

## Supporting Information

### **On the Rearrangements of Biologically-Relevant Vinyl Allene Oxides to *cis*-Cyclopentenones, Ketols, Cyclopropylcarbinols and Favorskii-type Carboxylic Acids**

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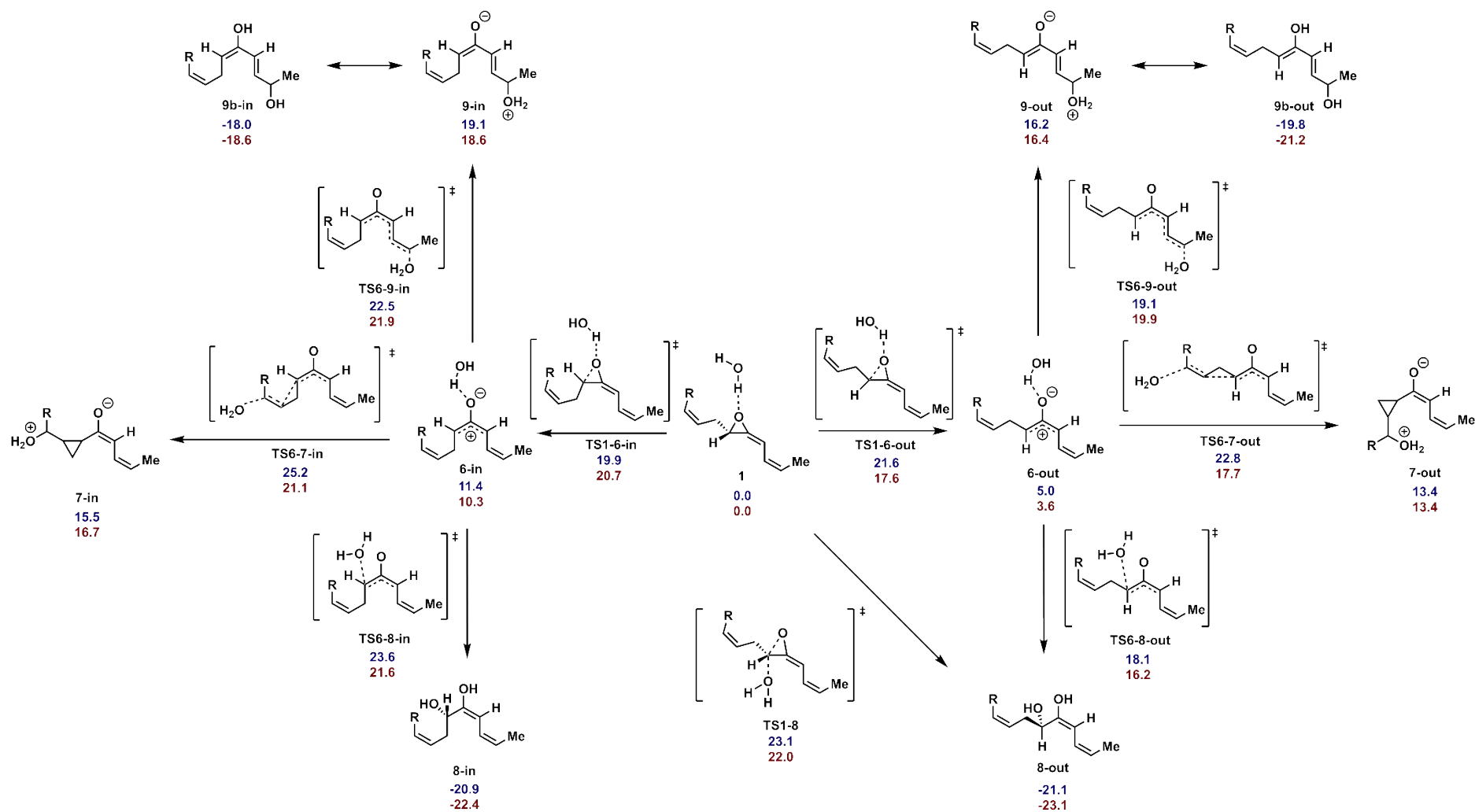
## **Diradical nature of intermediates**

In our previous calculations of allene oxides rearrangements<sup>1</sup> it was found that the intermediates formed after the oxirane ring opening had diradical nature. Thus, we followed the same procedure in order to evaluate this phenomenon in the mechanisms studied herein. Wave function stability analysis was carried out in order to determine the nature of the species involved in the rearrangement.<sup>2</sup> To corroborate these results, a TDDFT<sup>2, 3</sup> treatment of the characterized intermediates and transition states was made with both singlet and triplet excitation analysis. The finding of a low energy triplet “excitation” concurs with instability of the wavefunction. Broken symmetry calculations were carried out to evaluate the diradical character of the transition states and intermediates of the rearrangement, both for triplet and singlets (the latter mixing the HOMO and LUMO during the optimization process). Singlet energies were obtained after spin purification with the Yamaguchi correction for the broken symmetry mixing optimization energies.<sup>4, 5</sup>

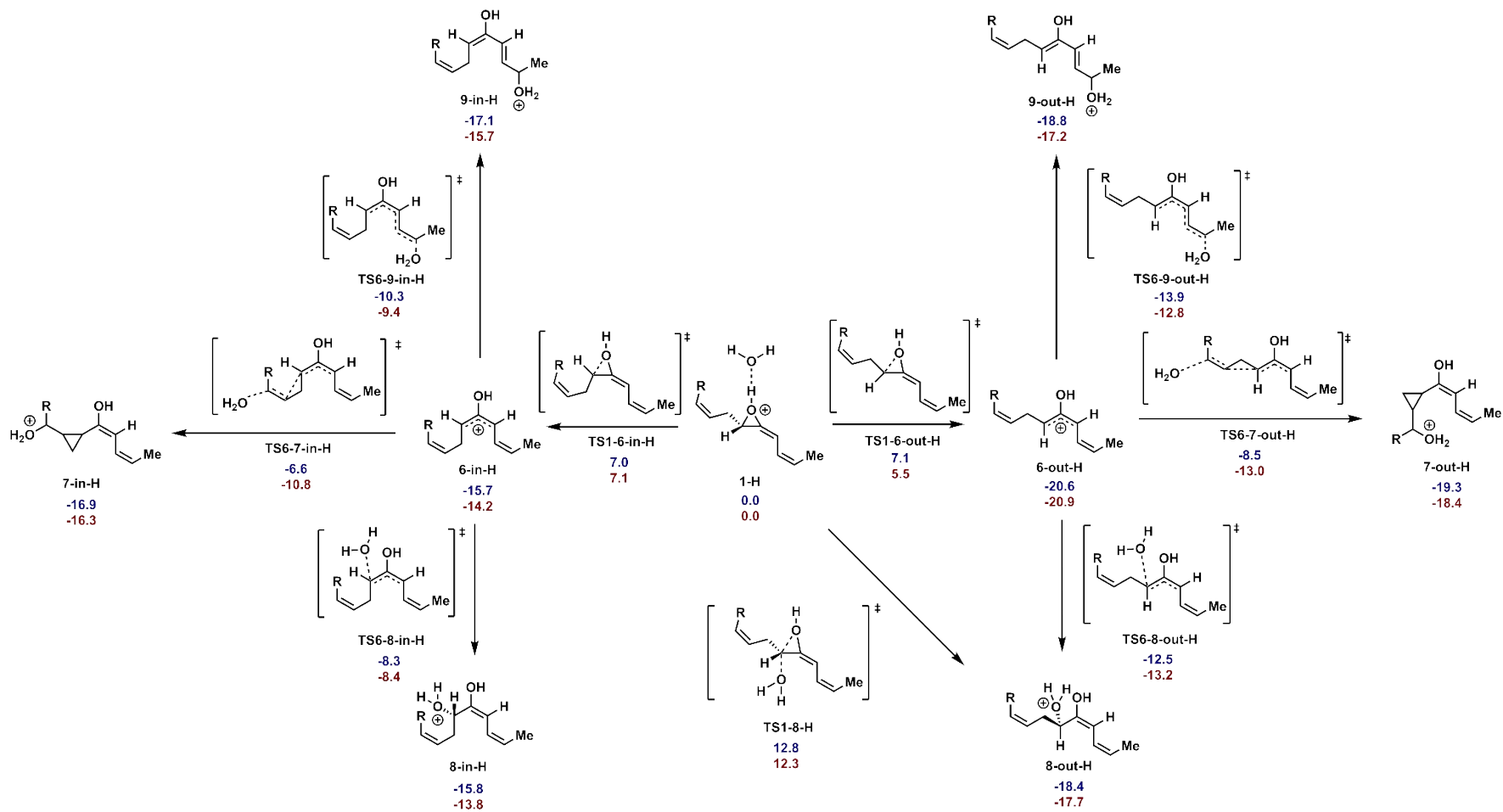
In this case, the closed shell wave function was found to be stable in most of the cases. The presence of H-bonds between a water molecule or a proton and the oxygen atom seem to stabilize the electron pair in the oxygen atom. The only exception is when an OH<sup>-</sup> anion is included in the calculation (the Favorskii rearrangement under basic conditions). In this case, the wavefunction was found to be unstable and, therefore, the corresponding open-shell calculations were carried out leading to intermediates with diradical nature. These intermediates are shown in the complete mechanistic picture of the Favorskii process shown in Scheme S3.

## **System comparison**

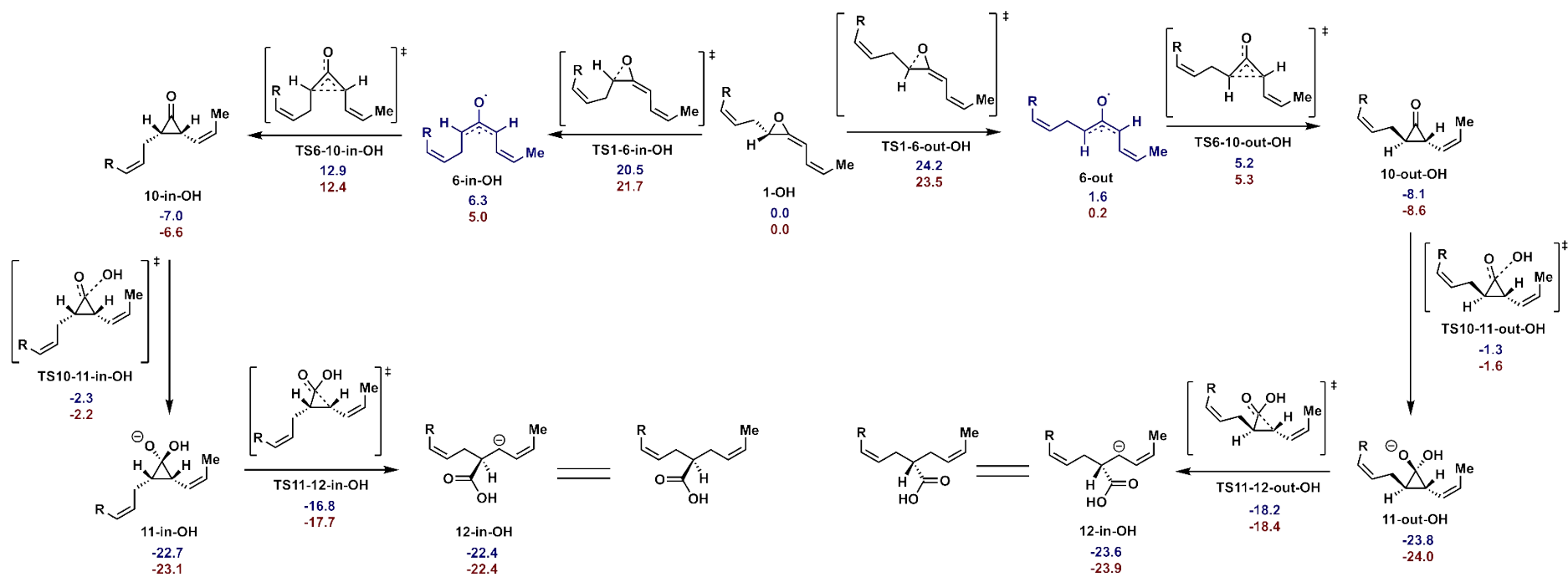
During this investigation, two main different systems were studied. They differ in the substitution chosen for the oxide, specifically an allyl and a crotyl substituent. In the final form of the manuscript, only the results for the crotyl-substituted system were shown. In the following schemes, all results obtained for both systems are shown.



Scheme S1: Complete paths for the concerted and stepwise for the  $\alpha$ - and  $\gamma$ -ketol and Cyclopropyl carbinol formation in neutral conditions. All energies are given in kcal/mol (Blue R=H, Red R=Me) and computed at the  $\omega$ b97xd/6-311++G(3df,2p)(SMD,H2O)// $\omega$ B97XD/6-31++G(d,p)(SMD,H2O) level of theory.



Scheme S2: Complete paths for the concerted and stepwise for the  $\alpha$ - and  $\gamma$ -ketol and Cyclopropyl carbinol formation in acid conditions. All energies are given in kcal/mol (Blue R=H, Red R=Me) and computed at the  $\omega$ b97xd/6-311++G(3df,2p)(SMD,H2O)// $\omega$ B97XD/6-31++G(d,p)(SMD,H2O) level of theory.



Scheme S3: Complete paths for Favorskii-type rearrangements under basic conditions. Free energy values (in kcal/mol, (Blue R=H, Red R=Me)), have been computed at the  $U\omega B97XD/6-311++G(3df,2p)(SMD,H_2O)/U\omega B97XD/6-31++G(d,p)(SMD,H_2O)$  level of theory. Intermediates highlighted in blue have diradical nature.

## Energies and XYZ coordinates

### Ketol formation with H<sub>2</sub>O (R=H)

m1-Allyl.out

```
Zero-point correction= 0.209692
(Hartree/Particle)
Thermal correction to Energy= 0.224727
Thermal correction to Enthalpy= 0.225671
Thermal correction to Gibbs Free Energy= 0.164706
Sum of electronic and zero-point Energies= -501.409209
Sum of electronic and thermal Energies= -501.394174
Sum of electronic and thermal Enthalpies= -501.393230
Sum of electronic and thermal Free Energies= -501.454195
E(ωB97XD/6-311++G(3df,2p))= -501.753733984
```

C	-2.372985	-0.744545	-0.536166
C	-1.510618	0.115588	0.272186
C	-0.207232	0.193897	0.041281
C	-3.699757	-0.898502	-0.395077
O	0.879924	0.844592	0.569430
C	1.046324	-0.094071	-0.587960
H	-1.870678	-1.309031	-1.320278
H	-1.918909	0.707875	1.085999
H	-4.194260	-1.585852	-1.079558
H	1.297193	0.440467	-1.502702
C	-4.594520	-0.227611	0.602505
H	-5.091145	-0.973565	1.234015
H	-4.065123	0.469910	1.255614
H	-5.389120	0.326231	0.089168
C	1.825580	-1.350457	-0.304276
H	1.496275	-1.784093	0.644890
H	1.570165	-2.058666	-1.103111
C	3.307109	-1.097394	-0.298343
H	3.728614	-0.696715	-1.220151
C	4.101202	-1.323933	0.747993
H	3.708556	-1.720338	1.682223
H	5.168206	-1.124707	0.701070
O	1.095709	3.547466	-0.338292
H	1.036958	2.643107	0.014786
H	1.347576	4.091073	0.416065

m6-in-Allyl.out

```
Zero-point correction= 0.209163
(Hartree/Particle)
Thermal correction to Energy= 0.223701
Thermal correction to Enthalpy= 0.224645
Thermal correction to Gibbs Free Energy= 0.166106
Sum of electronic and zero-point Energies= -501.395787
Sum of electronic and thermal Energies= -501.381249
Sum of electronic and thermal Enthalpies= -501.380305
```

Sum of electronic and thermal Free Energies= -501.438844  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -501.736976592

C	1.072534	0.100590	-0.246549
C	0.011992	0.973935	-0.463357
C	-1.330013	0.532316	-0.236340
C	-1.871302	-0.757270	-0.393801
C	-3.152786	-1.073230	-0.028947
C	-4.162475	-0.226614	0.640524
O	0.203145	2.250559	-0.709348
H	-1.282977	-1.535549	-0.863181
H	-2.007265	1.334719	0.051091
H	-3.476351	-2.090469	-0.242101
H	2.042811	0.597260	-0.207567
C	1.103087	-1.378418	-0.016801
H	-3.850126	0.799899	0.830165
H	-4.427099	-0.699281	1.595050
H	-5.081490	-0.229479	0.042826
H	0.888937	-1.910548	-0.954905
H	0.310454	-1.672506	0.684660
C	2.430604	-1.835047	0.526086
H	2.761298	-1.349393	1.444120
C	3.188899	-2.777388	-0.033149
H	2.886068	-3.278092	-0.950824
H	4.133411	-3.078714	0.411039
O	2.282527	3.394505	0.491922
H	1.963355	3.650710	1.363372
H	1.510367	2.947689	0.049676

m6-out-Allyl.out

Zero-point correction= 0.209897  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.224063  
 Thermal correction to Enthalpy= 0.225007  
 Thermal correction to Gibbs Free Energy= 0.168380  
 Sum of electronic and zero-point Energies= -501.406765  
 Sum of electronic and thermal Energies= -501.392599  
 Sum of electronic and thermal Enthalpies= -501.391655  
 Sum of electronic and thermal Free Energies= -501.448281  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -501.749391288

C	-4.385749	0.323278	0.577955
C	-3.512757	-0.826862	0.253555
C	-2.202162	-0.836856	-0.134265
C	-1.441711	0.339786	-0.286373
C	-0.066500	0.484570	-0.667303
C	0.685724	-0.680174	-0.746387
C	2.134689	-0.708651	-1.066203
O	0.412673	1.687691	-0.859101
H	-1.751410	-1.803084	-0.332993

H	-1.945967	1.287580	-0.106001
H	-3.993234	-1.800004	0.337938
H	0.213522	-1.636798	-0.551879
H	-5.274525	0.282237	-0.063001
H	-4.752451	0.205220	1.604949
H	-3.916015	1.301186	0.476740
H	2.288891	-1.410029	-1.898597
H	2.472786	0.273917	-1.412619
C	3.015095	-1.155599	0.078162
H	4.050988	-1.346706	-0.196232
C	2.635006	-1.303193	1.348806
H	1.612530	-1.118081	1.672085
H	3.345533	-1.615986	2.108282
O	2.351873	2.108797	0.960950
H	1.656303	1.964371	0.269494
H	2.706873	1.226475	1.129366

m7-in-Allyl.out

Zero-point correction=	0.215982
(Hartree/Particle)	
Thermal correction to Energy=	0.228487
Thermal correction to Enthalpy=	0.229431
Thermal correction to Gibbs Free Energy=	0.175709
Sum of electronic and zero-point Energies=	-501.391681
Sum of electronic and thermal Energies=	-501.379176
Sum of electronic and thermal Enthalpies=	-501.378232
Sum of electronic and thermal Free Energies=	-501.431954
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.740035627

C	0.689644	0.138328	-0.463496
C	-0.391710	1.128291	-0.064559
C	-1.702163	0.705702	0.024835
C	-2.164863	-0.645116	-0.225420
C	-3.430392	-1.118289	-0.158548
C	-4.663654	-0.336886	0.199122
O	-0.013287	2.356276	0.136447
H	-1.398731	-1.367604	-0.505601
H	-2.436286	1.467494	0.284331
H	-3.588280	-2.171233	-0.389213
H	0.752423	-0.043628	-1.535432
C	1.070033	-1.024846	0.406818
H	-4.436860	0.687216	0.508356
H	-5.210615	-0.817452	1.019884
H	-5.360487	-0.279746	-0.647475
H	1.345122	-1.958494	-0.076671
H	0.560910	-1.130699	1.359391
C	2.010224	0.149969	0.267205
H	2.088997	0.827524	1.112491
C	3.248996	-0.010343	-0.536409
H	3.106520	-0.602163	-1.439231
H	3.763362	0.922036	-0.760444



O	4.294344	-0.794577	0.218768
H	3.938932	-1.644724	0.539507
H	4.629852	-0.302982	0.991104

m7-out-Allyl.out

Zero-point correction=	0.216156
(Hartree/Particle)	
Thermal correction to Energy=	0.228571
Thermal correction to Enthalpy=	0.229515
Thermal correction to Gibbs Free Energy=	0.175799
Sum of electronic and zero-point Energies=	-501.394783
Sum of electronic and thermal Energies=	-501.382368
Sum of electronic and thermal Enthalpies=	-501.381424
Sum of electronic and thermal Free Energies=	-501.435140
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.743417389

C	-2.214538	-0.781233	0.252901
C	-1.737261	0.530926	-0.127580
C	-0.437209	1.003693	-0.072171
C	-3.498956	-1.203355	0.192681
O	-0.101531	2.198181	-0.451682
C	0.672421	0.126296	0.450219
H	-1.485276	-1.503808	0.616798
H	-2.474394	1.238054	-0.508222
H	-3.721997	-2.221463	0.505175
H	0.388968	-0.855291	0.812821
C	-4.651318	-0.356659	-0.281768
H	-5.597492	-0.899808	-0.206852
H	-4.753391	0.565974	0.305472
H	-4.532508	-0.046663	-1.329088
C	1.855200	0.742696	1.148770
H	1.875559	1.823057	1.242638
H	2.290174	0.188306	1.975375
C	2.025884	0.183028	-0.236453
H	2.118270	0.896526	-1.049947
C	2.743836	-1.104424	-0.422126
H	2.619339	-1.545904	-1.408749
O	4.238962	-0.920552	-0.326827
H	4.586730	-0.350786	-1.037789
H	4.497979	-0.520400	0.524500
H	2.540236	-1.834632	0.359110

m8-in-Allyl.out

Zero-point correction=	0.214915
(Hartree/Particle)	
Thermal correction to Energy=	0.227668
Thermal correction to Enthalpy=	0.228613
Thermal correction to Gibbs Free Energy=	0.175581

Sum of electronic and zero-point Energies=	-501.448744
Sum of electronic and thermal Energies=	-501.435991
Sum of electronic and thermal Enthalpies=	-501.435047
Sum of electronic and thermal Free Energies=	-501.488079
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.797880735

C	4.340558	-0.542608	0.158685
C	3.084920	-1.239732	-0.270818
C	1.842733	-0.725945	-0.329083
C	1.461027	0.639934	0.011523
C	0.200224	1.103916	0.001670
C	-1.046532	0.306192	-0.325918
C	-1.574771	-0.399864	0.925787
O	-0.044956	2.397963	0.382050
H	1.048512	-1.392697	-0.659729
H	2.236127	1.338897	0.314648
H	3.207211	-2.280202	-0.567808
H	-0.809712	-0.431838	-1.099159
H	4.818905	-1.086385	0.981642
H	5.066618	-0.519158	-0.662827
H	4.171357	0.485054	0.488211
H	-0.765903	-1.017641	1.334993
H	-1.797914	0.355412	1.689562
C	-2.786615	-1.270165	0.721311
H	-3.261155	-1.602928	1.643443
C	-3.305978	-1.668174	-0.442259
H	-2.888363	-1.382329	-1.405398
H	-4.181233	-2.311058	-0.465212
O	-1.990852	1.245523	-0.846486
H	-0.971149	2.590439	0.161456
H	-2.880240	0.885221	-0.743716

m8-out-Allyl.out

Zero-point correction=	0.214866
(Hartree/Particle)	
Thermal correction to Energy=	0.227589
Thermal correction to Enthalpy=	0.228533
Thermal correction to Gibbs Free Energy=	0.175499
Sum of electronic and zero-point Energies=	-501.449318
Sum of electronic and thermal Energies=	-501.436595
Sum of electronic and thermal Enthalpies=	-501.435651
Sum of electronic and thermal Free Energies=	-501.488685
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.798214530

C	-4.309914	-0.572806	0.133237
C	-3.037644	-1.246171	-0.285478
C	-1.804428	-0.709777	-0.328392
C	-1.447157	0.661492	0.017930
C	-0.189283	1.134455	0.023896
C	1.072326	0.346600	-0.299401

C	1.569751	-0.410809	0.929270
O	0.046059	2.430972	0.397809
H	-0.995161	-1.362138	-0.651979
H	-2.235484	1.352039	0.306422
H	-3.137683	-2.287557	-0.587510
H	0.859628	-0.355515	-1.111020
H	-5.023919	-0.547421	-0.698804
H	-4.792794	-1.134658	0.941239
H	-4.159938	0.452267	0.479946
H	1.871738	0.317963	1.692927
H	0.723137	-0.959356	1.359435
C	2.691248	-1.385918	0.697757
H	3.052683	-1.869280	1.605065
C	3.247279	-1.721381	-0.467445
H	2.944771	-1.276733	-1.412224
H	4.040011	-2.463220	-0.508106
O	2.097648	1.253642	-0.709536
H	0.978182	2.616837	0.192664
H	1.972108	1.465752	-1.642483

m9b-in-Allyl.out

Zero-point correction=	0.214816
(Hartree/Particle)	
Thermal correction to Energy=	0.227761
Thermal correction to Enthalpy=	0.228706
Thermal correction to Gibbs Free Energy=	0.174575
Sum of electronic and zero-point Energies=	-501.443823
Sum of electronic and thermal Energies=	-501.430878
Sum of electronic and thermal Enthalpies=	-501.429933
Sum of electronic and thermal Free Energies=	-501.484064
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.792262772

