-0.048770
C	0.715655	-0.979883	0.759346
C	-0.629579	-0.488543	0.288398
C	2.982928	-1.026037	-0.258794
C	-1.572557	-1.349793	-0.071650
O	-1.865031	1.546151	0.109540
H	3.134509	-2.033271	0.108348
H	3.797470	-0.566888	-0.805086
H	1.229892	0.927645	-1.619076
H	2.505696	1.586163	-0.616088
H	0.842615	-0.674751	1.803567
H	-1.453128	-2.425632	-0.054348
F	-2.772124	-0.983584	-0.515430
H	0.832804	1.827051	1.273149
H	0.337732	2.754060	-0.142289
H	0.762535	-2.067531	0.742304

6 H

SCF Energy: -386.038472841

Num. Imaginary Frequencies: 0

C	0.274032	-1.588563	0.340812
C	-1.009188	-1.260743	-0.428977
C	-1.595257	0.071967	-0.016810
C	-0.623497	1.037300	0.627603
C	0.773427	0.879965	0.089315
C	1.514615	1.867963	-0.397096
C	1.312774	-0.520672	0.096853
O	2.480676	-0.774664	-0.097639
C	-2.872273	0.377706	-0.203167
H	-3.264585	1.350177	0.066323
H	-3.563563	-0.337322	-0.631913
H	-0.770272	-1.225285	-1.495865
H	-1.744292	-2.053404	-0.299618
H	-0.596788	0.819664	1.701896
H	1.144816	2.884147	-0.440313
H	2.512893	1.671529	-0.765719
H	0.066952	-1.613236	1.415506
H	0.688080	-2.553453	0.057977
H	-0.966450	2.064949	0.521641

6 Me E

SCF Energy: -425.351352129

2 *CARTESIAN COORDINATES*

Num. Imaginary Frequencies: 0

C	-0.351964	1.436532	0.095060
C	1.136187	1.633419	0.266682
C	1.901414	0.544156	-0.490227
C	1.537164	-0.842035	-0.005567
C	0.222794	-0.944027	0.737715
C	-0.807786	0.015294	0.198829
C	2.314162	-1.896924	-0.212835
C	-2.044381	-0.285713	-0.201800
O	-1.102908	2.362849	-0.129674
H	2.020307	-2.887002	0.112325
H	3.269003	-1.800635	-0.715083
H	1.652573	0.623651	-1.552308
H	2.975438	0.704113	-0.408124
H	0.409645	-0.684185	1.786427
C	-2.704860	-1.620641	-0.212947
H	-2.643619	0.544516	-0.563330
H	1.362924	1.572358	1.335779
H	1.399248	2.631816	-0.074484
H	-0.134585	-1.970282	0.733480
H	-3.068523	-1.847995	-1.216466
H	-2.053137	-2.426369	0.112698
H	-3.582393	-1.603142	0.437023

6 Me Z

SCF Energy: -425.348815421

Num. Imaginary Frequencies: 0

C	-0.730200	1.008810	0.234960
C	0.589536	1.743639	0.130018
C	1.606743	0.936049	-0.678331
C	1.870530	-0.414362	-0.053096
C	0.746272	-0.948330	0.809216
C	-0.604824	-0.473073	0.330249
C	2.999632	-1.084734	-0.240866
C	-1.576186	-1.315363	-0.032506
O	-1.790856	1.599254	0.248549
H	3.150756	-2.066569	0.190088
H	3.806884	-0.670721	-0.832450
H	1.203578	0.784361	-1.684138
H	2.536793	1.490465	-0.793022
H	0.902415	-0.581691	1.830351
H	-1.353741	-2.375485	0.057107
C	-2.932346	-0.987942	-0.565409
H	0.959496	1.897983	1.149081
H	0.403566	2.724519	-0.302200
H	0.777572	-2.035641	0.856167
H	-3.234269	-1.736782	-1.296572
H	-3.668172	-1.014083	0.242514
H	-2.972969	0.001445	-1.010728

6 NH2 E

SCF Energy: -441.414436781

Num. Imaginary Frequencies: 0

C	-0.449100	1.366526	0.071526
C	1.004662	1.657222	0.381060
C	1.906817	0.677480	-0.374146
C	1.597513	-0.762922	-0.028395
C	0.256269	-1.004891	0.631794
C	-0.803267	-0.042779	0.154773
C	2.445474	-1.751260	-0.283464
C	-2.068999	-0.400862	-0.176616
O	-1.223170	2.267163	-0.235818
H	2.196548	-2.781133	-0.059451
H	3.416045	-1.559485	-0.724748
H	1.749490	0.823464	-1.446523
H	2.956885	0.893965	-0.180285
H	0.388140	-0.892175	1.714879
N	-2.604762	-1.629214	-0.133265
H	-2.741214	0.379966	-0.511740
H	1.155869	1.541888	1.458950
H	1.220869	2.690196	0.118390
H	-0.037866	-2.042056	0.471692
H	-3.543941	-1.787948	-0.448280
H	-2.078353	-2.430578	0.167329

6 NH2 Z

SCF Energy: -441.417568915

Num. Imaginary Frequencies: 0

C	-0.720187	0.962407	0.150782
C	0.577732	1.708102	0.372575
C	1.707604	1.037931	-0.417585
C	1.866935	-0.426578	-0.062113
C	0.717757	-1.028052	0.715099
C	-0.614754	-0.470914	0.273993
C	2.938184	-1.129182	-0.408509
C	-1.673453	-1.285553	-0.007779
O	-1.758741	1.562574	-0.144161
H	3.022003	-2.182500	-0.171439
H	3.764330	-0.672188	-0.940002
H	1.475538	1.118614	-1.482894
H	2.647014	1.567725	-0.262125
H	0.878369	-0.795320	1.775134
H	-1.543561	-2.360409	0.062591
N	-2.896235	-0.890767	-0.374535
H	0.811253	1.683632	1.441523
H	0.444100	2.747121	0.079858
H	0.731071	-2.114661	0.632493
H	-3.605532	-1.563898	-0.598517
H	-3.079924	0.097697	-0.460367

6 NO2 E

SCF Energy: -590.550669141

Num. Imaginary Frequencies: 0

C	0.797305	1.558943	0.157918
C	2.245362	1.166028	0.248198
C	2.492722	-0.092828	-0.586361
C	1.663586	-1.257491	-0.099369
C	0.405544	-0.914634	0.674887
C	-0.182457	0.397205	0.249699
C	2.005484	-2.519220	-0.318199
C	-1.434284	0.697192	-0.068749
O	0.417144	2.694121	0.017830
H	1.380052	-3.339602	0.009567
H	2.925457	-2.767079	-0.832516
H	2.229512	0.122748	-1.625918
H	3.549764	-0.351580	-0.577946
H	0.672125	-0.803140	1.733525
N	-2.534580	-0.255065	-0.072108
H	-1.742145	1.671815	-0.412049
H	2.472901	0.967895	1.300284
H	2.853982	2.006308	-0.075662
H	-0.314640	-1.722356	0.619736
O	-3.433646	-0.020880	-0.852573
O	-2.514064	-1.199581	0.686942

6 NO2 Z

SCF Energy: -590.548071538

Num. Imaginary Frequencies: 0

C	-0.127439	-0.526397	0.318412
C	0.110453	0.947018	0.537559
C	1.034492	1.555240	-0.489183
C	1.880086	0.474181	-1.187020
C	2.303146	-0.558916	-0.177078
C	1.146765	-1.321067	0.452893
O	-0.293630	1.518304	1.516195
C	3.562329	-0.773349	0.175350
C	-1.276888	-1.082889	-0.021942
N	-2.481169	-0.293108	-0.237517
H	3.820861	-1.496509	0.938633
H	4.372895	-0.234497	-0.297917
H	1.278713	-0.006186	-1.963619
H	2.742898	0.926840	-1.669952
H	1.349449	-1.498399	1.511077
H	-1.450607	-2.137938	-0.159776
H	1.659397	2.284981	0.024848
H	0.412224	2.093071	-1.208488
H	1.018163	-2.292971	-0.025448
O	-3.533972	-0.892279	-0.179229
O	-2.376583	0.890278	-0.479551

6 OH E

SCF Energy: -461.280155789

Num. Imaginary Frequencies: 0

C	-0.512429	1.362596	0.084842
C	0.938322	1.702533	0.336882
C	1.843324	0.728516	-0.424763
C	1.605009	-0.710302	-0.019445
C	0.285047	-0.987554	0.667929
C	-0.810626	-0.078221	0.178208
C	2.493954	-1.668452	-0.246745
C	-2.026913	-0.497135	-0.186687
O	-1.338317	2.214932	-0.191144
H	2.292878	-2.698709	0.018928
H	3.450527	-1.450291	-0.705729
H	1.635744	0.832273	-1.493557
H	2.890674	0.991689	-0.283334
H	0.422230	-0.820630	1.742689
O	-2.384016	-1.788667	-0.136099
H	-2.770426	0.208245	-0.538580
H	1.124303	1.616696	1.412111
H	1.114069	2.735230	0.045142
H	0.002945	-2.031571	0.548614
H	-3.278406	-1.904945	-0.469671

6 OH Z

SCF Energy: -461.275012386

Num. Imaginary Frequencies: 0

C	-0.730207	1.027564	0.162971
C	0.603286	1.731960	0.302952
C	1.681334	0.996820	-0.499516
C	1.837634	-0.441632	-0.053867
C	0.685285	-0.986924	0.758297
C	-0.642435	-0.439359	0.289397
C	2.905888	-1.170195	-0.350237
C	-1.645143	-1.275154	-0.017415
O	-1.757607	1.641595	-0.055936
H	2.982944	-2.206997	-0.047760
H	3.736246	-0.750667	-0.905123
H	1.394951	1.010888	-1.554750
H	2.633553	1.520748	-0.427504
H	0.839524	-0.690008	1.802014
H	-1.495727	-2.347409	0.062638
O	-2.856564	-0.887151	-0.436088
H	0.872826	1.741559	1.363650
H	0.486438	2.762869	-0.022790
H	0.685113	-2.076027	0.741349
H	-3.396350	-1.658979	-0.631016

