Supporting Information

for

Origin of Stereoselectivity in the Imidazolidinone-Catalyzed Reductions of Cyclic α,β-Unsaturated Ketones

Osvaldo Gutierrez, Robert Iafe, K. N. Houk

Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095-1569

houk@chem.ucla.edu

Full Gaussian Reference:

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.;Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.;Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.;Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.;Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.;Fukuda, R.;Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.;Klene, M.; Li, X.; Knox, J. E.; Hratchian, H.P.;Cross, J. B.; Bakken, V.;Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin,A. J.;Cammi,R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.;Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich,S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.;Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.;Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M.A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson,B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

3-phenyl-cyclopent-2-enone

E (0 K) = -500.4118286
ZPE = 0.179888
H (298 K) = -500.2212756
G (298 K) = -500.2688566

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.333462
C	2.323729	0.000000	0.681425
C	1.415552	-0.000407	-0.556451
H	-0.850635	-0.000020	1.985744
H	2.963696	0.873093	0.735631
H	2.964380	-0.872567	0.735878
H	1.578687	0.870980	-1.182459
H	1.578446	-0.872494	-1.181555
C	-1.180766	0.000219	-0.892152
C	-2.479625	0.002173	-0.377768
C	-1.023967	-0.001494	-2.275874
C	-3.575876	0.002364	-1.216667
H	-2.637037	0.003666	0.684069
C	-2.123496	-0.001370	-3.119789
H	-0.041118	-0.002993	-2.707788
C	-3.402046	0.000540	-2.593779
H	-4.566357	0.003885	-0.798456
H	-1.976887	-0.002714	-4.184919
H	-4.256494	0.000640	-3.246412
C	1.372042	-0.000042	1.869236
O	1.693261	-0.000511	3.018033

imidazolidinone 2

E (0 K) = -499.5866432
ZPE = 0.255813
H (298 K) = -499.3176872
G (298 K) = -499.3680932

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.468130
H	1.061467	0.000000	-0.268197
H	1.077167	0.024314	2.692748
C	-0.374858	1.370413	0.560275
O	-0.561802	2.356935	-0.114905
N	-0.458909	1.273390	1.936494
N	-0.138532	-0.884544	1.222760
H	-1.067663	-1.324232	1.214838
C	-0.556906	2.498673	2.732738
H	0.329251	2.625767	3.362786
H	-0.617522	3.326027	2.023839
H	-1.454201	2.499439	3.355072
C	-0.750673	-0.634085	3.674423
C	-2.276420	-0.608651	3.465370
H	-2.602587	-1.190668	2.591342
H	-2.771845	-1.057658	4.331360
H	-2.659519	0.409041	3.350152
C	-0.255764	-2.093361	3.826207
H	0.837142	-2.148828	3.908490
H	-0.668445	-2.523732	4.742782
H	-0.579139	-2.749470	3.007524
C	-0.374710	0.122416	4.968361
H	-0.791371	-0.411108	5.828089
H	0.711740	0.169333	5.107362
H	-0.769696	1.139417	4.997024
H	0.537541	-1.653147	1.223337
H	-0.600824	-0.343834	-0.815898

imidazolidinone 3

E (0 K) = -880.867159
ZPE = 0.33022
H (298 K) = -880.517496
G (298 K) = -880.586823

C	0.899194	1.519554	0.147660
C	-1.291805	0.753679	0.993359
H	1.375949	1.954292	1.032171
H	-1.266376	1.048673	2.051331
C	-0.239161	2.433522	-0.324512
O	-0.081594	3.441859	-0.974971
N	-1.429088	1.889658	0.100226
C	1.939996	1.175993	-0.923987
H	2.460929	2.111081	-1.155725
H	1.421395	0.876756	-1.843158
C	2.889235	0.087635	-0.463670
C	2.752566	-1.221043	-0.948147
C	3.885894	0.357938	0.486402
C	3.593500	-2.240411	-0.493524
H	2.013090	-1.439171	-1.717649
C	4.725107	-0.659117	0.940808
H	4.023588	1.372665	0.855051
C	4.578362	-1.961096	0.453980
H	3.486726	-3.245772	-0.890288
H	5.501706	-0.433336	1.665640
H	5.238082	-2.749787	0.802897
C	-2.255043	-0.348096	0.817875
C	-3.142618	-0.963253	1.651910
C	-3.244447	-1.918964	-0.382421
C	-3.784382	-1.973267	0.872606
H	-3.326205	-0.724763	2.691167
H	-4.554409	-2.655584	1.203308
C	-3.473899	-2.687506	-1.633888
H	-3.803790	-2.031564	-2.447710
H	-2.560361	-3.195377	-1.964788
H	-4.244583	-3.443462	-1.467207
O	-2.300293	-0.920918	-0.431197
C	-2.712467	2.556418	-0.099070
H	-3.113456	2.928686	0.850146
H	-2.531208	3.398970	-0.767814
H	-3.429983	1.869904	-0.555124
N	0.139914	0.295137	0.624711
H	0.603225	-0.187283	1.401445
H	0.064801	-0.387942	-0.141187

iminium ion 2-*E*

E (0 K) = -923.609021
ZPE = 0.409897
H (298 K) = -923.176931
G (298 K) = -923.250093

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.420556
H	0.799551	0.000000	-0.750301
H	0.761605	-0.037154	3.200673
N	-0.189464	-1.349844	0.519925
C	-0.149313	-2.566698	-0.285989
H	0.194124	-3.376899	0.360443
H	-1.131796	-2.835528	-0.683040
H	0.549545	-2.437363	-1.117764
C	-0.256837	-1.414015	1.887944
O	-0.436258	-2.401044	2.567582
C	-1.279241	0.660545	-0.629562
C	-1.680162	-0.161299	-1.874483
H	-2.079964	-1.143164	-1.611236
H	-2.463952	0.370869	-2.422766
H	-0.837778	-0.301837	-2.562932
C	-0.965518	2.097880	-1.088099
H	-0.177254	2.121063	-1.850363
H	-1.859620	2.536589	-1.541998
H	-0.679187	2.749334	-0.254882
C	-2.455794	0.691383	0.363020
H	-2.272406	1.376287	1.198669
H	-3.355038	1.048705	-0.148796
H	-2.683882	-0.302091	0.762580
N	0.493595	0.705232	1.226375
H	-0.912673	0.450323	2.821714
C	1.457602	1.607036	1.268654
C	2.265229	2.074512	0.080645
C	1.923926	2.243668	2.448618
C	3.285505	3.059975	0.688927
H	2.753665	1.220643	-0.404335
H	1.636829	2.550819	-0.674791
C	2.974388	3.092191	2.168931
H	1.488329	2.089786	3.426239
H	4.316928	2.733037	0.514876
H	3.197267	4.060153	0.250478
C	3.703681	3.916918	3.111225
C	4.759866	4.742562	2.664360
C	3.383233	3.920361	4.488997
C	5.465048	5.539788	3.557902
H	5.030611	4.760253	1.613774
C	4.089319	4.718030	5.377956
H	2.579272	3.296312	4.865300
C	5.131682	5.529825	4.915153
H	6.273889	6.168599	3.199489
H	3.832288	4.710702	6.432498
H	5.683023	6.152762	5.613190

iminium ion 2-*Z*

E (0 K) = -923.609647
ZPE = 0.409739
H (298 K) = -923.177722
G (298 K) = -923.250709

C	-2.038722	0.518252	-0.304314
C	-2.412444	-1.779351	0.363130
H	-1.366659	0.977906	-1.038915
H	-2.030335	-2.758942	0.073889
N	-3.197717	-0.041847	-0.990711
C	-3.853142	0.578611	-2.139130
H	-4.338081	-0.219302	-2.704764
H	-4.612976	1.305630	-1.843267
H	-3.108269	1.075984	-2.768822
C	-3.490757	-1.332597	-0.628762
O	-4.397309	-2.022870	-1.040420
C	-2.361092	1.566346	0.817759
C	-3.109064	2.753427	0.173249
H	-4.125832	2.486798	-0.124793
H	-3.187473	3.568438	0.899780
H	-2.580594	3.146816	-0.703768
C	-1.050679	2.099521	1.429686
H	-0.423015	2.597349	0.680237
H	-1.285874	2.844348	2.196482
H	-0.461380	1.313995	1.913777
C	-3.234578	0.959058	1.930657
H	-2.693788	0.203835	2.512641
H	-3.534296	1.745512	2.630601
H	-4.151831	0.511429	1.534012
N	-1.391044	-0.730467	0.220797
C	-0.093825	-0.962499	0.284547
C	0.965563	-0.084454	-0.064276
C	0.469204	-2.282982	0.754089
C	2.188445	-0.684254	0.151356
H	0.822657	0.916976	-0.442284
C	1.995864	-2.071698	0.722809
H	0.092440	-2.540445	1.750138
H	0.160890	-3.093562	0.082539
H	2.432321	-2.138220	1.726205
H	2.502303	-2.825853	0.111174
C	3.495900	-0.113493	-0.108578
C	3.638089	1.173515	-0.677176
C	4.664961	-0.842486	0.204384
C	4.896189	1.705590	-0.920676
H	2.760289	1.757529	-0.933799
C	5.923687	-0.305730	-0.039572
H	4.589324	-1.831902	0.643348
C	6.042477	0.967816	-0.602453
H	4.989743	2.694114	-1.359226
H	6.812238	-0.877934	0.207767
H	7.026059	1.386267	-0.794058
H	-2.804523	-1.833170	1.383482

iminium ion 3-*E*-a

E (0 K) = -1304.880953
ZPE = 0.484766
H (298 K) = -1304.367771
G (298 K) = -1304.457577

C	2.584787	-0.382316	-1.033577
C	0.971491	1.429821	-0.627959
H	2.636232	-1.065983	-1.891070
H	0.194124	1.754439	-1.326700
C	0.617248	1.900732	0.818643
H	1.507331	2.366994	1.254500
N	3.137127	0.916650	-1.379071
C	4.524670	1.072134	-1.788959
H	4.714881	0.522443	-2.717160
H	4.691755	2.137006	-1.956272