C	1.653946	0.898647	-0.255009
C	0.500101	1.563591	-0.090200
C	-0.843761	1.002362	0.121612
C	-1.341292	-0.041059	-0.548966
C	-2.705474	-0.652766	-0.354169
C	-3.502217	-0.107016	0.813707
O	0.448123	2.949280	-0.072412
H	-0.743406	-0.513577	-1.328088
H	-1.448372	1.523132	0.862240
H	-3.277499	-0.498006	-1.279874
H	2.554079	1.494329	-0.409136
C	1.850628	-0.594914	-0.217602
H	-2.961930	-0.242899	1.756029
H	-4.460353	-0.629186	0.880274
H	-3.705133	0.958476	0.676770
H	1.959987	-0.996407	-1.233570
H	0.966956	-1.074637	0.218714
C	3.061991	-0.970469	0.594264
H	3.057509	-0.639897	1.633583
C	4.105548	-1.659733	0.131009

H	4.144991	-2.001281	-0.901942
H	4.950770	-1.906214	0.767915
O	-2.562162	-2.069421	-0.145401
H	-2.144378	-2.452913	-0.925844
H	1.342262	3.308350	-0.142437

m9b-out-Allyl.out

Zero-point correction=	0.215069
(Hartree/Particle)	
Thermal correction to Energy=	0.227873
Thermal correction to Enthalpy=	0.228817
Thermal correction to Gibbs Free Energy=	0.174554
Sum of electronic and zero-point Energies=	-501.446084
Sum of electronic and thermal Energies=	-501.433280
Sum of electronic and thermal Enthalpies=	-501.432336
Sum of electronic and thermal Free Energies=	-501.486600
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.795145039

C	-3.609409	0.808773	0.750711
C	-3.137472	-0.208874	-0.274545
C	-1.662531	-0.180977	-0.584696
C	-0.764683	0.654515	-0.052777
C	0.679862	0.614419	-0.333827
C	1.389348	-0.491488	-0.605413
C	2.858173	-0.523116	-0.923637
O	1.230767	1.879221	-0.257842
H	-1.338745	-0.934690	-1.301589
H	-1.078201	1.442052	0.629851
H	-3.682232	-0.051506	-1.211947
H	0.859265	-1.437840	-0.565531
H	-3.411222	1.828926	0.409063
H	-4.686857	0.702087	0.901634
H	-3.106434	0.659610	1.712356
H	3.066876	-1.395799	-1.553307
H	3.146831	0.342306	-1.537937
C	3.788513	-0.575020	0.267210
H	4.842901	-0.684867	0.014451
C	3.434751	-0.489409	1.550096
H	2.395398	-0.375861	1.850963
H	4.179997	-0.531337	2.339509
O	-3.504147	-1.542641	0.121504
H	-3.053799	-1.737939	0.953616
H	2.193938	1.829267	-0.309160

m9-in-Allyl.out

Zero-point correction=	0.214978
(Hartree/Particle)	
Thermal correction to Energy=	0.227589

Thermal correction to Enthalpy=	0.228533
Thermal correction to Gibbs Free Energy=	0.175595
Sum of electronic and zero-point Energies=	-501.386413
Sum of electronic and thermal Energies=	-501.373801
Sum of electronic and thermal Enthalpies=	-501.372857
Sum of electronic and thermal Free Energies=	-501.425795
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.734150750

C	1.704597	0.961231	-0.331094
C	0.569273	1.674353	-0.076587
C	-0.741366	1.008086	0.193189
C	-1.330768	0.117725	-0.611281
C	-2.672121	-0.487829	-0.364683
C	-3.437829	-0.066792	0.861530
O	0.504015	2.992757	-0.019443
H	-0.839614	-0.205834	-1.527137
H	-1.260512	1.367668	1.081254
H	-3.296197	-0.455924	-1.258123
H	2.612742	1.544464	-0.495002
C	1.883714	-0.539093	-0.351731
H	-2.854189	-0.217398	1.773294
H	-4.371710	-0.627212	0.931528
H	-3.678847	0.995217	0.771880
H	2.127880	-0.901389	-1.360855
H	0.951124	-1.033730	-0.057941
C	2.974638	-0.975417	0.591291
H	2.803497	-0.751553	1.645559
C	4.111693	-1.573932	0.229399
H	4.322491	-1.804505	-0.813782
H	4.866815	-1.850558	0.960504
O	-2.475486	-2.009839	-0.219413
H	-1.812772	-2.210403	0.468634
H	-2.169924	-2.422187	-1.049167

m9-out-Allyl.out

Zero-point correction=	0.214550
(Hartree/Particle)	
Thermal correction to Energy=	0.227387
Thermal correction to Enthalpy=	0.228332
Thermal correction to Gibbs Free Energy=	0.174029
Sum of electronic and zero-point Energies=	-501.389794
Sum of electronic and thermal Energies=	-501.376957
Sum of electronic and thermal Enthalpies=	-501.376013
Sum of electronic and thermal Free Energies=	-501.430316
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.737296345

C	-3.627539	-0.545114	-0.850661
C	-3.028011	0.117274	0.361997
C	-1.572753	-0.068254	0.635737
C	-0.731974	-0.725629	-0.172291

C	0.723343	-0.956463	0.075881
C	1.475072	0.053781	0.603868
C	2.946284	-0.049579	0.882698
O	1.154239	-2.150756	-0.275848
H	-1.218212	0.362504	1.570038
H	-1.113906	-1.201277	-1.075422
H	-3.627325	-0.065052	1.254162
H	0.992485	1.007237	0.805562
H	-3.542909	-1.627872	-0.732099
H	-4.685391	-0.289580	-0.933892
H	-3.111126	-0.251783	-1.768533
H	3.170708	0.320875	1.893943
H	3.255178	-1.103572	0.889767
C	3.858222	0.687340	-0.071319
H	4.915568	0.672969	0.196869
C	3.487307	1.330027	-1.180587
H	2.445268	1.370988	-1.491230
H	4.217276	1.829845	-1.811786
O	-3.286666	1.624822	0.164545
H	-2.761282	1.979947	-0.577803
H	-3.056621	2.141941	0.958905

ts1-6-in-Allyl.out

Zero-point correction=	0.207139
(Hartree/Particle)	
Thermal correction to Energy=	0.221796
Thermal correction to Enthalpy=	0.222740
Thermal correction to Gibbs Free Energy=	0.162257
Sum of electronic and zero-point Energies=	-501.378672
Sum of electronic and thermal Energies=	-501.364016
Sum of electronic and thermal Enthalpies=	-501.363071
Sum of electronic and thermal Free Energies=	-501.423554
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.719501640

C	-1.089399	-1.221345	-0.025354
C	0.298020	-0.981988	0.260576
C	1.015085	0.171441	0.238827
C	0.436598	1.462796	-0.078287
C	1.089182	2.641338	-0.107650
C	2.542347	2.886494	0.156320
O	0.649123	-2.206141	0.605537
H	-0.625324	1.475768	-0.320343
H	2.074512	0.090995	0.469794
H	0.503718	3.524886	-0.356416
H	-1.288801	-1.990230	-0.769999
C	-2.233153	-0.661873	0.707849
H	3.103036	1.974694	0.373490
H	2.664356	3.570648	1.004537
H	3.007907	3.374735	-0.707782
H	-1.927290	0.150772	1.369919
H	-2.657055	-1.476420	1.316376
C	-3.264555	-0.220808	-0.312740

H	-3.757657	-1.012448	-0.872038
C	-3.551599	1.060408	-0.534369
H	-4.307488	1.344798	-1.260614
O	3.008557	-2.706954	-0.734572
H	3.378894	-1.821227	-0.815371
H	2.169088	-2.579552	-0.242515
H	-3.054480	1.858564	0.012220

ts1-6-out-Allyl.out

Zero-point correction=	0.208361
(Hartree/Particle)	
Thermal correction to Energy=	0.222590
Thermal correction to Enthalpy=	0.223534
Thermal correction to Gibbs Free Energy=	0.165081
Sum of electronic and zero-point Energies=	-501.377965
Sum of electronic and thermal Energies=	-501.363736
Sum of electronic and thermal Enthalpies=	-501.362792
Sum of electronic and thermal Free Energies=	-501.421244
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.719690521

C	1.692342	0.427537	-0.437184
C	0.368924	0.807416	0.103119
C	-0.823412	0.167582	0.124797
C	-1.100481	-1.131135	-0.471502
C	-2.240583	-1.840379	-0.362897
C	-3.461975	-1.472687	0.426723
O	0.654291	2.038173	0.468170
H	-0.316043	-1.556353	-1.094916
H	-1.637209	0.717964	0.592412
H	-2.296277	-2.782415	-0.906290
H	1.867760	0.611970	-1.497061
C	2.829229	0.079382	0.380465
H	-3.743548	-2.289579	1.101569
H	-4.320074	-1.304725	-0.235937
H	-3.322472	-0.572330	1.030345
H	2.654382	0.091364	1.453665
H	3.783233	0.502907	0.074626
C	2.615959	-1.301459	-0.254646
H	3.174610	-1.520455	-1.157918
C	1.763913	-2.194278	0.276255
H	1.653867	-3.183851	-0.156361
O	-1.374076	3.685797	-0.305277
H	-2.142398	3.108160	-0.366978
H	-0.641622	3.095071	-0.013953
H	1.180578	-1.961360	1.162877

ts1-8-Allyl.out

```

Zero-point correction=                                0.210227
(Hartree/Particle)
Thermal correction to Energy=                        0.223742
Thermal correction to Enthalpy=                     0.224686
Thermal correction to Gibbs Free Energy=            0.169853
Sum of electronic and zero-point Energies=          -501.378359
Sum of electronic and thermal Energies=             -501.364843
Sum of electronic and thermal Enthalpies=           -501.363899
Sum of electronic and thermal Free Energies=        -501.418733
E( $\omega$ B97XD/6-311++G(3df,2p))= -501.722059565

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C      1.041041   -0.658126    0.433603
C     -0.292355   -1.221759    0.208484
C     -1.543524   -0.754740    0.003870
C     -1.916527    0.650773   -0.055161
C     -3.157717    1.147481   -0.222602
C     -4.434401    0.370871   -0.363259
O      0.184548   -2.446900    0.191988
H     -1.102806    1.366487    0.028475
H     -2.304569   -1.516445   -0.151568
H     -3.259282    2.230921   -0.266753
H      1.485833   -0.913064    1.389214
C      1.933437   -0.342877   -0.725578
H     -4.301168   -0.701223   -0.197434
H     -4.867051    0.503677   -1.362832
H     -5.184449    0.729382    0.351506
H      1.455113    0.428825   -1.338016
H      1.961273   -1.255928   -1.333914
C      3.325052    0.048181   -0.317783
H      3.885689   -0.699096    0.242449
C      3.878611    1.227166   -0.598709
H      3.336472    1.990189   -1.153475
H      4.892529    1.461582   -0.287437
O      0.910196    1.296456    1.128954
H      1.816600    1.537722    1.370574
H      0.426165    1.238705    1.964492

```

ts6-7-in-Allyl.out

```

Zero-point correction=                                0.210147
(Hartree/Particle)
Thermal correction to Energy=                        0.223786
Thermal correction to Enthalpy=                     0.224730
Thermal correction to Gibbs Free Energy=            0.169011
Sum of electronic and zero-point Energies=          -501.375191
Sum of electronic and thermal Energies=             -501.361553
Sum of electronic and thermal Enthalpies=           -501.360609
Sum of electronic and thermal Free Energies=        -501.416328
E( $\omega$ B97XD/6-311++G(3df,2p))= -501.717849000

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C      0.645667    0.326436   -0.675162

```



C	-0.468677	1.183708	-0.119026
C	-1.728616	0.652637	0.033744
C	-2.177994	-0.681863	-0.324932
C	-3.415575	-1.193640	-0.152231
C	-4.597912	-0.511419	0.473758
O	-0.149030	2.420125	0.115227
H	-1.455640	-1.336301	-0.808600
H	-2.478007	1.358162	0.389733
H	-3.591439	-2.207908	-0.508008
H	1.016303	0.643631	-1.645944
C	1.025519	-0.991001	-0.220280
H	-5.388377	-0.331516	-0.266322
H	-4.341872	0.449939	0.926742
H	-5.040220	-1.140867	1.255174
H	1.553282	-1.645432	-0.906311
H	0.418708	-1.475598	0.537228
C	1.883828	0.128810	0.418451
H	1.638829	0.419672	1.431938
C	3.065193	0.529535	-0.154125
H	3.286501	0.300427	-1.191380
H	3.733814	1.207948	0.364309
O	4.700004	-1.145906	0.315088
H	4.199737	-1.916897	0.019165
H	4.651989	-1.178239	1.278575

ts6-7-out-Allyl.out

Zero-point correction=	0.211004
(Hartree/Particle)	
Thermal correction to Energy=	0.224233
Thermal correction to Enthalpy=	0.225177
Thermal correction to Gibbs Free Energy=	0.170148
Sum of electronic and zero-point Energies=	-501.379361
Sum of electronic and thermal Energies=	-501.366132
Sum of electronic and thermal Enthalpies=	-501.365188
Sum of electronic and thermal Free Energies=	-501.420217
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.722783233

C	-2.147963	-0.753889	0.268803
C	-1.742549	0.579478	-0.133371
C	-0.483044	1.135512	-0.053931
C	-3.394195	-1.273353	0.212934
O	-0.172524	2.314493	-0.497547
C	0.614936	0.353009	0.609426
H	-1.375190	-1.424842	0.639985
H	-2.501247	1.226264	-0.570788
H	-3.519678	-2.306337	0.534284
H	0.353026	-0.562534	1.123092
C	-4.642950	-0.584969	-0.256926
H	-5.448133	-0.700427	0.478284
H	-4.499752	0.484930	-0.428940
H	-5.009297	-1.026561	-1.192778
C	1.887676	0.960240	0.968441

H	1.990548	2.030758	0.829064
H	2.446303	0.520590	1.787728
C	1.950635	0.190350	-0.353058
H	1.898770	0.761034	-1.271679
C	2.342196	-1.137426	-0.381969
H	2.439844	-1.662756	-1.325168
O	4.550452	-1.201166	-0.231602
H	4.841033	-0.765229	-1.043525
H	4.724107	-0.558715	0.469414
H	2.327798	-1.736500	0.522120

ts6-8-in-Allyl.out

Zero-point correction=	0.211208
(Hartree/Particle)	
Thermal correction to Energy=	0.224281
Thermal correction to Enthalpy=	0.225226
Thermal correction to Gibbs Free Energy=	0.171134
Sum of electronic and zero-point Energies=	-501.378457
Sum of electronic and thermal Energies=	-501.365384
Sum of electronic and thermal Enthalpies=	-501.364440
Sum of electronic and thermal Free Energies=	-501.418532
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.722607745

C	-1.614094	0.396476	0.523450
C	-1.119808	-0.739229	-0.218069
C	0.165316	-1.206939	-0.436560
C	-2.909079	0.782202	0.557779
O	0.409708	-2.379912	-0.976641
C	1.343022	-0.396154	-0.214157
H	-0.926874	0.971911	1.131460
H	-1.874312	-1.361516	-0.696824
H	-3.147305	1.632329	1.194801
H	2.097241	-0.532997	-0.986621
C	-4.072336	0.195916	-0.175110
H	-4.566580	0.973118	-0.769339
H	-3.804544	-0.624379	-0.843705
H	-4.819819	-0.171661	0.537964
C	1.577373	0.791889	0.651227
H	0.976913	0.766813	1.561702
H	2.633944	0.786075	0.931861
C	1.300756	2.031893	-0.177155
H	0.259218	2.234711	-0.416446
C	2.257711	2.844712	-0.623258
H	3.308021	2.663110	-0.406528
H	2.012704	3.721625	-1.215716
O	2.394640	-1.959519	0.814190
H	1.993567	-1.992634	1.693559
H	1.849884	-2.555652	0.254560

ts6-8-out-Allyl.out

Zero-point correction= 0.211113  
(Hartree/Particle)  
Thermal correction to Energy= 0.224475  
Thermal correction to Enthalpy= 0.225419  
Thermal correction to Gibbs Free Energy= 0.170329  
Sum of electronic and zero-point Energies= -501.386773  
Sum of electronic and thermal Energies= -501.373412  
Sum of electronic and thermal Enthalpies= -501.372467  
Sum of electronic and thermal Free Energies= -501.427557  
E( $\omega$ B97XD/6-311++G(3df,2p))= -501.730570210

C	1.934445	0.126949	-0.705988
C	1.280765	-0.138563	0.554566
C	-0.040403	-0.497815	0.790228
C	3.224579	0.501258	-0.850581
O	-0.504048	-0.836299	1.961149
C	-0.952847	-0.399376	-0.331511
H	1.364633	-0.003047	-1.622159
H	1.895890	-0.075640	1.450703
H	3.584213	0.640477	-1.868786
H	-0.564457	-0.105430	-1.299006
C	4.238188	0.755597	0.219521
H	4.633930	1.773779	0.126301
H	3.847030	0.634910	1.231573
H	5.092192	0.078476	0.098927
C	-2.405195	-0.155381	-0.113742
H	-2.961830	-0.334427	-1.035760
H	-2.781562	-0.803978	0.682052
C	-2.533675	1.296840	0.301008
H	-2.144666	1.547333	1.286006
C	-3.073143	2.240617	-0.469870
H	-3.463523	2.013975	-1.459472
H	-3.148809	3.267783	-0.124389
O	-1.031855	-2.377748	-0.961568
H	-1.730142	-2.440705	-1.629067
H	-1.371962	-2.861881	-0.195346

ts6-9-in-Allyl.out

Zero-point correction= 0.210403  
(Hartree/Particle)  
Thermal correction to Energy= 0.223886  
Thermal correction to Enthalpy= 0.224830  
Thermal correction to Gibbs Free Energy= 0.169462  
Sum of electronic and zero-point Energies= -501.380079  
Sum of electronic and thermal Energies= -501.366596  
Sum of electronic and thermal Enthalpies= -501.365652  
Sum of electronic and thermal Free Energies= -501.421020  
E( $\omega$ B97XD/6-311++G(3df,2p))= -501.722602833

C	1.645364	1.061890	-0.203877
C	0.485646	1.745887	0.035723
C	-0.806995	1.043954	0.152697
C	-1.305739	0.129642	-0.724994
C	-2.582847	-0.468413	-0.567455
C	-3.599995	-0.069890	0.430331
O	0.396036	3.044243	0.240970
H	-0.730480	-0.162569	-1.597563
H	-1.424171	1.378667	0.985341
H	-2.956278	-1.022940	-1.422860
H	2.557012	1.661206	-0.179686
C	1.851766	-0.416834	-0.422854
H	-3.178233	0.190090	1.401679
H	-4.356724	-0.846420	0.542341
H	-4.098463	0.820223	0.022390
H	2.133996	-0.624059	-1.464691
H	0.927310	-0.971924	-0.230296
C	2.923882	-0.959918	0.486508
H	2.734875	-0.850643	1.555363
C	4.055986	-1.536612	0.078947
H	4.281108	-1.656529	-0.979524
H	4.790553	-1.908341	0.788399
O	-2.099411	-2.344139	0.277619
H	-1.675613	-2.101091	1.113455
H	-1.380296	-2.684742	-0.273208

ts6-9-out-Allyl.out

Zero-point correction=	0.210701
(Hartree/Particle)	
Thermal correction to Energy=	0.224114
Thermal correction to Enthalpy=	0.225058
Thermal correction to Gibbs Free Energy=	0.169420
Sum of electronic and zero-point Energies=	-501.384816
Sum of electronic and thermal Energies=	-501.371404
Sum of electronic and thermal Enthalpies=	-501.370460
Sum of electronic and thermal Free Energies=	-501.426097
E( $\omega$ B97XD/6-311++G(3df,2p))=	-501.728012500

C	-3.689454	-0.683754	-0.591004
C	-2.940605	-0.042422	0.519156
C	-1.544194	-0.192080	0.751888
C	-0.698538	-0.743513	-0.162334
C	0.755559	-0.950324	-0.025066
C	1.454058	-0.088091	0.779668
C	2.943665	-0.131072	0.935204
O	1.267737	-1.922968	-0.743670
H	-1.171317	0.154345	1.710769
H	-1.111159	-1.124234	-1.095972
H	-3.534788	0.211484	1.391536
H	0.918658	0.703439	1.295180

H	-3.824950	-1.736766	-0.313461
H	-4.679182	-0.238949	-0.695938
H	-3.162247	-0.648302	-1.545353
H	3.220648	0.199450	1.944856
H	3.305119	-1.165300	0.853310
C	3.732876	0.703753	-0.049209
H	4.809991	0.711084	0.120071
C	3.235508	1.399412	-1.072847
H	2.167935	1.418915	-1.283086
H	3.884965	1.969633	-1.731493
O	-3.146304	1.873042	-0.096814
H	-2.678542	1.904150	-0.944673
H	-2.609847	2.409005	0.505388

### Ketol formation with H<sub>2</sub>O (R=Me)

m1-Crotyl.out

Zero-point correction=	0.238551
(Hartree/Particle)	
Thermal correction to Energy=	0.254847
Thermal correction to Enthalpy=	0.255791
Thermal correction to Gibbs Free Energy=	0.191681
Sum of electronic and zero-point Energies=	-540.689481
Sum of electronic and thermal Energies=	-540.673185
Sum of electronic and thermal Enthalpies=	-540.672241
Sum of electronic and thermal Free Energies=	-540.736351
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.072010391

C	-2.662840	-0.768702	-0.617815
C	-1.809277	0.015744	0.272703
C	-0.548680	0.281355	-0.042044
C	-3.945327	-1.101614	-0.398387
O	0.516810	0.945938	0.511938
C	0.656926	0.257997	-0.814544
H	-2.194210	-1.106546	-1.540932
H	-2.190211	0.398047	1.215388
H	-4.442654	-1.693551	-1.165061
H	0.761115	0.976050	-1.626411
C	-4.785019	-0.750067	0.791923
H	-5.155795	-1.659362	1.279241
H	-4.246493	-0.161777	1.538402
H	-5.667663	-0.178705	0.481473
C	1.581851	-0.930096	-0.836832
H	1.373622	-1.565112	0.027575
H	1.323517	-1.505795	-1.734759
C	3.023264	-0.503542	-0.905513
H	3.309393	0.012643	-1.821406
C	3.956682	-0.679145	0.036629
H	4.956603	-0.303593	-0.179103
O	0.190515	3.771085	0.092777
H	0.323789	2.825632	0.275808

H	-0.766235	3.881267	0.066997
C	3.801537	-1.341699	1.372914
H	2.779225	-1.669422	1.574235
H	4.461745	-2.213758	1.445184
H	4.100952	-0.653597	2.171450

m6-in-Crotyl.out

Zero-point correction=	0.237345
(Hartree/Particle)	
Thermal correction to Energy=	0.253535
Thermal correction to Enthalpy=	0.254479
Thermal correction to Gibbs Free Energy=	0.190962
Sum of electronic and zero-point Energies=	-540.676446
Sum of electronic and thermal Energies=	-540.660255
Sum of electronic and thermal Enthalpies=	-540.659311
Sum of electronic and thermal Free Energies=	-540.722828
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.054909684

C	0.567750	0.702976	-0.138303
C	-0.741540	1.058204	-0.447636
C	-1.801650	0.120387	-0.243789
C	-1.764238	-1.284089	-0.337840
C	-2.830896	-2.076890	-0.009681
C	-4.138296	-1.681738	0.555336
O	-1.066847	2.289315	-0.774419
H	-0.882907	-1.775786	-0.730073
H	-2.763185	0.588890	-0.040051
H	-2.703536	-3.145973	-0.170612
H	1.251110	1.552554	-0.106235
C	1.181822	-0.619312	0.199847
H	-4.271302	-0.609374	0.694942
H	-4.261337	-2.183631	1.523354
H	-4.935451	-2.073517	-0.087365
H	1.261393	-1.227659	-0.710704
H	0.523633	-1.184407	0.874097
C	2.528085	-0.453863	0.855296
H	2.533096	0.191846	1.733104
C	3.683154	-1.014785	0.481376
H	4.561517	-0.787976	1.084972
O	0.347920	4.250912	0.322175
H	-0.119108	4.481975	1.131786
H	-0.172551	3.501062	-0.077760
C	3.929868	-1.935282	-0.676485
H	4.701284	-1.519113	-1.334309
H	4.307872	-2.900284	-0.319640
H	3.036534	-2.124066	-1.276292

m6-out-Crotyl.out

```

Zero-point correction=                                0.237902
(Hartree/Particle)
Thermal correction to Energy=                        0.253808
Thermal correction to Enthalpy=                     0.254752
Thermal correction to Gibbs Free Energy=            0.192128
Sum of electronic and zero-point Energies=          -540.687138
Sum of electronic and thermal Energies=              -540.671232
Sum of electronic and thermal Enthalpies=           -540.670288
Sum of electronic and thermal Free Energies=        -540.732912
E( $\omega$ B97XD/6-311++G(3df,2p)) = -541.066748681