6 OMe E

SCF Energy: -500.571717684

Num. Imaginary Frequencies: 0

C	0.419553	1.520048	0.090391
C	1.912020	1.347466	0.255719
C	2.382959	0.106848	-0.510058
C	1.693685	-1.154178	-0.035041
C	0.401573	-0.948144	0.726444
C	-0.345329	0.272269	0.257928
C	2.188788	-2.363240	-0.265580
C	-1.655202	0.290214	-0.021117
O	-0.080193	2.598919	-0.178473
H	1.665958	-3.256796	0.051710
H	3.133434	-2.495003	-0.779003
H	2.158396	0.253048	-1.570439
H	3.463838	-0.002003	-0.432078
H	0.651301	-0.818854	1.786119
O	-2.432250	-0.785065	0.103932
H	-2.132868	1.203527	-0.363535
H	2.122892	1.225788	1.322893
H	2.410975	2.251083	-0.086328
H	-0.227292	-1.833559	0.660895
C	-3.790208	-0.616706	-0.299596
H	-4.287577	-1.563109	-0.116074
H	-4.264196	0.169286	0.287540
H	-3.842349	-0.371706	-1.359909

6 OMe Z

SCF Energy: -500.566524800

Num. Imaginary Frequencies: 0

C	-0.019223	1.295806	0.180142
C	1.454669	1.646213	0.173333
C	2.245336	0.613129	-0.635218
C	2.082736	-0.784900	-0.078512
C	0.893470	-0.972878	0.835926
C	-0.287758	-0.135867	0.404526
C	2.920721	-1.772216	-0.366165
C	-1.486622	-0.709949	0.211700
O	-0.876431	2.138982	-0.007868
H	2.766728	-2.772550	0.018715
H	3.786902	-1.609118	-0.995859
H	1.877995	0.627919	-1.665211
H	3.299432	0.884461	-0.675564
H	1.193730	-0.664661	1.844035
H	-1.598879	-1.783060	0.355503
O	-2.590148	-0.065170	-0.158900
H	1.807054	1.654346	1.209496
H	1.569054	2.650743	-0.227328
H	0.621810	-2.025692	0.900817
C	-3.726114	-0.893873	-0.399598
H	-4.547375	-0.229071	-0.645275
H	-3.534646	-1.567393	-1.234651
H	-3.972460	-1.469212	0.492660

6 tBut E

SCF Energy: -543.273816412

Num. Imaginary Frequencies: 0

C	1.238397	1.582484	0.089233
C	2.667377	1.092885	0.157146
C	2.806599	-0.251003	-0.563379
C	1.886912	-1.302045	0.020213
C	0.751515	-0.766040	0.862858
C	0.202797	0.516246	0.286951
C	2.053171	-2.600471	-0.194702
C	-1.046209	0.781386	-0.101867
O	0.967113	2.743984	-0.130183
H	1.361930	-3.331334	0.206103
H	2.887108	-2.971028	-0.778269
H	2.553721	-0.106184	-1.617264
H	3.839965	-0.593502	-0.534428
H	1.144785	-0.542933	1.861776
C	-2.273961	-0.105027	-0.081475
H	-1.197433	1.781872	-0.500124
H	2.932809	0.978822	1.212783
H	3.316542	1.854832	-0.267639
H	-0.010377	-1.525764	0.994935
C	-3.445649	0.686536	-0.672028
C	-2.053923	-1.355284	-0.945819
C	-2.636713	-0.502582	1.356291
H	-3.553024	-1.095721	1.350563
H	-1.855363	-1.092311	1.831933
H	-2.809574	0.384804	1.966497
H	-2.964753	-1.956712	-0.955350
H	-1.821809	-1.072296	-1.973344
H	-1.240988	-1.978641	-0.577136
H	-4.350449	0.077567	-0.676717
H	-3.640979	1.585460	-0.085041
H	-3.230903	0.988692	-1.698345

6 tBut Z

SCF Energy: -543.269292847

Num. Imaginary Frequencies: 0

2 CARTESIAN COORDINATES

C	-0.480274	1.308834	-0.294522
C	-1.887533	1.646716	0.158235
C	-2.535542	0.480710	0.903649
C	-2.602625	-0.753167	0.036238
C	-1.509993	-0.847432	-1.008566
C	-0.247799	-0.143928	-0.554850
C	-3.539312	-1.682562	0.170848
C	0.894323	-0.814115	-0.375238
O	0.350858	2.173322	-0.468787
H	-3.541903	-2.573727	-0.444372
H	-4.331686	-1.579210	0.901833
H	-1.927070	0.256237	1.785374
H	-3.526832	0.750795	1.263607
H	-1.872296	-0.363297	-1.922597
H	0.840003	-1.870986	-0.631347
C	2.255378	-0.391339	0.144415
H	-2.465645	1.889755	-0.739401
H	-1.838909	2.550007	0.763404
H	-1.302784	-1.885989	-1.260000
C	3.032654	-1.671273	0.478549
C	3.016397	0.371632	-0.949184
C	2.165763	0.455885	1.418026
H	3.171545	0.626682	1.806410
H	1.707969	1.423408	1.234073
H	1.591176	-0.065579	2.185512
H	4.024265	0.603793	-0.598495
H	3.103733	-0.233697	-1.853074
H	2.503370	1.298374	-1.195516
H	4.029670	-1.421884	0.843293
H	2.520303	-2.247875	1.250911
H	3.139607	-2.303139	-0.404922

TS 2 BH2 E boat

SCF Energy: -298.013997014
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -685.1039

C	0.031690	1.365852	0.015976
C	-1.298681	1.295970	0.393681
C	-2.210462	0.565750	-0.363739
C	-1.491930	-1.327860	-0.304417
C	-0.332734	-1.336238	0.475832
C	0.762594	-0.564933	0.184537
C	2.072675	-0.631030	-0.077218
B	3.077637	0.514873	-0.203218
H	-0.426279	-1.610297	1.525096
H	-1.367445	-1.346621	-1.378461
H	-2.120151	0.613442	-1.440913
H	-1.537479	1.481592	1.436142
H	0.733617	1.900012	0.638929
H	-2.338421	-1.895660	0.058480
H	-3.225313	0.456779	-0.003857
H	2.439285	-1.648545	-0.205060
H	0.268122	1.355864	-1.042320
H	4.232190	0.256946	-0.342500
H	2.754773	1.657051	-0.177367

TS 2 BH2 E chair

SCF Energy: -298.045800963
 Num. Imaginary Frequencies: 1
 Imaginary Frequency: -376.3349

C	0.204180	-1.338115	0.188549
C	-0.989457	-1.196515	-0.478577
C	-2.116652	-0.529004	0.178554
C	-1.847183	1.005352	0.027123
C	-0.397135	1.290530	0.172274
C	0.636830	0.467463	-0.032109
C	1.992219	0.589568	-0.336100
B	3.106867	-0.207354	0.232079
H	-1.041139	-1.410030	-1.540189
H	0.210805	-1.389171	1.270228
H	1.021268	-1.841712	-0.300275
H	-0.121522	2.298773	0.464709
H	-2.441516	1.572400	0.743170
H	-2.185212	1.290828	-0.970184
H	-2.145297	-0.772550	1.238837
H	-3.073204	-0.769530	-0.277546
H	2.190112	1.396063	-1.039663
H	4.244751	0.084476	-0.002379
H	2.909791	-1.158443	0.934622

TS 2 BH2 Z boat

SCF Energy: -298.018949577
 Num. Imaginary Frequencies: 1

Imaginary Frequency: -698.2037

C	0.569616	-1.493960	-0.138795
C	1.770032	-0.973751	0.318382
C	2.341743	0.125882	-0.320979
C	0.932824	1.557793	-0.217395
C	-0.151244	1.076179	0.526620
C	-0.822053	-0.070812	0.191415
C	-2.026373	-0.597470	-0.048667
B	-3.253551	0.301900	-0.192947
H	-2.104613	-1.677996	-0.124083
H	-0.206676	1.341893	1.579865
H	0.822750	1.573914	-1.293070
H	2.332239	0.135306	-1.402871
H	2.038229	-1.159161	1.353574
H	0.106627	-2.322510	0.380947
H	1.469799	2.406932	0.184812
H	3.216513	0.586830	0.119335
H	0.372439	-1.453715	-1.205418
H	-4.342937	-0.169291	-0.303357
H	-3.123890	1.485123	-0.188479

TS 2 BH2 Z chair

SCF Energy: -298.041859368

Num. Imaginary Frequencies: 1

Imaginary Frequency: -500.7100

C	0.355240	1.427769	0.260376
C	1.507255	0.971719	-0.471407
C	2.302311	-0.033967	0.073614
C	1.145829	-1.458019	-0.157766
C	-0.105979	-1.061640	0.377511
C	-0.695441	0.187797	0.172711
C	-2.020946	0.528585	0.040038
B	-3.093587	-0.465812	-0.306885
H	1.561363	1.172056	-1.535098
H	0.529509	1.586289	1.322341
H	-0.143049	2.286341	-0.175978
H	-0.566024	-1.700248	1.120714
H	1.607082	-2.321806	0.314930
H	1.261347	-1.492212	-1.233407
H	2.427884	-0.050363	1.149393
H	3.174233	-0.360365	-0.479691
H	-2.258500	1.578831	0.189898
H	-4.248913	-0.154895	-0.305123
H	-2.806619	-1.588028	-0.604012

TS 2 CH3 E boat

SCF Energy: -311.890896144

Num. Imaginary Frequencies: 1

Imaginary Frequency: -673.5077

C	-0.028403	-1.335746	0.056973
C	1.311619	-1.329476	0.399875
C	2.239166	-0.645940	-0.385093
C	1.629934	1.290582	-0.327538
C	0.501984	1.361390	0.494818
C	-0.636708	0.645942	0.216183
C	-1.923252	0.716559	-0.061148
C	-2.894466	-0.423680	-0.199303
H	0.661393	1.616868	1.540277
H	1.467858	1.308762	-1.396914
H	2.120545	-0.697733	-1.459463
H	1.566857	-1.519294	1.437766
H	-0.743978	-1.828143	0.701882
H	2.525910	1.802311	-0.000726
H	3.267874	-0.592041	-0.052705
H	-2.322522	1.713322	-0.227593
H	-0.292616	-1.317892	-0.995006
H	-2.915002	-1.048852	0.693387
H	-3.900423	-0.046923	-0.368039
H	-2.635143	-1.068168	-1.041468

TS 2 CH3 E chair

SCF Energy: -311.906548327

Num. Imaginary Frequencies: 1

Imaginary Frequency: -606.8077

C	0.063639	-1.216163	0.453300
C	-1.102827	-1.350137	-0.307758
C	-2.245393	-0.604219	0.044039
C	-1.747517	1.099837	-0.354572
C	-0.550969	1.345490	0.363002
C	0.575905	0.567187	0.148509
C	1.853217	0.711973	-0.174087
H	-1.009675	-1.692744	-1.332599
H	-0.037476	-1.164067	1.531749
H	0.928098	-1.782111	0.132517
H	-0.628372	1.844886	1.324530
H	-2.606708	1.694926	-0.060953
H	-1.667904	1.008128	-1.431616
H	-2.466504	-0.513926	1.101836
H	-3.137883	-0.739996	-0.557174
H	2.149359	1.699576	-0.513597
C	2.946371	-0.320433	-0.137479
H	3.918609	0.167017	-0.090801
H	2.863726	-0.981623	0.723266
H	2.940177	-0.941281	-1.036883