H	5.206582	0.713958	-1.010786
C	2.315337	1.977123	-1.110787
O	2.587314	3.156610	-1.220439
C	0.166406	-0.900149	-0.749541
N	1.152856	-0.028482	-0.775334
C	-0.550330	2.866954	0.854919
C	-1.701614	2.567824	1.595547
C	-0.492439	4.078775	0.149907
C	-2.777702	3.459086	1.631522
H	-1.749019	1.643617	2.168891
C	-1.568626	4.965350	0.182575
H	0.402881	4.326534	-0.415835
C	-2.714054	4.658300	0.921714
H	-3.657658	3.219877	2.222510
H	-1.509132	5.902346	-0.363812
H	-3.547413	5.354321	0.950283
H	0.397238	1.020541	1.430796
C	3.569013	-2.541771	1.389804
C	3.247293	-1.044151	0.127247
C	4.777649	-2.217403	1.433256
O	2.716372	-2.059796	0.696477
C	3.126268	-3.029019	2.723455
H	2.041193	-3.183391	2.753730
H	3.614452	-3.979453	2.951655
H	3.381240	-2.312515	3.512955
C	4.619983	-1.168868	0.503839
H	5.393085	-1.060704	-0.245597
H	5.385442	-2.853110	2.040016
C	-1.199263	-0.585562	-0.527376
H	-1.560895	0.415465	-0.332724
C	-1.972945	-1.724719	-0.585079
C	-1.103674	-2.933953	-0.859030
H	-1.197545	-3.671962	-0.054463
H	-1.415769	-3.436808	-1.781264
C	0.333952	-2.382287	-0.965273
H	0.785069	-2.585933	-1.944014
H	1.010300	-2.806385	-0.215067
C	-3.411082	-1.804448	-0.415900
C	-4.183566	-0.649961	-0.148794
C	-4.072370	-3.048397	-0.518764
C	-5.559881	-0.741974	0.005342
H	-3.706423	0.320601	-0.057406
C	-5.450935	-3.135356	-0.363793
H	-3.505602	-3.951173	-0.722242
C	-6.197497	-1.983258	-0.102587
H	-6.141029	0.151989	0.208999
H	-5.944687	-4.098454	-0.446839
H	-7.274723	-2.050994	0.017327

iminium ion 3-*E*-b

E (0 K) = -1304.882851
ZPE = 0.484828
H (298 K) = -1304.36964
G (298 K) = -1304.458663

C	2.488120	-0.494048	-1.110380
C	1.152512	1.549003	-1.058081
H	2.391160	-1.401073	-1.719285
H	0.310665	1.869845	-1.677698
C	1.194918	2.368451	0.257604
H	1.518388	3.370539	-0.048009
N	3.135442	0.564754	-1.853890
C	4.416923	0.379629	-2.520742
H	4.338371	-0.388685	-3.298204
H	4.679325	1.334009	-2.979646
H	5.192718	0.090276	-1.805822
C	2.454340	1.754201	-1.846636
O	2.808511	2.802537	-2.343866
C	0.023131	-0.664777	-0.828887
N	1.111094	0.078259	-0.909202
C	-0.115098	2.448722	1.008598
C	-0.341247	1.668842	2.149835
C	-1.129276	3.314098	0.570085
C	-1.556066	1.742335	2.834746
H	0.444901	1.010840	2.513564
C	-2.345052	3.388558	1.252047
H	-0.957876	3.951015	-0.295618
C	-2.561815	2.599625	2.385718
H	-1.711671	1.139533	3.725015
H	-3.112513	4.078905	0.912752
H	-3.502011	2.667259	2.925424
H	1.980408	1.957320	0.899601
C	3.680140	-2.197248	1.838966
C	3.194426	-0.830037	0.166262
C	4.389889	-1.049602	2.043869
O	2.941850	-2.075228	0.685777
C	3.568224	-3.484939	2.574937
H	3.876152	-4.330857	1.949200
H	4.210229	-3.462175	3.458776
H	2.539340	-3.672304	2.905401
C	4.079320	-0.164344	0.963062
H	4.478771	0.826921	0.798089
H	5.068463	-0.859438	2.863445
C	-1.310900	-0.193293	-0.717991
H	-1.573424	0.852308	-0.646263
C	-2.196851	-1.247967	-0.689427
C	-1.452636	-2.562096	-0.775155
H	-1.656066	-3.180442	0.106600
H	-1.778980	-3.143528	-1.644768
C	0.036094	-2.174626	-0.875559
H	0.486653	-2.527835	-1.811142
H	0.643537	-2.585267	-0.063398
C	-3.642310	-1.164881	-0.588279
C	-4.294144	0.074684	-0.395115
C	-4.430932	-2.332688	-0.682315
C	-5.678102	0.138408	-0.308249
H	-3.714947	0.986323	-0.292406
C	-5.816799	-2.263577	-0.597237
H	-3.958634	-3.298421	-0.830124
C	-6.443553	-1.028578	-0.411824
H	-6.165869	1.096460	-0.157157
H	-6.409102	-3.169837	-0.675962
H	-7.526166	-0.974373	-0.345122

iminium ion 3-*E*-c

E (0 K) = -1304.881753
ZPE = 0.484898
H (298 K) = -1304.36861
G (298 K) = -1304.457077

C	-1.567498	0.733480	-1.415279
C	-0.555355	-1.522719	-1.517617
H	-1.260781	1.498804	-2.143997
H	0.163246	-1.760409	-2.311874
C	-0.443008	-2.601829	-0.411043
H	0.602871	-2.699260	-0.104575
N	-2.449479	-0.234870	-2.037919
C	-3.746956	0.152824	-2.571801
H	-3.631472	0.904775	-3.360907
H	-4.202004	-0.745596	-2.990709
H	-4.384245	0.555379	-1.779412
C	-1.952986	-1.501325	-2.139197
O	-2.506870	-2.470178	-2.621594
C	0.791187	0.399672	-0.718284
N	-0.356932	-0.114220	-1.109595
C	-1.315551	-2.410174	0.811682
C	-2.663717	-2.800638	0.802350
C	-0.777694	-1.875568	1.990442
C	-3.452845	-2.650553	1.944182
H	-3.090238	-3.237102	-0.096690
C	-1.564324	-1.728025	3.134194
H	0.272871	-1.593359	2.022680
C	-2.905732	-2.114310	3.113004
H	-4.491129	-2.969617	1.925324
H	-1.127000	-1.324485	4.043169
H	-3.517249	-2.012630	4.005002
H	-0.707670	-3.533329	-0.924496
C	-2.727290	3.328684	0.779088
C	-2.161862	1.454050	-0.251162
C	-3.169748	2.294560	1.556629
O	-2.104725	2.827321	-0.332335
C	-2.803994	4.810142	0.898166
H	-3.346637	5.249740	0.053089
H	-3.327131	5.080715	1.818490
H	-1.807016	5.266039	0.923564
C	-2.809725	1.082054	0.891255
H	-3.014514	0.072453	1.218381
H	-3.703199	2.386787	2.492396
C	2.024781	-0.296399	-0.604293
H	2.146962	-1.346843	-0.824367
C	3.034529	0.557768	-0.217118
C	2.489487	1.956588	-0.032923
H	2.677279	2.322216	0.982715
H	2.989603	2.655672	-0.713132
C	0.981656	1.846070	-0.334694
H	0.657643	2.522614	-1.133068
H	0.363572	2.084523	0.536875
C	4.431383	0.220360	-0.016972
C	4.900972	-1.102334	-0.188022
C	5.358090	1.218582	0.357294
C	6.240177	-1.409732	0.006444
H	4.215293	-1.893730	-0.472586
C	6.698922	0.907138	0.551334
H	5.028622	2.243112	0.495910
C	7.142995	-0.406166	0.376438
H	6.585659	-2.429889	-0.128518
H	7.398450	1.685941	0.838266
H	8.190495	-0.649231	0.527930

iminium ion 3-*E*-d

E (0 K) = -1304.879283
ZPE = 0.484924
H (298 K) = -1304.366143
G (298 K) = -1304.454546

C	-1.396980	-1.402496	1.286156
C	-0.502255	0.826105	1.886917
H	-1.007993	-2.295996	1.797756
H	0.228149	0.886791	2.704179
C	-0.457568	2.161486	1.104227
H	0.578351	2.386999	0.834577
N	-2.293721	-0.668601	2.159563
C	-3.568277	-1.226986	2.585716
H	-3.417084	-2.176361	3.111037
H	-4.021609	-0.503766	3.264832
H	-4.228719	-1.388959	1.728541
C	-1.876728	0.581179	2.511537
O	-2.471390	1.383988	3.204288
C	0.910492	-0.769644	0.620638
N	-0.252484	-0.429263	1.140187
C	-1.336968	2.290576	-0.121718
C	-2.694944	2.620497	0.000530
C	-0.787417	2.159953	-1.403532
C	-3.480161	2.817397	-1.135206
H	-3.130265	2.745456	0.988216
C	-1.570358	2.361173	-2.541477
H	0.270968	1.931449	-1.515648
C	-2.919582	2.694150	-2.408658
H	-4.525569	3.091814	-1.024646
H	-1.121884	2.280074	-3.528028
H	-3.526554	2.874452	-3.291644
H	-0.750524	2.905245	1.854513
C	-3.232248	-1.657696	-1.809481
C	-2.023821	-1.875998	0.021980
C	-2.980793	-2.993888	-1.662067
O	-2.651532	-0.963901	-0.780275
C	-3.982044	-0.866690	-2.820140
H	-3.332575	-0.133274	-3.309387
H	-4.395515	-1.534605	-3.579722
H	-4.806762	-0.313338	-2.356689
C	-2.203569	-3.137390	-0.472763
H	-1.840240	-4.059194	-0.037261
H	-3.320134	-3.781711	-2.319591
C	2.093554	0.017693	0.630190
H	2.159425	1.001743	1.069693
C	3.137554	-0.657238	0.035532
C	2.672742	-2.013232	-0.445504
H	2.812880	-2.112652	-1.527907
H	3.260392	-2.812983	0.019131
C	1.184376	-2.092653	-0.051893
H	0.980855	-2.927024	0.629825
H	0.522669	-2.231261	-0.912009
C	4.500503	-0.186324	-0.123534
C	4.891838	1.098718	0.317917
C	5.472148	-1.012595	-0.730593
C	6.199696	1.534704	0.159335
H	4.168989	1.759937	0.784449
C	6.781495	-0.572958	-0.887217
H	5.202566	-2.003660	-1.080606