```

```

C      -4.583456   -0.114703    0.681456
C      -3.604296   -1.119672    0.203165
C      -2.325311   -0.935243   -0.232689
C      -1.711125    0.336901   -0.299743
C      -0.396023    0.681214   -0.731782
C       0.502671   -0.367983   -0.909192
C       1.933550   -0.156704   -1.238795
O      -0.072211    1.942181   -0.873997
H      -1.776498   -1.816604   -0.547502
H      -2.312459    1.195950   -0.006911
H      -3.967728   -2.145718    0.201962
H       0.163007   -1.393042   -0.808388
H      -5.485741   -0.176788    0.061489
H      -4.895831   -0.382895    1.697774
H      -4.221367    0.913107    0.681169
H       2.001759   -0.071830   -2.334344
H       2.249827    0.823337   -0.860422
C       2.849581   -1.259715   -0.759896
H       3.385644   -1.816449   -1.524918
C       3.043490   -1.585140    0.523002
H       3.734985   -2.397870    0.741997
O       1.620023    2.779656    1.048946
H       1.021585    2.453809    0.329753
H       2.281636    2.086653    1.151482
C       2.407317   -0.933650    1.714094
H       1.719164   -0.128972    1.440998
H       1.846937   -1.670936    2.300438
H       3.174185   -0.518272    2.378113

```

m7-in-Crotyl.out

```

Zero-point correction=                                0.243741
(Hartree/Particle)
Thermal correction to Energy=                        0.257431
Thermal correction to Enthalpy=                     0.258375
Thermal correction to Gibbs Free Energy=            0.203119
Sum of electronic and zero-point Energies=          -540.673847
Sum of electronic and thermal Energies=              -540.660157
Sum of electronic and thermal Enthalpies=           -540.659213
Sum of electronic and thermal Free Energies=        -540.714469
E( $\omega$ B97XD/6-311++G(3df,2p)) = -541.057344486

```

C	1.941336	0.366922	0.666746
C	1.572986	-0.724550	-0.207100
C	0.372329	-1.406805	-0.156646
C	3.099130	1.066475	0.627757
O	0.042115	-2.353809	-0.976236
C	-0.615664	-1.068053	0.950047
H	1.214203	0.657588	1.425208
H	2.274623	-1.023322	-0.985397
H	3.242496	1.870098	1.347245
H	-0.218171	-1.257779	1.944351
C	4.212744	0.805637	-0.353247
H	5.040953	1.504640	-0.207159
H	4.618669	-0.210500	-0.255042
H	3.876312	0.906258	-1.394098
C	-2.089427	-1.282400	0.795290
H	-2.440214	-1.588178	-0.186244
H	-2.650222	-1.693043	1.628118
C	-1.559099	0.123668	0.938655
H	-1.696203	0.592874	1.909938
C	-1.638162	1.126732	-0.172689
H	-1.036345	2.007401	0.052241
O	-3.054148	1.730530	-0.123229
H	-3.735380	1.040992	-0.241754
H	-3.231145	2.171101	0.728702
C	-1.457953	0.695775	-1.603864
H	-0.417235	0.397819	-1.746323
H	-2.105558	-0.145041	-1.864263
H	-1.669839	1.534914	-2.269486

m7-out-Crotyl.out

```

Zero-point correction= 0.244751
(Hartree/Particle)
Thermal correction to Energy= 0.258205
Thermal correction to Enthalpy= 0.259149
Thermal correction to Gibbs Free Energy= 0.204274
Sum of electronic and zero-point Energies= -540.677297
Sum of electronic and thermal Energies= -540.663843
Sum of electronic and thermal Enthalpies= -540.662899
Sum of electronic and thermal Free Energies= -540.717773
E( $\omega$ B97XD/6-311++G(3df,2p))= -541.063195471

```

C	-2.414438	-0.776872	0.185259
C	-2.021291	0.588901	-0.086022
C	-0.753896	1.137297	0.010088
C	-3.669840	-1.271490	0.080297
O	-0.498429	2.378660	-0.267029
C	0.412703	0.291741	0.457319
H	-1.642031	-1.477888	0.499380
H	-2.802960	1.277297	-0.407614
H	-3.831629	-2.322127	0.312360



H	0.188260	-0.724698	0.756767
C	-4.869433	-0.462008	-0.339266
H	-5.776504	-1.072779	-0.343344
H	-5.048296	0.388434	0.332742
H	-4.751457	-0.041523	-1.347348
C	1.565604	0.927125	1.189199
H	1.524641	1.997339	1.361686
H	2.036530	0.343746	1.974459
C	1.745356	0.486713	-0.237969
H	1.763577	1.282598	-0.977329
C	2.609962	-0.681551	-0.599512
H	2.517828	-0.932351	-1.655798
O	4.074051	-0.205991	-0.548031
H	4.262421	0.458341	-1.236494
H	4.284334	0.203394	0.313350
C	2.567157	-1.916683	0.263193
H	1.584747	-2.382262	0.156399
H	3.319720	-2.632382	-0.072752
H	2.734525	-1.685538	1.318493

m8-in-Crotyl.out

Zero-point correction=	0.243127
(Hartree/Particle)	
Thermal correction to Energy=	0.257579
Thermal correction to Enthalpy=	0.258523
Thermal correction to Gibbs Free Energy=	0.200818
Sum of electronic and zero-point Energies=	-540.730729
Sum of electronic and thermal Energies=	-540.716277
Sum of electronic and thermal Enthalpies=	-540.715333
Sum of electronic and thermal Free Energies=	-540.773039
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.116903701

C	4.335583	-0.971970	0.255052
C	2.984353	-1.441356	-0.193743
C	1.856503	-0.715197	-0.299039
C	1.715290	0.706251	-0.003608
C	0.554331	1.381682	-0.047128
C	-0.804968	0.797592	-0.361110
C	-1.464908	0.229845	0.908878
O	0.535844	2.710132	0.294012
H	0.964542	-1.240919	-0.634868
H	2.597207	1.268918	0.291363
H	2.921998	-2.495262	-0.460715
H	-0.700542	-0.005896	-1.097194
H	4.675447	-1.556864	1.117922
H	5.077537	-1.124426	-0.537832
H	4.353641	0.083603	0.535821
H	-0.796847	-0.544131	1.301007
H	-1.519704	1.026789	1.657820
C	-2.840824	-0.328354	0.641515
H	-3.683667	0.318530	0.878679
C	-3.097729	-1.530074	0.110030

H	-4.140406	-1.802136	-0.050487
O	-1.573189	1.858303	-0.931222
H	-0.342920	3.056838	0.072509
H	-2.496083	1.579834	-0.978533
C	-2.088644	-2.560083	-0.300946
H	-1.066735	-2.284577	-0.027436
H	-2.320473	-3.528127	0.156981
H	-2.118156	-2.709678	-1.386762

m8-out-Crotyl.out

Zero-point correction=	0.243367
(Hartree/Particle)	
Thermal correction to Energy=	0.257712
Thermal correction to Enthalpy=	0.258656
Thermal correction to Gibbs Free Energy=	0.200673
Sum of electronic and zero-point Energies=	-540.731517
Sum of electronic and thermal Energies=	-540.717173
Sum of electronic and thermal Enthalpies=	-540.716229
Sum of electronic and thermal Free Energies=	-540.774211
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.117862586

C	-4.295297	-0.998065	0.229563
C	-2.936258	-1.438533	-0.225223
C	-1.818016	-0.694520	-0.306479
C	-1.695902	0.720664	0.025481
C	-0.542447	1.409844	-0.008751
C	0.829080	0.856387	-0.358304
C	1.500168	0.226482	0.869283
O	-0.533433	2.730364	0.358044
H	-0.918075	-1.199068	-0.653341
H	-2.584527	1.263942	0.336860
H	-2.858949	-2.484188	-0.519326
H	0.734934	0.099359	-1.142346
H	-5.032989	-1.143502	-0.568606
H	-4.629667	-1.605656	1.078824
H	-4.328626	0.050949	0.532623
H	1.610846	1.001550	1.635865
H	0.812000	-0.525549	1.266959
C	2.840208	-0.381672	0.545202
H	3.709332	0.257518	0.686781
C	3.037078	-1.618456	0.073009
H	4.061897	-1.924340	-0.135491
O	1.665756	1.917529	-0.820985
H	0.343793	3.081016	0.130129
H	1.449269	2.104105	-1.742535
C	1.984404	-2.645469	-0.222299
H	2.216555	-3.591151	0.280220
H	0.984542	-2.328940	0.085404
H	1.952967	-2.859155	-1.297376

m9b-in-Crotyl.out

```
Zero-point correction= 0.243134
(Hartree/Particle)
Thermal correction to Energy= 0.257579
Thermal correction to Enthalpy= 0.258523
Thermal correction to Gibbs Free Energy= 0.199908
Sum of electronic and zero-point Energies= -540.724117
Sum of electronic and thermal Energies= -540.709672
Sum of electronic and thermal Enthalpies= -540.708728
Sum of electronic and thermal Free Energies= -540.767343
E( $\omega$ B97XD/6-311++G(3df,2p)) = -541.109877052
```

C	1.088868	1.223161	-0.163660
C	-0.155686	1.722677	-0.120285
C	-1.418274	0.988563	0.059332
C	-1.717192	-0.162514	-0.550518
C	-2.990797	-0.952285	-0.382741
C	-3.923399	-0.458303	0.705011
O	-0.401839	3.084813	-0.217626
H	-1.007927	-0.597647	-1.254271
H	-2.138807	1.468055	0.719911
H	-3.524082	-0.938297	-1.343645
H	1.903867	1.932552	-0.310425
C	1.496506	-0.218556	0.005703
H	-3.424999	-0.458943	1.679694
H	-4.801102	-1.107814	0.758948
H	-4.265655	0.556886	0.487508
H	1.729520	-0.660367	-0.969573
H	0.658647	-0.795162	0.413521
C	2.672318	-0.343189	0.940957
H	2.475601	-0.024945	1.965123
C	3.903667	-0.780115	0.650532
H	4.629793	-0.799466	1.463180
O	-2.662567	-2.318538	-0.071068
H	-2.168721	-2.691386	-0.811277
C	4.423139	-1.256075	-0.674283
H	5.301250	-0.670263	-0.969434
H	4.751282	-2.299755	-0.604483
H	3.684346	-1.185560	-1.475875
H	0.437332	3.561722	-0.259635

m9b-out-Crotyl.out

```
Zero-point correction= 0.242649
(Hartree/Particle)
Thermal correction to Energy= 0.257448
Thermal correction to Enthalpy= 0.258392
Thermal correction to Gibbs Free Energy= 0.197204
Sum of electronic and zero-point Energies= -540.725819
Sum of electronic and thermal Energies= -540.711021
Sum of electronic and thermal Enthalpies= -540.710076
```

Sum of electronic and thermal Free Energies= -540.771264  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.111389551

C	-4.211228	0.569372	0.223328
C	-3.372552	-0.579390	-0.313936
C	-1.884672	-0.343488	-0.326985
C	-1.267468	0.805907	-0.034230
C	0.190721	1.002487	-0.111194
C	0.993168	0.458809	-1.037042
C	2.491035	0.606499	-1.084921
O	0.722474	1.853927	0.842249
H	-1.291874	-1.211692	-0.613830
H	-1.840304	1.673864	0.291456
H	-3.683533	-0.796904	-1.342333
H	0.525375	-0.152509	-1.803519
H	-4.080019	1.468510	-0.385602
H	-5.268197	0.291847	0.198517
H	-3.936201	0.805324	1.257167
H	2.778725	1.047591	-2.047567
H	2.827443	1.294033	-0.305872
C	3.171543	-0.736632	-0.952255
H	3.171406	-1.352309	-1.851366
C	3.728839	-1.242426	0.154447
H	4.168405	-2.237404	0.086410
O	-3.653663	-1.796153	0.397953
H	-3.401187	-1.665728	1.320976
C	3.811203	-0.597359	1.506446
H	4.855586	-0.493381	1.822922
H	3.343563	0.389602	1.536526
H	3.317230	-1.227022	2.255678
H	0.059555	2.041306	1.516866

m9-in-Crotyl.out

Zero-point correction= 0.243223  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.257484  
 Thermal correction to Enthalpy= 0.258428  
 Thermal correction to Gibbs Free Energy= 0.200600  
 Sum of electronic and zero-point Energies= -540.666207  
 Sum of electronic and thermal Energies= -540.651946  
 Sum of electronic and thermal Enthalpies= -540.651002  
 Sum of electronic and thermal Free Energies= -540.708830  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.051263842

C	1.125281	1.300105	-0.239379
C	-0.116172	1.851646	-0.114883
C	-1.328646	1.018400	0.147957
C	-1.734661	-0.002498	-0.613452
C	-2.989507	-0.779785	-0.392176
C	-3.844279	-0.440560	0.799496

O	-0.380937	3.144904	-0.191484
H	-1.150305	-0.308376	-1.479516
H	-1.944894	1.356489	0.980897
H	-3.582702	-0.849061	-1.304694
H	1.947686	1.997326	-0.411539
C	1.518251	-0.155440	-0.120065
H	-3.272926	-0.487905	1.730293
H	-4.694274	-1.122672	0.858923
H	-4.226291	0.575484	0.674211
H	1.838443	-0.555973	-1.090184
H	0.650768	-0.751935	0.184605
C	2.608695	-0.349362	0.903772
H	2.326095	-0.080002	1.922671
C	3.861983	-0.776776	0.702199
H	4.516303	-0.838782	1.572015
O	-2.600479	-2.257373	-0.208732
H	-1.955233	-2.376656	0.514416
H	-2.201807	-2.628516	-1.017440
C	4.493834	-1.187405	-0.596518
H	5.389687	-0.586717	-0.792251
H	4.821038	-2.232941	-0.551774
H	3.821064	-1.079963	-1.450623

m9-out-Crotyl.out

Zero-point correction=	0.242809
(Hartree/Particle)	
Thermal correction to Energy=	0.257216
Thermal correction to Enthalpy=	0.258161
Thermal correction to Gibbs Free Energy=	0.200477
Sum of electronic and zero-point Energies=	-540.669763
Sum of electronic and thermal Energies=	-540.655356
Sum of electronic and thermal Enthalpies=	-540.654412
Sum of electronic and thermal Free Energies=	-540.712095
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.054638603

C	-3.969092	1.221215	0.631337
C	-3.591873	0.093307	-0.291961
C	-2.146210	-0.150150	-0.569278
C	-1.144869	0.563894	-0.041529
C	0.308194	0.364314	-0.324411
C	0.814540	-0.903698	-0.362220
C	2.279394	-1.192074	-0.598651
O	0.995211	1.472996	-0.494960
H	-1.937989	-0.958549	-1.267613
H	-1.367663	1.411075	0.607029
H	-4.176024	0.116244	-1.212398
H	0.149546	-1.740124	-0.163881
H	-3.658043	2.163368	0.173633
H	-5.051348	1.246706	0.770516
H	-3.479894	1.125372	1.604236
H	2.388914	-2.228862	-0.940692
H	2.670082	-0.554505	-1.399538

C	3.101972	-1.014444	0.655854
H	2.833744	-1.685270	1.473327
C	4.072689	-0.119819	0.883639
H	4.536831	-0.124031	1.870286
O	-4.171746	-1.175583	0.363851
H	-3.694578	-1.406689	1.183043
H	-4.123082	-1.947192	-0.230049
C	4.612152	0.910169	-0.066612
H	5.685168	0.756073	-0.231817
H	4.114863	0.894839	-1.039075
H	4.500382	1.915960	0.354861

ts1-6-in-Crotyl.out

Zero-point correction=	0.236576
(Hartree/Particle)	
Thermal correction to Energy=	0.252212
Thermal correction to Enthalpy=	0.253157
Thermal correction to Gibbs Free Energy=	0.191941
Sum of electronic and zero-point Energies=	-540.660181
Sum of electronic and thermal Energies=	-540.644545
Sum of electronic and thermal Enthalpies=	-540.643601
Sum of electronic and thermal Free Energies=	-540.704816
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.039268064

C	0.196407	-1.717788	0.034212
C	-0.981442	-0.937764	-0.242943
C	-1.168892	0.408723	-0.189082
C	-0.129283	1.347679	0.178010
C	-0.232554	2.691342	0.182564
C	-1.428553	3.513120	-0.184472
O	-1.814303	-1.891738	-0.610490
H	0.819975	0.922262	0.494534
H	-2.168227	0.769556	-0.420757
H	0.648496	3.253523	0.488234
H	0.053919	-2.531019	0.744377
C	1.493475	-1.642953	-0.652294
H	-2.295920	2.910773	-0.464071
H	-1.190226	4.175735	-1.025061
H	-1.716797	4.160833	0.651706
H	1.510906	-0.857617	-1.407157
H	1.695094	-2.613913	-1.125170
C	2.505010	-1.430993	0.465894
H	2.577425	-2.245273	1.182456
C	3.286759	-0.355252	0.617742
H	3.975182	-0.377422	1.461788
O	-4.200606	-1.318904	0.623558
H	-4.152616	-0.359597	0.698959
H	-3.368557	-1.571433	0.165803
C	3.373402	0.866692	-0.241425
H	3.159576	1.761693	0.354521
H	4.394980	0.978892	-0.621503
H	2.690090	0.851304	-1.092435

ts1-6-out-Crotyl.out

Zero-point correction=	0.236598
(Hartree/Particle)	
Thermal correction to Energy=	0.252392
Thermal correction to Enthalpy=	0.253336
Thermal correction to Gibbs Free Energy=	0.191797
Sum of electronic and zero-point Energies=	-540.665090
Sum of electronic and thermal Energies=	-540.649296
Sum of electronic and thermal Enthalpies=	-540.648352
Sum of electronic and thermal Free Energies=	-540.709891
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.044118628

C	-1.112743	-1.287661	-0.546158
C	0.178272	-1.013573	0.104351
C	1.018822	0.043203	0.126420
C	0.804038	1.296585	-0.580939
C	1.598673	2.383177	-0.556119
C	2.863665	2.562476	0.230571
O	0.350024	-2.237432	0.563074
H	-0.081458	1.344635	-1.212580
H	1.943588	-0.105717	0.679664
H	1.302350	3.232257	-1.170311
H	-1.067955	-1.650676	-1.572466
C	-2.395195	-1.339077	0.120066
H	3.093233	1.705740	0.869032
H	2.796870	3.449750	0.871511
H	3.718841	2.723276	-0.437342
H	-2.371727	-1.190864	1.196688
H	-3.045801	-2.153887	-0.191506
C	-2.696522	-0.068304	-0.679279
H	-3.094110	-0.211290	-1.677945
C	-2.539819	1.184906	-0.198941
H	-2.853849	1.994930	-0.855320
O	2.917924	-2.971509	-0.055122
H	3.363908	-2.126779	-0.180070
H	1.995614	-2.729293	0.184909
C	-2.054883	1.600220	1.142458
H	-1.280838	2.366366	1.033433
H	-2.887169	2.071036	1.680316
H	-1.660932	0.780334	1.743788

ts1-8-Crotyl.out

Zero-point correction=	0.238716
(Hartree/Particle)	
Thermal correction to Energy=	0.253676
Thermal correction to Enthalpy=	0.254620
Thermal correction to Gibbs Free Energy=	0.195691

Sum of electronic and zero-point Energies=	-540.659667
Sum of electronic and thermal Energies=	-540.644707
Sum of electronic and thermal Enthalpies=	-540.643763
Sum of electronic and thermal Free Energies=	-540.702691
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.040939990

C	-0.616448	1.063729	0.399303
C	0.772784	1.404443	0.083875
C	1.933950	0.735155	-0.089930
C	2.090053	-0.708802	0.004970
C	3.236390	-1.406153	-0.115344
C	4.613507	-0.856898	-0.347662
O	0.477280	2.675013	-0.081701
H	1.179580	-1.279669	0.170544
H	2.792581	1.350311	-0.350559
H	3.170248	-2.490686	-0.040822
H	-0.998449	1.508320	1.311406
C	-1.569442	0.698263	-0.692653
H	4.642325	0.235568	-0.348936
H	5.015760	-1.204477	-1.307338
H	5.305263	-1.209308	0.426769
H	-1.190726	-0.199145	-1.190049
H	-1.489272	1.509032	-1.428674
C	-2.992771	0.569072	-0.227530
H	-3.457735	1.498106	0.098623
C	-3.710566	-0.557744	-0.170667
H	-4.733915	-0.475962	0.193971
O	-0.717737	-0.775295	1.407107
H	-1.585652	-0.781902	1.835777
H	-0.077232	-0.698979	2.127967
C	-3.275770	-1.942739	-0.544155
H	-3.339740	-2.603457	0.328124
H	-3.945620	-2.359278	-1.304751
H	-2.253874	-1.986179	-0.926555

ts6-7-in-Crotly.out

Zero-point correction=	0.239228
(Hartree/Particle)	
Thermal correction to Energy=	0.253666
Thermal correction to Enthalpy=	0.254610
Thermal correction to Gibbs Free Energy=	0.197349
Sum of electronic and zero-point Energies=	-540.664060
Sum of electronic and thermal Energies=	-540.649621
Sum of electronic and thermal Enthalpies=	-540.648677
Sum of electronic and thermal Free Energies=	-540.705938
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.044100456

C	2.147912	-0.419676	0.682404
C	1.636963	0.659661	-0.140047
C	0.445381	1.332852	0.006476



C	3.294617	-1.098352	0.458834
O	0.089033	2.351832	-0.717042
C	-0.535830	0.966297	1.096048
H	1.579197	-0.693416	1.568417
H	2.280496	1.025083	-0.940179
H	3.582286	-1.866938	1.173413
H	-0.640855	1.754406	1.839018
C	4.221220	-0.859645	-0.704264
H	4.748196	0.100606	-0.619618
H	4.981417	-1.642974	-0.768455
H	3.682562	-0.839414	-1.659733
C	-0.957672	-0.367976	1.518147
H	-0.574044	-1.233093	0.988150
H	-1.209959	-0.532047	2.560380
C	-1.998802	0.458672	0.742111
H	-2.778715	0.941680	1.317105
C	-2.331889	0.137087	-0.596796
H	-3.221690	0.618844	-0.991235
O	-3.628944	-1.610671	-0.306241
H	-4.239925	-1.358290	0.398793
H	-3.030911	-2.251064	0.103072
C	-1.451376	-0.494963	-1.593266
H	-2.040494	-0.942471	-2.393801
H	-0.866370	0.325055	-2.036505
H	-0.755051	-1.218986	-1.170441

ts6-7-out-Crotyl.out

Zero-point correction=	0.239530
(Hartree/Particle)	
Thermal correction to Energy=	0.253960
Thermal correction to Enthalpy=	0.254904
Thermal correction to Gibbs Free Energy=	0.197488
Sum of electronic and zero-point Energies=	-540.669016
Sum of electronic and thermal Energies=	-540.654586
Sum of electronic and thermal Enthalpies=	-540.653642
Sum of electronic and thermal Free Energies=	-540.711058
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.049626592

C	-2.329041	-0.753642	0.208574
C	-2.007549	0.633489	-0.058134
C	-0.776466	1.248465	0.055887
C	-3.552757	-1.312264	0.075118
O	-0.546031	2.483627	-0.258718
C	0.391940	0.456840	0.586395
H	-1.526120	-1.415616	0.529519
H	-2.816634	1.273000	-0.409659
H	-3.658569	-2.372329	0.296169
H	0.181879	-0.504007	1.038485
C	-4.788689	-0.573067	-0.365721
H	-5.665838	-1.225282	-0.344025
H	-5.002143	0.290352	0.277747
H	-4.692361	-0.184838	-1.388533

C	1.636915	1.103018	0.993223
H	1.693559	2.184189	0.933135
H	2.235221	0.631124	1.765520
C	1.660471	0.428520	-0.383498
H	1.584915	1.085511	-1.241267
C	2.247285	-0.838670	-0.589208
H	2.417211	-1.126447	-1.622614
O	4.393022	-0.373669	-0.540184
H	4.496078	0.331615	-1.192974
H	4.491262	0.065930	0.315589
C	2.295799	-1.929788	0.401315
H	1.347913	-2.477146	0.290346
H	3.097751	-2.629668	0.166800
H	2.372498	-1.583454	1.433268

ts6-8-in-Crotyl.out

Zero-point correction=	0.239325
(Hartree/Particle)	
Thermal correction to Energy=	0.253918
Thermal correction to Enthalpy=	0.254862
Thermal correction to Gibbs Free Energy=	0.196537
Sum of electronic and zero-point Energies=	-540.661053
Sum of electronic and thermal Energies=	-540.646459
Sum of electronic and thermal Enthalpies=	-540.645515
Sum of electronic and thermal Free Energies=	-540.703840
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.042389895

C	1.922232	-0.628712	0.472973
C	1.595233	0.555576	-0.285624
C	0.406402	1.242677	-0.443259
C	3.128050	-1.238405	0.459999
O	0.332714	2.399312	-1.067947
C	-0.881188	0.713516	-0.033127
H	1.175096	-1.059853	1.127249
H	2.410734	0.999299	-0.854385
H	3.243432	-2.105144	1.108719
H	-1.672967	0.925076	-0.749133
C	4.340313	-0.879411	-0.338116
H	4.659389	-1.739884	-0.937637
H	4.189471	-0.033365	-1.011303
H	5.174883	-0.640738	0.331857
C	-1.249602	-0.297971	0.988321
H	-0.531306	-0.355090	1.805236
H	-2.217504	-0.006809	1.404550
C	-1.376021	-1.621543	0.248495
H	-0.492841	-2.254201	0.250886
C	-2.458607	-2.027166	-0.425626
H	-2.401864	-2.999917	-0.912226
O	-1.501784	2.587562	0.846238
H	-1.038184	2.637160	1.692904
H	-0.878037	2.956733	0.176860
C	-3.754028	-1.296176	-0.593703