TS 2 CH3 Z boat

SCF Energy: -311.893089344

Num. Imaginary Frequencies: 1

Imaginary Frequency: -665.8530

C	-0.703303	-1.525755	0.103138
C	-1.898532	-0.962380	-0.304873
C	-2.426434	0.133052	0.379063
C	-1.007425	1.578394	0.219014
C	0.022316	1.076755	-0.582781
C	0.720088	-0.052521	-0.231124
C	1.895107	-0.577443	0.041265
C	3.162978	0.217423	0.184943
H	1.979814	-1.649550	0.189789
H	-0.022770	1.296977	-1.647400
H	-0.843923	1.592463	1.288274
H	-2.360187	0.128633	1.459237
H	-2.199934	-1.109633	-1.337333
H	-0.263617	-2.336169	-0.463590
H	-1.579959	2.415728	-0.158374
H	-3.314491	0.614052	-0.010316
H	-0.467195	-1.516434	1.160363
H	3.603301	0.067581	1.172456
H	3.904066	-0.108426	-0.547468
H	2.976125	1.279619	0.042503

TS 2 CH3 Z chair

SCF Energy: -311.909900923

Num. Imaginary Frequencies: 1

Imaginary Frequency: -597.3680

C	0.632193	1.477460	0.385304
C	1.640108	1.013406	-0.463153
C	2.356464	-0.146083	-0.097088
C	1.117003	-1.467605	-0.240580
C	0.016246	-1.077713	0.564485
C	-0.654385	0.099992	0.282865
C	-1.854913	0.560260	-0.025165
H	1.593711	1.280241	-1.513347
H	0.817088	1.442913	1.452982
H	0.060061	2.343353	0.075614
H	-0.019856	-1.438162	1.588802
H	1.651857	-2.355245	0.082628
H	0.967215	-1.453149	-1.314166
H	2.636399	-0.236769	0.946863
H	3.141057	-0.481741	-0.766560
C	-3.044760	-0.314808	-0.299874
H	-2.022219	1.630008	-0.084552
H	-3.488935	-0.073441	-1.267445
H	-2.762971	-1.365872	-0.294312
H	-3.821135	-0.161590	0.452727

TS 2 CHO E boat

SCF Energy: -385.914570083

Num. Imaginary Frequencies: 1

Imaginary Frequency: -663.6600

2 CARTESIAN COORDINATES

C	-0.408080	-1.380596	-0.072452
C	-1.757801	-1.319209	-0.372176
C	-2.635025	-0.613926	0.446208
C	-1.983245	1.305490	0.353111
C	-0.878874	1.344539	-0.499599
C	0.247921	0.601501	-0.267278
C	1.549300	0.737250	-0.036469
C	2.528626	-0.344500	0.046901
H	-1.041874	1.622425	-1.538705
H	-1.790389	1.318336	1.416888
H	-2.474330	-0.663536	1.514919
H	-2.054417	-1.499653	-1.400191
H	0.250689	-1.905624	-0.750028
H	-2.869389	1.845614	0.047979
H	-3.672003	-0.523737	0.150678
H	1.957587	1.732172	0.113114
H	-0.108865	-1.379217	0.969791
O	3.708088	-0.144746	0.245391
H	2.161360	-1.372102	-0.077051

TS 2 CHO E chair

SCF Energy: -385.943003419

Num. Imaginary Frequencies: 1

Imaginary Frequency: -359.6078

C	-0.284501	-1.328137	0.208740
C	-1.478322	-1.202249	-0.472723
C	-2.606164	-0.524250	0.164606
C	-2.318276	1.011908	-0.000313
C	-0.874381	1.288750	0.182158
C	0.156078	0.450228	-0.000834
C	1.488251	0.606644	-0.334756
C	2.541207	-0.169638	0.212300
H	-1.517492	-1.423527	-1.532996
H	-0.300878	-1.401239	1.289203
H	0.523150	-1.855955	-0.273997
H	-0.599890	2.290199	0.496381
H	-2.928717	1.596893	0.686687
H	-2.625536	1.274681	-1.013209
H	-2.651918	-0.752476	1.227502
H	-3.559744	-0.754133	-0.302332
H	1.750134	1.373532	-1.054398
O	3.741436	-0.022902	-0.024507
H	2.236049	-0.964299	0.918152

TS 2 CHO Z boat

SCF Energy: -385.920439264

Num. Imaginary Frequencies: 1

Imaginary Frequency: -683.0209

C	1.037440	-1.500848	-0.160453
C	2.245944	-0.991995	0.288319
C	2.807188	0.123556	-0.342375
C	1.440706	1.536234	-0.239846
C	0.362940	1.085001	0.541027
C	-0.297915	-0.079416	0.249329
C	-1.516870	-0.578330	0.070233
H	-1.713464	-1.641519	0.005888
H	0.323209	1.385761	1.585067
H	1.291680	1.541306	-1.311098
H	2.812015	0.125816	-1.424558
H	2.524921	-1.191841	1.317745
H	0.584789	-2.342455	0.347826
H	1.984504	2.397060	0.127382
H	3.688119	0.570995	0.099971
C	-2.657873	0.326801	-0.068763
H	0.826675	-1.440483	-1.223535
O	-3.806055	-0.041407	-0.186791
H	-2.403368	1.400610	-0.055181

TS 2 CHO Z chair

SCF Energy: -385.943721196

Num. Imaginary Frequencies: 1

Imaginary Frequency: -440.9563

C	-0.896817	-1.448911	0.280616
C	-1.979793	-0.944467	-0.515453
C	-2.755252	0.106052	-0.013605
C	-1.568035	1.471578	-0.161766
C	-0.356476	1.037316	0.442844
C	0.192383	-0.231839	0.247844
C	1.494997	-0.611024	0.139502
C	2.520582	0.346359	-0.179374
H	-1.982524	-1.144775	-1.580325
H	-1.133492	-1.592814	1.331863
H	-0.400762	-2.322705	-0.126770
H	0.072452	1.641821	1.232160
H	-2.025971	2.346484	0.292952
H	-1.603310	1.533112	-1.242258
H	-2.955082	0.110552	1.051326
H	-3.586837	0.454525	-0.614194
H	1.793340	-1.644605	0.264123
O	3.720233	0.113660	-0.203441
H	2.150785	1.358732	-0.425002

TS 2 CN E boat

SCF Energy: -364.839422993

Num. Imaginary Frequencies: 1

Imaginary Frequency: -682.8561

C	0.035487	-1.242523	0.014445
C	1.346230	-1.413558	0.422937
C	2.390439	-0.858430	-0.321868
C	2.043631	1.089507	-0.353257
C	0.916731	1.366699	0.434830
C	-0.286324	0.761877	0.196994
C	-1.559929	1.047193	-0.044557
C	-2.595926	0.064504	-0.090605
H	1.070344	1.704023	1.457043
H	1.898430	1.092223	-1.424951
H	2.329837	-0.947533	-1.398533
H	1.523385	-1.623897	1.472497
H	-0.770202	-1.636641	0.619988
H	2.983447	1.521165	-0.034917
H	3.396707	-0.928811	0.070418
H	-1.872671	2.064225	-0.245465
H	-0.169304	-1.194681	-1.050612
N	-3.447429	-0.705956	-0.145570

TS 2 CN E chair

SCF Energy: -364.864565855

Num. Imaginary Frequencies: 1

Imaginary Frequency: -351.6555

C	0.017447	-1.213486	0.163269
C	-1.212236	-1.262893	-0.468551
C	-2.384206	-0.720262	0.205486
C	-2.276878	0.851697	0.014944
C	-0.884690	1.298478	0.228710
C	0.233536	0.590736	-0.020663
C	1.513688	0.907271	-0.386517
C	2.629958	0.134156	-0.013493
N	3.545093	-0.510139	0.276946
H	-1.261888	-1.480831	-1.529057
H	0.051938	-1.298024	1.242904
H	0.872606	-1.634591	-0.346146
H	-0.730920	2.283770	0.653857
H	-2.969785	1.362132	0.682452
H	-2.602073	1.041812	-1.007672
H	-2.370516	-0.931064	1.272431
H	-3.325071	-1.048780	-0.226596
H	1.700335	1.762368	-1.019911

TS 2 CN Z boat

SCF Energy: -364.839863886

Num. Imaginary Frequencies: 1

Imaginary Frequency: -681.7536

C	1.060590	-1.477702	-0.211840
C	2.204552	-0.870279	0.278070
C	2.665370	0.316905	-0.306537
C	1.180960	1.576098	-0.211413
C	0.136369	1.019573	0.549730
C	-0.404260	-0.195983	0.235543
C	-1.560438	-0.824744	0.051988
C	-2.776096	-0.087468	-0.083751
H	-1.637893	-1.900939	-0.024401
H	0.043136	1.309121	1.593446
H	1.039688	1.583081	-1.283822
H	2.705824	0.345695	-1.387636
H	2.482108	-1.075844	1.306638
H	0.682607	-2.375587	0.260405
H	1.631364	2.482995	0.171042
H	3.488413	0.831275	0.173102
H	0.859847	-1.397925	-1.275444
N	-3.762483	0.494246	-0.192010

TS 2 CN Z chair

SCF Energy: -364.864658755

Num. Imaginary Frequencies: 1

Imaginary Frequency: -332.9121

C	0.922556	1.563075	0.191779
C	1.732658	0.851506	-0.674292
C	2.519724	-0.262253	-0.162677
C	1.494926	-1.470152	-0.020549
C	0.226693	-0.992886	0.566147
C	-0.315747	0.227924	0.396323
C	-1.572188	0.758922	0.352630
C	-2.649235	-0.006945	-0.138955
H	1.602952	0.963047	-1.744480
H	1.236418	1.681785	1.221626
H	0.347037	2.387658	-0.202845
H	-0.315966	-1.663467	1.223199
H	1.936596	-2.271224	0.570228
H	1.350922	-1.844732	-1.033568
H	2.926648	-0.052464	0.823832
H	3.314333	-0.575932	-0.833465
H	-1.783853	1.773194	0.656717
N	-3.538773	-0.630431	-0.534812