C	7.148339	0.700176	-0.442990
H	6.484955	2.524053	0.502970
H	7.516621	-1.220434	-1.354733
H	8.171283	1.043445	-0.565611

iminium ion 3-*E*-e

E (0 K) = -1304.88269
ZPE = 0.484705
H (298 K) = -1304.369549
G (298 K) = -1304.459493

C	2.367695	-0.988141	-1.152118
C	1.020351	1.025828	-0.867830
H	2.294876	-1.762792	-1.905064
H	0.252203	1.366668	-1.547735
C	0.841806	1.677680	0.531490
H	1.801215	2.057444	0.861005
N	3.028247	0.172025	-1.688709
C	4.387585	0.105839	-2.193632
H	4.458007	-0.647879	-2.968387
H	4.630338	1.069660	-2.610701
H	5.087114	-0.128781	-1.401068
C	2.369632	1.334395	-1.490469
O	2.755382	2.431042	-1.751048
C	-0.047170	-1.169483	-0.714113
N	1.019826	-0.448770	-0.862842
C	-0.187266	2.791499	0.550657
C	-1.283903	2.719573	1.400790
C	-0.042739	3.910079	-0.266639
C	-2.225311	3.739231	1.432329
H	-1.398556	1.874304	2.058358
C	-0.983982	4.924384	-0.238325
H	0.811017	3.991335	-0.916010
C	-2.078990	4.841839	0.609602
H	-3.061931	3.673484	2.104658
H	-0.858386	5.783552	-0.871894
H	-2.804326	5.634603	0.633382
H	0.559512	0.907433	1.237533
C	3.856084	-1.434067	2.069173
C	3.037753	-1.563010	0.052253
C	4.130105	-2.673362	1.630383
O	3.188781	-0.746747	1.115261
C	4.137729	-0.712322	3.340762
H	3.215867	-0.398023	3.818474
H	4.676454	-1.358301	4.020755
H	4.736998	0.172158	3.154420
C	3.591487	-2.757673	0.298574
H	3.637031	-3.595525	-0.367702
H	4.652662	-3.437743	2.166203
C	-1.354134	-0.667089	-0.479701
H	-1.578218	0.373477	-0.381415
C	-2.247431	-1.688108	-0.398641
C	-1.558030	-3.019899	-0.579748
H	-1.709472	-3.647832	0.290044
H	-1.968464	-3.546664	-1.432939
C	-0.076179	-2.672404	-0.783069
H	0.297216	-3.013229	-1.742222
H	0.562110	-3.094636	-0.017360
C	-3.684757	-1.572442	-0.170140
C	-4.287567	-0.323459	0.027123
C	-4.487957	-2.715807	-0.145830
C	-5.646170	-0.226872	0.238784
H	-3.699988	0.574846	0.020609
C	-5.849987	-2.617654	0.065526
H	-4.057254	-3.688107	-0.292987
C	-6.429486	-1.373922	0.257333
H	-6.097194	0.736270	0.388393
H	-6.455111	-3.504756	0.080181
H	-7.488535	-1.295889	0.421470

iminium ion 3-*E*-f

E (0 K) = -1304.884373
ZPE = 0.484833
H (298 K) = -1304.371189
G (298 K) = -1304.460579

C	2.367625	-1.145712	-0.936436
C	1.178114	0.923916	-1.505376
H	2.204518	-2.158660	-1.326007
H	0.361727	1.078022	-2.216611
C	1.265791	2.108784	-0.508361
H	1.631714	2.947131	-1.112649
N	3.110346	-0.352286	-1.898606
C	4.433861	-0.744891	-2.356479
H	4.395087	-1.713304	-2.867896
H	4.770605	0.021255	-3.056223
H	5.135006	-0.808274	-1.518081
C	2.505589	0.818186	-2.266115
O	2.940891	1.661458	-3.022696
C	-0.076657	-1.021822	-0.568725
N	1.050941	-0.424864	-0.908185
C	-0.025969	2.486967	0.179302
C	-0.274784	2.102417	1.503199
C	-0.996548	3.241960	-0.496992
C	-1.467877	2.454790	2.137243
H	0.478566	1.533779	2.043997
C	-2.190849	3.595390	0.133897
H	-0.805900	3.577295	-1.514617
C	-2.429907	3.200116	1.453451
H	-1.640390	2.158580	3.168189
H	-2.922856	4.198678	-0.396142
H	-3.352375	3.486736	1.950188
H	2.042618	1.878945	0.226869
C	3.946946	-0.508798	2.250117
C	3.015944	-1.285393	0.400444
C	4.066199	-1.868689	2.288949
O	3.304444	-0.139169	1.093780
C	4.360988	0.586824	3.166706
H	3.497254	1.159160	3.525873
H	4.877968	0.168422	4.033566
H	5.039000	1.288281	2.666858
C	3.465876	-2.372732	1.092228
H	3.396804	-3.407533	0.783203
H	4.534214	-2.443945	3.075225
C	-1.379291	-0.461156	-0.610925
H	-1.584908	0.560755	-0.895525
C	-2.319403	-1.391374	-0.224097
C	-1.650110	-2.701472	0.127510

H	-1.870888	-2.986117	1.162447
H	-2.022836	-3.514886	-0.505273
C	-0.145189	-2.453701	-0.094166
H	0.277523	-3.136084	-0.841297
H	0.447556	-2.583302	0.817965
C	-3.755199	-1.194956	-0.147985
C	-4.334026	0.076944	-0.362273
C	-4.607987	-2.282643	0.142594
C	-5.710308	0.245985	-0.296995
H	-3.703216	0.937698	-0.557765
C	-5.985811	-2.108937	0.204256
H	-4.192445	-3.270545	0.312730
C	-6.540251	-0.845562	-0.017317
H	-6.141757	1.228645	-0.460784
H	-6.628234	-2.955978	0.423667
H	-7.616646	-0.709666	0.031047

iminium ion 3-*Z*-a

E (0 K) = -1304.879486
ZPE = 0.4844
H (298 K) = -1304.366529
G (298 K) = -1304.457656

C	-0.316795	1.875999	-0.941625
C	-2.081280	0.179881	-0.704386
H	0.483021	1.907868	-1.693751
H	-2.281700	-0.676109	-1.355048
C	-2.734286	-0.055045	0.697204
H	-3.288424	0.850070	0.972905
N	-1.574675	2.333770	-1.494519
C	-1.715372	3.648526	-2.105352
H	-1.065052	3.736549	-2.982948
H	-2.756835	3.748292	-2.414232
H	-1.465867	4.437648	-1.390184
C	-2.610320	1.444309	-1.384416
O	-3.760475	1.619922	-1.734359
C	0.289111	-0.507439	-0.537169
C	1.696745	-0.321516	-0.516792
C	2.339802	-1.533158	-0.382627
H	2.175125	0.646521	-0.561554
N	-0.627559	0.428321	-0.670082
C	-3.658472	-1.256192	0.736702
C	-3.450195	-2.281241	1.667525
C	-4.741691	-1.351210	-0.149807
C	-4.303957	-3.385856	1.713282
H	-2.627938	-2.207761	2.377480
C	-5.590896	-2.456869	-0.106610
H	-4.923699	-0.551949	-0.864948
C	-5.374258	-3.476809	0.823390
H	-4.134228	-4.169877	2.445931
H	-6.428783	-2.517573	-0.795326
H	-6.040430	-4.333964	0.857644
H	-1.938269	-0.167807	1.440580
H	-1.613887	3.344902	1.404235
C	-0.542167	3.276351	1.276130
C	0.464228	3.839985	2.121492
C	0.118922	2.649189	0.260913
C	1.673330	3.524817	1.570519
H	0.307173	4.419271	3.020476
O	1.474642	2.793250	0.425483
C	3.082534	3.819108	1.945026
H	3.653232	2.899212	2.120890
H	3.595207	4.385206	1.158354
H	3.104363	4.412863	2.861969
C	1.329627	-2.655921	-0.281140
H	1.491676	-3.403831	-1.065227
H	1.431350	-3.180936	0.675681
H	6.746943	-0.086726	-0.552909
C	6.056129	-0.915409	-0.432305
C	6.544472	-2.211439	-0.229713
C	4.688017	-0.687825	-0.482952
C	5.656563	-3.279832	-0.079897
H	7.615495	-2.386778	-0.191128
C	3.773144	-1.755176	-0.332221
H	4.325829	0.321847	-0.647216
C	4.285480	-3.055897	-0.132044
H	6.034285	-4.285416	0.076149
H	3.608340	-3.895497	-0.014036
C	-0.046267	-1.972588	-0.412618
H	-0.591539	-2.311118	-1.302639
H	-0.705984	-2.167381	0.439027

iminium ion 3-*Z*-b

E (0 K) = -1304.882448
ZPE = 0.484594
H (298 K) = -1304.369351
G (298 K) = -1304.459703

C	1.653223	-1.425936	-0.957545
C	2.404614	0.913787	-1.044775
H	0.976475	-1.937162	-1.655453
H	2.189119	1.659980	-1.814844
C	2.844639	1.626594	0.275962
H	3.773116	2.174690	0.076378
N	2.987895	-1.314396	-1.508650
C	3.742880	-2.481960	-1.942571
H	3.226640	-2.990057	-2.764868
H	4.713574	-2.124852	-2.289315
H	3.882419	-3.183623	-1.115148
C	3.479455	-0.037729	-1.574337
O	4.582475	0.298361	-1.957152
C	-0.012279	0.424896	-0.847963
C	-1.165928	-0.394443	-0.728824
C	-2.306705	0.379003	-0.726232
H	-1.130298	-1.468777	-0.617087
N	1.239575	0.020362	-0.900982
C	1.796471	2.573426	0.826678
C	1.320209	2.421374	2.134574
C	1.298755	3.621823	0.038369
C	0.360643	3.296336	2.649212
H	1.716378	1.627007	2.765109
C	0.337088	4.492149	0.551425
H	1.675001	3.760399	-0.972872
C	-0.135008	4.331618	1.856593
H	0.005988	3.170450	3.668351
H	-0.037951	5.302748	-0.066915
H	-0.880198	5.014187	2.254670
H	3.091216	0.863185	1.021196

H	3.447940	-1.759685	1.494145
C	2.473046	-2.221102	1.414335
C	1.836645	-3.062571	2.379775
C	1.612435	-2.130890	0.359704
C	0.631818	-3.434424	1.855420
H	2.232378	-3.364225	3.339364
O	0.482251	-2.868641	0.613127
C	-0.478385	-4.297938	2.339684
H	-1.418507	-3.738760	2.419199
H	-0.649402	-5.144950	1.664792
H	-0.233851	-4.693523	3.328381
C	-1.947484	1.845769	-0.830664
H	-2.429191	2.308555	-1.699116
H	-2.301764	2.393290	0.050359
H	-5.506831	-2.973090	-0.467917
C	-5.290796	-1.909617	-0.496907
C	-6.336193	-0.980217	-0.446141
C	-3.976421	-1.473484	-0.587994
C	-6.059976	0.388782	-0.488988
H	-7.363796	-1.324258	-0.375504
C	-3.675957	-0.092613	-0.631209
H	-3.177985	-2.207022	-0.632952
C	-4.744676	0.829273	-0.582209
H	-6.870033	1.110289	-0.450793
H	-4.545799	1.895470	-0.614527
C	-0.409860	1.876799	-0.940492
H	-0.073023	2.299397	-1.895486
H	0.064767	2.478601	-0.158806