H	-4.589955	-1.928736	-0.275513
H	-3.795523	-0.358574	-0.033996
H	-3.918971	-1.065263	-1.652404

ts6-8-out-Crotyl.out

Zero-point correction=	0.239279
(Hartree/Particle)	
Thermal correction to Energy=	0.254352
Thermal correction to Enthalpy=	0.255296
Thermal correction to Gibbs Free Energy=	0.195615
Sum of electronic and zero-point Energies=	-540.669208
Sum of electronic and thermal Energies=	-540.654135
Sum of electronic and thermal Enthalpies=	-540.653191
Sum of electronic and thermal Free Energies=	-540.712872
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.050162310

C	-2.006298	-0.507615	-0.576206
C	-1.566269	0.402534	0.457615
C	-0.333395	1.020164	0.605631
C	-3.220579	-1.097056	-0.631987
O	-0.063817	1.895969	1.534265
C	0.728970	0.607440	-0.299099
H	-1.325233	-0.733457	-1.392612
H	-2.292327	0.657933	1.227796
H	-3.413217	-1.746133	-1.484656
H	0.514594	-0.139413	-1.054146
C	-4.351537	-0.971474	0.340022
H	-4.631897	-1.960250	0.721878
H	-4.122698	-0.330710	1.193946
H	-5.239446	-0.568217	-0.161370
C	2.155188	0.733707	0.087524
H	2.801033	0.648388	-0.788013
H	2.343020	1.680137	0.595925
C	2.365300	-0.428920	1.046365
H	2.226349	-0.199873	2.099554
C	2.647494	-1.684892	0.679740
H	2.769128	-2.420510	1.473710
O	0.600223	2.098111	-1.745351
H	1.423224	2.081401	-2.254456
H	0.636068	2.919912	-1.235473
C	2.819213	-2.201911	-0.714641
H	2.712341	-1.424412	-1.475033
H	3.803828	-2.668734	-0.829520
H	2.075459	-2.980556	-0.918627

ts6-9-in-Crotyl.out

Zero-point correction=	0.238927
(Hartree/Particle)	

Thermal correction to Energy=	0.253920
Thermal correction to Enthalpy=	0.254864
Thermal correction to Gibbs Free Energy=	0.194484
Sum of electronic and zero-point Energies=	-540.659914
Sum of electronic and thermal Energies=	-540.644921
Sum of electronic and thermal Enthalpies=	-540.643977
Sum of electronic and thermal Free Energies=	-540.704357
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.039953831

C	-1.059968	1.336528	0.025736
C	0.193345	1.882910	-0.037787
C	1.396015	1.031726	-0.073779
C	1.653415	-0.037138	0.730562
C	2.856333	-0.788159	0.651923
C	4.046555	-0.420057	-0.147889
O	0.450417	3.173085	-0.137214
H	0.934872	-0.343431	1.483474
H	2.160048	1.371651	-0.771699
H	3.037773	-1.477076	1.471117
H	-1.883126	2.049343	-0.047070
C	-1.472944	-0.112943	0.121386
H	3.802076	-0.012918	-1.129585
H	4.720059	-1.270963	-0.249985
H	4.575412	0.354753	0.423667
H	-1.780674	-0.358823	1.145398
H	-0.629569	-0.772307	-0.111349
C	-2.587490	-0.421931	-0.846680
H	-2.321118	-0.306758	-1.897999
C	-3.840787	-0.795672	-0.560451
H	-4.513183	-0.972087	-1.400040
O	2.288452	-2.455034	-0.478233
H	1.997363	-2.065185	-1.315321
H	1.476981	-2.775296	-0.059269
C	-4.450959	-1.004195	0.794795
H	-4.790842	-2.040392	0.907715
H	-3.761978	-0.782410	1.613105
H	-5.336148	-0.368921	0.914525

ts6-9-out-Crotyl.out

Zero-point correction=	0.239921
(Hartree/Particle)	
Thermal correction to Energy=	0.254555
Thermal correction to Enthalpy=	0.255500
Thermal correction to Gibbs Free Energy=	0.196568
Sum of electronic and zero-point Energies=	-540.663936
Sum of electronic and thermal Energies=	-540.649301
Sum of electronic and thermal Enthalpies=	-540.648357
Sum of electronic and thermal Free Energies=	-540.707289
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.045224108

C	-3.999662	-0.468541	-0.775422
C	-3.297999	0.063071	0.421805
C	-1.936169	-0.198269	0.744946
C	-1.073057	-0.793215	-0.125394
C	0.339715	-1.135742	0.112563
C	1.063746	-0.312595	0.935546
C	2.542917	-0.444363	1.167070
O	0.793418	-2.177470	-0.548685
H	-1.607718	0.085548	1.740185
H	-1.446341	-1.117642	-1.096359
H	-3.939219	0.304782	1.263995
H	0.562405	0.521872	1.418439
H	-4.200632	-1.529498	-0.580823
H	-4.957702	0.032817	-0.913169
H	-3.407254	-0.394852	-1.688583
H	2.734289	-0.690254	2.219603
H	2.924642	-1.284689	0.577170
C	3.296446	0.826173	0.826253
H	3.608656	1.448094	1.664097
C	3.575349	1.249915	-0.412340
H	4.110468	2.192738	-0.523039
O	-3.338673	2.006523	-0.085197
H	-2.687104	2.095075	-0.796958
H	-2.958193	2.486066	0.665245
C	3.205242	0.556165	-1.689986
H	4.081587	0.444092	-2.338348
H	2.771848	-0.433459	-1.520862
H	2.473142	1.151289	-2.249781

### Ketol formation with H<sub>3</sub>O (R=H)

m1-H-Allyl.out

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Zero-point correction= 0.223603
(Hartree/Particle)
Thermal correction to Energy= 0.237758
Thermal correction to Enthalpy= 0.238702
Thermal correction to Gibbs Free Energy= 0.181421
Sum of electronic and zero-point Energies= -501.822590
Sum of electronic and thermal Energies= -501.808435
Sum of electronic and thermal Enthalpies= -501.807491
Sum of electronic and thermal Free Energies= -501.864772
E( $\omega$ B97XD/6-311++G(3df,2p))= -502.180498091

```

C	-2.424966	-0.778968	-0.509508
C	-1.535280	0.147848	0.188170
C	-0.237108	0.174115	-0.062241
C	-3.748054	-0.897760	-0.314738
O	0.869123	0.870750	0.415211
C	1.012610	-0.192211	-0.653033
H	-1.949915	-1.426901	-1.243785
H	-1.919810	0.834300	0.936747

H	-4.268851	-1.644803	-0.911448
H	1.271765	0.250919	-1.612848
C	-4.607301	-0.122945	0.636083
H	-5.075709	-0.799259	1.360648
H	-4.059953	0.641964	1.191527
H	-5.423142	0.368736	0.094108
C	1.784536	-1.411137	-0.232161
H	1.449615	-1.738962	0.756395
H	1.523516	-2.197114	-0.952631
C	3.267236	-1.166064	-0.251730
H	3.690699	-0.858326	-1.207553
C	4.058049	-1.298757	0.812605
H	3.661299	-1.602499	1.779182
H	5.126652	-1.113611	0.748653
H	1.074562	2.254982	0.007886
O	1.246783	3.246487	-0.268277
H	0.502344	3.799922	0.023620
H	2.051346	3.568040	0.173339

m4-H-Allyl.out

Zero-point correction=	0.222245
(Hartree/Particle)	
Thermal correction to Energy=	0.237300
Thermal correction to Enthalpy=	0.238244
Thermal correction to Gibbs Free Energy=	0.179481
Sum of electronic and zero-point Energies=	-501.848361
Sum of electronic and thermal Energies=	-501.833306
Sum of electronic and thermal Enthalpies=	-501.832361
Sum of electronic and thermal Free Energies=	-501.891125
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.204491920

C	-2.533761	0.568998	-0.957425
C	-1.632719	1.292448	-0.147676
C	-0.540758	0.794429	0.589781
C	-2.992069	-0.707836	-0.770737
O	0.019580	1.529398	1.590541
C	0.106601	-0.340940	0.174464
H	-3.016495	1.149597	-1.738664
H	-1.787478	2.370738	-0.099646
H	-3.728014	-1.037105	-1.501954
H	-0.297153	-0.866736	-0.684730
C	-2.749980	-1.670222	0.328862
H	-2.179732	-2.522958	-0.060695
H	-2.205859	-1.252924	1.177533
H	-3.713786	-2.071596	0.657257
C	1.339784	-0.873059	0.793242
H	1.840921	-0.116849	1.403510
H	0.985476	-1.654106	1.491365
C	2.278022	-1.500976	-0.202088
H	1.839824	-2.228109	-0.884252
C	3.578172	-1.215942	-0.270044
H	4.037190	-0.494040	0.402436

H	4.223149	-1.703255	-0.995303
H	-0.550594	2.265255	1.847225
O	2.333277	1.865308	-1.183733
H	2.008487	1.985832	-0.283480
H	2.601462	0.937211	-1.215352

m5-H-Allyl.out

Zero-point correction= (Hartree/Particle)	0.226388
Thermal correction to Energy=	0.240034
Thermal correction to Enthalpy=	0.240978
Thermal correction to Gibbs Free Energy=	0.185867
Sum of electronic and zero-point Energies=	-501.907638
Sum of electronic and thermal Energies=	-501.893993
Sum of electronic and thermal Enthalpies=	-501.893048
Sum of electronic and thermal Free Energies=	-501.948160
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.267634414

C	-0.176083	0.109465	-0.058172
C	-1.142804	1.213874	0.183449
C	-2.425990	0.936378	-0.348096
C	-2.385286	-0.325732	-0.844263
C	-1.081556	-1.014541	-0.626906
O	-0.768873	2.290187	0.781071
H	-3.220952	-0.819875	-1.329767
H	-3.260323	1.625553	-0.343209
H	-0.701040	-1.371316	-1.590428
C	-1.283764	-2.234426	0.286807
H	0.452181	0.491550	-0.879590
C	0.736063	-0.198266	1.131997
H	1.111186	0.747278	1.540473
H	0.158495	-0.663434	1.938443
H	-0.331733	-2.745501	0.446789
H	-1.695324	-1.938001	1.255637
H	-1.977013	-2.936320	-0.183622
C	1.923244	-1.063192	0.816670
H	2.550204	-1.285509	1.678850
C	2.277274	-1.550137	-0.375047
H	1.697553	-1.380126	-1.279248
H	3.174359	-2.153200	-0.479764
H	-1.479562	2.951414	0.851516
O	3.026836	1.682105	-0.883717
H	2.874554	0.767558	-0.603802
H	3.937122	1.691064	-1.199740

m6-in-H-Allyl.out

Zero-point correction= (Hartree/Particle)	0.222606
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Thermal correction to Energy=	0.237681
Thermal correction to Enthalpy=	0.238625
Thermal correction to Gibbs Free Energy=	0.179458
Sum of electronic and zero-point Energies=	-501.847660
Sum of electronic and thermal Energies=	-501.832586
Sum of electronic and thermal Enthalpies=	-501.831641
Sum of electronic and thermal Free Energies=	-501.890808
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.203510350

C	-1.870833	-0.806027	-0.344154
C	-1.363334	0.494575	-0.274258
C	-0.061303	0.926886	-0.624632
C	-3.124582	-1.123185	0.126431
O	0.157700	2.281154	-0.773767
C	1.053839	0.142969	-0.723931
H	-1.299295	-1.596947	-0.811012
H	-2.038583	1.284347	0.049356
H	-3.436441	-2.156531	-0.013762
H	1.970036	0.692757	-0.939015
C	-4.100986	-0.268623	0.820213
H	-3.816849	0.777304	0.926321
H	-5.064399	-0.349409	0.303081
H	-4.268175	-0.698043	1.817331
C	1.203128	-1.323105	-0.517359
H	0.553023	-1.680763	0.288802
H	0.864533	-1.829438	-1.436262
C	2.633662	-1.705841	-0.244683
H	3.363332	-1.393227	-0.990734
C	3.024866	-2.394269	0.826005
H	4.067475	-2.661235	0.973141
H	-0.669337	2.779441	-0.763881
O	2.216341	2.858121	1.157968
H	2.606157	1.976517	1.163644
H	1.494127	2.795589	0.511472
H	2.315335	-2.714846	1.586114

m6-out-H-Allyl.out

Zero-point correction=	0.222774
(Hartree/Particle)	
Thermal correction to Energy=	0.237654
Thermal correction to Enthalpy=	0.238598
Thermal correction to Gibbs Free Energy=	0.179567
Sum of electronic and zero-point Energies=	-501.858667
Sum of electronic and thermal Energies=	-501.843787
Sum of electronic and thermal Enthalpies=	-501.842843
Sum of electronic and thermal Free Energies=	-501.901874
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.214751202

C	1.259764	-0.349232	-0.241086
C	0.112291	0.397150	-0.184469



C	-1.165653	-0.202032	-0.087957
C	-1.463039	-1.567219	0.050520
C	-2.751617	-2.025241	0.120045
C	-4.018344	-1.268239	0.068730
O	0.223107	1.749616	-0.262719
H	-0.665114	-2.299151	0.110636
H	-2.003201	0.491075	-0.116611
H	-2.868519	-3.101982	0.228376
H	1.179289	-1.430515	-0.215976
C	2.607813	0.255605	-0.364572
H	-3.914147	-0.188701	-0.033586
H	-4.593433	-1.495461	0.974585
H	-4.615404	-1.654984	-0.766432
H	2.701377	1.088925	0.344060
H	2.656628	0.722124	-1.363284
C	3.729238	-0.731233	-0.205419
H	3.701508	-1.597667	-0.865508
C	4.724212	-0.593561	0.669442
H	5.519888	-1.329874	0.738778
O	-2.026664	3.129727	0.237158
H	-2.787886	2.742057	-0.211996
H	-0.636847	2.207993	-0.089327
H	-2.228538	3.054639	1.177825
H	4.774864	0.260795	1.341542

m7-in-H-Allyl.out

Zero-point correction=	0.230522
(Hartree/Particle)	
Thermal correction to Energy=	0.242866
Thermal correction to Enthalpy=	0.243811
Thermal correction to Gibbs Free Energy=	0.191861
Sum of electronic and zero-point Energies=	-501.854256
Sum of electronic and thermal Energies=	-501.841911
Sum of electronic and thermal Enthalpies=	-501.840967
Sum of electronic and thermal Free Energies=	-501.892917
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.217876409

C	2.063365	-0.572218	0.401944
C	1.393682	0.652436	-0.022926
C	0.149717	1.014632	0.340122
C	3.298305	-0.966270	0.042070
O	-0.401607	2.220480	-0.032342
C	-0.791236	0.251768	1.205250
H	1.515484	-1.214911	1.086419
H	1.946149	1.345766	-0.654482
H	3.659406	-1.904773	0.460127
H	-0.797110	0.583985	2.240750
C	4.255847	-0.263400	-0.872452
H	3.858287	0.667814	-1.282320
H	5.187671	-0.029983	-0.343711
H	4.527775	-0.912981	-1.712768
C	-1.108274	-1.195202	0.970748

H	-0.656592	-1.671504	0.105330
H	-1.240597	-1.835275	1.835586
C	-2.162780	-0.152668	0.693159
H	-2.978607	-0.056104	1.402311
C	-2.523543	0.144623	-0.720702
H	-3.113224	1.049526	-0.848749
H	0.240636	2.737198	-0.537255
H	-1.678268	0.133184	-1.406618
O	-3.424888	-0.921789	-1.281965
H	-4.285792	-0.954104	-0.825843
H	-3.023766	-1.809577	-1.227594

m7-out-H-Allyl.out

Zero-point correction=	0.230297
(Hartree/Particle)	
Thermal correction to Energy=	0.242897
Thermal correction to Enthalpy=	0.243841
Thermal correction to Gibbs Free Energy=	0.190331
Sum of electronic and zero-point Energies=	-501.856544
Sum of electronic and thermal Energies=	-501.843944
Sum of electronic and thermal Enthalpies=	-501.843000
Sum of electronic and thermal Free Energies=	-501.896509
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.220220917

C	-2.252562	-0.807495	0.242505
C	-1.722679	0.504006	-0.110244
C	-0.431552	0.882841	-0.022739
C	-3.541620	-1.186599	0.165502
O	-0.024960	2.142750	-0.382424
C	0.695013	0.050345	0.455864
H	-1.544325	-1.551208	0.600607
H	-2.424144	1.250999	-0.476838
H	-3.777480	-2.206080	0.466798
H	0.418122	-0.947383	0.774739
C	-4.710776	-0.365567	-0.289612
H	-5.459200	-0.289564	0.508193
H	-4.434918	0.648133	-0.589317
H	-5.208497	-0.845729	-1.140463
C	1.861611	0.663947	1.188536
H	1.866005	1.738089	1.333984
H	2.290179	0.078925	1.996605
C	2.052780	0.163907	-0.216769
H	2.143992	0.908856	-1.000879
C	2.792499	-1.105968	-0.449641
H	2.669153	-1.512723	-1.451041
O	4.278826	-0.897151	-0.351237
H	4.619651	-0.311688	-1.052958
H	4.536136	-0.511124	0.507205
H	-0.782297	2.655430	-0.693137
H	2.600405	-1.866229	0.305387

m8-in-H-Allyl.out

Zero-point correction=	0.229097
(Hartree/Particle)	
Thermal correction to Energy=	0.242203
Thermal correction to Enthalpy=	0.243147
Thermal correction to Gibbs Free Energy=	0.188730
Sum of electronic and zero-point Energies=	-501.849607
Sum of electronic and thermal Energies=	-501.836501
Sum of electronic and thermal Enthalpies=	-501.835557
Sum of electronic and thermal Free Energies=	-501.889974
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.212916760

C	1.682135	0.212607	0.665286
C	1.127459	-0.429336	-0.520868
C	-0.121754	-0.892252	-0.697004
C	2.916039	0.741103	0.752956
O	-0.518942	-1.514247	-1.859523
C	-1.293413	-0.836474	0.246628
H	1.068058	0.253434	1.560161
H	1.804173	-0.575541	-1.360570
H	3.197852	1.173445	1.711599
H	-2.152362	-1.274190	-0.259471
C	3.965331	0.814010	-0.312364
H	4.876035	0.301353	0.018196
H	3.652852	0.375886	-1.262424
H	4.243115	1.858396	-0.495725
C	-1.678142	0.502986	0.861574
H	-2.590294	0.351241	1.445947
H	-0.893417	0.846765	1.540828
C	-1.910377	1.531907	-0.211826
H	-1.035177	1.836113	-0.784267
C	-3.098869	2.072719	-0.476457
H	-3.989365	1.788137	0.080108
H	-3.215148	2.821806	-1.254473
H	0.219419	-1.552925	-2.482115
O	-1.039650	-1.846971	1.343209
H	-1.860352	-2.073068	1.821819
H	-0.387095	-1.544736	2.003335

m8-out-H-Allyl.out

Zero-point correction=	0.228378
(Hartree/Particle)	
Thermal correction to Energy=	0.241642
Thermal correction to Enthalpy=	0.242586
Thermal correction to Gibbs Free Energy=	0.188002
Sum of electronic and zero-point Energies=	-501.853697
Sum of electronic and thermal Energies=	-501.840433
Sum of electronic and thermal Enthalpies=	-501.839489
Sum of electronic and thermal Free Energies=	-501.894073

E( $\omega$ B97XD/6-311++G(3df,2p)) = -502.216447197

C	-4.462805	-0.414528	0.195808
C	-3.243901	-1.249441	-0.047646
C	-1.959890	-0.850977	-0.081765
C	-1.498528	0.518044	0.116253
C	-0.226690	0.949788	0.069425
C	0.979780	0.098202	-0.162321
C	2.070556	0.247849	0.876860
O	0.135676	2.262085	0.234474
H	-1.212049	-1.614786	-0.278353
H	-2.250688	1.276914	0.323465
H	-3.434468	-2.307069	-0.222253
H	0.711824	-0.942718	-0.323696
H	-5.128199	-0.453285	-0.674669
H	-5.031953	-0.816255	1.041831
H	-4.240174	0.634062	0.404274
H	2.454254	1.274184	0.862771
H	1.579710	0.130151	1.850800
C	3.216496	-0.722622	0.792295
H	3.964833	-0.576406	1.569470
C	3.393639	-1.704154	-0.092049
H	2.697542	-1.910591	-0.901247
H	4.267913	-2.345611	-0.029690
H	-0.649611	2.817615	0.322988
O	1.594779	0.479761	-1.500010
H	1.790707	1.434629	-1.570553
H	1.024778	0.231440	-2.252011

m9-in-H-Allyl.out

Zero-point correction=	0.228194
(Hartree/Particle)	
Thermal correction to Energy=	0.241437
Thermal correction to Enthalpy=	0.242382
Thermal correction to Gibbs Free Energy=	0.187610
Sum of electronic and zero-point Energies=	-501.851746
Sum of electronic and thermal Energies=	-501.838503
Sum of electronic and thermal Enthalpies=	-501.837559
Sum of electronic and thermal Free Energies=	-501.892330
E( $\omega$ B97XD/6-311++G(3df,2p)) =	-502.213954265

C	1.227206	-0.288689	-0.320856
C	0.701019	0.755876	0.324486
C	-0.555820	1.413123	-0.069512
C	2.486113	-0.981848	0.092409
O	-0.502075	2.800328	-0.065195
C	-1.725507	0.829309	-0.361692
H	0.739042	-0.695866	-1.203499
H	1.209262	1.191631	1.183567
H	2.347818	-2.063278	0.095384

H	-2.546935	1.493646	-0.626584
C	3.189824	-0.508733	1.337245
H	3.440134	0.554015	1.279614
H	2.528850	-0.668890	2.192206
H	4.102042	-1.087246	1.492522
C	-2.052871	-0.638801	-0.300998
H	-2.200862	-1.034327	-1.313810
H	-1.219379	-1.194375	0.142109
C	-3.297409	-0.883157	0.512635
H	-3.249774	-0.570489	1.556253
C	-4.418795	-1.430797	0.042536
H	-5.286638	-1.580365	0.679120
H	0.416886	3.091657	-0.101292
H	-4.502160	-1.748657	-0.995265
O	3.502012	-0.822069	-1.038064
H	3.693677	0.118176	-1.218400
H	3.205988	-1.229410	-1.873383

m9-out-H-Allyl.out

Zero-point correction=	0.228297
(Hartree/Particle)	
Thermal correction to Energy=	0.241621
Thermal correction to Enthalpy=	0.242565
Thermal correction to Gibbs Free Energy=	0.186995
Sum of electronic and zero-point Energies=	-501.853579
Sum of electronic and thermal Energies=	-501.840256
Sum of electronic and thermal Enthalpies=	-501.839312
Sum of electronic and thermal Free Energies=	-501.894882
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.215961889

C	1.498803	-0.326590	0.391509
C	0.879407	0.781649	-0.026388
C	-0.578362	0.900950	-0.193806
C	2.979818	-0.452971	0.537449
O	-1.111577	2.147485	0.074810
C	-1.370407	-0.086007	-0.634226
H	0.926168	-1.209558	0.667374
H	1.451815	1.681578	-0.248319
H	3.241253	-0.863032	1.513399
H	-0.894504	-1.028064	-0.891555
C	3.840109	0.731255	0.184178
H	3.663874	1.065469	-0.841704
H	3.600451	1.549757	0.867178
H	4.894368	0.477618	0.307668
C	-2.861209	0.003389	-0.808775
H	-3.232549	0.986856	-0.508223
H	-3.100446	-0.125973	-1.873697
C	-3.566733	-1.073896	-0.025898
H	-3.279407	-2.099268	-0.260812
C	-4.488324	-0.849461	0.911504
H	-4.796114	0.161123	1.173623
H	-4.965354	-1.667981	1.443854

H	-0.460164	2.700265	0.522714
O	3.445577	-1.590126	-0.377611
H	3.243455	-1.412495	-1.316300
H	3.036542	-2.445067	-0.146072

ts1-6-in-H-Allyl.out

Zero-point correction=(Hartree/Particle)	0.219361
Thermal correction to Energy	0.233876
Thermal correction to Enthalpy	0.234821
Thermal correction to Gibbs Free Energy	0.177105
Sum of electronic and zero-point Energies	-501.811772
Sum of electronic and thermal Energies	-501.797256
Sum of electronic and thermal Enthalpies	-501.796312
Sum of electronic and thermal Free Energies	-501.854028
E( $\omega$ B97XD/6-311++G(3df,2p))	-502.165021898

C	-2.081139	-0.863250	-0.410868
C	-1.407123	0.223142	0.287501
C	-0.089764	0.395521	0.250286
C	-3.409029	-1.068336	-0.426128
O	0.698734	1.304190	0.945627
C	1.071932	-0.256059	-0.302151
H	-1.444620	-1.559172	-0.954045
H	-1.976953	0.945704	0.864776
H	-3.765912	-1.930694	-0.986538
H	1.626596	0.310976	-1.052468
C	-4.472976	-0.249310	0.232182
H	-5.062412	-0.875495	0.911339
H	-4.083509	0.599186	0.798343
H	-5.169752	0.133047	-0.522596
C	1.558231	-1.552410	0.105457
H	1.111786	-1.893514	1.044694
H	0.992205	-2.128666	-0.673743
C	3.025422	-1.840326	-0.013753
H	3.280619	-2.894224	-0.081734
C	3.981617	-0.913187	-0.006579
H	3.762972	0.148439	0.084722
H	5.026635	-1.196527	-0.084345
H	0.833389	2.155015	0.403266
O	1.070941	3.429787	-0.456911
H	1.407993	3.169409	-1.323663
H	0.240540	3.889991	-0.633408

ts1-6-out-H-Allyl.out

Zero-point correction=(Hartree/Particle)	0.221534
Thermal correction to Energy	0.235659

Thermal correction to Enthalpy=	0.236603
Thermal correction to Gibbs Free Energy=	0.180097
Sum of electronic and zero-point Energies=	-501.812635
Sum of electronic and thermal Energies=	-501.798509
Sum of electronic and thermal Enthalpies=	-501.797565
Sum of electronic and thermal Free Energies=	-501.854071
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.167851054

C	1.629694	-0.088766	-0.153937
C	0.406806	0.533432	0.300028
C	-0.916509	0.455094	0.285093
C	-1.668759	-0.601744	-0.382224
C	-3.005533	-0.731463	-0.364374
C	-4.004831	0.132935	0.337465
O	1.224305	1.525078	0.843564
H	-1.087060	-1.326258	-0.946602
H	-1.441868	1.259798	0.792448
H	-3.424701	-1.565972	-0.924048
H	2.041182	0.266604	-1.099107
C	2.375581	-1.095207	0.590932
H	-3.556043	0.973036	0.871343
H	-4.575755	-0.464012	1.057981
H	-4.728708	0.530444	-0.382869
H	1.992167	-1.262621	1.596187
H	3.452128	-0.928225	0.567855
C	1.981890	-2.214857	-0.375888
H	2.628372	-2.360864	-1.235475
C	0.879201	-2.947949	-0.196219
H	0.626666	-3.750217	-0.882815
O	1.175130	3.558961	-0.709805
H	0.508004	3.404707	-1.391187
H	1.216226	2.347543	0.235509
H	0.868515	4.337103	-0.226662
H	0.220156	-2.782228	0.652122

ts1-8-out-H-Allyl.out

Zero-point correction=	0.221868
(Hartree/Particle)	
Thermal correction to Energy=	0.236399
Thermal correction to Enthalpy=	0.237343
Thermal correction to Gibbs Free Energy=	0.179987
Sum of electronic and zero-point Energies=	-501.802098
Sum of electronic and thermal Energies=	-501.787567
Sum of electronic and thermal Enthalpies=	-501.786623
Sum of electronic and thermal Free Energies=	-501.843978
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.158727233

C	1.067995	-0.450029	0.425515
C	-0.281850	-0.906244	0.304560
C	-1.561033	-0.711063	0.046689

C	-2.106492	0.598462	-0.294453
C	-3.412908	0.864204	-0.455896
C	-4.567786	-0.072183	-0.302277
O	0.443343	-2.106194	0.549745
H	-1.387391	1.400928	-0.434871
H	-2.206021	-1.583834	0.095014
H	-3.674626	1.885574	-0.726633
H	1.428982	-0.241889	1.429918
C	1.967373	-0.280165	-0.741937
H	-5.119778	-0.146301	-1.246085
H	-5.270340	0.323912	0.439471
H	-4.277534	-1.078357	0.006811
H	1.682826	0.695095	-1.161656
H	1.696887	-1.024873	-1.499153
C	3.429704	-0.320379	-0.401411
H	3.798448	-1.252321	0.023505
C	4.259348	0.701225	-0.604810
H	3.909885	1.639301	-1.030923
H	5.313976	0.628090	-0.355958
H	0.384577	-2.369944	1.488086
O	0.757880	2.144168	0.955367
H	1.424551	2.210553	1.649182
H	-0.080333	2.067307	1.426526

ts4-5-H-Allyl.out

Zero-point correction=	0.221519
(Hartree/Particle)	
Thermal correction to Energy=	0.235969
Thermal correction to Enthalpy=	0.236913
Thermal correction to Gibbs Free Energy=	0.178322
Sum of electronic and zero-point Energies=	-501.841182
Sum of electronic and thermal Energies=	-501.826732
Sum of electronic and thermal Enthalpies=	-501.825787
Sum of electronic and thermal Free Energies=	-501.884378
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.196585961

C	-0.407397	-0.486140	0.435874
C	-1.455691	-1.011673	-0.308819
O	-1.168094	-1.830298	-1.341361
C	-2.780214	-0.675072	0.054909
C	-2.916930	0.524657	0.725283
C	-1.965437	1.544389	0.605574
C	-1.315084	2.055737	-0.633073
H	-3.745002	0.675173	1.414686
H	-3.611340	-1.343179	-0.150997
H	-1.909725	2.236473	1.446214
H	-0.606317	-0.188967	1.458873
C	0.997224	-0.486598	-0.039412
H	-1.809230	3.010521	-0.857906
H	-0.261549	2.294303	-0.454006
H	-1.409887	1.391305	-1.492058
H	1.205433	-1.396981	-0.614011



H	1.072550	0.339769	-0.770466
C	2.006668	-0.281593	1.053035
H	1.827454	0.563162	1.717538
C	3.086251	-1.045116	1.225582
H	3.288696	-1.895672	0.577898
H	3.797707	-0.842183	2.020726
H	-1.957488	-2.011115	-1.869184
O	4.146947	1.125392	-1.144585
H	3.772616	0.592271	-0.428208
H	5.018922	1.382816	-0.825247

ts6-4-H-Allyl.out

Zero-point correction=	0.221496
(Hartree/Particle)	
Thermal correction to Energy=	0.236289
Thermal correction to Enthalpy=	0.237233
Thermal correction to Gibbs Free Energy=	0.178896
Sum of electronic and zero-point Energies=	-501.833391
Sum of electronic and thermal Energies=	-501.818598
Sum of electronic and thermal Enthalpies=	-501.817654
Sum of electronic and thermal Free Energies=	-501.875991
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.188850307

C	2.399332	0.188065	-1.043994
C	1.337537	-0.806017	-0.817035
C	0.146997	-0.568715	-0.182337
C	3.477831	0.340655	-0.270988
O	-0.846988	-1.492454	-0.083277
C	-0.040968	0.652881	0.484838
H	2.268792	0.799090	-1.936759
H	1.495474	-1.810232	-1.215474
H	4.201079	1.097925	-0.565328
H	0.765897	1.376877	0.405872
C	3.772077	-0.417324	0.983826
H	3.761909	0.261068	1.844673
H	3.049191	-1.216358	1.170112
H	4.775151	-0.853844	0.935920
C	-1.239366	1.044914	1.215411
H	-1.927506	0.225206	1.411824
H	-1.003448	1.605927	2.120184
C	-1.753628	1.998956	0.130566
H	-1.470331	3.041205	0.241678
C	-2.452296	1.577441	-0.927550
H	-2.697613	0.528622	-1.071428
H	-2.814003	2.285253	-1.667145
H	-0.627791	-2.294244	-0.577017
O	-3.773816	-1.639324	0.188971
H	-3.880028	-2.544825	0.500446
H	-2.815433	-1.512592	0.120474

ts6-7-in-H-Allyl.out