TS 2 F E boat

SCF Energy: -371.833609516

Num. Imaginary Frequencies: 1

Imaginary Frequency: -657.0264

2 *CARTESIAN COORDINATES*

C	-0.047366	-1.379070	0.016208
C	1.278492	-1.314704	0.400412
C	2.200697	-0.584379	-0.354013
C	1.553639	1.311974	-0.323623
C	0.421452	1.365459	0.498262
C	-0.671922	0.587768	0.221371
C	-1.943504	0.638756	-0.080985
F	-2.711905	-0.471937	-0.192031
H	0.556480	1.670233	1.532748
H	1.383617	1.312004	-1.391811
H	2.123944	-0.652072	-1.431264
H	1.508416	-1.495077	1.445616
H	-0.767058	-1.893375	0.638098
H	2.430678	1.863253	-0.010391
H	3.215193	-0.496127	0.012737
H	-2.506568	1.536910	-0.292518
H	-0.286482	-1.353144	-1.040729

TS 2 F E chair

SCF Energy: -371.850534675

Num. Imaginary Frequencies: 1

Imaginary Frequency: -572.8072

C	0.096538	-1.257270	0.465150
C	-1.056864	-1.340134	-0.316878
C	-2.185560	-0.563747	0.032245
C	-1.674521	1.118304	-0.351815
C	-0.482615	1.348055	0.386114
C	0.611444	0.532959	0.176297
C	1.866622	0.658083	-0.190838
F	2.753820	-0.367672	-0.150446
H	-0.959477	-1.670901	-1.344910
H	-0.021081	-1.195470	1.540662
H	0.967882	-1.820044	0.156914
H	-0.553421	1.860301	1.340134
H	-2.527629	1.728413	-0.072340
H	-1.572933	1.035843	-1.427787
H	-2.415254	-0.489847	1.089569
H	-3.076106	-0.683284	-0.575340
H	2.323379	1.566540	-0.554535

TS 2 F Z boat

SCF Energy: -371.832142326

Num. Imaginary Frequencies: 1

Imaginary Frequency: -647.4482

C	0.614537	-1.540438	-0.139067
C	1.795595	-1.001911	0.333527
C	2.377476	0.090951	-0.316904
C	1.019345	1.559780	-0.254535
C	-0.041231	1.122336	0.547810
C	-0.741278	-0.009008	0.223338
C	-1.918320	-0.519095	-0.030909
F	-3.016910	0.266442	-0.185576
H	-2.154583	-1.563783	-0.168733
H	-0.036732	1.406210	1.597132
H	0.868332	1.530825	-1.325079
H	2.386358	0.077218	-1.398969
H	2.040177	-1.161737	1.378640
H	0.136905	-2.352579	0.393691
H	1.599691	2.404703	0.092268
H	3.252740	0.548345	0.126067
H	0.422560	-1.502879	-1.204395

TS 2 F Z chair

SCF Energy: -371.849893739

Num. Imaginary Frequencies: 1

Imaginary Frequency: -561.0557

C	0.534952	1.498372	0.385653
C	1.559227	1.048210	-0.445606
C	2.297852	-0.097347	-0.064702
C	1.130255	-1.447267	-0.258413
C	0.004736	-1.116034	0.544849
C	-0.684650	0.047380	0.281909
C	-1.878950	0.488385	-0.037226
F	-2.893238	-0.370321	-0.320354
H	1.526859	1.314055	-1.496242
H	0.695339	1.466898	1.456636
H	-0.058875	2.344300	0.060142
H	-0.054517	-1.521647	1.549891
H	1.685836	-2.327345	0.049447
H	0.986209	-1.416947	-1.332156
H	2.559498	-0.176439	0.984885
H	3.112897	-0.397679	-0.714381
H	-2.194641	1.517487	-0.113804

TS 2 H boat

SCF Energy: -272.581930680

Num. Imaginary Frequencies: 1

Imaginary Frequency: -678.7790

2 CARTESIAN COORDINATES

C	-0.065508	-1.489630	-0.086653
C	1.187154	-1.131991	0.378436
C	1.937058	-0.170472	-0.297397
C	0.783906	1.510268	-0.250086
C	-0.360533	1.216676	0.495339
C	-1.224042	0.217723	0.122810
C	-2.450625	-0.109247	-0.217614
H	-0.341900	1.450436	1.557358
H	0.688846	1.520084	-1.327501
H	1.925452	-0.193157	-1.379201
H	1.403498	-1.299665	1.428842
H	-0.672385	-2.191734	0.470155
H	1.470813	2.245466	0.148015
H	2.873139	0.161775	0.132444
H	-2.753276	-1.138400	-0.363057
H	-3.199701	0.657056	-0.380029
H	-0.238949	-1.471822	-1.156040

TS 2 H chair

SCF Energy: -272.598837466

Num. Imaginary Frequencies: 1

Imaginary Frequency: -604.9913

C	0.255085	-1.370015	0.409644
C	-0.920084	-1.229826	-0.334632
C	-1.863809	-0.259679	0.063125
C	-1.018182	1.306900	-0.293990
C	0.226771	1.261643	0.383943
C	1.133289	0.256247	0.096873
H	-0.917692	-1.553507	-1.369619
H	0.175832	-1.307751	1.489192
H	0.989062	-2.092159	0.073901
H	0.296998	1.722221	1.364610
H	-1.715325	2.065026	0.048915
H	-0.989447	1.244693	-1.375745
H	-2.044888	-0.162596	1.128010
H	-2.773345	-0.176505	-0.521713
C	2.379622	0.075106	-0.305440
H	2.975515	0.918220	-0.631511
H	2.847138	-0.899896	-0.323173

TS 2 NH2 E boat

SCF Energy: -327.943561703

Num. Imaginary Frequencies: 1

Imaginary Frequency: -668.9221

C	-0.005498	-1.370273	0.070041
C	1.338049	-1.311046	0.390603
C	2.227671	-0.588048	-0.407027
C	1.584350	1.311876	-0.324167
C	0.455296	1.355822	0.505072
C	-0.655081	0.601949	0.220052
C	-1.947252	0.647119	-0.055334
H	0.617944	1.631536	1.545904
H	1.411184	1.342187	-1.391785
H	2.095657	-0.650715	-1.479469
H	1.613246	-1.483834	1.426277
H	-0.680121	-1.882999	0.745005
H	2.470076	1.844227	-0.000674
H	3.260807	-0.510423	-0.093237
N	-2.858093	-0.409097	-0.127641
H	-2.400001	1.619714	-0.218327
H	-0.290309	-1.379962	-0.977125
H	-3.623809	-0.234102	-0.759911
H	-2.453231	-1.316347	-0.298623

TS 2 NH2 E chair

SCF Energy: -327.958729355

Num. Imaginary Frequencies: 1

Imaginary Frequency: -601.1082

C	0.064916	-1.251478	0.373718
C	-1.143846	-1.339228	-0.322735
C	-2.243079	-0.558309	0.092797
C	-1.720900	1.125668	-0.330405
C	-0.499791	1.342681	0.359017
C	0.598717	0.537706	0.113557
C	1.887986	0.656345	-0.178171
H	-1.112842	-1.662677	-1.357561
H	0.030009	-1.231165	1.457477
H	0.897522	-1.821184	-0.021735
H	-0.554750	1.844050	1.322191
H	-2.558844	1.740508	-0.016141
H	-1.670522	1.032241	-1.409111
H	-2.406195	-0.470405	1.161434
H	-3.170882	-0.668242	-0.458530
H	2.248955	1.617679	-0.524691
N	2.865813	-0.351035	-0.171293
H	3.803109	0.020117	-0.175413
H	2.769740	-1.023994	0.574466

TS 2 NH2 Z boat

SCF Energy: -327.943285400

Num. Imaginary Frequencies: 1

Imaginary Frequency: -670.8535

C	-0.633607	1.512072	-0.183847
C	-1.808543	1.010954	0.345613
C	-2.422170	-0.099396	-0.254103
C	-1.075169	-1.528674	-0.269509
C	0.025423	-1.118241	0.503486
C	0.716570	0.026056	0.188132
C	1.925723	0.526214	-0.003460
H	2.081723	1.595830	-0.080049
H	0.045085	-1.435694	1.545247
H	-0.948826	-1.491003	-1.343796
H	-2.515571	-0.085634	-1.332696
H	-1.997535	1.187544	1.399967
H	-0.128305	2.335131	0.305787
H	-1.637496	-2.387783	0.074871
H	-3.276104	-0.538748	0.246745
N	3.080011	-0.233543	-0.242304
H	-0.492670	1.456023	-1.256642
H	3.926696	0.208469	0.083714
H	3.013573	-1.183238	0.095111

TS 2 NH2 Z chair

SCF Energy: -327.960702009

Num. Imaginary Frequencies: 1

Imaginary Frequency: -576.0270

C	0.592101	1.489278	0.381146
C	1.615572	1.035386	-0.448597
C	2.331429	-0.128346	-0.077265
C	1.132027	-1.452281	-0.260576
C	0.013996	-1.095731	0.545434
C	-0.668759	0.072275	0.266844
C	-1.881037	0.515086	-0.028982
H	1.585471	1.305426	-1.498624
H	0.753093	1.453591	1.452298
H	0.009173	2.344295	0.059731
H	-0.009144	-1.470609	1.566366
H	1.678278	-2.337952	0.049962
H	0.981741	-1.428551	-1.334278
H	2.597172	-0.216219	0.970991
H	3.139680	-0.440576	-0.730289
N	-3.008838	-0.306436	-0.202525
H	-2.094031	1.574470	-0.097627
H	-3.629025	0.021659	-0.929664
H	-2.762525	-1.274487	-0.359216

TS 2 NO2 E boat

SCF Energy: -477.099834721

Num. Imaginary Frequencies: 1

Imaginary Frequency: -650.7281

C	-0.634393	-1.351272	0.053741
C	-1.984142	-1.337673	-0.248713
C	-2.875853	-0.573250	0.502390
C	-2.277244	1.317165	0.262628
C	-1.169440	1.331118	-0.588777
C	-0.037785	0.600375	-0.329485
C	1.225797	0.910296	-0.091613
N	2.323806	-0.031020	0.041560
H	-1.310115	1.612123	-1.629565
H	-2.078159	1.407202	1.321471
H	-2.727021	-0.545800	1.573423
H	-2.275694	-1.614209	-1.256564
H	0.045506	-1.911089	-0.566573
H	-3.165217	1.836579	-0.071967
H	-3.912088	-0.527377	0.193997
H	1.578508	1.915555	0.075078
H	-0.329530	-1.238772	1.089832
O	3.358190	0.428448	0.492098
O	2.195002	-1.190652	-0.289733