iminium ion 3-*Z*-c

E (0 K) = -1304.881396
ZPE = 0.485124
H (298 K) = -1304.368108
G (298 K) = -1304.456036

C	-0.894694	0.427030	-1.529502
C	-1.764466	-1.852118	-1.104349
H	-0.116787	0.601054	-2.287371
H	-1.423890	-2.701335	-1.709853
C	-2.465529	-2.414191	0.158109
H	-1.796925	-3.121698	0.657295
N	-2.182874	0.208303	-2.156713
C	-2.822205	1.236226	-2.965537
H	-2.185164	1.510378	-3.814124
H	-3.758613	0.816098	-3.334834
H	-3.027407	2.127053	-2.365261
C	-2.727169	-1.027756	-1.962086
O	-3.795682	-1.431911	-2.377786
C	0.574569	-1.276044	-0.494224
C	1.723481	-0.441527	-0.441930
C	2.827057	-1.162062	-0.039617
H	1.713601	0.610505	-0.687763
N	-0.625062	-0.927397	-0.914337
C	-2.991363	-1.401837	1.154152
C	-4.238349	-0.787322	0.958856
C	-2.262686	-1.089866	2.309656
C	-4.736007	0.121133	1.894936
H	-4.826067	-1.033641	0.078788
C	-2.759056	-0.183520	3.248038
H	-1.306880	-1.576799	2.494238
C	-3.997970	0.425669	3.041788
H	-5.709239	0.577050	1.736162
H	-2.184995	0.036108	4.143779
H	-4.393085	1.121495	3.776401
H	-3.293610	-3.006164	-0.248502
C	0.045984	3.449139	0.179262
C	-0.865462	1.580074	-0.581485
C	-1.101259	3.243469	0.891523
C	2.447561	-2.603111	0.220367
H	2.995941	-3.273072	-0.452128
H	2.708166	-2.904304	1.240793
H	6.034608	2.189387	-0.201520
C	5.802615	1.148643	0.002193
C	6.814485	0.272361	0.411600
C	4.501706	0.688516	-0.145982
C	6.518276	-1.068086	0.671928
H	7.831643	0.635171	0.525911
C	4.181515	-0.664183	0.112903
H	3.728759	1.380034	-0.465474
C	5.216462	-1.532715	0.524203
H	7.302333	-1.748631	0.988664
H	5.002595	-2.576689	0.728491
C	0.927405	-2.667376	-0.029327
H	0.650881	-3.418611	-0.778399
H	0.378361	-2.918219	0.883650
O	0.204425	2.435646	-0.730552
C	1.086326	4.512969	0.190471
H	0.843227	5.259273	0.950623
H	2.079106	4.106103	0.418617
H	1.149940	5.020052	-0.779556
C	-1.692858	2.038097	0.400828
H	-2.613795	1.579727	0.732524
H	-1.487311	3.883778	1.672265

iminium ion 3-*Z*-d

E (0 K) = -1304.878321
ZPE = 0.484642
H (298 K) = -1304.365358
G (298 K) = -1304.454391

C	-0.732836	0.192089	-1.786182
C	-1.501044	-2.014949	-0.973034
H	0.022556	0.229014	-2.585830
H	-1.108829	-2.907357	-1.478468
C	-2.154796	-2.472782	0.353866
H	-1.453263	-3.108193	0.901997
N	-2.028910	-0.171522	-2.330236
C	-2.742902	0.702378	-3.248859
H	-2.135177	0.908070	-4.137026
H	-3.652890	0.178711	-3.544525
H	-3.004659	1.647692	-2.764008
C	-2.522858	-1.370625	-1.911827
O	-3.587576	-1.872174	-2.217170
C	0.783028	-1.207307	-0.417215
C	1.888572	-0.316301	-0.475625
C	3.014440	-0.900990	0.062442
H	1.832020	0.682012	-0.882120
N	-0.418961	-1.002662	-0.919924

C	-2.708172	-1.400484	1.269423
C	-3.963253	-0.823959	1.022121
C	-2.007596	-1.016139	2.419548
C	-4.498291	0.114218	1.904634
H	-4.531703	-1.129731	0.148150
C	-2.542364	-0.080814	3.306806
H	-1.048292	-1.477062	2.648866
C	-3.792044	0.485747	3.051040
H	-5.479636	0.537160	1.708451
H	-1.994184	0.186963	4.206068
H	-4.221522	1.198067	3.750043
H	-2.964662	-3.131808	0.018980
C	-1.375158	3.033273	0.343345
C	-0.699831	1.515746	-1.105921
C	-0.480298	3.652658	-0.484306
C	2.703894	-2.307310	0.523533
H	3.286932	-3.036645	-0.051406
H	2.974590	-2.450749	1.574925
H	5.995360	2.630223	-0.364884
C	5.831389	1.595987	-0.078756
C	6.894603	0.825724	0.406629
C	4.565210	1.039548	-0.192992
C	6.683996	-0.503960	0.780877
H	7.884672	1.263300	0.493845
C	4.331843	-0.304599	0.178419
H	3.749570	1.652829	-0.561957
C	5.416384	-1.063890	0.670559
H	7.507889	-1.101735	1.157776
H	5.268959	-2.098563	0.962429
C	1.190747	-2.480018	0.283819
H	0.948618	-3.364064	-0.317004
H	0.647591	-2.582345	1.228325
O	-1.519323	1.723342	-0.033159
C	-2.177615	3.492738	1.507131
H	-1.950661	2.902398	2.401288
H	-1.961699	4.543763	1.713796
H	-3.251206	3.388925	1.312955
C	-0.045206	2.671761	-1.427452
H	0.646499	2.814352	-2.248003
H	-0.175640	4.688279	-0.431052

iminium ion 3-*Z*-e

E (0 K) = -1304.88039
ZPE = 0.484488
H (298 K) = -1304.367376
G (298 K) = -1304.458141

C	-0.295020	1.787150	-1.135776
C	-1.823512	-0.096853	-0.887110
H	0.511178	1.920866	-1.846555
H	-1.880662	-0.975918	-1.512310
C	-2.494165	-0.361423	0.491192
H	-3.153976	0.467383	0.717903
N	-1.562991	2.045023	-1.766231
C	-1.868088	3.333171	-2.361350
H	-1.127798	3.580184	-3.112863
H	-2.837373	3.258333	-2.826892
H	-1.889280	4.112482	-1.610080
C	-2.473566	1.058683	-1.626517
O	-3.605057	1.067283	-1.999712
C	0.590469	-0.434329	-0.591658
C	1.959614	-0.060776	-0.520779
C	2.737250	-1.152164	-0.293542
H	2.304448	0.946498	-0.603582
N	-0.419391	0.348264	-0.808839
C	-3.266580	-1.665053	0.550554
C	-2.973758	-2.609139	1.525959
C	-4.294092	-1.927920	-0.352294
C	-3.682313	-3.800025	1.596885
H	-2.201505	-2.411796	2.250752
C	-4.998172	-3.117419	-0.284035
H	-4.550910	-1.197805	-1.099419
C	-4.693454	-4.058211	0.689020
H	-3.446558	-4.517543	2.362022
H	-5.790697	-3.306566	-0.985160
H	-5.245490	-4.978829	0.741810
H	-1.728087	-0.352709	1.255836
C	-0.484267	3.435015	2.033162
C	-0.020375	2.642919	0.055871
C	0.608889	4.091258	1.612071
C	1.892944	-2.399118	-0.179748
H	2.197427	-3.136903	-0.912089
H	2.015902	-2.847010	0.799309
H	6.899673	0.851355	-0.286425
C	6.326085	-0.049628	-0.173624
C	6.964498	-1.252740	0.100589
C	4.954589	-0.012692	-0.302257
C	6.226777	-2.416187	0.244353
H	8.033980	-1.280252	0.200471
C	4.191709	-1.178235	-0.159790
H	4.480075	0.925752	-0.516710
C	4.851217	-2.379157	0.114231
H	6.719464	-3.346668	0.455899
H	4.297572	-3.291562	0.229100
C	0.453432	-1.922040	-0.410410
H	0.017152	-2.356536	-1.303253
H	-0.208451	-2.159613	0.411239
O	-0.878087	2.548110	1.091831
C	-1.302319	3.499970	3.275629
H	-1.308672	2.541720	3.784128
H	-0.895971	4.244310	3.947023
H	-2.328691	3.764065	3.045376
C	0.913755	3.569289	0.306284
H	1.711636	3.870696	-0.342333
H	1.138157	4.853818	2.143870

iminium ion 3-*Z*-f

E (0 K) = -1304.883391
ZPE = 0.484646
H (298 K) = -1304.370267
G (298 K) = -1304.46029

C	1.544647	-1.464921	-1.097458
C	2.094337	0.925328	-1.280142
H	0.897223	-2.058041	-1.757071
H	1.776784	1.620981	-2.062369
C	2.525331	1.719528	-0.003937
H	3.429873	2.288817	-0.245179

N	2.843905	-1.256204	-1.715670
C	3.709796	-2.370808	-2.068342
H	3.223348	-3.017298	-2.807130
H	4.618264	-1.947328	-2.498744
H	3.965947	-2.963028	-1.183843
C	3.228288	0.052114	-1.821001
O	4.289803	0.467130	-2.243071
C	-0.253324	0.237904	-0.911340
C	-1.321248	-0.670297	-0.686117
C	-2.521182	0.004024	-0.611716
H	-1.188224	-1.734961	-0.557649
N	1.020985	-0.061795	-1.048515
C	1.443826	2.643919	0.519704
C	0.998221	2.532301	1.842701
C	0.880436	3.628016	-0.306465
C	0.005656	3.382696	2.335125
H	1.444060	1.788958	2.501978
C	-0.114174	4.473785	0.184619
H	1.230313	3.734157	-1.330686
C	-0.554903	4.353396	1.504889
H	-0.324380	3.288186	3.365905
H	-0.540364	5.234132	-0.463757
H	-1.326285	5.016764	1.885228
H	2.815634	1.004297	0.772181
C	2.225987	-2.303465	2.341181
C	1.586931	-2.134774	0.233229
C	1.538777	-3.445970	2.044124
C	-2.297518	1.490915	-0.785538
H	-2.878840	1.880082	-1.628756
H	-2.633647	2.037437	0.103079
H	-5.389454	-3.583399	0.060327
C	-5.270310	-2.509346	-0.042630
C	-6.386923	-1.669040	0.036135
C	-4.008885	-1.970855	-0.253960
C	-6.235005	-0.286577	-0.098325
H	-7.373033	-2.092895	0.201155
C	-3.833521	-0.574746	-0.391807
H	-3.154340	-2.636724	-0.315191
C	-4.972865	0.256062	-0.310655
H	-7.100380	0.365851	-0.037934
H	-4.871281	1.331495	-0.412737
C	-0.780525	1.647336	-1.011175
H	-0.549451	2.065656	-1.998984
H	-0.305250	2.311785	-0.282763
O	2.263543	-1.491459	1.234762
C	2.905427	-1.800426	3.564857
H	2.463741	-0.858021	3.909770
H	2.814476	-2.535674	4.367918
H	3.971156	-1.619893	3.382317
C	1.125234	-3.339085	0.678492
H	0.573732	-4.072091	0.104109
H	1.354321	-4.270690	2.717912