```
Zero-point correction= 0.222712
(Hartree/Particle)
Thermal correction to Energy= 0.237175
Thermal correction to Enthalpy= 0.238120
Thermal correction to Gibbs Free Energy= 0.180455
Sum of electronic and zero-point Energies= -501.833721
Sum of electronic and thermal Energies= -501.819257
Sum of electronic and thermal Enthalpies= -501.818313
Sum of electronic and thermal Free Energies= -501.875978
E( $\omega$ B97XD/6-311++G(3df,2p)) = -502.190122603
```

C	-1.909148	0.419172	0.680287
C	-1.422035	-0.635317	-0.196313
C	-0.265641	-1.319889	-0.080526
C	-3.033610	1.129484	0.474559
O	0.081322	-2.360149	-0.903773
C	0.747262	-1.112867	0.959392
H	-1.341258	0.637462	1.579749
H	-2.080579	-0.955947	-1.000991
H	-3.283057	1.877526	1.225157
H	1.032646	-1.997164	1.525885
C	-3.994587	1.030902	-0.667652
H	-4.028238	1.982858	-1.210421
H	-3.748306	0.243093	-1.382488
H	-5.007611	0.850372	-0.290882
C	1.227526	0.161727	1.400884
H	0.804702	1.059154	0.961819
H	1.589329	0.248254	2.420040
C	2.324237	-0.498462	0.499633
H	3.134376	-0.996803	1.015877
C	2.373213	-0.266321	-0.834683
H	1.534426	0.174004	-1.367201
H	3.256817	-0.527771	-1.408753
H	-0.637335	-2.558201	-1.519191
O	3.179025	2.593790	-0.777849
H	2.477126	2.510143	-0.121597
H	3.930894	2.133319	-0.387505

ts6-7-out-H-Allyl.out

```
Zero-point correction= 0.223034
(Hartree/Particle)
Thermal correction to Energy= 0.237209
Thermal correction to Enthalpy= 0.238153
Thermal correction to Gibbs Free Energy= 0.181097
Sum of electronic and zero-point Energies= -501.835220
Sum of electronic and thermal Energies= -501.821045
Sum of electronic and thermal Enthalpies= -501.820101
Sum of electronic and thermal Free Energies= -501.877157
E( $\omega$ B97XD/6-311++G(3df,2p)) = -502.195293861
```

C	-2.344878	-0.733218	0.078903
C	-1.591462	0.510921	0.082506
C	-0.295725	0.655665	0.429925
C	-3.644810	-0.851828	-0.249979
O	0.370405	1.848930	0.341724
C	0.534871	-0.421829	0.978703
H	-1.818658	-1.645880	0.346545
H	-2.107854	1.413193	-0.238380
H	-4.070112	-1.853422	-0.214700
H	0.003491	-1.308720	1.302713
C	-4.594609	0.228396	-0.662959
H	-5.436642	0.276278	0.037449
H	-4.136842	1.218531	-0.711672
H	-5.019772	-0.000461	-1.646949
C	1.877314	-0.243160	1.472076
H	2.322508	0.743698	1.412385
H	2.202085	-0.868335	2.296474
C	1.882115	-1.033305	0.136062
H	1.953072	-2.111173	0.202676
C	2.145250	-0.395242	-1.049207
H	2.012342	0.675934	-1.156816
H	2.352796	-0.967587	-1.946312
H	-0.191600	2.511256	-0.081020
O	4.473660	0.130402	-1.062240
H	4.535629	0.539152	-0.189660
H	4.838634	-0.755514	-0.944792

ts6-8-in-H-Allyl.out

Zero-point correction=	0.224124
(Hartree/Particle)	
Thermal correction to Energy=	0.238136
Thermal correction to Enthalpy=	0.239081
Thermal correction to Gibbs Free Energy=	0.182950
Sum of electronic and zero-point Energies=	-501.837732
Sum of electronic and thermal Energies=	-501.823719
Sum of electronic and thermal Enthalpies=	-501.822775
Sum of electronic and thermal Free Energies=	-501.878906
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.195328972

C	-1.532366	-0.522239	0.546506
C	-1.132272	0.503616	-0.368121
C	0.114414	1.013138	-0.642293
C	-2.816224	-0.938272	0.675294
O	0.246697	2.066411	-1.530623
C	1.368364	0.599977	-0.139184
H	-0.798671	-0.995549	1.184273
H	-1.933269	0.964528	-0.942815
H	-2.993529	-1.714373	1.417548
H	2.209297	1.045113	-0.663538

C	-4.030396	-0.490606	-0.057350
H	-4.771026	-0.127446	0.664450
H	-3.854687	0.287563	-0.800578
H	-4.485622	-1.354389	-0.555496
C	1.703608	-0.611169	0.660792
H	2.729650	-0.507126	1.017982
H	1.050191	-0.722119	1.527740
C	1.604006	-1.814840	-0.255966
H	0.604778	-2.085360	-0.592070
C	2.661867	-2.521843	-0.649741
H	3.669890	-2.264038	-0.333179
H	2.545529	-3.387169	-1.295858
H	-0.620869	2.409799	-1.778433
O	1.685854	2.103461	1.369104
H	2.530069	1.895429	1.793310
H	1.011850	1.889588	2.029193

ts6-8-out-H-Allyl.out

Zero-point correction=	0.224201
(Hartree/Particle)	
Thermal correction to Energy=	0.237961
Thermal correction to Enthalpy=	0.238906
Thermal correction to Gibbs Free Energy=	0.183132
Sum of electronic and zero-point Energies=	-501.844615
Sum of electronic and thermal Energies=	-501.830855
Sum of electronic and thermal Enthalpies=	-501.829911
Sum of electronic and thermal Free Energies=	-501.885685
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.202208479

C	1.961188	0.133162	-0.754996
C	1.305071	-0.036178	0.510631
C	-0.019440	-0.320012	0.721902
C	3.266137	0.464449	-0.885052
O	-0.531783	-0.536756	1.976751
C	-0.965642	-0.376729	-0.327642
H	1.392368	-0.024315	-1.665871
H	1.916169	0.058760	1.405885
H	3.643347	0.547431	-1.902694
H	-0.620632	-0.119923	-1.321030
C	4.269703	0.744504	0.178736
H	4.663764	1.758480	0.044263
H	3.886158	0.654522	1.195779
H	5.121796	0.065202	0.062541
C	-2.429110	-0.259560	-0.082992
H	-2.976635	-0.560635	-0.977388
H	-2.732903	-0.878097	0.764791
C	-2.678258	1.207166	0.217122
H	-2.361675	1.555833	1.197717
C	-3.228908	2.049636	-0.655966
H	-3.543548	1.720894	-1.643907
H	-3.392145	3.092499	-0.399751
H	0.165745	-0.476969	2.642004

O	-0.878376	-2.413473	-0.882898
H	-1.547237	-2.539446	-1.570994
H	-1.217756	-2.891021	-0.112625

ts6-9-in-H-Allyl.out

Zero-point correction=	0.223322
(Hartree/Particle)	
Thermal correction to Energy=	0.237336
Thermal correction to Enthalpy=	0.238280
Thermal correction to Gibbs Free Energy=	0.182076
Sum of electronic and zero-point Energies=	-501.841091
Sum of electronic and thermal Energies=	-501.827077
Sum of electronic and thermal Enthalpies=	-501.826133
Sum of electronic and thermal Free Energies=	-501.882337
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.197598921

C	1.091771	-0.497729	0.014331
C	0.766013	0.812174	0.223894
C	-0.488151	1.448966	-0.103258
C	2.324264	-1.043434	0.444909
O	-0.456026	2.827468	-0.230330
C	-1.698523	0.855535	-0.195672
H	0.427595	-1.163210	-0.522533
H	1.510368	1.475585	0.661695
H	2.428822	-2.117568	0.329271
H	-2.529439	1.529675	-0.398312
C	3.302123	-0.396153	1.339244
H	3.391639	0.681123	1.193844
H	2.937937	-0.571657	2.361937
H	4.277149	-0.875716	1.254250
C	-2.049536	-0.589069	0.003989
H	-1.883557	-1.145992	-0.928193
H	-1.387778	-1.036976	0.756464
C	-3.479988	-0.758962	0.441280
H	-3.765653	-0.231550	1.351353
C	-4.380100	-1.502904	-0.200713
H	-5.397692	-1.600865	0.166912
H	0.446159	3.135083	-0.379316
H	-4.125542	-2.039521	-1.112760
O	3.550284	-0.927677	-1.385750
H	3.623816	0.026900	-1.522527
H	2.964881	-1.234178	-2.091470

ts6-9-out-H-Allyl.out

Zero-point correction=	0.223925
(Hartree/Particle)	
Thermal correction to Energy=	0.237926
Thermal correction to Enthalpy=	0.238870

Thermal correction to Gibbs Free Energy=	0.181260
Sum of electronic and zero-point Energies=	-501.845111
Sum of electronic and thermal Energies=	-501.831110
Sum of electronic and thermal Enthalpies=	-501.830165
Sum of electronic and thermal Free Energies=	-501.887776
E( $\omega$ B97XD/6-311++G(3df,2p))=	-502.202557837

C	1.498599	-0.479190	0.444710
C	0.854961	0.655944	0.051172
C	-0.551538	0.787272	-0.272312
C	2.882448	-0.490291	0.755074
O	-1.028731	2.058352	-0.507706
C	-1.392332	-0.259636	-0.399088
H	0.969710	-1.420839	0.544371
H	1.431454	1.576617	-0.020552
H	3.244014	-1.387976	1.246311
H	-0.993274	-1.257173	-0.245636
C	3.747568	0.703151	0.888740
H	3.545596	1.477775	0.147975
H	3.547281	1.118829	1.885685
H	4.799268	0.418684	0.857234
C	-2.841958	-0.159722	-0.754773
H	-3.181782	0.878516	-0.739796
H	-2.962165	-0.530619	-1.783646
C	-3.687633	-1.005650	0.162709
H	-3.440697	-2.066637	0.197562
C	-4.687542	-0.533936	0.907010
H	-4.954516	0.520989	0.896133
H	-5.272442	-1.188896	1.546911
H	-0.373002	2.725609	-0.273102
O	3.766412	-1.255100	-0.997461
H	3.579303	-0.582591	-1.668123
H	3.224357	-2.015950	-1.249442

### Ketol formation with H<sub>3</sub>O<sup>+</sup> (R=Me)

m1-H-Crotyl.out

Zero-point correction=	0.251781
(Hartree/Particle)	
Thermal correction to Energy=	0.267639
Thermal correction to Enthalpy=	0.268583
Thermal correction to Gibbs Free Energy=	0.206083
Sum of electronic and zero-point Energies=	-541.103574
Sum of electronic and thermal Energies=	-541.087715
Sum of electronic and thermal Enthalpies=	-541.086771
Sum of electronic and thermal Free Energies=	-541.149271
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.498828937

C	-2.785759	-0.774543	-0.492032
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C	-1.839339	0.120577	0.171179
C	-0.572116	0.184171	-0.201808
C	-4.087318	-0.905947	-0.189581
O	0.563167	0.873863	0.208909
C	0.619607	-0.117069	-0.934326
H	-2.377258	-1.381658	-1.297766
H	-2.155964	0.755869	0.993174
H	-4.660725	-1.622132	-0.775826
H	0.774422	0.391090	-1.884287
C	-4.857406	-0.180101	0.870199
H	-5.280543	-0.893576	1.586822
H	-4.254809	0.541928	1.425829
H	-5.703561	0.354420	0.423421
C	1.460601	-1.334300	-0.663475
H	1.216138	-1.724115	0.327741
H	1.154525	-2.089393	-1.396843
C	2.928447	-1.031819	-0.818252
H	3.293616	-0.986883	-1.842966
C	3.791927	-0.789851	0.174447
H	4.823843	-0.577275	-0.103386
H	0.709265	2.285919	-0.110689
O	0.857341	3.296308	-0.329088
H	0.085118	3.810422	-0.038005
H	1.633614	3.620454	0.158750
C	3.510178	-0.768430	1.646805
H	2.470017	-0.998062	1.888229
H	4.153315	-1.485160	2.169944
H	3.741989	0.220654	2.058354

m4-H-Crotyl.out

Zero-point correction=	0.251062
(Hartree/Particle)	
Thermal correction to Energy=	0.267504
Thermal correction to Enthalpy=	0.268448
Thermal correction to Gibbs Free Energy=	0.206028
Sum of electronic and zero-point Energies=	-541.129493
Sum of electronic and thermal Energies=	-541.113051
Sum of electronic and thermal Enthalpies=	-541.112107
Sum of electronic and thermal Free Energies=	-541.174526
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.523401561

C	-2.965550	0.552287	-0.887522
C	-2.036907	1.276693	-0.110540
C	-0.915961	0.777255	0.580185
C	-3.410694	-0.726616	-0.684509
O	-0.326431	1.504116	1.570164
C	-0.277391	-0.346287	0.120680
H	-3.480391	1.132168	-1.648540
H	-2.194853	2.353807	-0.049074
H	-4.173257	-1.058456	-1.386747
H	-0.711333	-0.856974	-0.733108
C	-3.122757	-1.688389	0.404856

H	-2.564124	-2.538656	-0.006189
H	-2.548271	-1.268798	1.232094
H	-4.071661	-2.093480	0.769987
C	0.984054	-0.882199	0.675590
H	1.453016	-0.164948	1.350527
H	0.668703	-1.736803	1.302652
C	1.917242	-1.391948	-0.392894
H	1.466233	-2.064598	-1.120572
C	3.219268	-1.105715	-0.507073
H	3.754518	-1.575085	-1.331434
H	-0.900588	2.223131	1.864089
O	1.839159	1.895429	-1.287847
H	1.607299	2.010177	-0.358476
H	2.074026	0.959323	-1.355520
C	4.051013	-0.220669	0.372600
H	4.803317	-0.816481	0.902394
H	4.596610	0.508924	-0.235157
H	3.465016	0.323930	1.116297

m5-H-Crotyl.out

Zero-point correction=	0.254925
(Hartree/Particle)	
Thermal correction to Energy=	0.270006
Thermal correction to Enthalpy=	0.270950
Thermal correction to Gibbs Free Energy=	0.212339
Sum of electronic and zero-point Energies=	-541.189457
Sum of electronic and thermal Energies=	-541.174377
Sum of electronic and thermal Enthalpies=	-541.173432
Sum of electronic and thermal Free Energies=	-541.232044
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.586798914

C	-0.923912	0.200847	-0.631640
C	-1.965391	1.057987	-0.004526
C	-3.119734	0.325151	0.363361
C	-2.855239	-0.981709	0.110038
C	-1.470659	-1.228854	-0.383883
O	-1.779735	2.324847	0.122497
H	-3.557253	-1.792235	0.279114
H	-4.024964	0.757113	0.769259
H	-1.514946	-1.800238	-1.317328
C	-0.701675	-2.066717	0.652493
H	-1.017475	0.416381	-1.707976
C	0.516236	0.537048	-0.214192
H	0.644143	1.620284	-0.322109
H	0.663373	0.300971	0.841859
H	0.297111	-2.299802	0.280126
H	-0.610532	-1.532397	1.602443
H	-1.229934	-3.006579	0.832742
C	1.522864	-0.150616	-1.094453
H	1.403415	0.040842	-2.160829
C	2.533941	-0.939229	-0.708489
H	3.177865	-1.339134	-1.490877



H	-2.542822	2.778566	0.520102
O	3.557976	2.025085	0.496995
H	3.289131	1.393045	-0.184707
H	3.174158	1.665733	1.305441
C	2.896664	-1.351367	0.687078
H	2.861627	-2.443271	0.778223
H	3.924573	-1.049065	0.916913
H	2.238032	-0.924924	1.446936

m6-in-H-Crotyl.out

Zero-point correction=	0.251128
(Hartree/Particle)	
Thermal correction to Energy=	0.267440
Thermal correction to Enthalpy=	0.268384
Thermal correction to Gibbs Free Energy=	0.207042
Sum of electronic and zero-point Energies=	-541.129193
Sum of electronic and thermal Energies=	-541.112882
Sum of electronic and thermal Enthalpies=	-541.111938
Sum of electronic and thermal Free Energies=	-541.173280
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.522481822

C	-2.183527	-0.842421	0.270901
C	-1.774739	0.410379	-0.199792
C	-0.473749	0.836614	-0.552338
C	-3.503476	-1.117368	0.542626
O	-0.295614	2.166260	-0.887513
C	0.652259	0.065726	-0.669272
H	-1.470207	-1.632665	0.453504
H	-2.546158	1.170731	-0.307799
H	-3.708797	-2.117311	0.920632
H	1.529062	0.612775	-1.014546
C	-4.689527	-0.258653	0.390079
H	-4.493241	0.752741	0.037453
H	-5.381604	-0.758504	-0.299985
H	-5.213009	-0.221715	1.353284
C	0.848877	-1.387193	-0.410928
H	0.613617	-1.585857	0.645251
H	0.114310	-1.962865	-0.987421
C	2.246329	-1.865455	-0.731471
H	2.340611	-2.540843	-1.578089
C	3.346553	-1.513786	-0.058662
H	4.298439	-1.922181	-0.394709
H	-1.060042	2.699937	-0.636037
O	2.006014	2.983821	0.683934
H	2.404270	2.112590	0.795544
H	1.228488	2.822675	0.124899
C	3.414854	-0.592019	1.121724
H	3.945787	-1.072461	1.950840
H	3.982809	0.310895	0.866351
H	2.429334	-0.283540	1.482254

m6-out-H-Crotyl.out

```
Zero-point correction= 0.251811
(Hartree/Particle)
Thermal correction to Energy= 0.267894
Thermal correction to Enthalpy= 0.268838
Thermal correction to Gibbs Free Energy= 0.207548
Sum of electronic and zero-point Energies= -541.139457
Sum of electronic and thermal Energies= -541.123374
Sum of electronic and thermal Enthalpies= -541.122430
Sum of electronic and thermal Free Energies= -541.183719
E( $\omega$ B97XD/6-311++G(3df,2p))= -541.533523936
```

C	-0.813367	1.177569	-0.685458
C	0.054345	0.133887	-0.878613
C	1.396795	0.188142	-0.438426
C	2.004704	1.205640	0.316703
C	3.319370	1.154320	0.693161
C	4.329778	0.109556	0.431658
O	-0.364472	-0.979744	-1.552944
H	1.426191	2.069600	0.624785
H	1.999709	-0.675160	-0.712278
H	3.681073	2.002414	1.271840
H	-0.431424	2.085215	-0.229211
C	-2.263144	1.149943	-0.990590
H	3.976957	-0.748387	-0.139364
H	4.729944	-0.232423	1.393807
H	5.174540	0.572007	-0.093535
H	-2.541627	0.234265	-1.514851
H	-2.519136	2.008675	-1.618585
C	-2.974527	1.280916	0.349540
H	-3.385123	2.259945	0.582100
C	-3.071147	0.300146	1.255763
H	-3.592694	0.528808	2.184110
O	0.434303	-3.012538	0.022239
H	1.364835	-2.859464	0.227904
H	-0.051377	-1.785069	-1.073251
C	-2.522090	-1.088967	1.135386
H	-1.598947	-1.182503	1.722174
H	-3.231450	-1.818773	1.537053
H	-2.287940	-1.361380	0.103417
H	-0.036480	-2.826419	0.844784

m7-in-H-Crotyl.out