TS 2 NO2 E chair

SCF Energy: -477.138341653

Num. Imaginary Frequencies: 1

Imaginary Frequency: -371.4507

C	0.474838	1.352871	-0.068394
C	1.669264	1.095784	-0.682747
C	2.798208	0.575516	0.104220
C	2.586702	-0.965693	0.192980
C	1.142767	-1.295906	0.295941
C	0.102816	-0.539516	-0.036330
C	-1.187786	-0.763911	-0.458217
N	-2.255794	-0.055983	0.058283
H	1.736132	1.108799	-1.764768
H	0.440908	1.544505	0.994943
H	-0.355661	1.741898	-0.637568
H	0.886663	-2.286214	0.659095
H	3.150404	-1.395009	1.019790
H	2.974553	-1.410486	-0.725174
H	2.784578	0.990439	1.110160
H	3.760424	0.778368	-0.358288
H	-1.440790	-1.430330	-1.264370
O	-3.380238	-0.247103	-0.424866
O	-2.078200	0.746483	0.984052

TS 2 NO2 Z boat

SCF Energy: -477.105647728

Num. Imaginary Frequencies: 1

Imaginary Frequency: -661.4761

C	1.363340	-1.516748	-0.194905
C	2.541497	-0.979191	0.302251
C	3.082295	0.172778	-0.286124
C	1.672788	1.500818	-0.279742
C	0.586939	1.042381	0.490841
C	-0.001266	-0.164435	0.255185
C	-1.182296	-0.751047	0.144467
N	-2.399427	0.016617	-0.041392
H	-1.377898	-1.809830	0.126554
H	0.439181	1.441859	1.490309
H	1.545268	1.452107	-1.352568
H	3.164445	0.176654	-1.365076
H	2.793975	-1.194725	1.335050
H	0.937821	-2.396379	0.270639
H	2.152536	2.412212	0.053307
H	3.918097	0.646711	0.212955
H	1.178483	-1.428500	-1.261364
O	-3.415717	-0.634217	-0.224283
O	-2.376245	1.228747	-0.002204

TS 2 NO2 Z chair

SCF Energy: -477.136495552

Num. Imaginary Frequencies: 1

Imaginary Frequency: -380.5027

C	-1.197984	-1.686413	0.121266
C	-1.914988	-0.916742	-0.753914
C	-2.863010	0.081368	-0.241040
C	-2.019574	1.354490	0.099135
C	-0.714822	0.970387	0.689230
C	-0.055816	-0.170382	0.519156
C	1.229781	-0.629326	0.514356
N	2.247425	0.099307	-0.106855
H	-1.655184	-0.912011	-1.806169
H	-1.575546	-1.863973	1.119711
H	-0.493931	-2.412772	-0.255474
H	-0.207759	1.699220	1.313802
H	-2.570326	2.025191	0.756496
H	-1.844006	1.887385	-0.836590
H	-3.341508	-0.272307	0.670040
H	-3.624118	0.350271	-0.968568
H	1.552615	-1.586635	0.882212
O	3.377225	-0.403809	-0.114274
O	2.028558	1.200082	-0.612802

TS 2 OH E boat

SCF Energy: -347.815388698

Num. Imaginary Frequencies: 1

Imaginary Frequency: -666.8307

C	-0.033780	-1.366865	0.026945
C	1.297539	-1.317348	0.395585
C	2.218276	-0.591239	-0.366275
C	1.580238	1.301991	-0.324910
C	0.445187	1.362835	0.496128
C	-0.655206	0.593885	0.217880
C	-1.939513	0.628617	-0.065850
O	-2.720574	-0.491452	-0.164934
H	0.592922	1.661176	1.531903
H	1.411281	1.314309	-1.393499
H	2.132768	-0.660832	-1.442979
H	1.535944	-1.497042	1.439345
H	-0.751680	-1.873622	0.657096
H	2.461162	1.846073	-0.008304
H	3.237944	-0.515705	-0.010328
H	-2.442790	1.569358	-0.258905
H	-0.286704	-1.347141	-1.027038
H	-3.602711	-0.236215	-0.444844

TS 2 OH E chair

SCF Energy: -347.831649615

Num. Imaginary Frequencies: 1

Imaginary Frequency: -591.3124

C	0.064709	-1.248216	0.494837
C	-1.068384	-1.346221	-0.313899
C	-2.206765	-0.568876	-0.003275
C	-1.679370	1.123977	-0.366929
C	-0.505040	1.346116	0.399399
C	0.599427	0.543497	0.189037
C	1.866432	0.644229	-0.167326
O	2.755788	-0.399277	-0.132167
H	-0.941369	-1.682009	-1.337406
H	-0.080874	-1.170801	1.566107
H	0.948959	-1.806576	0.216956
H	-0.615718	1.815636	1.373011
H	-2.543458	1.725246	-0.101380
H	-1.553059	1.047497	-1.441028
H	-2.468575	-0.489186	1.046335
H	-3.079086	-0.688389	-0.637013
H	2.272253	1.590330	-0.504273
H	3.588564	-0.114567	-0.515040

TS 2 OH Z boat

SCF Energy: -347.813522290

Num. Imaginary Frequencies: 1

Imaginary Frequency: -661.8626

C	0.604924	-1.524253	-0.158563
C	1.791770	-1.022042	0.340441
C	2.406593	0.068659	-0.288049
C	1.076436	1.538254	-0.267283
C	-0.011544	1.132587	0.520551
C	-0.726342	0.007058	0.201138
C	-1.928646	-0.485005	-0.010786
O	-3.030069	0.323964	-0.145545
H	-2.116300	-1.547040	-0.111426
H	-0.014045	1.436411	1.565471
H	0.937412	1.506202	-1.339826
H	2.457057	0.050972	-1.369178
H	2.005375	-1.189454	1.391417
H	0.100787	-2.332224	0.356263
H	1.661189	2.381635	0.077445
H	3.279376	0.504315	0.181866
H	0.439603	-1.479526	-1.228157
H	-3.789053	-0.214554	-0.384206

TS 2 OH Z chair

SCF Energy: -347.830700929

Num. Imaginary Frequencies: 1

Imaginary Frequency: -575.5888

C	0.552584	1.488689	0.397894
C	1.574559	1.058498	-0.445653
C	2.320126	-0.089660	-0.086224
C	1.149774	-1.444806	-0.268001
C	0.034827	-1.117572	0.551446
C	-0.674917	0.034236	0.285082
C	-1.880624	0.464000	-0.032665
O	-2.912260	-0.409746	-0.282458
H	1.527923	1.333028	-1.493770
H	0.722533	1.446107	1.467174
H	-0.050995	2.333718	0.088281
H	0.020092	-1.502274	1.567845
H	1.718684	-2.319807	0.030873
H	0.989254	-1.413692	-1.339732
H	2.596784	-0.177816	0.959018
H	3.127684	-0.382486	-0.748822
H	-2.132285	1.514099	-0.104625
H	-3.679565	0.086772	-0.577854

TS 2 OMe E boat

SCF Energy: -387.106752835

Num. Imaginary Frequencies: 1

Imaginary Frequency: -667.4095

C	-0.430624	-1.351463	-0.092412
C	-1.785184	-1.337603	-0.368057
C	-2.671219	-0.646545	0.464482
C	-2.091241	1.262441	0.404900
C	-1.017194	1.366926	-0.490937
C	0.119827	0.625013	-0.301645
C	1.422677	0.694794	-0.120130
O	2.244277	-0.392395	-0.112244
H	-1.243473	1.676336	-1.509172
H	-1.849138	1.267668	1.459382
H	-2.510513	-0.726939	1.531830
H	-2.089586	-1.511912	-1.395438
H	0.256780	-1.829167	-0.776777
H	-3.005969	1.786010	0.157041
H	-3.714659	-0.596673	0.180050
H	1.913905	1.649167	0.048662
H	-0.105948	-1.336093	0.941838
C	3.564762	-0.120890	0.328003
H	4.116339	-1.054239	0.266258
H	4.041673	0.624762	-0.311088
H	3.565544	0.234207	1.360146

TS 2 OMe E chair

SCF Energy: -387.123174616

Num. Imaginary Frequencies: 1

Imaginary Frequency: -583.5143

C	0.443831	-1.231979	-0.559186
C	1.512493	-1.361859	0.329358
C	2.684561	-0.601337	0.114270
C	2.161369	1.087372	0.470362
C	1.052424	1.348732	-0.378536
C	-0.077798	0.560536	-0.282735
C	-1.376293	0.692196	-0.071837
H	1.304244	-1.706535	1.336445
H	0.669782	-1.152556	-1.616432
H	-0.470270	-1.772735	-0.352063
H	1.242281	1.851927	-1.322459
H	3.050602	1.682115	0.284989
H	1.952532	0.994090	1.530148
H	3.023346	-0.512491	-0.912367
H	3.506614	-0.748558	0.806710
H	-1.793638	1.642505	0.247400
O	-2.289611	-0.305238	-0.260816
C	-3.512357	-0.102449	0.426848
H	-4.167794	-0.926177	0.159654
H	-3.355506	-0.097225	1.507267
H	-3.974684	0.840262	0.125974

TS 2 OMe Z boat

SCF Energy: -387.105035123

Num. Imaginary Frequencies: 1

Imaginary Frequency: -663.2344

C	-1.036931	-1.523407	0.113724
C	-2.278662	-1.067550	-0.287348
C	-2.894619	-0.019374	0.408620
C	-1.635511	1.507868	0.328576
C	-0.588467	1.169834	-0.542628
C	0.194115	0.070080	-0.303778
C	1.431117	-0.374572	-0.208325
O	2.507663	0.467136	-0.171491
H	1.672034	-1.431785	-0.149643
H	-0.669409	1.499209	-1.576540
H	-1.419658	1.459833	1.387667
H	-2.866833	-0.061740	1.489896
H	-2.559856	-1.223447	-1.324087
H	-0.536691	-2.297954	-0.453526
H	-2.278142	2.332115	0.046285
H	-3.817366	0.385123	0.012011
H	-0.797463	-1.492599	1.169772
C	3.681996	-0.118465	0.368025
H	4.474860	0.617807	0.274166
H	3.542658	-0.371365	1.420775
H	3.956334	-1.018766	-0.186041