Hantzsh ester 4

E (0 K) = -862.4955938
ZPE = 0.310709
H (298 K) = -862.1637678
G (298 K) = -862.2367938

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.339822
C	2.390636	0.000000	1.420844
C	2.481354	0.000000	0.084099
C	1.269845	-0.103824	-0.818520
H	1.289223	-1.049983	-1.390295
H	1.295984	0.684799	-1.589927
N	1.171011	-0.115790	2.097487
H	1.138999	0.239963	3.042239
C	-1.297737	0.086382	2.164453
H	-1.326828	-0.718357	2.869045
H	-1.326616	1.019472	2.687338
H	-2.141441	0.018048	1.509935
C	3.629555	0.086390	2.331458
H	3.622206	1.018869	2.856176
H	3.611614	-0.719178	3.035474
H	4.515652	0.019502	1.735423
C	3.877217	0.080983	-0.561354
O	4.201428	0.095579	-1.748045
O	4.868855	0.144067	0.362813
C	-1.348958	0.081014	-0.738478
O	-1.592081	0.095616	-1.944396
O	-2.400881	0.144258	0.116431
C	6.146850	0.218026	-0.274493
H	6.189190	1.093446	-0.888290
H	6.293425	-0.650732	-0.881680
C	7.251254	0.288085	0.796479
H	8.207516	0.343425	0.319614
H	7.104688	1.156851	1.403657
H	7.208904	-0.587328	1.410286
C	-3.632793	0.218241	-0.605940
H	-3.633488	1.093693	-1.221149
H	-3.737911	-0.650487	-1.221702
C	-4.807177	0.288235	0.387803
H	-5.728958	0.343593	-0.152712
H	-4.806471	-0.587208	1.003025
H	-4.702069	1.156973	1.003553

Water

E (0 K) = -76.408953
ZPE = 0.021168
H (298 K) = -76.384006
G (298 K) = -76.405452

O	0.000000	0.000000	0.119720
H	0.000000	0.761560	-0.478879
H	0.000000	-0.761560	-0.478879

Transition Structure TS-2-*E* (bottom, *anti*)

E (0 K) = -1786.095142
ZPE = 0.717722
H (298 K) = -1785.334335
G (298 K) = -1785.4562
One imaginary frequency at = -801.1 cm^{-1}

C	-4.385664	-0.002888	0.046954
C	-3.140732	-1.861450	-0.854337
H	-4.147213	1.064576	0.137058
H	-2.159761	-1.951891	-1.329212
N	-4.804518	-0.292534	-1.325049
C	-5.660719	0.561375	-2.134868
H	-5.406750	0.379079	-3.181426
H	-6.724048	0.343850	-1.998117
H	-5.479842	1.612865	-1.889096
C	-4.161207	-1.368777	-1.879774
O	-4.335070	-1.822982	-2.994374
C	-5.446388	-0.367513	1.147222
C	-6.705084	0.503584	0.952382
H	-7.271243	0.221884	0.061086
H	-7.373556	0.382155	1.811535
H	-6.457105	1.570164	0.880022
C	-4.868359	-0.061776	2.543050
H	-4.653549	1.006691	2.668531
H	-5.600576	-0.333686	3.310804
H	-3.955128	-0.630891	2.746089
C	-5.835632	-1.855064	1.078142
H	-4.989233	-2.506794	1.321045
H	-6.626501	-2.065173	1.806244
H	-6.218352	-2.131648	0.090107
N	-3.140195	-0.796934	0.149564
H	-3.427943	-2.839034	-0.449956
C	-1.991243	-0.376833	0.730729
C	-1.787015	1.015810	1.290088
C	-0.830619	-1.111815	0.820625
C	-0.409905	0.925664	1.976634
H	-1.764941	1.736185	0.461862
H	-2.570368	1.329399	1.983631
C	0.258698	-0.322401	1.369701
H	-0.714926	-2.117812	0.443893
H	0.177451	1.840027	1.847258
H	-0.527083	0.765959	3.054585
C	1.400066	-0.961831	2.106343
C	2.178683	-0.208379	3.002466
C	1.751386	-2.305805	1.890744
C	3.254634	-0.783241	3.677842
H	1.931382	0.832288	3.190943
C	2.827560	-2.881887	2.566713
H	1.171923	-2.912279	1.202916
C	3.583055	-2.123865	3.463755
H	3.828138	-0.187907	4.383112
H	3.066662	-3.928973	2.402288
H	4.412949	-2.576135	3.999196
C	2.066114	1.953855	-0.581771
C	3.355254	2.230855	-0.173541
C	2.719097	-0.415434	-0.932709
C	3.995034	-0.110747	-0.510664
N	4.235889	1.179346	-0.099349
H	5.171750	1.387065	0.227261
C	1.673391	0.577142	-0.807285
H	0.905133	0.146298	0.360781
H	0.781928	0.422982	-1.412566
C	0.998931	2.967954	-0.809395
O	-0.155938	2.648054	-1.034598
O	1.425099	4.239471	-0.767452
C	2.289062	-1.736263	-1.475709
O	1.113636	-2.037804	-1.580728
O	3.302166	-2.527871	-1.855024
C	2.927730	-3.818844	-2.423237
H	2.352796	-4.368893	-1.672503
H	2.273516	-3.635650	-3.279879
C	0.416345	5.261691	-1.025268
H	-0.371744	5.161115	-0.273335
H	-0.025619	5.062260	-2.005300
C	1.103493	6.610600	-0.964962
H	0.371034	7.400081	-1.162130
H	1.540022	6.791087	0.022523
H	1.894446	6.685250	-1.717735
C	4.204245	-4.535610	-2.813257
H	4.846229	-4.706584	-1.943279
H	3.955435	-5.508590	-3.249163
H	4.766820	-3.963266	-3.557414
C	3.941756	3.570225	0.179792
H	4.065335	4.185446	-0.716860
H	3.286808	4.123427	0.853827
H	4.920251	3.453176	0.656503
C	5.184763	-1.027480	-0.453088
H	4.923839	-1.968449	0.034319
H	5.536899	-1.270987	-1.459588
H	6.006970	-0.563882	0.101473

Transition Structure TS-2-*E* (bottom, *syn*)

E (0 K) = -1786.093032
ZPE = 0.718234
H (298 K) = -1785.331964
G (298 K) = -1785.451959
One imaginary frequency at = -1015.2 cm^{-1}

C	3.646908	-0.963951	-0.521063
C	2.027148	-1.974298	0.907418
H	3.665768	-0.040133	-1.109125
H	0.985607	-1.846047	1.195992
N	3.906074	-0.610460	0.890640
C	4.850223	0.420327	1.305067
H	4.612312	0.682771	2.337388
H	5.881844	0.067007	1.261335
H	4.754287	1.306849	0.666973
C	2.932222	-1.058193	1.728332
O	2.763389	-0.735656	2.902623
C	4.646197	-1.966222	-1.183082
C	6.071745	-1.376619	-1.155098
H	6.505631	-1.395474	-0.151113
H	6.726463	-1.972918	-1.798966
H	6.100260	-0.345044	-1.527708
C	4.219795	-2.147724	-2.654512
H	4.269433	-1.201917	-3.208806
H	4.895043	-2.850781	-3.152671
H	3.204480	-2.548779	-2.738533
C	4.649081	-3.333501	-0.476050
H	3.692867	-3.854300	-0.593771
H	5.421900	-3.973522	-0.914455

H	4.873346	-3.238647	0.592487
N	2.261029	-1.483797	-0.455879
H	2.304635	-3.025314	1.038612
C	1.219242	-0.940869	-1.153469
C	1.373421	0.212948	-2.123811
C	-0.097561	-1.322957	-1.043534
C	-0.070761	0.488643	-2.603970
H	1.818161	1.083697	-1.625240
H	2.037224	-0.040799	-2.957984
C	-0.974741	-0.404016	-1.734699
H	-0.450473	-2.155641	-0.448334
H	-0.337862	1.545513	-2.543904
H	-0.200513	0.183598	-3.647456
C	-2.308034	-0.798597	-2.265916
C	-3.153945	0.182003	-2.815503
C	-2.736667	-2.135759	-2.252273
C	-4.395002	-0.168622	-3.336764
H	-2.844848	1.224219	-2.810165
C	-3.978184	-2.484478	-2.781403
H	-2.086190	-2.911031	-1.858549
C	-4.811071	-1.503009	-3.320828
H	-5.041517	0.598604	-3.752318
H	-4.291971	-3.524454	-2.778414
H	-5.779872	-1.775706	-3.729125
C	-1.905316	0.136794	1.435895
C	-0.896258	-0.083439	2.349622
C	-0.673329	2.129591	0.607812
C	0.303900	1.890683	1.548964
N	0.191589	0.760497	2.323975
H	0.985704	0.505418	2.909403
C	-1.718852	1.134837	0.387639
H	-1.360667	0.435345	-0.713434
H	-2.640358	1.506122	-0.058841
C	-3.232182	-0.549096	1.418275
O	-4.090126	-0.266719	0.605045
O	-3.394630	-1.470534	2.384502
C	-0.754124	3.329439	-0.268775
O	-1.457203	3.353872	-1.265636
O	-0.011773	4.369391	0.142838
C	-0.841573	-1.115166	3.445582
H	-1.451590	-0.795739	4.298162
H	-1.242373	-2.071198	3.112548
H	0.188690	-1.249450	3.789766
C	1.491641	2.754808	1.877982
H	1.949490	3.168446	0.979290
H	1.181897	3.605900	2.493945
H	2.237997	2.182574	2.437148
C	-4.696824	-2.124674	2.417928
H	-4.853727	-2.623456	1.457136
H	-5.463844	-1.352380	2.522620
C	-4.693630	-3.095601	3.581401
H	-5.663641	-3.600413	3.636686
H	-3.919344	-3.860190	3.460062
H	-4.526199	-2.575659	4.529880
C	-0.101272	5.578817	-0.668520
H	0.237881	5.339156	-1.680696
H	-1.153201	5.870406	-0.728103
C	0.754712	6.639264	-0.006322
H	0.701870	7.564670	-0.588994
H	0.402219	6.854065	1.007212
H	1.803618	6.329944	0.045982

Transition Structure TS-2-*E* (top, *syn*)

E (0 K) = -1786.086917
ZPE = 0.717628
H (298 K) = -1785.326146
G (298 K) = -1785.448119
One imaginary frequency at = -897.1 cm^{-1}