```
Zero-point correction= 0.257811
(Hartree/Particle)
Thermal correction to Energy= 0.271748
Thermal correction to Enthalpy= 0.272692
Thermal correction to Gibbs Free Energy= 0.216830
Sum of electronic and zero-point Energies= -541.135894
```

Sum of electronic and thermal Energies= -541.121957  
 Sum of electronic and thermal Enthalpies= -541.121013  
 Sum of electronic and thermal Free Energies= -541.176875  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.535580843

C	2.205158	-0.429369	0.648620
C	1.587089	0.692816	-0.049912
C	0.369139	1.199875	0.212932
C	3.374338	-1.012583	0.328057
O	-0.110734	2.316160	-0.435808
C	-0.617947	0.728824	1.219022
H	1.680512	-0.812793	1.519581
H	2.160854	1.182840	-0.834676
H	3.710297	-1.830824	0.963359
H	-0.670691	1.382834	2.087145
C	4.283220	-0.672896	-0.814527
H	3.917017	0.156708	-1.423756
H	5.281496	-0.409494	-0.445672
H	4.411676	-1.542042	-1.470617
C	-0.926939	-0.716712	1.472034
H	-0.453512	-1.450517	0.827754
H	-1.075311	-1.036187	2.497432
C	-1.980080	0.161877	0.847084
H	-2.782705	0.489238	1.501828
C	-2.463088	-0.068823	-0.556803
H	-3.117943	0.738835	-0.882140
H	0.556111	2.653520	-1.048748
O	-3.460614	-1.235133	-0.487185
H	-4.206506	-1.042231	0.109404
H	-3.032824	-2.051651	-0.164850
C	-1.499758	-0.458420	-1.649137
H	-2.061376	-0.731887	-2.544824
H	-0.875041	0.401457	-1.893448
H	-0.858051	-1.293563	-1.358055

m7-out-H-Crotyl.out

Zero-point correction= 0.258436  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.272173  
 Thermal correction to Enthalpy= 0.273117  
 Thermal correction to Gibbs Free Energy= 0.217825  
 Sum of electronic and zero-point Energies= -541.139363  
 Sum of electronic and thermal Energies= -541.125626  
 Sum of electronic and thermal Enthalpies= -541.124682  
 Sum of electronic and thermal Free Energies= -541.179974  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.544715477

C	-2.441714	-0.801658	0.181376
C	-2.006527	0.567022	-0.068490
C	-0.743883	1.025396	0.047684

C	-3.699495	-1.265759	0.063577
O	-0.423311	2.330374	-0.227755
C	0.437903	0.239435	0.470651
H	-1.681879	-1.517521	0.486786
H	-2.758220	1.288517	-0.382671
H	-3.861410	-2.320256	0.281696
H	0.219255	-0.780177	0.761287
C	-4.923469	-0.499056	-0.339427
H	-5.692332	-0.569550	0.438972
H	-4.728233	0.559805	-0.524389
H	-5.360828	-0.925475	-1.250187
C	1.583742	0.887807	1.207263
H	1.534317	1.953659	1.398576
H	2.053558	0.296820	1.986890
C	1.767050	0.465245	-0.224754
H	1.777480	1.268133	-0.955807
C	2.642531	-0.691928	-0.604768
H	2.539968	-0.932043	-1.662451
O	4.095261	-0.200997	-0.560061
H	4.277343	0.466057	-1.247819
H	4.314541	0.201103	0.302611
C	2.616513	-1.936334	0.245080
H	1.638160	-2.410760	0.140193
H	3.372915	-2.640415	-0.106162
H	2.791508	-1.716178	1.301421
H	-1.207656	2.802252	-0.535566

m8-in-H-Crotyl.out

Zero-point correction=	0.259420
(Hartree/Particle)	
Thermal correction to Energy=	0.273286
Thermal correction to Enthalpy=	0.274230
Thermal correction to Gibbs Free Energy=	0.218958
Sum of electronic and zero-point Energies=	-541.131075
Sum of electronic and thermal Energies=	-541.117209
Sum of electronic and thermal Enthalpies=	-541.116265
Sum of electronic and thermal Free Energies=	-541.171537
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.533703538

C	-1.659102	-0.866482	0.152516
C	-1.762004	0.586113	0.049151
C	-0.759670	1.481428	0.017609
C	-2.687206	-1.724662	0.029664
O	-0.979345	2.839268	-0.042216
C	0.721924	1.226414	0.012053
H	-0.681014	-1.295050	0.359257
H	-2.766055	1.003905	0.012994
H	-2.459569	-2.783393	0.141777
H	1.236567	2.183026	-0.070463
C	-4.122191	-1.407749	-0.258032
H	-4.768626	-1.846486	0.510270
H	-4.331354	-0.337154	-0.309603

H	-4.421738	-1.856200	-1.212747
C	1.257117	0.246310	-1.022546
H	0.728548	-0.704562	-0.963877
H	1.003539	0.694109	-1.989458
C	2.747743	0.060834	-0.914396
H	3.359690	0.836087	-1.371447
C	3.357997	-0.953290	-0.289128
H	4.447264	-0.959022	-0.286922
H	-1.927883	3.024517	-0.062895
O	1.122101	0.809506	1.413957
H	2.091770	0.870638	1.527027
H	0.863288	-0.104428	1.640022
C	2.708321	-2.098457	0.427921
H	3.028370	-2.113726	1.475927
H	1.616256	-2.052943	0.408855
H	3.021328	-3.052262	-0.011518

m8-out-H-Crotyl.out

Zero-point correction=	0.257329
(Hartree/Particle)	
Thermal correction to Energy=	0.271872
Thermal correction to Enthalpy=	0.272816
Thermal correction to Gibbs Free Energy=	0.215099
Sum of electronic and zero-point Energies=	-541.135526
Sum of electronic and thermal Energies=	-541.120984
Sum of electronic and thermal Enthalpies=	-541.120039
Sum of electronic and thermal Free Energies=	-541.177756
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.536071539

C	4.515307	-0.877377	-0.198232
C	3.232108	-1.359008	0.404738
C	2.032630	-0.750946	0.393845
C	1.749325	0.539643	-0.223369
C	0.558988	1.163427	-0.260477
C	-0.716845	0.610510	0.285767
C	-1.884103	0.576261	-0.688177
O	0.359574	2.389077	-0.841354
H	1.214382	-1.265568	0.891062
H	2.576270	1.055186	-0.707609
H	3.290905	-2.320007	0.913075
H	-0.566108	-0.360145	0.750102
H	5.279055	-0.763603	0.579984
H	4.900221	-1.618390	-0.908164
H	4.419809	0.076215	-0.721788
H	-2.104978	1.593630	-1.022605
H	-1.517430	0.026935	-1.561847
C	-3.117446	-0.071928	-0.108841
H	-3.891346	0.602315	0.250359
C	-3.311341	-1.390081	0.009154
H	-4.247346	-1.725274	0.454104
H	1.193870	2.740529	-1.179286
O	-1.169970	1.447716	1.468572

H	-1.348441	2.378338	1.233799
H	-0.520021	1.439757	2.196716
C	-2.362980	-2.477324	-0.397910
H	-2.858478	-3.185181	-1.071585
H	-1.466035	-2.098738	-0.894666
H	-2.045011	-3.049406	0.481622

m9-in-H-Crotyl.out

Zero-point correction=	0.256908
(Hartree/Particle)	
Thermal correction to Energy=	0.271546
Thermal correction to Enthalpy=	0.272490
Thermal correction to Gibbs Free Energy=	0.214070
Sum of electronic and zero-point Energies=	-541.131939
Sum of electronic and thermal Energies=	-541.117300
Sum of electronic and thermal Enthalpies=	-541.116356
Sum of electronic and thermal Free Energies=	-541.174776
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.531847473

C	1.600127	-0.344077	-0.231876
C	1.261838	0.868315	0.215918
C	0.051069	1.592921	-0.201424
C	2.797828	-1.106031	0.237995
O	0.245566	2.948384	-0.435756
C	-1.193838	1.109381	-0.311992
H	0.982073	-0.856530	-0.965907
H	1.901759	1.395185	0.922571
H	2.507321	-2.090206	0.608143
H	-1.960341	1.814076	-0.631734
C	3.755620	-0.422516	1.177982
H	4.124665	0.518013	0.760155
H	3.234459	-0.211719	2.114747
H	4.598916	-1.080411	1.394636
C	-1.668531	-0.282317	0.014236
H	-1.888023	-0.823437	-0.912522
H	-0.874934	-0.842069	0.520922
C	-2.882595	-0.242597	0.908084
H	-2.712911	0.207769	1.886374
C	-4.116089	-0.680601	0.629107
H	-4.872138	-0.565789	1.405726
H	1.182630	3.126792	-0.580369
C	-4.601895	-1.321506	-0.637382
H	-5.435735	-0.747200	-1.057226
H	-3.827077	-1.402800	-1.403092
H	-4.985427	-2.327951	-0.433296
O	3.622532	-1.491947	-0.983031
H	3.921524	-0.712953	-1.490062
H	3.137253	-2.078090	-1.592649

m9-out-H-Crotyl.out

Zero-point correction=	0.257199
(Hartree/Particle)	
Thermal correction to Energy=	0.271791
Thermal correction to Enthalpy=	0.272735
Thermal correction to Gibbs Free Energy=	0.213695
Sum of electronic and zero-point Energies=	-541.133488
Sum of electronic and thermal Energies=	-541.118896
Sum of electronic and thermal Enthalpies=	-541.117952
Sum of electronic and thermal Free Energies=	-541.176992
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.533809805

C	1.831529	-0.296361	0.343429
C	1.220703	0.775522	-0.170476
C	-0.218933	0.835185	-0.471433
C	3.288467	-0.354841	0.668552
O	-0.822348	2.058368	-0.246045
C	-0.929591	-0.184474	-0.971532
H	1.262447	-1.189403	0.593287
H	1.781624	1.689745	-0.362618
H	3.440371	-0.652710	1.706818
H	-0.394885	-1.107315	-1.178208
C	4.154831	0.819876	0.298181
H	4.078997	1.054775	-0.766832
H	3.827173	1.688320	0.874647
H	5.195457	0.612034	0.552967
C	-2.408466	-0.163374	-1.247838
H	-2.817984	0.829433	-1.051327
H	-2.576657	-0.375918	-2.311297
C	-3.119138	-1.217953	-0.431768
H	-2.975412	-2.243726	-0.770563
C	-3.864836	-1.016297	0.660968
H	-4.301174	-1.893374	1.138652
H	-0.220609	2.639825	0.233702
O	3.887957	-1.557160	-0.058952
H	3.778338	-1.489681	-1.026539
H	3.484832	-2.397909	0.226386
C	-4.171858	0.292573	1.326569
H	-3.841417	0.270660	2.371497
H	-3.689304	1.142753	0.838768
H	-5.252915	0.473685	1.342734

ts1-6-in-H-Crotyl.out

Zero-point correction=	0.247906
(Hartree/Particle)	
Thermal correction to Energy=	0.263892
Thermal correction to Enthalpy=	0.264836
Thermal correction to Gibbs Free Energy=	0.203053
Sum of electronic and zero-point Energies=	-541.093632
Sum of electronic and thermal Energies=	-541.077646
Sum of electronic and thermal Enthalpies=	-541.076702

Sum of electronic and thermal Free Energies= -541.138486  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.484457017

C	-2.110002	-1.205113	-0.537751
C	-1.794877	-0.043329	0.284959
C	-0.648751	0.618802	0.177452
C	-3.250182	-1.913195	-0.480910
O	-0.158109	1.675590	0.935946
C	0.593195	0.545447	-0.552599
H	-1.345857	-1.512604	-1.249207
H	-2.507344	0.328557	1.015805
H	-3.336660	-2.759019	-1.160812
H	0.776370	1.340718	-1.277663
C	-4.431371	-1.684236	0.407424
H	-4.636961	-2.585923	0.995253
H	-4.303734	-0.848060	1.097617
H	-5.324755	-1.495613	-0.198928
C	1.595687	-0.470409	-0.345786
H	1.456287	-1.002336	0.597669
H	1.148658	-1.166933	-1.110978
C	3.005461	-0.138229	-0.727306
H	3.115003	0.607349	-1.512117
C	4.098839	-0.690667	-0.193974
H	5.057876	-0.346106	-0.577529
H	-0.441156	2.568720	0.536659
O	-0.916384	3.903415	-0.109722
H	-0.569467	4.655921	0.386181
H	-0.537522	3.985875	-0.994255
C	4.174160	-1.742177	0.869299
H	4.771729	-1.382420	1.714053
H	3.196691	-2.051467	1.245172
H	4.683826	-2.630060	0.478435

ts1-6-out-H-Crotyl.out

Zero-point correction= 0.250138  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.265686  
 Thermal correction to Enthalpy= 0.266630  
 Thermal correction to Gibbs Free Energy= 0.206725  
 Sum of electronic and zero-point Energies= -541.097851  
 Sum of electronic and thermal Energies= -541.082303  
 Sum of electronic and thermal Enthalpies= -541.081359  
 Sum of electronic and thermal Free Energies= -541.141264  
 E( $\omega$ B97XD/6-311++G(3df,2p))= -541.490747879

C	-1.612730	0.197271	-0.235781
C	-0.582018	-0.667218	0.279973
C	0.708859	-0.963239	0.258459
C	1.685997	-0.213601	-0.522738
C	3.010548	-0.433064	-0.528445



C	3.775985	-1.452094	0.255038
O	-1.644816	-1.319637	0.910743
H	1.288210	0.578481	-1.152677
H	1.015740	-1.824952	0.844856
H	3.611052	0.204510	-1.175189
H	-2.115900	-0.130859	-1.145769
C	-2.051167	1.443428	0.387157
H	3.144337	-2.080835	0.885871
H	4.512257	-0.954937	0.897027
H	4.340550	-2.101974	-0.423170
H	-1.665954	1.579786	1.396046
H	-3.132983	1.569293	0.341989
C	-1.372799	2.347231	-0.641714
H	-1.934100	2.524006	-1.553756
C	-0.168027	2.916908	-0.478914
H	0.165534	3.579130	-1.276456
O	-2.190566	-3.443025	-0.390532
H	-3.024699	-3.363312	-0.870662
H	-1.890504	-2.169092	0.389429
C	0.750543	2.804263	0.691250
H	1.766643	2.586856	0.347725
H	0.793292	3.768422	1.212015
H	0.453653	2.032503	1.403828
H	-1.515226	-3.575025	-1.068507

ts1-8-out-H-Crotyl.out

Zero-point correction=	0.249925
(Hartree/Particle)	
Thermal correction to Energy=	0.266046
Thermal correction to Enthalpy=	0.266990
Thermal correction to Gibbs Free Energy=	0.205316
Sum of electronic and zero-point Energies=	-541.084778
Sum of electronic and thermal Energies=	-541.068657
Sum of electronic and thermal Enthalpies=	-541.067713
Sum of electronic and thermal Free Energies=	-541.129387
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.478490884

C	-0.657449	0.612688	0.401794
C	0.726105	0.969412	0.320196
C	1.993239	0.672525	0.101831
C	2.447024	-0.680036	-0.200675
C	3.728356	-1.031249	-0.396583
C	4.940234	-0.157477	-0.344094
O	0.100232	2.225255	0.551424
H	1.676182	-1.442077	-0.274704
H	2.701301	1.494400	0.161058
H	3.919607	-2.079110	-0.621346
H	-1.063385	0.426006	1.393239
C	-1.549732	0.546283	-0.780030
H	5.466554	-0.191683	-1.304666
H	5.639768	-0.536021	0.409723
H	4.717618	0.885710	-0.111460

H	-1.460470	-0.502336	-1.096958
H	-1.117254	1.143436	-1.588446
C	-2.972468	0.935391	-0.482149
H	-3.160168	2.006125	-0.443852
C	-3.985593	0.094431	-0.249907
H	-4.957493	0.538137	-0.037957
H	0.154624	2.475881	1.493419
O	-0.556269	-1.986495	0.830186
H	-1.411862	-2.061103	1.269687
H	0.093759	-2.024538	1.541646
C	-3.948888	-1.403019	-0.234153
H	-4.743467	-1.808145	-0.869646
H	-2.995256	-1.815601	-0.570818
H	-4.136741	-1.772849	0.780829

ts4-5-H-Crotyl.out

Zero-point correction=	0.250417
(Hartree/Particle)	
Thermal correction to Energy=	0.265909
Thermal correction to Enthalpy=	0.266853
Thermal correction to Gibbs Free Energy=	0.207334
Sum of electronic and zero-point Energies=	-541.123105
Sum of electronic and thermal Energies=	-541.107614
Sum of electronic and thermal Enthalpies=	-541.106669
Sum of electronic and thermal Free Energies=	-541.166188
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.516371262

C	0.644764	-0.693440	-0.541956
C	1.691683	-1.123088	0.264211
O	1.402545	-1.942895	1.296955
C	3.001627	-0.690886	-0.031586
C	3.088402	0.494923	-0.741014
C	2.070922	1.451165	-0.711421
C	1.283555	1.941524	0.456962
H	3.942901	0.678582	-1.388914
H	3.870001	-1.276942	0.255535
H	2.036080	2.123167	-1.569256
H	0.866503	-0.412346	-1.564967
C	-0.771024	-0.805085	-0.126613
H	1.689282	2.933156	0.697698
H	0.237035	2.099861	0.179826
H	1.346228	1.303875	1.338839
H	-0.991669	-1.875036	0.019017
H	-0.874181	-0.368546	0.879030
C	-1.739947	-0.180057	-1.098628
H	-1.304806	0.380203	-1.924608
C	-3.072205	-0.256220	-1.005272
H	-3.662920	0.247104	-1.768816
H	2.164369	-2.040837	1.883690
O	-2.322391	2.105554	1.279441
H	-2.366821	1.552050	0.485446
H	-1.513532	1.820693	1.720416

C	-3.845400	-0.971982	0.060174
H	-4.534436	-0.281676	0.559428
H	-4.458849	-1.765116	-0.382606
H	-3.200689	-1.420589	0.819936

ts6-4-H-Crotyl.out

Zero-point correction=	0.249595
(Hartree/Particle)	
Thermal correction to Energy=	0.265588
Thermal correction to Enthalpy=	0.266533
Thermal correction to Gibbs Free Energy=	0.205062
Sum of electronic and zero-point Energies=	-541.117301
Sum of electronic and thermal Energies=	-541.101308
Sum of electronic and thermal Enthalpies=	-541.100363
Sum of electronic and thermal Free Energies=	-541.161834
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.509832128

C	-2.977322	-0.475643	-0.745431
C	-2.249957	0.791232	-0.589605
C	-0.891619	0.964625	-0.744135
C	-3.302739	-1.281633	0.268584
O	-0.273908	2.171467	-0.630262
C	-0.087121	-0.151400	-0.965306
H	-3.282237	-0.706603	-1.765637
H	-2.838461	1.679532	-0.349584
H	-3.869815	-2.178836	0.031675
H	-0.594250	-1.110862	-1.037321
C	-2.936507	-1.074661	1.703295
H	-2.284413	-1.886161	2.045458
H	-2.418777	-0.126540	1.873671
H	-3.834232	-1.102953	2.329695
C	1.362595	-0.114751	-1.139343
H	1.452530	-0.043760	-2.246125
H	1.792626	0.811367	-0.754408
C	2.058315	-1.366701	-0.672058
H	1.566910	-2.299510	-0.941943
C	3.200201	-1.411921	0.019538
H	3.575464	-2.400971	0.279074
H	-0.910401	2.871146	-0.428300
O	1.151355	1.583894	1.954090
H	1.627903	0.782530	1.707769
H	0.800080	1.922440	1.117639
C	4.047250	-0.265819	0.482832
H	4.163437	-0.297614	1.571952
H	5.053222	-0.347080	0.056034
H	3.642270	0.711009	0.209501

ts6-7-in-H-Crotyl.out

```

Zero-point correction= 0.252055
(Hartree/Particle)
Thermal correction to Energy= 0.267127
Thermal correction to Enthalpy= 0.268071
Thermal correction to Gibbs Free Energy= 0.209846
Sum of electronic and zero-point Energies= -541.125616
Sum of electronic and thermal Energies= -541.110545
Sum of electronic and thermal Enthalpies= -541.109601
Sum of electronic and thermal Free Energies= -541.167825
E( $\omega$ B97XD/6-311++G(3df,2p))= -541.519762582

```

C	2.105549	-0.417837	0.743340
C	1.620392	0.671056	-0.095763
C	0.454152	1.325413	0.046316
C	3.211428	-1.147676	0.510288
O	0.093154	2.386542	-0.749760
C	-0.592868	1.086508	1.064202
H	1.540754	-0.645552	1.642760
H	2.268373	1.012873	-0.900511
H	3.455046	-1.918588	1.239635
H	-0.774454	1.945365	1.706288
C	4.160535	-1.037695	-0.643160
H	3.910610	-0.232183	-1.337082
H	5.181240	-0.871994	-0.279847
H	4.178655	-1.976935	-1.208567
C	-1.035796	-0.206590	1.562627
H	-0.610662	-1.111142	1.143249
H	-1.372055	-0.272363	2.590964
C	-2.036364	0.522803	0.639026
H	-2.851950	1.051976	1.113947
C	-2.252871	0.084618	-0.679547
H	-3.153356	0.456907	-1.159808
H	0.797066	2.586121	-1.381096
O	-3.603032	-1.816222	-0.254539
H	-4.261970	-1.473300	0.362132
H	-2.987174	-2.313961	0.298575
C	-1.309271	-0.629596	-1.546598
H	-1.848705	-1.193280	-2.308240
H	-0.740763	0.151754	-2.077635
H	-0.600949	-1.264285	-1.014761

ts6-7-out-H-Crotyl.out

```

Zero-point correction= 0.252391
(Hartree/Particle)
Thermal correction to Energy= 0.267404
Thermal correction to Enthalpy= 0.268348
Thermal correction to Gibbs Free Energy= 0.209848
Sum of electronic and zero-point Energies= -541.128948
Sum of electronic and thermal Energies= -541.113935
Sum of electronic and thermal Enthalpies= -541.112991
Sum of electronic and thermal Free Energies= -541.171491
E( $\omega$ B97XD/6-311++G(3df,2p))= -541.523342663

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C	-2.306958	-0.777730	0.197336
C	-1.986774	0.622076	-0.044058
C	-0.772888	1.186813	0.117208
C	-3.520149	-1.340766	0.047388
O	-0.513136	2.497482	-0.183210
C	0.413722	0.479543	0.631951
H	-1.497013	-1.430351	0.514814
H	-2.783559	1.273404	-0.396779
H	-3.598981	-2.405201	0.262538
H	0.215496	-0.451742	1.146956
C	-4.793281	-0.680471	-0.383211
H	-5.553996	-0.778133	0.400275
H	-4.676609	0.381099	-0.611557
H	-5.195734	-1.178088	-1.273155
C	1.680248	1.138026	0.926970
H	1.755320	2.210997	0.796097
H	2.304371	0.705309	1.701350
C	1.647141	0.377171	-0.407482
H	1.531629	0.978830	-1.300408
C	2.183667	-0.911847	-0.556273
H	2.335851	-1.254300	-1.575846
O	4.458234	-0.438288	-0.618428
H	4.519131	0.267639	-1.274647
H	4.553514	0.010130	0.232078
C	2.286887	-1.933393	0.495892
H	1.345730	-2.503276	0.451181
H	3.089824	-2.635839	0.271779
H	2.394147	-1.525766	1.502193
H	-1.289601	2.905208	-0.588094

ts6-8-in-H-Crotyl.out

Zero-point correction=	0.252564
(Hartree/Particle)	
Thermal correction to Energy=	0.268004
Thermal correction to Enthalpy=	0.268949
Thermal correction to Gibbs Free Energy=	0.209179
Sum of electronic and zero-point Energies=	-541.120338
Sum of electronic and thermal Energies=	-541.104897
Sum of electronic and thermal Enthalpies=	-541.103953
Sum of electronic and thermal Free Energies=	-541.163723
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.515278285

C	-1.917163	-0.631130	0.544300
C	-1.541347	0.367679	-0.414586
C	-0.334090	0.979281	-0.628290
C	-3.159155	-1.167115	0.603485
O	-0.206299	1.944650	-1.612752
C	0.901211	0.776985	0.041173
H	-1.195422	-0.985126	1.267201

H	-2.330570	0.687314	-1.092993
H	-3.324355	-1.909901	1.381739
H	1.742818	1.241449	-0.466900
C	-4.342739	-0.886824	-0.254613
H	-5.172859	-0.545550	0.374439
H	-4.168598	-0.145614	-1.035607
H	-4.675426	-1.819050	-0.725310
C	1.282506	-0.272966	1.016218
H	2.211289	0.030127	1.501825
H	0.532361	-0.437228	1.786915
C	1.489852	-1.516478	0.165798
H	0.617299	-2.153648	0.045799
C	2.624812	-1.833944	-0.468404
H	2.626581	-2.757819	-1.045083
H	-1.046588	2.077542	-2.068792
O	0.891042	2.437924	1.399664
H	0.648122	3.205877	0.863884
H	1.820011	2.578155	1.631486
C	3.908560	-1.065246	-0.476531
H	4.729286	-1.695037	-0.115846
H	4.161964	-0.774406	-1.502179
H	3.871454	-0.159130	0.132817

ts6-8-out-H-Crotyl.out

Zero-point correction=	0.252329
(Hartree/Particle)	
Thermal correction to Energy=	0.267881
Thermal correction to Enthalpy=	0.268826
Thermal correction to Gibbs Free Energy=	0.208414
Sum of electronic and zero-point Energies=	-541.127513
Sum of electronic and thermal Energies=	-541.111960
Sum of electronic and thermal Enthalpies=	-541.111016
Sum of electronic and thermal Free Energies=	-541.171428
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.522226005