TS 2 OMe Z chair

SCF Energy: -387.122296741

Num. Imaginary Frequencies: 1

Imaginary Frequency: -570.8918

C	1.043563	1.478014	0.432578
C	1.994466	1.093225	-0.510975
C	2.803826	-0.036972	-0.244121
C	1.661869	-1.420494	-0.345458
C	0.616987	-1.144073	0.579118
C	-0.143393	-0.005986	0.414399
C	-1.392202	0.396395	0.264137
H	1.841842	1.382798	-1.544830
H	1.316851	1.427924	1.479971
H	0.389873	2.309181	0.195661
H	0.695637	-1.562348	1.578956
H	2.277219	-2.285734	-0.118834
H	1.403270	-1.374728	-1.397257
H	3.179016	-0.133431	0.769162
H	3.554785	-0.293242	-0.983932
O	-2.428099	-0.490365	0.143867
H	-1.681030	1.442358	0.256263
C	-3.572965	0.051595	-0.493440
H	-4.343542	-0.713487	-0.467469
H	-3.927301	0.939832	0.034695
H	-3.354738	0.313572	-1.530742

TS 2 tBut E boat

SCF Energy: -429.811001489

Num. Imaginary Frequencies: 1

Imaginary Frequency: -670.9043

2 CARTESIAN COORDINATES

C	1.036835	-1.274383	0.002324
C	2.360589	-1.296416	0.401412
C	3.328364	-0.626534	-0.345256
C	2.717160	1.311524	-0.348661
C	1.592637	1.405271	0.471299
C	0.423973	0.724148	0.214551
C	-0.862657	0.931773	-0.000903
H	1.758096	1.677598	1.511870
H	2.554372	1.302096	-1.418129
H	3.259150	-0.682616	-1.423378
H	2.573103	-1.505319	1.445080
H	0.292114	-1.786045	0.593901
H	3.616822	1.824090	-0.033924
H	4.340992	-0.576641	0.034009
C	-2.074488	0.008073	-0.045094
H	-1.115265	1.981328	-0.144776
H	0.826899	-1.210257	-1.058847
C	-3.298745	0.887656	-0.329795
C	-1.991022	-1.045730	-1.157185
C	-2.282784	-0.672702	1.312915
H	-3.168636	-1.310548	1.278580
H	-1.430307	-1.289176	1.592944
H	-2.429331	0.073046	2.095564
H	-2.967724	-1.518368	-1.278984
H	-1.716175	-0.586191	-2.107859
H	-1.273774	-1.831033	-0.934610
H	-4.207769	0.284981	-0.327893
H	-3.402186	1.666507	0.427623
H	-3.209559	1.370467	-1.304817

TS 2 tBut E chair

SCF Energy: -429.828030261

Num. Imaginary Frequencies: 1

Imaginary Frequency: -608.0608

C	0.989274	-1.136989	-0.556404
C	2.085345	-1.317324	0.292102
C	3.271250	-0.597310	0.041143
C	2.793877	1.114487	0.407814
C	1.646677	1.395511	-0.374103
C	0.482542	0.657659	-0.215912
C	-0.786056	0.891445	0.096176
C	-2.036426	0.022816	0.059620
H	1.901367	-1.677723	1.298588
H	1.178543	-1.044593	-1.619943
H	0.095983	-1.697979	-0.332353
H	1.787027	1.897939	-1.326816
H	3.683240	1.688175	0.165937
H	2.647072	1.026277	1.478334
H	3.578455	-0.508282	-0.995080
H	4.109484	-0.763186	0.709204
H	-0.975292	1.905457	0.440923
C	-3.237032	0.954140	0.277076
C	-2.235304	-0.667619	-1.295676
C	-2.033934	-1.001172	1.203999
H	-3.183979	-1.208558	-1.296313
H	-2.268586	0.074846	-2.094429
H	-1.447474	-1.377790	-1.533759
H	-2.968037	-1.566937	1.198344
H	-1.210819	-1.710053	1.132909
H	-1.951582	-0.491909	2.165432
H	-4.167135	0.384157	0.266316
H	-3.160917	1.467289	1.237231
H	-3.288636	1.709007	-0.509533

TS 2 tBut Z boat

SCF Energy: -429.819420060

Num. Imaginary Frequencies: 1

Imaginary Frequency: -659.5983

2 CARTESIAN COORDINATES

C	-1.848857	1.579036	-0.085335
C	-3.021672	0.941923	0.278053
C	-3.455210	-0.181499	-0.425557
C	-1.953879	-1.540812	-0.210262
C	-0.990582	-0.975425	0.629512
C	-0.352366	0.195844	0.301621
C	0.799817	0.782841	0.061442
H	-1.057086	-1.200679	1.692199
H	-1.748449	-1.540379	-1.272581
H	-3.345989	-0.172348	-1.502170
H	-3.369184	1.067065	1.298849
H	-1.480241	2.412930	0.497777
H	-2.486770	-2.413403	0.144449
H	-4.325215	-0.718585	-0.070338
H	0.831181	1.857878	-0.093135
C	2.131397	0.042308	-0.050626
H	-1.574104	1.587635	-1.133112
C	3.238439	1.066135	-0.305196
C	2.426594	-0.714707	1.246446
C	2.076571	-0.951156	-1.214964
H	3.379884	-1.241572	1.167532
H	2.482513	-0.027893	2.092470
H	1.645209	-1.448016	1.449922
H	3.025213	-1.485014	-1.302809
H	1.281405	-1.680548	-1.054668
H	1.884508	-0.434407	-2.156631
H	4.205468	0.568423	-0.393036
H	3.052401	1.616579	-1.229269
H	3.297747	1.785404	0.513744

TS 2 tBut Z chair

SCF Energy: -429.836093635
Num. Imaginary Frequencies: 1
Imaginary Frequency: -596.3446

C	-1.790503	1.527868	-0.413974
C	-2.712011	0.993930	0.491594
C	-3.360280	-0.215071	0.166307
C	-2.011120	-1.444467	0.234823
C	-0.994674	-0.970128	-0.629965
C	-0.402726	0.258316	-0.385340
C	0.775788	0.807345	-0.143793
H	-2.622605	1.265160	1.537878
H	-2.036238	1.476947	-1.468760
H	-1.269523	2.436443	-0.138144
H	-0.981364	-1.332201	-1.654407
H	-2.494339	-2.371151	-0.058295
H	-1.802447	-1.412098	1.298329
H	-3.690906	-0.332880	-0.859855
H	-4.074119	-0.610609	0.880624
C	2.065573	0.022207	0.074469
H	0.863556	1.888272	-0.098840
C	3.182389	1.010779	0.414765
C	1.897553	-0.967875	1.230288
C	2.439570	-0.744165	-1.197774
H	3.374513	-1.289574	-1.051111
H	1.659364	-1.461597	-1.455274
H	2.569256	-0.060851	-2.038723
H	4.122970	0.482969	0.580202
H	3.329930	1.724284	-0.398231
H	2.941368	1.571389	1.319886
H	2.820736	-1.531241	1.381723
H	1.659242	-0.442767	2.156724
H	1.093252	-1.672933	1.017877

TS 5 BH2 E

SCF Energy: -411.355072299
Num. Imaginary Frequencies: 1
Imaginary Frequency: -529.7631

O	-0.837802	-0.848981	-1.323663
C	-0.163040	-1.089338	-0.241398
C	-0.978810	-1.226127	0.991000
C	-1.651892	0.231434	1.241562
C	-1.156280	1.117350	0.154593
C	-1.641900	0.781833	-1.124466
C	0.179686	1.467565	0.225608
C	1.084270	-0.524556	-0.112447
C	2.405796	-0.599821	-0.127833
H	-1.225500	1.281870	-1.989263
H	0.655946	1.603473	1.188211
H	-2.667552	0.454430	-1.230101
B	3.356119	0.570339	0.172395
H	2.812732	-1.579252	-0.373754
H	0.659759	1.952888	-0.615491
H	-0.393075	-1.519369	1.858526
H	-1.778241	-1.943111	0.820591
H	-1.341437	0.573801	2.225661
H	-2.733075	0.118661	1.226787
H	4.532183	0.395376	0.156001
H	2.933112	1.651340	0.420456

TS 5 BH2 Z

SCF Energy: -411.357444029

Num. Imaginary Frequencies: 1

Imaginary Frequency: -532.0026

O	0.428688	-0.688860	1.413335
C	-0.205143	-0.829979	0.282673
C	0.604286	-1.415164	-0.812330
C	1.780191	-0.327192	-1.120877
C	1.555980	0.811501	-0.193177
C	1.764257	0.484407	1.166640
C	0.442660	1.588051	-0.458611
C	-1.114701	0.138406	-0.064413
C	-2.341504	0.599757	-0.232147
H	1.502233	1.215456	1.920812
H	0.125943	1.756545	-1.481084
H	2.593557	-0.160420	1.426151
H	-2.460682	1.606883	-0.620738
B	-3.546631	-0.291114	0.116464
H	0.100279	2.313196	0.270636
H	0.029437	-1.604685	-1.715169
H	1.078429	-2.331727	-0.470333
H	1.690559	-0.034449	-2.164111
H	2.740853	-0.811392	-0.964806
H	-4.658355	0.100021	-0.045665
H	-3.354752	-1.381705	0.548757

TS 5 CHO E

SCF Energy: -499.254446922

Num. Imaginary Frequencies: 1

Imaginary Frequency: -525.8087

O	-1.310874	-0.844883	-1.313952
C	-0.641259	-1.102460	-0.236300
C	-1.449910	-1.205785	1.001480
C	-2.046830	0.287508	1.254266
C	-1.535048	1.145584	0.153940
C	-2.047703	0.820929	-1.117367
C	-0.192014	1.470401	0.208423
C	0.623516	-0.576734	-0.119484
C	1.931017	-0.736158	-0.161547
H	-1.622097	1.297153	-1.990862
H	0.288089	1.610098	1.169118
H	-3.084873	0.528095	-1.208483
C	2.882880	0.350203	0.102780
H	2.363418	-1.702444	-0.402384
H	0.284382	1.941780	-0.643150
H	-0.871677	-1.523934	1.864789
H	-2.286887	-1.879890	0.838671
H	-1.700781	0.619778	2.229665
H	-3.131710	0.222241	1.260811
O	4.081539	0.199017	0.067058
H	2.448912	1.333123	0.339820

TS 5 CHO Z

SCF Energy: -499.256934013

Num. Imaginary Frequencies: 1

Imaginary Frequency: -522.8061

O	0.868925	-0.688583	1.408507
C	0.235892	-0.836024	0.276599
C	1.046310	-1.422969	-0.811799
C	2.209492	-0.312165	-1.124455
C	1.985370	0.817357	-0.189348
C	2.183293	0.473086	1.172156
C	0.881579	1.608179	-0.452022
C	-0.652973	0.149227	-0.077038
C	-1.884948	0.583810	-0.233773
H	1.925963	1.202829	1.929228
H	0.574997	1.792579	-1.474771
H	3.017381	-0.167680	1.426696
H	-2.113272	1.572669	-0.613051
C	-3.016317	-0.293501	0.115256
H	0.544766	2.329877	0.283075
H	0.476542	-1.621622	-1.715420
H	1.537872	-2.328283	-0.465829
H	2.104248	-0.015658	-2.164911
H	3.173569	-0.792637	-0.980141
O	-4.173443	0.027697	-0.006010
H	-2.732103	-1.286983	0.501696