C	3.725244	-1.176154	-0.962494
C	3.543695	1.128274	-0.284306
H	3.357774	-1.716909	-1.843170
H	3.102976	2.012023	-0.753136
N	4.935978	-0.437050	-1.313305
C	5.998841	-0.930933	-2.179016
H	6.474220	-0.062031	-2.639154
H	6.763738	-1.489118	-1.631393
H	5.577632	-1.575242	-2.957347
C	4.918308	0.870565	-0.900499
O	5.805439	1.689063	-1.037482
C	3.913176	-2.212024	0.203515
C	4.909332	-3.305056	-0.238306
H	5.933937	-2.930488	-0.295863
H	4.906041	-4.124695	0.488324
H	4.642910	-3.730974	-1.213600
C	2.564929	-2.893133	0.507131
H	2.182820	-3.443482	-0.361228
H	2.694663	-3.617603	1.318995
H	1.807402	-2.166573	0.821190
C	4.434349	-1.531016	1.481569
H	3.702986	-0.826091	1.893796
H	4.632580	-2.285383	2.250948
H	5.371578	-0.993943	1.303633
N	2.786314	-0.078016	-0.623343
H	3.618627	1.304340	0.795001
C	1.491049	0.006943	-1.022264
C	0.773799	-1.076455	-1.807965
C	0.656427	1.082430	-0.808428
C	-0.523866	-0.384344	-2.280080
H	1.369929	-1.437844	-2.653612
H	0.570623	-1.946657	-1.174937
C	-0.646070	0.891989	-1.422835
H	0.917380	1.963864	-0.238140
H	-0.435938	-0.082726	-3.328808
H	-1.403912	-1.029367	-2.209605
C	-1.411138	2.049205	-1.991850
C	-2.693603	1.850152	-2.532505
C	-0.852450	3.336803	-2.042619
C	-3.391647	2.909100	-3.108966
H	-3.157257	0.870923	-2.480499
C	-1.551061	4.392841	-2.623487
H	0.144015	3.513640	-1.651772
C	-2.823804	4.183867	-3.157387
H	-4.382972	2.737724	-3.518700
H	-1.097686	5.379163	-2.662933

H	-3.368524	5.008366	-3.608360
C	-1.865050	-2.208691	1.336951
C	-0.660784	-0.437233	2.525564
C	-2.551546	-1.271293	0.598232
C	-1.335272	0.525888	1.809242
C	-2.186115	0.135932	0.695513
H	-1.419867	0.491315	-0.440258
N	-0.905847	-1.754359	2.213890
H	-0.404557	-2.453444	2.747975
H	-2.954765	0.852401	0.409360
C	-2.048303	-3.702405	1.334592
H	-1.178527	-4.198955	1.777910
H	-2.935830	-3.982805	1.911287
H	-2.193585	-4.085397	0.324798
C	0.306091	-0.231717	3.660203
H	-0.224301	0.077223	4.566334
H	0.852599	-1.155467	3.877240
H	1.023197	0.556530	3.430903
C	-1.245176	1.994472	2.054467
O	-1.679317	2.802587	1.256867
O	-0.672033	2.325518	3.224179
C	-3.669786	-1.590661	-0.334705
O	-4.057849	-0.797970	-1.173622
O	-4.214894	-2.801897	-0.146788
C	-5.334636	-3.140299	-1.021380
H	-4.984254	-3.099279	-2.056711
H	-6.104337	-2.374157	-0.896076
C	-5.822473	-4.519728	-0.628482
H	-6.157290	-4.538662	0.413310
H	-6.669645	-4.798885	-1.263316
H	-5.038047	-5.272082	-0.759229
C	-0.604165	3.754061	3.514699
H	-0.028537	4.238735	2.720768
H	-1.620822	4.155097	3.483406
C	0.038970	3.915490	4.877104
H	0.096783	4.979752	5.127321
H	-0.548459	3.415055	5.653263
H	1.055229	3.508436	4.888918

Transition Structure TS-2-*E* (top, *anti*)

E (0 K) = -1786.094434
ZPE = 0.718329
H (298 K) = -1785.333204
G (298 K) = -1785.453807
One imaginary frequency at = -863.5 cm^{-1}

C	4.474125	-0.142641	0.261199
C	3.429543	-2.236560	-0.310079
H	4.432260	0.483577	1.161078
H	2.771168	-2.921445	0.230686
N	5.391270	-1.259990	0.489715
C	6.663589	-1.170806	1.191800
H	6.849990	-2.140848	1.658168
H	7.499985	-0.947620	0.522685
H	6.610333	-0.395220	1.962238
C	4.872528	-2.476540	0.131475
O	5.433263	-3.553532	0.196651
C	4.852494	0.775151	-0.955757
C	6.215285	1.445032	-0.679784
H	7.043676	0.733585	-0.720479
H	6.408511	2.209783	-1.439680
H	6.236354	1.943418	0.297764
C	3.797113	1.886480	-1.110975
H	3.738664	2.517756	-0.215805
H	4.073383	2.537749	-1.947323
H	2.799550	1.490248	-1.321856
C	4.934876	-0.032141	-2.263508
H	3.957584	-0.432388	-2.554662
H	5.275339	0.616495	-3.077898
H	5.645331	-0.862032	-2.187117
N	3.182717	-0.849575	0.086434
H	3.305853	-2.406503	-1.385576
C	1.997771	-0.482736	0.633121
C	1.790447	0.781147	1.440447
C	0.825146	-1.200776	0.543486
C	0.398843	0.576150	2.073337
H	2.566421	0.930003	2.199601
H	1.795524	1.656869	0.785223
C	-0.263702	-0.538878	1.241532
H	0.692248	-2.081166	-0.068928
H	0.494514	0.227589	3.107751
H	-0.185587	1.501549	2.098190
C	-1.390580	-1.314108	1.863956
C	-2.207527	-0.712176	2.837488
C	-1.685681	-2.631098	1.472985
C	-3.269496	-1.407176	3.414591
H	-2.000381	0.303277	3.163187
C	-2.748332	-3.327572	2.050030
H	-1.073301	-3.122569	0.725027
C	-3.544528	-2.719527	3.022837
H	-3.873361	-0.929677	4.181481
H	-2.944590	-4.352910	1.748935
H	-4.363346	-3.267158	3.480675
C	-4.062706	0.095028	-0.436819
C	-3.293131	2.348358	0.144441
C	-2.816194	-0.220494	-0.933329
C	-2.030526	2.056382	-0.329710
C	-1.716765	0.698984	-0.730610
H	-0.930789	0.100097	0.344524
N	-4.225852	1.339776	0.124989
H	-5.141918	1.554799	0.499391
H	-0.854086	0.575376	-1.383007
C	-0.912553	3.032356	-0.451822
O	0.224585	2.678765	-0.714897
O	-1.271436	4.311756	-0.268139
C	-2.472108	-1.487569	-1.641033
O	-1.318003	-1.819318	-1.843720
O	-3.537103	-2.193201	-2.048443
C	-0.211250	5.303614	-0.412616
H	0.558380	5.092429	0.335634
H	0.237346	5.179427	-1.401896
C	-3.248920	-3.431394	-2.763472
H	-2.617397	-3.189455	-3.622565
H	-2.676197	-4.084038	-2.098001
C	-3.799377	3.665123	0.666764
H	-3.103985	4.099212	1.386173
H	-3.904067	4.387971	-0.148102

H	-4.774580	3.543744	1.149118
C	-5.294477	-0.766335	-0.438244
H	-5.674062	-0.901307	-1.454778
H	-5.069483	-1.758789	-0.043087
H	-6.084283	-0.318033	0.173045
C	-0.834985	6.672057	-0.228249
H	-1.281962	6.775184	0.765630
H	-0.062338	7.440407	-0.334616
H	-1.606593	6.859138	-0.981499
C	-4.573023	-4.043230	-3.173482
H	-5.132062	-3.370170	-3.831027
H	-4.389411	-4.975462	-3.717438
H	-5.191444	-4.274765	-2.300462

Transition Structure TS-2-*Z* (top,*syn*)

E (0 K) = -1786.085924
ZPE = 0.717995
H (298 K) = -1785.324906
G (298 K) = -1785.446021
One imaginary frequency at = -832.5 cm^{-1}

C	3.811231	-1.076384	0.563287
C	4.007789	-1.261792	-1.824085
H	3.175983	-1.598529	1.290944
H	3.556561	-1.869367	-2.607676
N	4.937922	-1.940164	0.207869
C	5.560348	-2.883088	1.128763
H	6.197730	-3.532900	0.526220
H	6.174295	-2.389305	1.883791
H	4.795156	-3.487158	1.633212
C	5.112726	-2.072452	-1.148858
O	5.955081	-2.739180	-1.715586
C	4.225085	0.312274	1.161857
C	5.103713	0.096162	2.411541
H	6.098500	-0.274341	2.151414
H	5.240105	1.049004	2.934832
H	4.646304	-0.604707	3.121030
C	2.960133	1.079463	1.592357
H	2.406619	0.538685	2.370572
H	3.247671	2.049953	2.012864
H	2.284873	1.263417	0.751536
C	5.007214	1.155565	0.139003
H	4.385250	1.429540	-0.720725
H	5.349775	2.084581	0.607844
H	5.895302	0.628597	-0.225234
N	3.077081	-0.972865	-0.728053
C	1.733694	-1.125346	-0.836106
C	0.794171	-1.132107	0.175807
C	1.050336	-1.296541	-2.178526
C	-0.543175	-1.371293	-0.344073
H	1.015976	-0.991842	1.223793
C	-0.346916	-1.824464	-1.800045
H	0.994131	-0.321466	-2.679095
H	1.572353	-1.982421	-2.851209
H	-1.137096	-1.473711	-2.468021
H	-0.349919	-2.920658	-1.827432
C	-1.585004	-2.026191	0.512712
C	-1.575899	-1.871124	1.910886
C	-2.618465	-2.784150	-0.063668
C	-2.549845	-2.471252	2.706536
H	-0.795498	-1.284631	2.387089
C	-3.591564	-3.388904	0.732934
H	-2.664776	-2.903524	-1.140509
C	-3.561374	-3.236888	2.120227
H	-2.512765	-2.352639	3.785993
H	-4.368698	-3.988746	0.267544
H	-4.313700	-3.715866	2.740283
H	4.407492	-0.350677	-2.283087
C	-0.943121	2.035148	-0.124985
C	-1.274992	2.494312	1.132475
C	-3.119276	0.834847	-0.223837
C	-3.416592	1.296385	1.038782
C	-1.786204	1.034700	-0.751429
H	-1.105457	-0.203491	-0.514601
H	-1.686364	0.938109	-1.829485
N	-2.454154	2.045556	1.680096
H	-2.680837	2.376622	2.610011
C	-0.519785	3.476743	1.984993
H	-0.668836	4.497698	1.616694
H	-0.862946	3.433555	3.023975
H	0.551834	3.283009	1.958117
C	-4.688455	1.096768	1.814306
H	-4.556744	1.391068	2.860787
H	-5.501846	1.691148	1.387011
H	-5.000511	0.052034	1.780944
C	-4.050022	0.096651	-1.125767
O	-3.667695	-0.415723	-2.162790
O	-5.323510	0.081685	-0.707539
C	0.215860	2.489750	-0.941017
O	0.495774	1.977109	-2.010750
O	0.888735	3.526909	-0.414936
C	1.983230	4.053506	-1.221480
H	2.723845	3.259283	-1.354707
H	1.586293	4.311075	-2.207106
C	2.551862	5.255760	-0.495626
H	2.943132	4.978561	0.488555