C	2.041390	-0.692199	0.495012
C	1.602232	0.309315	-0.440466
C	0.360992	0.876830	-0.513214
C	3.291141	-1.205536	0.517973
O	0.051797	1.858449	-1.422130
C	-0.712825	0.507730	0.342192
H	1.338665	-1.061297	1.235335
H	2.330494	0.662703	-1.167910
H	3.489812	-1.956621	1.280354
H	-0.553448	-0.332928	1.006161
C	4.449491	-0.884926	-0.363508
H	4.768125	-1.792329	-0.889564
H	4.249407	-0.107473	-1.102261
H	5.299281	-0.569843	0.252441
C	-2.126536	0.827569	0.022493
H	-2.743787	0.729737	0.916359
H	-2.229063	1.833199	-0.385612

C	-2.490719	-0.212793	-1.027089
H	-2.360099	0.096939	-2.060270
C	-2.899056	-1.459754	-0.761362
H	-3.126501	-2.098504	-1.613657
H	0.818479	2.060664	-1.972644
O	-0.392985	1.791108	1.965637
H	-1.095596	1.601040	2.603635
H	-0.592047	2.675505	1.626565
C	-3.089148	-2.086497	0.584168
H	-2.879112	-1.404512	1.411568
H	-4.115886	-2.454398	0.688279
H	-2.431001	-2.956771	0.685965

ts6-9-in-H-Crotyl.out

Zero-point correction=	0.251624
(Hartree/Particle)	
Thermal correction to Energy=	0.267178
Thermal correction to Enthalpy=	0.268122
Thermal correction to Gibbs Free Energy=	0.207820
Sum of electronic and zero-point Energies=	-541.121736
Sum of electronic and thermal Energies=	-541.106181
Sum of electronic and thermal Enthalpies=	-541.105237
Sum of electronic and thermal Free Energies=	-541.165539
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.515519457

C	1.399260	-0.491900	0.102892
C	1.302457	0.870693	0.123407
C	0.148748	1.658433	-0.238652
C	2.558228	-1.165224	0.556671
O	0.390750	2.985575	-0.555001
C	-1.143907	1.266648	-0.194204
H	0.601826	-1.107455	-0.293570
H	2.174058	1.452824	0.419604
H	2.485425	-2.246942	0.606455
H	-1.869890	2.035040	-0.455730
C	3.679437	-0.561701	1.301755
H	3.919944	0.456229	0.991872
H	3.360656	-0.529432	2.353545
H	4.563546	-1.196914	1.249049
C	-1.702657	-0.058569	0.229682
H	-1.668006	-0.755548	-0.616517
H	-1.068632	-0.499179	1.010464
C	-3.107693	0.078203	0.756634
H	-3.234653	0.831782	1.533521
C	-4.180926	-0.629725	0.387687
H	-5.119955	-0.404338	0.892391
H	1.305295	3.106403	-0.837068
C	-4.258463	-1.717057	-0.641954
H	-5.024786	-1.479417	-1.388272
H	-3.313626	-1.884128	-1.164265
H	-4.557974	-2.661867	-0.173624
O	3.661420	-1.510442	-1.308820

H	3.874306	-0.608488	-1.585339
H	2.988188	-1.808443	-1.935447

ts6-9-out-H-Crotyl.out

Zero-point correction=	0.251990
(Hartree/Particle)	
Thermal correction to Energy=	0.267580
Thermal correction to Enthalpy=	0.268524
Thermal correction to Gibbs Free Energy=	0.207824
Sum of electronic and zero-point Energies=	-541.126475
Sum of electronic and thermal Energies=	-541.110886
Sum of electronic and thermal Enthalpies=	-541.109942
Sum of electronic and thermal Free Energies=	-541.170641
E( $\omega$ B97XD/6-311++G(3df,2p))=	-541.520918925

C	1.706292	-0.259376	0.545234
C	1.080592	0.597914	-0.310956
C	-0.295431	0.515708	-0.752761
C	3.061079	-0.092829	0.926840
O	-0.820948	1.625937	-1.376362
C	-1.042112	-0.603673	-0.651475
H	1.174747	-1.096921	0.984146
H	1.637759	1.450110	-0.696947
H	3.386293	-0.694584	1.769501
H	-0.582466	-1.480293	-0.206318
C	3.912403	1.076238	0.610120
H	3.778128	1.453381	-0.404612
H	3.625420	1.869369	1.313836
H	4.962411	0.843798	0.787341
C	-2.463060	-0.742820	-1.099672
H	-2.836725	0.209642	-1.483459
H	-2.502809	-1.463774	-1.924176
C	-3.326776	-1.250496	0.039399
H	-3.577674	-2.308978	0.022561
C	-3.761595	-0.504085	1.060795
H	-4.366042	-0.992142	1.824557
H	-0.270974	2.401102	-1.211618
C	-3.492605	0.954752	1.276726
H	-4.429648	1.498545	1.439961
H	-2.883394	1.098734	2.177181
H	-2.966732	1.416985	0.437489
O	4.080609	-1.487139	-0.283783
H	3.939152	-1.160871	-1.184012
H	3.562543	-2.302484	-0.229772

Favorskii rearrangement with  $\cdot$ OH (R=H)

m11-in-OH-Allyl.out



```

Zero-point correction=                                0.200830
(Hartree/Particle)
Thermal correction to Energy=                        0.213157
Thermal correction to Enthalpy=                     0.214101
Thermal correction to Gibbs Free Energy=            0.161852
Sum of electronic and zero-point Energies=          -500.965694
Sum of electronic and thermal Energies=              -500.953367
Sum of electronic and thermal Enthalpies=           -500.952423
Sum of electronic and thermal Free Energies=        -501.004672
E(UwB97XD/6-311++G(3df,2p))= -501.263025693

```

```

C      -2.989967   -0.778134    0.462554
C      -1.684233   -0.498031    0.602546
C      -0.834225    0.274541   -0.321945
C       0.359970    1.087330    0.209923
O       0.626063    1.200655    1.512545
C       0.637096   -0.141455   -0.601175
C       1.234329   -1.377125    0.024078
H      -1.198595   -0.854983    1.509596
H      -1.334835    0.691882   -1.191443
C      -3.888380   -0.400443   -0.679629
H      -3.468584   -1.342351    1.262677
H       0.936173    0.022012   -1.635637
H       0.926291   -1.462671    1.073548
H       0.842691   -2.277877   -0.468477
H      -3.360852    0.124855   -1.479500
H      -4.356180   -1.292557   -1.112680
H      -4.705192    0.244564   -0.333755
C       2.738282   -1.428034   -0.012626
H       3.176888   -2.363747    0.335035
C       3.552491   -0.448307   -0.411307
H       3.173157    0.508699   -0.762166
H       4.631611   -0.574799   -0.392583
O       0.608077    2.280512   -0.552788
H       0.112135    2.985583   -0.117186

```

m11-out-OH-Allyl.out

```

Zero-point correction=                                0.200395
(Hartree/Particle)
Thermal correction to Energy=                        0.212919
Thermal correction to Enthalpy=                     0.213863
Thermal correction to Gibbs Free Energy=            0.160565
Sum of electronic and zero-point Energies=          -500.966964
Sum of electronic and thermal Energies=              -500.954441
Sum of electronic and thermal Enthalpies=           -500.953496
Sum of electronic and thermal Free Energies=        -501.006794
E(UwB97XD/6-311++G(3df,2p))= -501.264417844

```

```

C      0.644211   -0.119898   -0.354912

```

C	0.121850	1.173362	0.194175
C	-0.816887	-0.047612	0.145144
C	-1.924525	-0.167612	-0.820286
C	-3.149028	-0.672432	-0.599037
C	-3.680432	-1.245141	0.683251
O	0.505685	1.700983	1.360958
H	-1.712938	0.208126	-1.821221
H	-0.971242	-0.502036	1.121695
H	-3.847531	-0.675008	-1.435389
H	0.738470	-0.176004	-1.439363
C	1.659959	-0.944823	0.407763
H	-4.558518	-0.683074	1.023339
H	-2.943327	-1.235627	1.489963
H	-4.009254	-2.281100	0.537457
H	1.550909	-2.007430	0.158275
H	1.462220	-0.839445	1.482062
C	3.064783	-0.492593	0.123216
H	3.285684	0.546553	0.370930
C	4.021624	-1.252961	-0.412398
H	3.836189	-2.292652	-0.677350
H	5.018610	-0.863552	-0.600988
O	-0.096530	2.133726	-0.847325
H	-0.771848	2.741838	-0.519971

m12-in-OH-Allyl.out

Zero-point correction=	0.199386
(Hartree/Particle)	
Thermal correction to Energy=	0.212123
Thermal correction to Enthalpy=	0.213067
Thermal correction to Gibbs Free Energy=	0.159773
Sum of electronic and zero-point Energies=	-500.959756
Sum of electronic and thermal Energies=	-500.947020
Sum of electronic and thermal Enthalpies=	-500.946075
Sum of electronic and thermal Free Energies=	-500.999370
E(UωB97XD/6-311++G(3df,2p))=	-501.297950128

C	-3.165906	-0.522999	0.599015
C	-1.796976	-0.626196	0.462997
C	-1.004190	-0.335033	-0.670000
C	0.723377	1.068289	0.242338
O	0.799924	1.133746	1.467777
C	0.512460	-0.182151	-0.567618
C	1.242787	-1.380844	0.040793
H	-1.262406	-1.005961	1.339816
H	-1.458633	0.224569	-1.488623
C	-4.038666	-0.061220	-0.535979
H	-3.641161	-0.880234	1.510224
H	0.908692	0.005564	-1.570687
H	0.887027	-1.559195	1.062915
H	0.948464	-2.271920	-0.528510
H	-3.760190	0.940879	-0.902727
H	-3.972717	-0.722997	-1.419097

H	-5.094041	-0.016401	-0.246257
C	2.745341	-1.311622	0.072864
H	3.226746	-2.153222	0.571559
C	3.522656	-0.357169	-0.444365
H	3.123559	0.512071	-0.962466
H	4.604776	-0.419089	-0.366911
O	0.735380	2.196260	-0.504374
H	0.762151	2.959553	0.093272

m12-out-OH-Allyl.out

Zero-point correction=	0.199008
(Hartree/Particle)	
Thermal correction to Energy=	0.211891
Thermal correction to Enthalpy=	0.212836
Thermal correction to Gibbs Free Energy=	0.158824
Sum of electronic and zero-point Energies=	-500.961478
Sum of electronic and thermal Energies=	-500.948594
Sum of electronic and thermal Enthalpies=	-500.947650
Sum of electronic and thermal Free Energies=	-501.001662
E(UωB97XD/6-311++G(3df,2p))=	-501.298552706

C	0.479659	-0.173563	-0.234754
C	0.561828	1.289860	0.105199
C	-0.942895	-0.576050	0.113592
C	-1.985652	-0.442695	-0.826912
C	-3.349300	-0.490044	-0.618017
C	-3.928267	-0.707424	0.753597
O	0.822409	1.761215	1.211119
H	-1.662502	-0.308886	-1.865545
H	-1.177619	-0.556939	1.180174
H	-4.021971	-0.477162	-1.473022
H	0.631265	-0.271325	-1.316118
C	1.555151	-0.988466	0.502058
H	-5.023188	-0.676142	0.743624
H	-3.588548	0.050780	1.478937
H	-3.637000	-1.679905	1.191620
H	1.406208	-2.042373	0.244106
H	1.384447	-0.889426	1.582190
C	2.960840	-0.572174	0.174965
H	3.236133	0.452616	0.428673
C	3.870815	-1.358756	-0.403192
H	3.640635	-2.388299	-0.672258
H	4.873577	-1.001758	-0.622784
O	0.229570	2.100292	-0.923876
H	0.189656	3.012634	-0.596746

m1-OH-Allyl.out

```

Zero-point correction=                                0.196878
(Hartree/Particle)
Thermal correction to Energy=                        0.211349
Thermal correction to Enthalpy=                    0.212294
Thermal correction to Gibbs Free Energy=           0.152590
Sum of electronic and zero-point Energies=         -500.921565
Sum of electronic and thermal Energies=            -500.907094
Sum of electronic and thermal Enthalpies=          -500.906149
Sum of electronic and thermal Free Energies=       -500.965853
E(UωB97XD/6-311++G(3df,2p))= -501.295399430

```

```

C      1.145141      0.101450     -0.166047
C     -0.190465      0.247583      0.331991
C     -1.501809      0.053910      0.395442
C     -2.188432     -0.797918     -0.573510
C     -3.504252     -1.065951     -0.605632
C     -4.558133     -0.558041      0.331390
O      0.770729      0.931858      1.022236
H     -1.553188     -1.249938     -1.334016
H     -2.051931      0.548541      1.190674
H     -3.858015     -1.724727     -1.397123
H      1.451143      0.720959     -1.007735
C      1.985801     -1.116890      0.114927
H     -4.161410      0.102299      1.106038
H     -5.065689     -1.394520      0.826056
H     -5.327859     -0.007125     -0.221686
H      1.873032     -1.797156     -0.736941
H      1.584797     -1.621368      1.001378
C      3.434499     -0.768364      0.317495
H      3.653912     -0.105035      1.153711
C      4.430048     -1.212736     -0.449490
H      4.244273     -1.877108     -1.291249
H      5.461304     -0.929955     -0.257252
O      0.344691      3.704166     -0.662703
H      0.511871      2.948684     -0.087504

```

m6-in-OH-Allyl.out

```

Zero-point correction=                                0.194674
(Hartree/Particle)
Thermal correction to Energy=                        0.209422
Thermal correction to Enthalpy=                    0.210366
Thermal correction to Gibbs Free Energy=           0.151586
Sum of electronic and zero-point Energies=         -500.915604
Sum of electronic and thermal Energies=            -500.900855
Sum of electronic and thermal Enthalpies=          -500.899911
Sum of electronic and thermal Free Energies=       -500.958692
E(UωB97XD/6-311++G(3df,2p))= -501.296483347
S**2 before annihilation      0.8027

```

```

C     -1.230987      1.243846     -0.243799
C      0.053904      1.631434      0.265340

```

C	1.236351	0.810968	0.103807
C	1.493492	-0.117132	-0.916399
C	2.639050	-0.875710	-1.010679
C	3.772830	-0.924560	-0.048919
O	0.144191	2.712621	0.932157
H	0.770411	-0.232366	-1.717275
H	2.023641	1.036588	0.818745
H	2.727852	-1.525334	-1.878712
H	-2.017182	1.969559	-0.039793
C	-1.648846	-0.015671	-0.923766
H	3.644526	-0.275472	0.818459
H	4.705449	-0.652850	-0.557993
H	3.905728	-1.953032	0.307796
H	-1.010256	-0.859192	-0.646460
H	-1.530966	0.123621	-2.012029
C	-3.089723	-0.345435	-0.629590
H	-3.822213	0.413303	-0.903794
C	-3.489437	-1.482989	-0.062526
H	-2.777177	-2.252875	0.227595
H	-4.541145	-1.679038	0.127124
O	-0.162367	-1.791665	2.150627
H	-0.353065	-1.029074	1.593252

m6-out-OH-Allyl.out

Zero-point correction=	0.194998
(Hartree/Particle)	
Thermal correction to Energy=	0.209859
Thermal correction to Enthalpy=	0.210803
Thermal correction to Gibbs Free Energy=	0.151439
Sum of electronic and zero-point Energies=	-500.922264
Sum of electronic and thermal Energies=	-500.907403
Sum of electronic and thermal Enthalpies=	-500.906459
Sum of electronic and thermal Free Energies=	-500.965823
E(UωB97XD/6-311++G(3df,2p))=	-501.252586350
S**2 before annihilation	0.6992

C	0.939560	-0.587713	-0.682240
C	-0.002840	-1.134034	0.244522
C	-1.381945	-0.714220	0.161396
C	-1.926091	0.287639	-0.660403
C	-3.254591	0.638229	-0.680798
C	-4.366843	0.064080	0.122569
O	0.344689	-1.985486	1.124979
H	-1.271890	0.840824	-1.327603
H	-2.042058	-1.240896	0.846522
H	-3.536487	1.433664	-1.367358
H	0.622698	0.157285	-1.403584
C	2.384600	-0.938836	-0.651069
H	-4.054609	-0.704326	0.831019
H	-5.119203	-0.366449	-0.549587
H	-4.872316	0.865489	0.673981
H	2.790502	-0.936110	-1.667191
H	2.520204	-1.932586	-0.211540

C	3.119670	0.087189	0.187489
H	2.844673	0.120916	1.240661
C	4.036499	0.927699	-0.291946
H	4.321827	0.919177	-1.341829
H	4.530757	1.647589	0.354441
O	0.358231	2.690484	0.969617
H	0.354425	1.775239	0.668187

m10-in-OH-Allyl.out

Zero-point correction=	0.196096
(Hartree/Particle)	
Thermal correction to Energy=	0.210699
Thermal correction to Enthalpy=	0.211643
Thermal correction to Gibbs Free Energy=	0.151922
Sum of electronic and zero-point Energies=	-500.933217
Sum of electronic and thermal Energies=	-500.918613
Sum of electronic and thermal Enthalpies=	-500.917669
Sum of electronic and thermal Free Energies=	-500.977390
E(UωB97XD/6-311++G(3df,2p))=	-501.241592263

C	-3.123781	-0.615475	-0.097981
C	-1.987867	-0.806138	-0.776758
C	-0.874341	0.186904	-0.885508
C	-0.078317	0.557893	0.288773
O	-0.083525	1.028523	1.406862
C	0.636366	-0.246447	-0.695814
C	1.022390	-1.674665	-0.374367
H	-1.841499	-1.741112	-1.315098
H	-0.984584	0.960369	-1.646023
C	-3.502669	0.606514	0.681689
H	-3.861199	-1.416989	-0.115789
H	1.315355	0.291034	-1.356314
H	0.247456	-2.142162	0.247064
H	1.047084	-2.256360	-1.304141
H	-2.755176	1.399942	0.606359
H	-4.461063	1.000221	0.324724
H	-3.637995	0.360006	1.740988
C	2.346075	-1.812235	0.326591
H	2.659235	-2.839658	0.509338
C	3.133871	-0.813929	0.729778
H	2.873727	0.231156	0.575202
H	4.075112	-1.016341	1.233125
O	2.308108	3.026676	-0.740217
H	2.096523	2.433762	-0.011006

m10-out-OH-Allyl.out

Zero-point correction=	0.196120
(Hartree/Particle)	

Thermal correction to Energy= 0.210923  
 Thermal correction to Enthalpy= 0.211867  
 Thermal correction to Gibbs Free Energy= 0.151484  
 Sum of electronic and zero-point Energies= -500.934723  
 Sum of electronic and thermal Energies= -500.919921  
 Sum of electronic and thermal Enthalpies= -500.918976  
 Sum of electronic and thermal Free Energies= -500.979360  
 E(UωB97XD/6-311++G(3df,2p))= -501.248899228

C	0.664087	-0.108912	-0.096674
C	0.111295	0.302268	1.185299
C	-0.830049	-0.431244	0.323704
C	-1.954017	0.267068	-0.346508
C	-3.165697	-0.242163	-0.601049
C	-3.673524	-1.612877	-0.270545
O	0.274825	0.881613	2.237752
H	-1.744614	1.291445	-0.652805
H	-0.981720	-1.471067	0.612156
H	-3.875813	0.409000	-1.108835
H	0.761969	0.695707	-0.827984
C	1.677525	-1.236487	-0.215497
H	-2.922530	-2.245826	0.207981
H	-4.018203	-2.119419	-1.179156
H	-4.538060	-1.546882	0.400099
H	1.588995	-1.694265	-1.206214
H	1.434320	-2.005305	0.528267
C	3.079862	-0.746879	0.014158
H	3.267597	-0.279127	0.980920
C	4.071138	-0.848763	-0.871693
H	3.914528	-1.306351	-1.846769
H	5.069003	-0.480677	-0.649634
O	0.002077	3.595451	-0.948258
H	-0.054412	2.884184	-0.301149

ts11-12-in-OH-Allyl.out

Zero-point correction= 0.198803  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.211083  
 Thermal correction to Enthalpy= 0.212027  
 Thermal correction to Gibbs Free Energy= 0.159902  
 Sum of electronic and zero-point Energies= -500.953404  
 Sum of electronic and thermal Energies= -500.941124  
 Sum of electronic and thermal Enthalpies= -500.940180  
 Sum of electronic and thermal Free Energies= -500.992304  
 E(UωB97XD/6-311++G(3df,2p))= -501.259978857

C	-3.063306	-0.787979	0.477764
C	-1.699790	-0.779958	0.387030
C	-0.902619	-0.095352	-0.572302
C	0.499630	1.031635	0.252150

O	0.563993	1.065508	1.516365
C	0.621857	-0.145601	-0.612439
C	1.330712	-1.366268	-0.055612
H	-1.165264	-1.339628	1.157335
H	-1.381584	0.429780	-1.393960
C	-3.952282	-0.064640	-0.499165
H	-3.533652	-1.355972	1.277361
H	0.996267	0.106802	-1.607060
H	0.976346	-1.584619	0.959062
H	1.049248	-2.239962	-0.658408
H	-3.744073	1.015995	-0.530405
H	-3.823409	-0.426133	-1.531572
H	-5.009898	-0.183990	-0.244110
C	2.830739	-1.269621	-0.004723
H	3.335361	-2.173232	0.337865
C	3.573563	-0.206447	-0.320623
H	3.137606	0.728338	-0.665651
H	4.656745	-0.239920	-0.241061
O	0.533785	2.239324	-0.437370
H	0.293053	2.929280	0.196160

ts11-12-out-OH-Allyl.out

Zero-point correction=	0.198231
(Hartree/Particle)	
Thermal correction to Energy=	0.210723
Thermal correction to Enthalpy=	0.211667
Thermal correction to Gibbs Free Energy=	0.158534
Sum of electronic and zero-point Energies=	-500.955198
Sum of electronic and thermal Energies=	-500.942707
Sum of electronic and thermal Enthalpies=	-500.941763
Sum of electronic and thermal Free Energies=	-500.994896
E(UωB97XD/6-311++G(3df,2p))=	-501.257856237

C	0.590956	-0.162972	-0.298288
C	0.319023	1.217096	0.112157
C	-0.860416	-0.364198	0.102500
C	-1.914202	-0.455313	-0.851328
C	-3.242759	-0.661135	-0.611570
C	-3.799907	-0.854536	0.773985
O	0.541379	1.734209	1.248343
H	-1.618787	-0.320472	-1.895614
H	-1.040969	-0.587493	1.151616
H	-3.929769	-0.704448	-1.453748
H	0.730238	-0.255057	-1.378873
C	1.648322	-0.942263	0.474537
H	-4.886856	-0.981030	0.756385
H	-3.580416	0.000230	1.432047
H	-3.377319	-1.738322	1.277376
H	1.549698	-2.006164	0.229103
H	1.445096	-0.833084	1.547485
C	3.040518	-0.462912	0.179793
H	3.245510	0.581376	0.420239



C	4.008476	-1.208024	-0.357076
H	3.842264	-2.252995	-0.613525
H	4.996226	-0.800159	-0.554855
O	-0.013681	2.062977	-0.938372
H	-0.336560	2.885686	-0.545668

ts1-6-in-OH-Allyl.out

Zero-point correction=(Hartree/Particle)	0.193497
Thermal correction to Energy=	0.207896
Thermal correction to Enthalpy=	0.208840
Thermal correction to Gibbs Free Energy=	0.149550
Sum of electronic and zero-point Energies=	-500.889970
Sum of electronic and thermal Energies=	-500.875571
Sum of electronic and thermal Enthalpies=	-500.874627
Sum of electronic and thermal Free Energies=	-500.933917
E(UωB97XD/6-311++G(3df,2p))=	-501.286660144

C	1.383291	0.555802	-0.407283
C	0.308958	0.798402	0.522213
C	-0.982082	0.356174	0.447511
C	-1.489924	-0.554196	-0.557398
C	-2.745742	-1.042014	-0.623100
C	-3.884068	-0.763925	0.307987
O	0.869178	1.560731	1.430191
H	-0.802345	-0.863238	-1.342554
H	-1.662485	0.755626	1.196235
H	-2.971271	-1.715764	-1.447949
H	1.871466	1.462073	-0.763312
C	1.985421	-0.714085	-0.813880
H	-3.626600	-0.073734	1.114194
H	-4.239541	-1.697283	0.760720
H	-4.732203	-0.342679	-0.244402
H	3.067169	-0.586046	-0.933865
H	1.610018	-0.793731	-1.859992
C	1.639014	-1.948676	-0.032745
H	0.584707	-2.154320	0.135789
C	2.565289	-2.784888	0.431768
H	3.626355	-2.605369	0.272048
H	2.287259	-3.676246	0.986403
O	0.586822	4.119857	-0.626298
H	0.658539	3.430452	0.045094

ts1-6-out-OH-Allyl.out

Zero-point correction=(Hartree/Particle)	0.194051
Thermal correction to Energy=	0.208401
Thermal correction to Enthalpy=	0.209345