TS 5 CN E

SCF Energy: -478.176010906

Num. Imaginary Frequencies: 1

Imaginary Frequency: -532.8264

O	1.327727	0.845334	-1.240691
C	0.665871	1.143927	-0.159944
C	1.443454	1.050126	1.093731
C	1.803248	-0.539448	1.252422
C	1.212533	-1.233108	0.081497
C	1.801751	-0.867575	-1.154269
C	-0.164378	-1.352462	0.078705
C	-0.648938	0.757735	-0.103693
C	-1.932530	1.043311	-0.154216
H	1.349047	-1.230009	-2.068180
H	-0.701878	-1.485362	1.010485
H	2.874957	-0.737695	-1.198655
C	-2.933045	0.034135	0.023859
H	-2.289496	2.049867	-0.336447
H	-0.680600	-1.675977	-0.818254
H	0.896133	1.391760	1.967861
H	2.379260	1.593325	0.993978
H	1.375104	-0.877156	2.192578
H	2.885326	-0.630962	1.292698
N	-3.742496	-0.768614	0.162986

TS 5 CN Z

SCF Energy: -478.175233260

Num. Imaginary Frequencies: 1

Imaginary Frequency: -526.8586

O	0.666835	-0.758962	1.372583
C	0.060765	-0.804568	0.219771
C	0.852886	-1.399036	-0.876892
C	2.102944	-0.364315	-1.105593
C	1.939623	0.731860	-0.119584
C	2.073020	0.308441	1.227663
C	0.912577	1.622569	-0.368459
C	-0.744116	0.256862	-0.105606
C	-1.921700	0.816486	-0.280308
H	1.849845	1.017659	2.014309
H	0.648803	1.878624	-1.387820
H	2.846658	-0.408243	1.469914
H	-2.031498	1.839437	-0.617373
C	-3.131373	0.091571	-0.025692
H	0.611383	2.330347	0.395098
H	0.294680	-1.510168	-1.802331
H	1.266396	-2.353923	-0.564001
H	2.047199	-0.009971	-2.131546
H	3.023822	-0.923624	-0.964102
N	-4.108533	-0.478238	0.173626

TS 5 F E

SCF Energy: -485.171689098

Num. Imaginary Frequencies: 1

Imaginary Frequency: -528.9916

O	-0.932859	-0.775762	-1.352508
C	-0.249990	-1.094993	-0.286676
C	-1.074058	-1.280348	0.925371
C	-1.659314	0.216723	1.257190
C	-1.148848	1.127832	0.203563
C	-1.639352	0.824455	-1.093230
C	0.193164	1.452535	0.277879
C	0.984924	-0.523949	-0.125458
C	2.285666	-0.584352	-0.146344
H	-1.219997	1.357808	-1.936846
H	0.678028	1.551467	1.241277
H	-2.682470	0.557263	-1.200974
F	3.051137	0.481852	0.177513
H	2.879751	-1.446614	-0.415142
H	0.677847	1.954791	-0.550857
H	-0.510969	-1.647095	1.778825
H	-1.922826	-1.926764	0.719483
H	-1.305712	0.491235	2.247704
H	-2.744171	0.149920	1.265214

TS 5 F Z

SCF Energy: -485.170067687

Num. Imaginary Frequencies: 1

Imaginary Frequency: -522.6968

O	0.552972	-0.641736	1.448079
C	-0.095187	-0.851341	0.337542
C	0.714649	-1.471800	-0.732455
C	1.814488	-0.325846	-1.134551
C	1.572411	0.840720	-0.249309
C	1.814566	0.573856	1.121408
C	0.444948	1.591845	-0.524809
C	-1.037658	0.068776	-0.042552
C	-2.255571	0.492317	-0.225914
H	1.539961	1.327149	1.848666
H	0.111935	1.717831	-1.547714
H	2.676364	-0.023097	1.389191
H	-2.538275	1.446039	-0.647535
F	-3.335109	-0.251609	0.115154
H	0.105672	2.336076	0.185286
H	0.134689	-1.742779	-1.610078
H	1.257517	-2.332642	-0.351719
H	1.665296	-0.084660	-2.183884
H	2.803177	-0.756703	-0.999394

TS 5 H

SCF Energy: -385.922289295

Num. Imaginary Frequencies: 1

Imaginary Frequency: -541.6310

C	0.185516	-1.445257	-0.690737
C	-1.054396	-0.904911	-0.399702
C	-1.409059	0.328793	-1.147244
C	-0.456128	1.519071	-0.562519
C	0.377852	0.879390	0.481795
C	1.455166	0.140074	0.061055
C	2.728933	-0.108797	-0.092291
C	-1.389673	-0.848988	0.973985
O	-0.294043	0.455866	1.517942
H	-1.053882	-1.650315	1.619941
H	0.582056	-1.387382	-1.697283
H	-2.330867	-0.398865	1.261617
H	3.074534	-0.989106	-0.619616
H	3.480182	0.560625	0.310375
H	0.596331	-2.225400	-0.061011
H	0.127918	1.951855	-1.370542
H	-1.101008	2.273173	-0.118448
H	-1.206430	0.239448	-2.211768
H	-2.445758	0.622793	-1.002854

TS 5 Me E

SCF Energy: -425.233460121

Num. Imaginary Frequencies: 1

Imaginary Frequency: -536.5215

2 CARTESIAN COORDINATES

O	-0.970936	-0.792630	-1.340354
C	-0.283084	-1.089496	-0.271468
C	-1.107453	-1.246413	0.949892
C	-1.722927	0.234694	1.253025
C	-1.206649	1.133185	0.188964
C	-1.700512	0.825149	-1.099713
C	0.142557	1.432971	0.262060
C	0.972901	-0.549283	-0.130256
C	2.279986	-0.638015	-0.154582
H	-1.278627	1.343090	-1.951695
H	0.618417	1.539285	1.229481
H	-2.741807	0.549979	-1.205602
C	3.272602	0.441520	0.152837
H	2.699124	-1.602182	-0.433439
H	0.631672	1.930021	-0.567680
H	-0.536714	-1.589367	1.808937
H	-1.940617	-1.918260	0.758847
H	-1.388675	0.532982	2.243825
H	-2.807653	0.159976	1.248145
H	3.919670	0.134868	0.975827
H	3.916576	0.617144	-0.710053
H	2.791595	1.377639	0.421689

TS 5 Me Z

SCF Energy: -425.233956287

Num. Imaginary Frequencies: 1

Imaginary Frequency: -531.0946

O	0.563558	-0.601598	1.456341
C	-0.088308	-0.819750	0.343544
C	0.725578	-1.471076	-0.708897
C	1.870443	-0.375506	-1.110976
C	1.637376	0.815662	-0.255537
C	1.857872	0.570548	1.122178
C	0.506445	1.554793	-0.555743
C	-1.017307	0.108233	-0.059469
C	-2.235231	0.542973	-0.259991
H	1.593811	1.345567	1.830722
H	0.182284	1.658490	-1.584248
H	2.707698	-0.034413	1.410896
H	-2.373417	1.518990	-0.715794
C	-3.481346	-0.214558	0.103709
H	0.165063	2.320516	0.130504
H	0.149854	-1.738640	-1.591118
H	1.231244	-2.346409	-0.308890
H	1.754251	-0.153277	-2.169061
H	2.844849	-0.828152	-0.944081
H	-4.096013	-0.380893	-0.782111
H	-3.238636	-1.176476	0.549383
H	-4.082576	0.359560	0.810162

TS 5 NH2 E

SCF Energy: -441.284812690

Num. Imaginary Frequencies: 1

Imaginary Frequency: -538.1627

2 CARTESIAN COORDINATES

O	-0.987302	-0.780332	-1.334741
C	-0.273709	-1.092533	-0.276841
C	-1.092624	-1.256981	0.943724
C	-1.676314	0.243992	1.265573
C	-1.173757	1.135885	0.193612
C	-1.680466	0.805438	-1.092240
C	0.179632	1.426357	0.243823
C	0.970678	-0.532628	-0.144638
C	2.285245	-0.601636	-0.143303
H	-1.275432	1.330906	-1.948322
H	0.666423	1.545876	1.205357
H	-2.730135	0.554570	-1.179073
N	3.179061	0.398781	0.230743
H	2.758071	-1.540779	-0.411243
H	0.651209	1.925130	-0.596305
H	-0.525341	-1.614849	1.798532
H	-1.946278	-1.903227	0.755065
H	-1.311589	0.530722	2.248974
H	-2.761523	0.180631	1.287136
H	4.075089	0.337110	-0.227007
H	2.812391	1.337733	0.191349

TS 5 NH2 Z

SCF Energy: -441.283737053

Num. Imaginary Frequencies: 1

Imaginary Frequency: -531.4973

O	0.585260	-0.666462	1.426439
C	-0.078114	-0.851770	0.309371
C	0.747024	-1.447341	-0.765074
C	1.846117	-0.290072	-1.142252
C	1.597344	0.851702	-0.228595
C	1.830543	0.536831	1.136591
C	0.448375	1.582080	-0.480550
C	-1.021622	0.076588	-0.052316
C	-2.256382	0.499211	-0.216277
H	1.563309	1.275106	1.882515
H	0.117717	1.736332	-1.500622
H	2.702830	-0.054369	1.385223
H	-2.436600	1.484592	-0.631574
N	-3.417336	-0.176249	0.172622
H	0.104371	2.307838	0.246286
H	0.176357	-1.706572	-1.652749
H	1.294148	-2.312228	-0.398323
H	1.695302	-0.024412	-2.185851
H	2.837103	-0.720388	-1.019367
H	-4.208256	0.003082	-0.427929
H	-3.286722	-1.166912	0.317145