H	3.374039	5.678877	-1.081845
H	1.792703	6.033057	-0.364318
C	-6.270229	-0.615094	-1.570833
H	-5.936701	-1.651539	-1.675020
H	-6.235351	-0.149385	-2.559483
C	-7.639144	-0.509514	-0.930228
H	-8.375302	-1.019383	-1.560151
H	-7.652532	-0.979939	0.058127
H	-7.947041	0.535550	-0.825485

Transition Structure TS-2-*Z* (top, *anti*)

E (0 K) = -1786.094755
ZPE = 0.717758
H (298 K) = -1785.333875
G (298 K) = -1785.45539
One imaginary frequency at = -784.8 cm^{-1}

C	-3.914117	-0.826598	-0.219111
C	-4.401827	1.098396	1.118088
H	-3.360973	-1.731848	-0.002627
H	-4.212321	1.368436	2.145025
N	-5.236016	-0.926148	0.376522
C	-6.098318	-2.092028	0.324896
H	-6.613658	-2.178060	1.270128
H	-6.839254	-2.017627	-0.460301
H	-5.499487	-2.978007	0.163157
C	-5.593891	0.165165	1.082564
O	-6.640610	0.361386	1.621672
C	-3.908275	-0.595955	-1.761135
C	-4.456836	-1.849375	-2.465677
H	-5.513100	-1.997961	-2.285060
H	-4.326391	-1.751003	-3.537671
H	-3.928332	-2.747615	-2.157023
C	-2.469787	-0.369738	-2.252708
H	-1.824952	-1.215515	-2.040653
H	-2.477106	-0.232817	-3.328956
H	-2.027079	0.517082	-1.815268
C	-4.760481	0.618447	-2.155543
H	-4.350001	1.541377	-1.760165
H	-4.778646	0.714864	-3.235849
H	-5.787991	0.524664	-1.822163
N	-3.333514	0.290506	0.543070
C	-2.078586	0.295757	1.021912
C	-1.109142	-0.650098	0.871906
C	-1.565105	1.480141	1.803744
C	0.130365	-0.233612	1.473935
H	-1.201759	-1.546847	0.300619
C	-0.157257	1.056171	2.240403
H	-1.555468	2.350543	1.159797
H	-2.185948	1.707733	2.660804
H	0.581469	1.826549	2.060910
H	-0.135063	0.832313	3.300242
C	1.115276	-1.201893	2.048318
C	0.988924	-2.574939	1.853110
C	2.191806	-0.734646	2.803197
C	1.904565	-3.454584	2.407225
H	0.171716	-2.965684	1.279809
C	3.106950	-1.611624	3.356292
H	2.313214	0.320089	2.971598
C	2.964469	-2.977258	3.160502
H	1.781262	-4.512098	2.260174
H	3.919963	-1.233378	3.949255
H	3.667113	-3.662046	3.599395
H	-4.601078	2.000405	0.553363
C	2.607441	-0.496509	-0.836942
C	3.891796	-0.280361	-0.462501
C	2.137273	1.909994	-0.425650
C	3.438512	2.073166	-0.076437
C	1.621166	0.563267	-0.659183
H	0.887510	0.192910	0.430291
H	0.758828	0.504956	-1.299683
N	4.240108	0.969627	-0.030997
H	5.188267	1.107890	0.237096
C	5.030406	-1.267840	-0.475311
H	5.332051	-1.481152	-1.491928
H	5.881767	-0.867448	0.061603
H	4.737534	-2.197080	-0.013114
C	4.147542	3.362015	0.255221
H	5.100523	3.155770	0.727113
H	4.326301	3.930960	-0.648006
H	3.559134	3.975020	0.918215
C	1.155340	3.006058	-0.618378
O	-0.010240	2.780318	-0.754467
O	1.669224	4.214833	-0.643511
C	2.077480	-1.767871	-1.392038
O	0.904062	-1.954801	-1.511236
O	2.993408	-2.637679	-1.753211
C	2.545321	-3.880609	-2.314643
H	1.931300	-4.385191	-1.582531
H	1.935310	-3.665072	-3.179326
C	3.774073	-4.686002	-2.675110
H	4.377434	-4.889961	-1.797875
H	3.472945	-5.633384	-3.108103
H	4.383191	-4.159193	-3.400421
C	0.773920	5.316606	-0.867301
H	0.042859	5.331463	-0.071739
H	0.257186	5.151284	-1.800938
C	1.605739	6.579668	-0.895415
H	0.961030	7.434046	-1.068310
H	2.120867	6.728689	0.046700
H	2.340574	6.541724	-1.691096

Transition Structure TS-2-*Z* (bottom, *syn*)

E (0 K) = -1786.089374
ZPE = 0.717882
H (298 K) = -1785.328478
G (298 K) = -1785.449442
One imaginary frequency at = -846.5 cm^{-1}

C	3.477781	0.351369	-0.718858
C	2.701591	-0.983409	-2.551582

H	3.022777	0.596145	0.249587
H	1.804379	-1.522077	-2.853244
N	4.022994	-1.012227	-0.638138
C	4.708255	-1.547396	0.529453
H	4.638630	-2.635739	0.471926
H	5.763815	-1.266969	0.557235
H	4.227402	-1.191442	1.448753
C	3.541778	-1.845537	-1.611085
O	3.709084	-3.050935	-1.694040
C	4.498009	1.479243	-1.079261
C	5.601366	1.545961	-0.003121
H	6.289518	0.698190	-0.061468
H	6.196322	2.454088	-0.145640
H	5.184626	1.585896	1.011321
C	3.748207	2.826731	-1.089784
H	3.333182	3.068174	-0.103555
H	4.441121	3.631647	-1.356207
H	2.931284	2.836849	-1.817782
C	5.141783	1.239106	-2.456481
H	4.406937	1.316912	-3.264928
H	5.910495	1.996286	-2.643446
H	5.627858	0.258752	-2.513480
N	2.403141	0.195066	-1.730485
C	1.120024	0.589610	-1.496438
C	0.630198	1.367022	-0.474842
C	0.006748	0.211610	-2.454992
C	-0.808936	1.565030	-0.598361
H	1.214599	1.778637	0.334421
C	-1.158307	1.126546	-2.029538
H	0.296237	0.353448	-3.501890
H	-0.254360	-0.850320	-2.341479
H	-1.190413	2.015842	-2.668384
H	-2.134302	0.638343	-2.105971
C	-1.481764	2.764706	-0.008788
C	-0.955867	3.407370	1.126024
C	-2.667153	3.266184	-0.572853
C	-1.577335	4.535370	1.655293
H	-0.071354	3.014786	1.614274
C	-3.285811	4.396631	-0.044411
H	-3.115230	2.771389	-1.428170
C	-2.740695	5.038433	1.068898
H	-1.153787	5.020958	2.529677
H	-4.196319	4.773809	-0.500686
H	-3.223607	5.919341	1.481880
H	3.271403	-0.730130	-3.452977
C	-2.352984	-2.436333	-0.524189
C	-2.754917	-1.257329	0.059977
C	-0.229524	-2.353999	0.701896
C	-0.612673	-1.182766	1.320958
N	-1.078146	-2.880904	-0.244258
H	-0.786416	-3.746675	-0.683611
C	-1.818828	-0.503059	0.877129
H	-2.261069	0.203151	1.577895
H	-1.337554	0.591993	0.098436
C	-3.145569	-3.330181	-1.438574
H	-2.498930	-4.078579	-1.908429
H	-3.928936	-3.852380	-0.881058
H	-3.644334	-2.757184	-2.221521
C	1.006140	-3.178159	0.933105
H	0.755433	-4.081316	1.504612
H	1.446272	-3.493543	-0.020542
H	1.751605	-2.629665	1.499743
C	-4.098713	-0.630330	-0.111080
O	-4.302087	0.531841	0.182563
O	-5.035260	-1.462051	-0.593755
C	0.112339	-0.509018	2.438374
O	-0.106324	0.651282	2.733360
O	0.969874	-1.297342	3.108439
C	-6.371237	-0.893873	-0.748195
H	-6.306168	-0.051920	-1.443452
H	-6.687464	-0.503694	0.222897
C	1.621778	-0.689101	4.263864
H	2.203271	0.171367	3.919243
H	0.842586	-0.317672	4.934693
C	2.485548	-1.750149	4.914779
H	2.974985	-1.328062	5.798476
H	1.884003	-2.606481	5.234145
H	3.264888	-2.106655	4.232922
C	-7.281948	-1.993869	-1.254005
H	-8.296215	-1.599124	-1.372578
H	-6.948819	-2.371608	-2.225961
H	-7.322252	-2.829143	-0.547898

Transition Structure TS-2-*Z* (bottom, *anti*)

E (0 K) = -1786.095128
ZPE = 0.718003
H (298 K) = -1785.334124
G (298 K) = -1785.455602
One imaginary frequency at = -801.9 cm^{-1}

C	3.999099	-0.436119	-0.259554
C	4.026990	1.874301	0.428395
H	3.245081	-1.021396	-0.802512
H	3.343905	2.718228	0.319404
N	4.747130	0.383294	-1.215156
C	5.169029	-0.061034	-2.536668
H	5.195722	0.817812	-3.184755
H	6.164881	-0.513361	-2.529372
H	4.452580	-0.788804	-2.930968
C	4.822573	1.705706	-0.865858
O	5.380364	2.592204	-1.483470
C	4.875417	-1.415073	0.595693
C	5.622908	-2.385884	-0.342365
H	6.422281	-1.888609	-0.897537
H	6.085301	-3.183982	0.248120
H	4.946302	-2.861896	-1.063352
C	3.963098	-2.247614	1.518187
H	3.262434	-2.865746	0.943077
H	4.574701	-2.927148	2.121504
H	3.385237	-1.622849	2.205585
C	5.896273	-0.645602	1.452890
H	5.401776	-0.030218	2.212473
H	6.547569	-1.351825	1.978929
H	6.538773	-0.001461	0.842886
N	3.315322	0.600050	0.553707
C	2.024887	0.521691	0.954240
C	1.155028	-0.541617	0.851562

C	1.346047	1.704857	1.610197
C	-0.158685	-0.202167	1.373508
H	1.377406	-1.479650	0.365791
C	0.032917	1.110540	2.152936
H	1.960377	2.157822	2.395892
H	1.140532	2.478240	0.859359
H	0.132314	0.871540	3.217808
H	-0.811796	1.800162	2.055579
C	-1.074350	-1.247136	1.943983
C	-0.966014	-2.600409	1.579706
C	-2.097012	-0.881631	2.836781
C	-1.833950	-3.556098	2.108695
H	-0.192879	-2.913756	0.886650
C	-2.965449	-1.835948	3.365703
H	-2.204857	0.155736	3.139560
C	-2.836650	-3.178940	3.004777
H	-1.717410	-4.599843	1.830184
H	-3.733459	-1.532821	4.072105
H	-3.503734	-3.925545	3.426111
H	4.696815	2.071687	1.273888
C	-3.806199	-0.744634	-0.618803
C	-2.489061	-0.696611	-1.019666
C	-3.756583	1.644388	-0.073274
C	-2.432638	1.720733	-0.455367
N	-4.358737	0.410193	-0.114965
H	-5.322441	0.359339	0.191987
C	-1.714864	0.503356	-0.781615
H	-0.812259	0.624710	-1.378350
H	-0.860137	0.154845	0.346716
C	-4.737111	-1.923590	-0.671310
H	-5.660223	-1.715623	-0.120804
H	-4.995662	-2.169630	-1.704995
H	-4.265047	-2.806658	-0.236574
C	-4.654852	2.768811	0.364465
H	-4.919906	3.404406	-0.486298
H	-5.578100	2.379667	0.805689
H	-4.159394	3.409568	1.094536
C	-1.741638	-1.825681	-1.643473
O	-0.526093	-1.826587	-1.723918
O	-2.525943	-2.802682	-2.121906
C	-1.639980	2.976957	-0.564226
O	-0.437273	2.961528	-0.765313
O	-2.361732	4.101075	-0.445646
C	-1.841635	-3.916052	-2.768258
H	-1.185735	-4.389085	-2.031334
H	-1.213927	-3.511977	-3.567130
C	-1.625484	5.353795	-0.586192
H	-0.879431	5.402153	0.212472
H	-1.095082	5.330517	-1.541766
C	-2.628194	6.486759	-0.508095
H	-2.104001	7.442230	-0.612389
H	-3.368167	6.415465	-1.311322
H	-3.152072	6.489843	0.453061
C	-2.901817	-4.864477	-3.290403
H	-2.419133	-5.712065	-3.787718
H	-3.521340	-5.255026	-2.476844
H	-3.550965	-4.367528	-4.017984

Transition Structure TS-3-*E*

E (0 K) = -2167.365316
ZPE = 0.792663
H (298 K) = -2166.523251
G (298 K) = -2166.662416
One imaginary frequency at = -863.5 cm^{-1}

C	-0.930610	-0.619007	1.157179
C	-0.797823	-2.150639	1.269660
C	0.385335	-2.503753	0.346670
C	1.117689	-1.186835	0.204119
C	0.374991	-0.151657	0.727611
H	-1.704453	-2.692328	0.994747
H	-0.558642	-2.396189	2.311086
H	1.019895	-3.296888	0.754534
H	0.023608	-2.843743	-0.633650
H	0.677379	0.885949	0.704620
H	-5.543519	1.694463	0.278448
N	-4.751495	1.202315	-0.115688
C	-3.675483	1.968297	-0.502880
C	-4.886067	-0.154263	-0.287669
C	-2.576094	1.309843	-1.010738
C	-3.802824	-0.842149	-0.792434
C	-2.555975	-0.138398	-1.004308
H	-1.706400	-0.465961	0.130798
H	-1.841771	-0.604749	-1.678852
C	3.075162	-2.202151	-0.972240
H	2.398644	-2.883392	-1.506589
N	2.314469	-1.071557	-0.404729
C	2.909374	0.224092	-0.741402
H	2.143504	0.851155	-1.212775
C	-1.738517	0.126514	2.173944
C	-1.521225	1.493782	2.424320
C	-2.776670	-0.520351	2.868453
C	-2.305348	2.184018	3.348563
H	-0.720733	2.020581	1.914350
C	-3.559210	0.169892	3.793232
H	-2.960656	-1.577387	2.700989
C	-3.328172	1.525866	4.035215
H	-2.107113	3.234440	3.543746
H	-4.341164	-0.354533	4.335650
H	-3.930254	2.061386	4.763809
C	3.950089	-0.155593	-1.794861
O	4.662906	0.622877	-2.405894
N	3.949936	-1.517038	-1.915852
C	4.870822	-2.236955	-2.776729
H	5.429502	-1.491368	-3.344368
H	5.567239	-2.845046	-2.189151
H	4.324417	-2.888219	-3.468526
C	3.817432	-3.009833	0.046738
C	5.280967	-3.258068	1.684173
C	4.796334	-4.501710	1.398270
C	3.539369	0.975589	0.473406
H	4.615492	0.769553	0.495290
H	3.124374	0.543818	1.389257
C	3.292398	2.471360	0.461381
C	2.621046	3.086596	1.527124
H	2.287358	2.483240	2.369390

C	3.736531	3.269642	-0.605063
H	4.259606	2.802580	-1.435719
C	3.516193	4.648050	-0.595987
H	3.879853	5.254043	-1.421807
C	2.400725	4.466622	1.536584
H	1.893368	4.927212	2.380414
C	2.849071	5.252009	0.473946
H	2.692329	6.327263	0.484201
O	4.688468	-2.334808	0.860036
C	6.275300	-2.740790	2.662675
H	6.675660	-3.566559	3.256101
H	7.111685	-2.243556	2.157183
H	5.823205	-2.012971	3.347103
H	5.083224	-5.423842	1.884002
C	3.848898	-4.342267	0.335563
H	3.276293	-5.119916	-0.152407
C	-3.776811	-2.295208	-1.120482
O	-2.739561	-2.877059	-1.389228
O	-4.981532	-2.885793	-1.109992
C	-1.355671	1.962625	-1.577142
O	-0.454778	1.315470	-2.079667
O	-1.352785	3.298978	-1.478740
C	-5.002507	-4.302614	-1.457571
H	-4.553305	-4.415478	-2.448050
H	-4.375072	-4.840013	-0.740520
C	-6.445680	-4.762515	-1.422081
H	-6.495260	-5.823313	-1.688459
H	-6.877589	-4.642663	-0.423350
H	-7.056136	-4.203109	-2.137802
C	-0.182142	3.980504	-2.028327
H	-0.070888	3.674363	-3.071908
H	0.700230	3.644359	-1.477547
C	-0.410960	5.470617	-1.882613
H	-0.526569	5.751323	-0.831083
H	0.454917	6.007898	-2.282251
H	-1.298656	5.794162	-2.435591
C	-6.238129	-0.704773	0.073699
H	-6.798513	-0.972665	-0.827370
H	-6.147016	-1.612033	0.671782
H	-6.819799	0.031406	0.637774
C	-3.869075	3.450323	-0.337724
H	-3.114459	3.864516	0.334873
H	-3.761785	3.966689	-1.294084
H	-4.860519	3.671918	0.069842

Transition Structure TS-3-*Z*

E (0 K) = -2167.363549
ZPE = 0.792611
H (298 K) = -2166.521506
G (298 K) = -2166.661178
One imaginary frequency at = -770.2 cm^{-1}

C	2.273198	-1.833189	-1.346564
C	3.513172	0.155864	-0.665671
H	1.326169	-1.878644	-1.904415
H	3.267350	1.196928	-0.900064
C	4.468930	0.110570	0.569876
H	5.226360	-0.663631	0.399172
N	3.387317	-1.568703	-2.248906
C	3.735376	-2.468140	-3.333278
H	2.919618	-2.530023	-4.062977
H	4.624440	-2.060239	-3.816523
H	3.952726	-3.473208	-2.955820
C	4.145747	-0.486346	-1.902902
O	5.161064	-0.107994	-2.462101
C	1.200510	-0.213557	0.191037
C	0.031808	-0.909052	0.403308
C	-0.944942	-0.092441	1.105735
H	-0.169272	-1.902214	0.029633
N	2.281893	-0.623011	-0.504509
C	5.132109	1.437154	0.884473
C	4.998039	2.006889	2.157340
C	5.892552	2.114651	-0.081078
C	5.607587	3.225193	2.465170
H	4.423711	1.485650	2.921269
C	6.497805	3.333740	0.225219
H	6.009696	1.678302	-1.069809
C	6.358294	3.893116	1.497714
H	5.497998	3.648011	3.460387
H	7.086628	3.844971	-0.531721
H	6.835696	4.840084	1.734198
H	3.885092	-0.223288	1.433601
H	0.787857	-4.467951	-1.150822
C	1.685007	-4.270416	-0.578997
C	2.353524	-5.159151	0.324321
C	2.411379	-3.116803	-0.589317
C	3.443378	-4.489593	0.801180
H	2.064331	-6.168253	0.582751
O	3.489943	-3.236406	0.245608
C	4.531756	-4.840061	1.753277
H	5.515977	-4.782502	1.273407
H	4.544845	-4.161937	2.615010
H	4.389201	-5.859228	2.121319
C	-0.162261	1.127241	1.634355
H	-0.728493	2.062430	1.574773
H	0.070245	0.958972	2.691835
H	-3.587612	-3.658362	2.621857
C	-3.339461	-2.604026	2.708255
C	-3.994514	-1.806487	3.648995
C	-2.351630	-2.058931	1.887186
C	-3.652920	-0.456779	3.761853
H	-4.754500	-2.235049	4.296130
C	-1.990276	-0.705487	1.995525
H	-1.848472	-2.696872	1.168901
C	-2.665748	0.086769	2.940689
H	-4.145476	0.170081	4.500287
H	-2.404928	1.135609	3.050370
C	1.128936	1.171152	0.794850
H	1.051878	1.909908	-0.013298
H	2.009930	1.431011	1.390089
C	-2.829415	2.295292	-0.638636
C	-3.997526	2.734709	-0.049810
C	-3.773100	0.000012	-0.727309
C	-4.921489	0.464915	-0.122419
N	-4.957599	1.792958	0.232812
H	-5.801020	2.120884	0.687438
C	-2.627812	0.875388	-0.842500
H	-1.870488	0.594655	-1.572013
H	-1.708146	0.407474	0.208039
C	-6.167750	-0.311882	0.198476

H	-6.851222	0.283764	0.812039
H	-6.688168	-0.608441	-0.716129
H	-5.921511	-1.226712	0.741416
C	-4.375277	4.146945	0.304278
H	-4.565332	4.733264	-0.599990
H	-5.277234	4.165535	0.924448
H	-3.569365	4.648754	0.841175
C	-3.575256	-1.384186	-1.245436
O	-2.475738	-1.805651	-1.557040
O	-4.708637	-2.092423	-1.360430
C	-1.706859	3.168231	-1.084423
O	-0.646531	2.703511	-1.466153
O	-1.974713	4.481842	-1.043163
C	-4.568775	-3.444498	-1.885947
H	-4.083601	-3.381568	-2.863899
H	-3.908029	-4.004325	-1.217437
C	-5.955094	-4.050880	-1.967550
H	-5.884368	-5.068802	-2.364490
H	-6.424820	-4.102336	-0.980188
H	-6.601162	-3.470309	-2.633430
C	-0.907036	5.367095	-1.499029
H	-0.033196	5.203868	-0.861728
H	-0.639100	5.078053	-2.518802
C	-1.423970	6.788860	-1.417554
H	-1.689418	7.057629	-0.390122
H	-0.644455	7.477934	-1.758336
H	-2.302698	6.927086	-2.055205