TS 5 NO2 E

SCF Energy: -590.439220850

Num. Imaginary Frequencies: 1

Imaginary Frequency: -504.0064

O	-1.558750	-1.019769	-1.217249
C	-0.903486	-1.146697	-0.115215
C	-1.712789	-1.112304	1.125614
C	-2.294021	0.403612	1.209471
C	-1.779085	1.135885	0.020693
C	-2.289068	0.680201	-1.209955
C	-0.443917	1.484423	0.041491
C	0.367177	-0.622373	-0.052959
C	1.640443	-0.923100	-0.100520
H	-1.853190	1.049566	-2.128684
H	0.053372	1.710320	0.974790
H	-3.323159	0.370869	-1.275068
N	2.701623	0.075234	0.025811
H	2.053823	-1.910410	-0.237623
H	0.048164	1.841875	-0.854407
H	-1.136381	-1.338923	2.018215
H	-2.553803	-1.794355	1.033537
H	-1.944414	0.840259	2.141184
H	-3.379158	0.346478	1.223720
O	3.836611	-0.352316	-0.045817
O	2.423621	1.242061	0.189557

TS 5 NO2 Z

SCF Energy: -590.440453509

Num. Imaginary Frequencies: 1

Imaginary Frequency: -509.6648

O	1.054905	-0.922448	1.252648
C	0.457807	-0.812039	0.107814
C	1.250145	-1.234101	-1.067591
C	2.470442	-0.151187	-1.158142
C	2.296886	0.799807	-0.029833
C	2.460140	0.213301	1.246691
C	1.266643	1.711270	-0.148851
C	-0.383043	0.254334	-0.066567
C	-1.565331	0.798769	-0.156454
H	2.216777	0.799643	2.123006
H	0.985044	2.094951	-1.121886
H	3.239033	-0.523693	1.388242
H	-1.794759	1.835700	-0.340740
N	-2.784723	-0.007276	0.002546
H	0.959410	2.300108	0.707249
H	0.682844	-1.228399	-1.994032
H	1.683287	-2.214899	-0.891611
H	2.399723	0.340505	-2.124717
H	3.405453	-0.701724	-1.099776
O	-3.831889	0.601973	-0.084350
O	-2.698752	-1.196048	0.203458

TS 5 OH E

SCF Energy: -461.155106156

Num. Imaginary Frequencies: 1

Imaginary Frequency: -531.8614

O	-0.967965	-0.763658	-1.347318
C	-0.269724	-1.094624	-0.286176
C	-1.096448	-1.271635	0.925951
C	-1.670242	0.231470	1.260685
C	-1.152802	1.135519	0.205637
C	-1.648594	0.824165	-1.090308
C	0.198194	1.428502	0.273027
C	0.969007	-0.532332	-0.132295
C	2.278181	-0.579187	-0.145921
H	-1.231315	1.358517	-1.934868
H	0.687682	1.525085	1.234494
H	-2.698591	0.580336	-1.191412
O	3.052690	0.496070	0.182775
H	2.808000	-1.482464	-0.427269
H	0.688670	1.925798	-0.555512
H	-0.536865	-1.643209	1.779878
H	-1.952809	-1.909583	0.723320
H	-1.311866	0.502226	2.250799
H	-2.755892	0.174310	1.271863
H	3.979747	0.258421	0.101450

TS 5 OH Z

SCF Energy: -461.153021060

Num. Imaginary Frequencies: 1

Imaginary Frequency: -528.3923

O	0.600398	-0.629308	1.449199
C	-0.071571	-0.851483	0.348063
C	0.738076	-1.469877	-0.724048
C	1.820097	-0.312988	-1.148562
C	1.576743	0.852372	-0.263213
C	1.833967	0.581088	1.106397
C	0.425813	1.576105	-0.520584
C	-1.027753	0.057339	-0.024768
C	-2.260393	0.460047	-0.212470
H	1.568779	1.336577	1.835365
H	0.079289	1.698915	-1.539539
H	2.711930	0.000916	1.360049
H	-2.480866	1.426376	-0.650928
O	-3.343834	-0.300032	0.134724
H	0.087710	2.318844	0.191699
H	0.154284	-1.756212	-1.594443
H	1.297931	-2.320156	-0.343233
H	1.651114	-0.077443	-2.196441
H	2.816086	-0.732043	-1.028676
H	-4.148645	0.183333	-0.070127

TS 5 OMe E

SCF Energy: -500.446348738

Num. Imaginary Frequencies: 1

Imaginary Frequency: -531.2574

O	-1.452142	-0.749867	-1.341880
C	-0.753391	-1.096977	-0.286127
C	-1.574191	-1.252344	0.933077
C	-2.107705	0.264856	1.270788
C	-1.577356	1.154674	0.210026
C	-2.091613	0.853717	-1.081258
C	-0.219001	1.414036	0.265233
C	0.499833	-0.565068	-0.143181
C	1.808498	-0.646488	-0.165681
H	-1.668812	1.376907	-1.930047
H	0.281683	1.499069	1.221988
H	-3.148086	0.635552	-1.173080
O	2.615873	0.398712	0.155245
H	2.313414	-1.565473	-0.450363
H	0.276747	1.897312	-0.568431
H	-1.017030	-1.637047	1.782759
H	-2.447597	-1.869187	0.737937
H	-1.733925	0.527832	2.257304
H	-3.194290	0.234534	1.291621
C	4.005008	0.124239	0.042095
H	4.527451	1.032950	0.324622
H	4.295301	-0.685961	0.712820
H	4.264803	-0.141118	-0.983888

TS 5 OMe Z

SCF Energy: -500.444323122
Num. Imaginary Frequencies: 1
Imaginary Frequency: -526.7581

O	1.090689	-0.586460	1.467429
C	0.432868	-0.868578	0.371588
C	1.273116	-1.475159	-0.683735
C	2.302026	-0.280504	-1.134940
C	2.001192	0.894825	-0.280876
C	2.266637	0.671810	1.095841
C	0.818328	1.556504	-0.559424
C	-0.563332	-0.015017	-0.025688
C	-1.813136	0.318558	-0.241888
H	1.963458	1.432495	1.804294
H	0.469671	1.635721	-1.581945
H	3.170227	0.140708	1.366411
H	-2.077326	1.264292	-0.706336
O	-2.861018	-0.489466	0.082249
H	0.443221	2.301094	0.132131
H	0.705315	-1.809465	-1.547588
H	1.870361	-2.289232	-0.281134
H	2.126602	-0.080305	-2.189085
H	3.315900	-0.649544	-1.001375
C	-4.126859	0.154829	0.042754
H	-4.872549	-0.606163	0.251454
H	-4.186010	0.940289	0.797777
H	-4.311272	0.583916	-0.943823

TS 5 tBut E

SCF Energy: -543.155884128
Num. Imaginary Frequencies: 1
Imaginary Frequency: -520.8730

2 CARTESIAN COORDINATES

C	2.773757	0.913996	0.991089	O	-1.506472	0.259469	1.525763
O	1.959725	-0.686112	1.435609	C	-0.870538	0.672515	0.462541
C	1.271808	-1.061303	0.405514	C	-1.674740	1.555593	-0.415757
C	2.085607	-1.374594	-0.797790	C	-2.870765	0.612615	-1.001679
C	2.732705	0.034591	-1.273914	C	-2.672628	-0.738675	-0.415112
C	2.259198	1.063072	-0.308116	C	-2.863429	-0.778577	0.986214
C	-0.001014	-0.561812	0.217707	C	-1.579515	-1.441350	-0.889725
C	-1.288527	-0.796319	0.322820	C	0.022519	-0.177384	-0.140447
C	-2.521371	0.013644	-0.015237	C	1.213888	-0.610237	-0.462797
C	0.923081	1.409222	-0.402426	H	-2.615843	-1.690347	1.514992
H	2.372239	1.524916	1.789011	H	-1.273853	-1.339154	-1.923909
H	0.436504	1.427745	-1.367392	H	-3.679024	-0.212085	1.416548
H	3.799229	0.595369	1.122250	H	1.298210	-1.479231	-1.112617
H	-1.537134	-1.766768	0.755403	C	2.539309	-0.021200	-0.014478
H	0.467597	2.004018	0.379621	H	-1.255068	-2.342603	-0.383563
H	1.498357	-1.803478	-1.605639	H	-1.100772	1.974785	-1.238392
H	2.898639	-2.044676	-0.528805	H	-2.132676	2.351180	0.166851
H	2.388388	0.234742	-2.285778	H	-2.785119	0.607818	-2.085746
H	3.815482	-0.065213	-1.279392	H	-3.822750	1.056033	-0.719872
C	-3.474139	-0.905796	-0.790885	C	3.325136	0.378951	-1.268631
C	-3.188558	0.423669	1.304350	C	2.352224	1.193414	0.886033
C	-2.244292	1.255886	-0.853391	C	3.310954	-1.111519	0.737759
H	-3.190905	1.733805	-1.110894	H	4.297490	-0.742778	1.024309
H	-1.643196	1.982515	-0.310566	H	2.778049	-1.409323	1.641649
H	-1.733164	0.997575	-1.781465	H	3.446332	-1.995302	0.111945
H	-4.126593	0.944460	1.103326	H	3.326025	1.584898	1.183947
H	-3.408642	-0.450819	1.918785	H	1.806345	1.984303	0.369344
H	-2.538263	1.088546	1.874282	H	1.794931	0.932141	1.786652
H	-4.407839	-0.382862	-1.003495	H	4.310501	0.755994	-0.989065
H	-3.029594	-1.214532	-1.738212	H	3.463500	-0.476867	-1.931538
H	-3.708446	-1.801994	-0.214255	H	2.801011	1.159907	-1.821171

TS 5 tBut Z

SCF Energy: -543.162760692

Num. Imaginary Frequencies: 1

Imaginary Frequency: -524.5402

3 NBO Secondary Interactions

Table 1: Main NBO Secondary Interactions for the [3,3] sigmatropic rearrangement (kcal/mol)

R	TS 5 E		TS 5 Z	
	$\pi\text{C}_2\text{-C}_8 \rightarrow \pi^*\text{C}_5\text{-C}_7$	$\pi\text{C}_5\text{-C}_7 \rightarrow \pi^*\text{C}_2\text{-C}_8$	$\pi\text{C}_2\text{-C}_8 \rightarrow \pi^*\text{C}_5\text{-C}_7$	$\pi\text{C}_5\text{-C}_7 \rightarrow \pi^*\text{C}_2\text{-C}_8$
NO₂	23.37	6.38	24.03	9.07
CHO	25.14	8.69	27.98	13.09
BH₂	25.72	8.84	27.24	11.59
CN	26.99	11.57	26.63	12.04
H	27.63	10.89	27.63	10.89
Me	28.07	10.23	28.22	11.36
tBu	25.77	6.20	27.33	10.07
NH₂	30.65	12.45	29.53	11.85
OH	29.05	12.45	28.28	11.15
OMe	28.98	12.47	28.18	11.25
F	30.27	11.20	26.01	10.06

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