Thermal correction to Gibbs Free Energy= 0.150430  
 Sum of electronic and zero-point Energies= -500.885160  
 Sum of electronic and thermal Energies= -500.870811  
 Sum of electronic and thermal Enthalpies= -500.869867  
 Sum of electronic and thermal Free Energies= -500.928781  
 E(U $\omega$ B97XD/6-311++G(3df,2p))= -501.287495126

C	0.754698	-0.282254	-0.094564
C	-0.275653	0.440345	0.613693
C	-1.623383	0.332744	0.462528
C	-2.221479	-0.543809	-0.525627
C	-3.537738	-0.742939	-0.734506
C	-4.676763	-0.140525	0.029817
O	0.456042	1.255944	1.332102
H	-1.528960	-1.093299	-1.164842
H	-2.249435	0.948933	1.102701
H	-3.817580	-1.417290	-1.542078
H	0.854973	-0.161643	-1.175776
C	1.780509	-1.094377	0.574307
H	-4.349884	0.492846	0.857786
H	-5.321850	-0.927028	0.438784
H	-5.305454	0.466060	-0.633277
H	1.617577	-2.097476	0.140166
H	1.603787	-1.141401	1.650874
C	3.193136	-0.657508	0.257892
H	3.480985	0.304662	0.676962
C	4.053168	-1.368382	-0.468006
H	3.779616	-2.329820	-0.896796
H	5.060511	-1.006459	-0.651970
O	2.018924	2.500278	-1.225266
H	1.697011	2.252361	-0.350422

ts6-10-in-OH-Allyl.out

Zero-point correction= 0.195523  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.209441  
 Thermal correction to Enthalpy= 0.210385  
 Thermal correction to Gibbs Free Energy= 0.153896  
 Sum of electronic and zero-point Energies= -500.905781  
 Sum of electronic and thermal Energies= -500.891863  
 Sum of electronic and thermal Enthalpies= -500.890919  
 Sum of electronic and thermal Free Energies= -500.947408  
 E(U $\omega$ B97XD/6-311++G(3df,2p))= -501.216803174

C	-1.027340	0.832459	0.370358
C	-0.050960	1.821385	0.124672
O	-0.053787	2.996948	0.604306
C	1.116320	1.058631	-0.161595
C	1.318162	0.081767	-1.189154
C	2.340583	-0.806520	-1.194931

C	3.380699	-1.013055	-0.151598
H	0.629853	0.070025	-2.027446
H	1.947065	1.282327	0.507955
H	2.410079	-1.465648	-2.058399
H	-1.553174	0.988800	1.315091
C	-1.473463	-0.351046	-0.434087
H	3.284854	-2.028467	0.251790
H	4.376341	-0.951816	-0.604770
H	3.320685	-0.308928	0.679483
H	-1.543087	-0.102366	-1.497886
H	-0.724628	-1.157006	-0.353133
C	-2.792989	-0.876495	0.064564
H	-2.827073	-1.149276	1.119379
C	-3.874791	-1.031639	-0.697402
H	-3.869253	-0.763863	-1.752196
H	-4.798046	-1.434463	-0.290511
O	0.667482	-1.754309	2.252717
H	0.819498	-1.213353	1.469504

ts6-10-out-OH-Allyl.out

Zero-point correction=	0.194729
(Hartree/Particle)	
Thermal correction to Energy=	0.209458
Thermal correction to Enthalpy=	0.210402
Thermal correction to Gibbs Free Energy=	0.149842
Sum of electronic and zero-point Energies=	-500.914066
Sum of electronic and thermal Energies=	-500.899338
Sum of electronic and thermal Enthalpies=	-500.898393
Sum of electronic and thermal Free Energies=	-500.958954
E(UωB97XD/6-311++G(3df,2p))=	-501.211895906

C	0.618474	-0.402657	-0.274032
C	-0.066759	-0.515658	0.947567
C	-1.405038	-0.429471	0.457708
C	-2.002805	0.656900	-0.268520
C	-3.283641	0.665909	-0.699193
C	-4.305371	-0.413721	-0.591838
O	0.313854	-1.083952	2.011810
H	-1.397474	1.544860	-0.433219
H	-2.034650	-1.273421	0.738689
H	-3.625388	1.578174	-1.184817
H	0.335244	0.354559	-0.995159
C	1.800935	-1.260587	-0.602856
H	-3.946824	-1.318078	-0.097671
H	-4.654540	-0.682183	-1.595678
H	-5.180951	-0.040293	-0.048799
H	1.795445	-1.519263	-1.665321
H	1.771623	-2.178436	-0.005914
C	3.051107	-0.477247	-0.269386
H	3.212763	-0.272300	0.787901
C	3.913571	-0.021969	-1.178512
H	3.768167	-0.205492	-2.241079

H	4.793376	0.543829	-0.885062
O	1.411181	2.921180	0.720510
H	1.440080	1.961218	0.641939

ts10-11-in-OH-Allyl.out

Zero-point correction=	0.196942
(Hartree/Particle)	
Thermal correction to Energy=	0.210215
Thermal correction to Enthalpy=	0.211159
Thermal correction to Gibbs Free Energy=	0.156330
Sum of electronic and zero-point Energies=	-500.929853
Sum of electronic and thermal Energies=	-500.916580
Sum of electronic and thermal Enthalpies=	-500.915636
Sum of electronic and thermal Free Energies=	-500.970466
E(UωB97XD/6-311++G(3df,2p))=	-501.233339187

C	-3.074053	-0.856810	0.328913
C	-1.766517	-0.683643	0.567425
C	-0.866480	0.254814	-0.140204
C	0.323602	0.771859	0.565192
O	0.686545	1.019867	1.711566
C	0.635597	-0.134889	-0.536474
C	1.236598	-1.490792	-0.243466
H	-1.312086	-1.272630	1.362709
H	-1.310920	0.887490	-0.899692
C	-3.918122	-0.162180	-0.696829
H	-3.597992	-1.584617	0.947335
H	0.902168	0.297423	-1.495867
H	0.878167	-1.871483	0.721214
H	0.887924	-2.210882	-0.994700
H	-3.350321	0.528605	-1.324352
H	-4.402351	-0.896761	-1.350346
H	-4.721474	0.403120	-0.210166
C	2.741458	-1.497757	-0.221342
H	3.193403	-2.482977	-0.109581
C	3.535391	-0.429480	-0.314724
H	3.139833	0.578398	-0.422114
H	4.616356	-0.533295	-0.281935
O	0.622121	2.847947	-0.584993
H	1.523116	2.588366	-0.806029

ts10-11-out-OH-Allyl.out

Zero-point correction=	0.196716
(Hartree/Particle)	
Thermal correction to Energy=	0.210033
Thermal correction to Enthalpy=	0.210978
Thermal correction to Gibbs Free Energy=	0.155725
Sum of electronic and zero-point Energies=	-500.928021

Sum of electronic and thermal Energies= -500.914703  
 Sum of electronic and thermal Enthalpies= -500.913759  
 Sum of electronic and thermal Free Energies= -500.969012  
 E(UωB97XD/6-311++G(3df,2p))= -501.241529483

C	-3.125579	-0.597167	-0.657981
C	-1.912054	-0.034649	-0.732410
C	-0.821609	-0.169718	0.259836
C	0.135022	0.879164	0.692541
O	0.414180	1.552863	1.673333
C	0.683605	-0.104366	-0.236892
C	1.715438	-1.119601	0.222845
H	-1.678831	0.574450	-1.602525
H	-0.996952	-0.881096	1.067990
C	-3.675073	-1.466412	0.433148
H	-3.807423	-0.403355	-1.485073
H	0.749734	0.198368	-1.279061
H	1.506209	-1.385495	1.266775
H	1.618026	-2.031332	-0.377074
H	-2.964429	-1.639495	1.244574
H	-4.575248	-1.012728	0.863669
H	-3.976342	-2.440157	0.029859
C	3.112005	-0.573546	0.117391
H	3.321887	0.312701	0.716823
C	4.071237	-1.087487	-0.653488
H	3.892630	-1.968161	-1.267893
H	5.063699	-0.646908	-0.693437
O	-0.255529	2.759883	-0.851505
H	-0.520110	2.463931	-1.729191

### Favorskii rearrangement with <sup>-</sup>OH (R=Me)

m10-in-OH-Crotyl.out

Zero-point correction= 0.224998  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.240867  
 Thermal correction to Enthalpy= 0.241811  
 Thermal correction to Gibbs Free Energy= 0.179039  
 Sum of electronic and zero-point Energies= -540.213349  
 Sum of electronic and thermal Energies= -540.197480  
 Sum of electronic and thermal Enthalpies= -540.196536  
 Sum of electronic and thermal Free Energies= -540.259308  
 E(UωB97XD/6-311++G(3df,2p))= -540.580970471

C	-2.011570	-2.063062	-0.158340
C	-1.229590	-1.400821	-1.017161
C	-0.984930	0.074709	-0.996529
C	-0.265826	0.702756	0.118992
O	-0.244245	0.921675	1.312005

C	0.479360	0.662732	-1.132440
C	1.697536	-0.244192	-1.253928
H	-0.731273	-1.951346	-1.813472
H	-1.731979	0.698748	-1.488790
C	-2.786025	-1.473766	0.980741
H	-2.114845	-3.138348	-0.298521
H	0.519779	1.586773	-1.706904
H	1.514328	-1.172420	-0.704336
H	1.819063	-0.515243	-2.307985
H	-2.702870	-0.385070	1.025196
H	-3.846692	-1.733951	0.891106
H	-2.439346	-1.884856	1.935752
C	2.942231	0.443089	-0.755706
H	3.407751	1.138005	-1.453485
C	3.490558	0.306064	0.457389
H	4.385557	0.889175	0.672912
O	-3.484416	2.610139	0.213556
H	-2.930715	1.845875	0.406697
C	3.004303	-0.557875	1.583155
H	2.125924	-1.151589	1.319371
H	3.795681	-1.240732	1.912758
H	2.742648	0.062666	2.448176

m10-out-OH-Crotyl.out

Zero-point correction=	0.224677
(Hartree/Particle)	
Thermal correction to Energy=	0.240910
Thermal correction to Enthalpy=	0.241855
Thermal correction to Gibbs Free Energy=	0.177190
Sum of electronic and zero-point Energies=	-540.215013
Sum of electronic and thermal Energies=	-540.198779
Sum of electronic and thermal Enthalpies=	-540.197835
Sum of electronic and thermal Free Energies=	-540.262499
E(UωB97XD/6-311++G(3df,2p))=	-540.582268266

C	0.282636	0.011515	0.169461
C	-0.491984	0.571660	1.265512
C	-1.237526	-0.366425	0.409316
C	-2.278378	0.117162	-0.530183
C	-3.411396	-0.518766	-0.853040
C	-3.895399	-1.843160	-0.345199
O	-0.536209	1.321842	2.217306
H	-2.073864	1.084313	-0.988574
H	-1.371676	-1.356446	0.844571
H	-4.066901	-0.024478	-1.568645
H	0.449614	0.696520	-0.664036
C	1.369727	-1.030027	0.392621
H	-3.199726	-2.315935	0.352017
H	-4.063568	-2.532649	-1.180313
H	-4.858564	-1.725832	0.164765
H	1.447509	-1.647665	-0.505928
H	1.058932	-1.687756	1.213136

C	2.681216	-0.382121	0.745111
H	2.698390	0.123320	1.710496
C	3.792595	-0.349788	0.000354
H	4.654665	0.172358	0.414895
O	-0.372856	3.436180	-1.390794
H	-0.550954	2.878310	-0.626051
C	4.005903	-0.948601	-1.358158
H	4.809374	-1.693679	-1.326263
H	3.111481	-1.429017	-1.761247
H	4.323443	-0.174234	-2.065680

m11-cis-OH-Crotyl.out

Zero-point correction=	0.229199
(Hartree/Particle)	
Thermal correction to Energy=	0.243111
Thermal correction to Enthalpy=	0.244056
Thermal correction to Gibbs Free Energy=	0.186834
Sum of electronic and zero-point Energies=	-540.245594
Sum of electronic and thermal Energies=	-540.231682
Sum of electronic and thermal Enthalpies=	-540.230738
Sum of electronic and thermal Free Energies=	-540.287959
E(UωB97XD/6-311++G(3df,2p))=	-540.615131054

C	-3.075581	-1.226792	0.567564
C	-1.822672	-0.744501	0.533915
C	-1.310007	0.349201	-0.310860
C	-0.160426	1.246464	0.187451
O	0.349715	1.142185	1.415894
C	0.116442	0.282223	-0.924360
C	1.012957	-0.922931	-0.713943
H	-1.104993	-1.189445	1.221682
H	-2.037394	0.833738	-0.956624
C	-4.247432	-0.788490	-0.262703
H	-3.283490	-2.027396	1.277112
H	0.170113	0.702008	-1.928211
H	0.984136	-1.234667	0.332714
H	0.629912	-1.763796	-1.308363
H	-3.988079	-0.017510	-0.992399
H	-4.673203	-1.639490	-0.807436
H	-5.047631	-0.393342	0.374846
C	2.425305	-0.623486	-1.139932
H	2.549178	-0.404416	-2.201363
C	3.517832	-0.573642	-0.367481
H	4.461805	-0.323295	-0.851934
O	-0.254986	2.594799	-0.303866
H	-0.763680	3.084664	0.355001
C	3.608740	-0.815232	1.110910
H	4.329373	-1.613047	1.325289
H	3.973621	0.084058	1.621093
H	2.651549	-1.090816	1.559006

m11-trans-OH-Crotyl.out

```
Zero-point correction= 0.228911
(Hartree/Particle)
Thermal correction to Energy= 0.242930
Thermal correction to Enthalpy= 0.243874
Thermal correction to Gibbs Free Energy= 0.186286
Sum of electronic and zero-point Energies= -540.246837
Sum of electronic and thermal Energies= -540.232818
Sum of electronic and thermal Enthalpies= -540.231874
Sum of electronic and thermal Free Energies= -540.289462
E(UωB97XD/6-311++G(3df,2p))= -540.615919950
```

```
C 0.268911 0.143094 -0.294072
C -0.530872 1.347847 0.100061
C -1.198981 -0.040578 0.152112
C -2.213577 -0.476972 -0.824099
C -3.338977 -1.166525 -0.575996
C -3.826788 -1.662522 0.754773
O -0.324348 2.052736 1.217753
H -2.019719 -0.192101 -1.858160
H -1.307727 -0.417797 1.167104
H -3.981334 -1.399579 -1.424758
H 0.425989 0.003355 -1.363755
C 1.392056 -0.377211 0.579634
H -4.804731 -1.227906 0.994472
H -3.143913 -1.421270 1.573143
H -3.963586 -2.750402 0.737372
H 1.486798 -1.460865 0.455722
H 1.126996 -0.199574 1.630063
C 2.688933 0.326051 0.282920
H 2.650577 1.410839 0.390380
C 3.850065 -0.218191 -0.102063
H 4.685699 0.459041 -0.279199
O -0.888609 2.136141 -1.041862
H -1.687595 2.621419 -0.799059
C 4.154881 -1.671642 -0.320592
H 4.515389 -1.837438 -1.342443
H 4.956362 -1.999639 0.351832
H 3.290535 -2.319192 -0.155914
```

m12-cis-OH-Crotyl.out

```
Zero-point correction= 0.227972
(Hartree/Particle)
Thermal correction to Energy= 0.242203
Thermal correction to Enthalpy= 0.243147
Thermal correction to Gibbs Free Energy= 0.185863
Sum of electronic and zero-point Energies= -540.240073
Sum of electronic and thermal Energies= -540.225843
Sum of electronic and thermal Enthalpies= -540.224898
```



Sum of electronic and thermal Free Energies= -540.282182  
 E(U $\omega$ B97XD/6-311++G(3df,2p))= -540.612973410

C	3.462005	-0.679042	-0.647941
C	2.091615	-0.520728	-0.660976
C	1.191793	-0.565060	0.427931
C	-0.110925	1.443944	0.120237
O	0.014480	2.032416	-0.952186
C	-0.236187	-0.044038	0.303916
C	-1.078315	-0.676221	-0.820300
H	1.644138	-0.362036	-1.647518
H	1.599622	-0.533031	1.439195
C	4.212770	-0.952782	0.626797
H	4.004278	-0.717369	-1.590423
H	-0.757108	-0.212022	1.252166
H	-0.565593	-0.548745	-1.778793
H	-1.113503	-1.752074	-0.619793
H	4.054214	-0.169347	1.386551
H	3.899037	-1.895715	1.111257
H	5.292560	-1.022971	0.456906
C	-2.467317	-0.096083	-0.918574
H	-2.604137	0.715082	-1.632774
C	-3.523461	-0.462026	-0.181252
H	-4.465673	0.060537	-0.345363
O	-0.055699	2.128186	1.286079
H	0.134354	3.058734	1.089126
C	-3.552607	-1.529405	0.872915
H	-4.329272	-2.270558	0.651400
H	-2.597609	-2.051601	0.972110
H	-3.801784	-1.095043	1.848297

m12-trans-OH-Crotyl.out

Zero-point correction= 0.227508  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.241856  
 Thermal correction to Enthalpy= 0.242801  
 Thermal correction to Gibbs Free Energy= 0.184861  
 Sum of electronic and zero-point Energies= -540.241920  
 Sum of electronic and thermal Energies= -540.227571  
 Sum of electronic and thermal Enthalpies= -540.226627  
 Sum of electronic and thermal Free Energies= -540.284567  
 E(U $\omega$ B97XD/6-311++G(3df,2p))= -540.614343245

C	-0.204971	-0.019671	-0.048614
C	-0.179098	1.463922	0.202200
C	1.226305	-0.400149	-0.374514
C	2.121360	-0.807122	0.635621
C	3.495030	-0.936002	0.573751
C	4.254836	-0.639616	-0.690489
O	-0.263856	2.342035	-0.655036

H	1.655186	-1.076381	1.590356
H	1.618108	0.019877	-1.303391
H	4.030439	-1.368150	1.416525
H	-0.504700	-0.504470	0.887982
C	-1.225780	-0.382442	-1.142366
H	5.335105	-0.760933	-0.555223
H	4.086953	0.388855	-1.052180
H	3.959174	-1.294643	-1.530926
H	-1.185839	-1.470422	-1.260802
H	-0.896724	0.052410	-2.092603
C	-2.628619	0.078167	-0.831368
H	-2.940739	1.022620	-1.275502
C	-3.495172	-0.549307	-0.026136
H	-4.470702	-0.089862	0.131760
O	0.038020	1.788034	1.496104
H	0.149388	2.749527	1.560047
C	-3.261726	-1.838102	0.706130
H	-3.286352	-1.671273	1.789645
H	-4.055289	-2.559831	0.481080
H	-2.300312	-2.295943	0.459395

m1-OH-Crotyl.out

Zero-point correction=	0.225490
(Hartree/Particle)	
Thermal correction to Energy=	0.241370
Thermal correction to Enthalpy=	0.242315
Thermal correction to Gibbs Free Energy=	0.179233
Sum of electronic and zero-point Energies=	-540.202035
Sum of electronic and thermal Energies=	-540.186155
Sum of electronic and thermal Enthalpies=	-540.185211
Sum of electronic and thermal Free Energies=	-540.248292
E(UωB97XD/6-311++G(3df,2p))=	-540.570654761

C	-0.714345	0.366339	-0.049027
C	0.664560	0.394057	-0.437207
C	1.947214	0.052974	-0.423751
C	2.454772	-0.939502	0.521358
C	3.725314	-1.362763	0.626013
C	4.900330	-0.919919	-0.192458
O	-0.156635	1.233829	-1.136594
H	1.714704	-1.364090	1.198282
H	2.611366	0.534710	-1.135550
H	3.938753	-2.110561	1.388111
H	-1.016801	0.954863	0.815914
C	-1.659672	-0.722530	-0.485623
H	4.638848	-0.178936	-0.951452
H	5.358835	-1.777281	-0.698992
H	5.673841	-0.486160	0.452204
H	-1.684287	-1.463377	0.319545
H	-1.240252	-1.215561	-1.369976
C	-3.030601	-0.181553	-0.790941
H	-3.075042	0.507599	-1.633483

C	-4.168748	-0.451786	-0.141479
H	-5.073840	0.035471	-0.503246
O	0.485878	3.637534	1.103953
H	0.301306	3.086717	0.334815
C	-4.364174	-1.356036	1.038514
H	-4.790320	-0.795048	1.878058
H	-5.080166	-2.149371	0.794988
H	-3.438798	-1.825569	1.379520

m6-in-OH-Crotyl.out

Zero-point correction=	0.222913
(Hartree/Particle)	
Thermal correction to Energy=	0.239333
Thermal correction to Enthalpy=	0.240277
Thermal correction to Gibbs Free Energy=	0.176623
Sum of electronic and zero-point Energies=	-540.196709
Sum of electronic and thermal Energies=	-540.180288
Sum of electronic and thermal Enthalpies=	-540.179344
Sum of electronic and thermal Free Energies=	-540.242999
E(UωB97XD/6-311++G(3df,2p))=	-540.560038911

C	-0.615964	1.533955	-0.481784
C	0.702291	1.700950	0.061871
C	1.700188	0.650980	0.034637
C	1.795255	-0.408861	-0.879032
C	2.773414	-1.378744	-0.855939
C	3.869649	-1.538954	0.137147
O	0.985388	2.798861	0.640990
H	1.081000	-0.466359	-1.693819
H	2.494574	0.788166	0.764091
H	2.743359	-2.122432	-1.649447
H	-1.240978	2.420945	-0.387065
C	-1.260099	0.324096	-1.069224
H	3.890139	-0.761289	0.902081
H	4.837563	-1.552657	-0.377730
H	3.772880	-2.511030	0.636166
H	-0.813226	-0.591426	-0.675926
H	-1.058618	0.320461	-2.154497
C	-2.752547	0.342713	-0.854958
H	-3.259651	1.236229	-1.217808
C	-3.488542	-0.610561	-0.273756
H	-4.561121	-0.431605	-0.202847
O	-0.568924	-0.449761	2.647091
H	-0.640716	-0.507745	1.688058
C	-3.025095	-1.917285	0.298061
H	-3.301374	-1.986862	1.356159
H	-3.520984	-2.750440	-0.213450
H	-1.945867	-2.066479	0.219256

m6-out-OH-Crotyl.out

Zero-point correction= 0.223569  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.239826  
 Thermal correction to Enthalpy= 0.240770  
 Thermal correction to Gibbs Free Energy= 0.177093  
 Sum of electronic and zero-point Energies= -540.203724  
 Sum of electronic and thermal Energies= -540.187466  
 Sum of electronic and thermal Enthalpies= -540.186522  
 Sum of electronic and thermal Free Energies= -540.250200  
 E(UωB97XD/6-311++G(3df,2p)) = -540.568157122

C	0.548323	-0.727468	-0.649185
C	-0.515077	-1.331951	0.089319
C	-1.817371	-0.711771	0.060673
C	-2.176901	0.498259	-0.559055
C	-3.441338	1.034281	-0.540415
C	-4.661776	0.477675	0.103783
O	-0.338998	-2.406361	0.752201
H	-1.417946	1.067247	-1.087809
H	-2.581349	-1.265977	0.600764
H	-3.576221	1.982676	-1.056256
H	0.384149	0.213665	-1.162661
C	1.925310	-1.286481	-0.667809
H	-4.503576	-0.478873	0.604066
H	-5.449118	0.352268	-0.649047
H	-5.049280	1.195396	0.836823
H	2.403528	-1.065359	-1.625291
H	1.901501	-2.370115	-0.525801
C	2.691345	-0.647251	0.479715
H	2.589403	-1.146527	1.440748
C	3.414046	0.477082	0.409160
H	3.897799	0.817712	1.323893
O	0.546709	2.358724	1.246164
H	1.084441	1.586814	1.034529
C	3.629353	1.341145	-0.795625
H	3.256879	2.353362	-0.600660
H	4.698825	1.434749	-1.016246
H	3.123792	0.962942	-1.687334

ts10-11-cis-OH-Crotyl.out

Zero-point correction= 0.225493  
 (Hartree/Particle)  
 Thermal correction to Energy= 0.240257  
 Thermal correction to Enthalpy= 0.241201  
 Thermal correction to Gibbs Free Energy= 0.182626  
 Sum of electronic and zero-point Energies= -540.210054  
 Sum of electronic and thermal Energies= -540.195289  
 Sum of electronic and thermal Enthalpies= -540.194345  
 Sum of electronic and thermal Free Energies= -540.252920  
 E(UωB97XD/6-311++G(3df,2p)) = -540.577612907

C	-3.090755	-1.378511	0.410607
C	-1.820219	-0.956106	0.474090
C	-1.273377	0.273628	-0.142078
C	-0.081608	0.902885	0.466725
O	0.446363	1.013183	1.569025
C	0.169359	0.307929	-0.841195
C	1.067165	-0.915618	-0.939664
H	-1.112458	-1.559468	1.040741
H	-1.970630	0.918934	-0.664636
C	-4.240505	-0.723321	-0.293371
H	-3.330362	-2.305743	0.929746
H	0.159046	0.953006	-1.714538
H	1.003000	-1.499991	-0.018054
H	0.696236	-1.551740	-1.752062
H	-3.955913	0.185594	-0.828379
H	-4.688865	-1.416828	-1.014026
H	-5.028143	-0.462852	0.423238
C	2.489646	-0.511987	-1.224013
H	2.678247	-0.157407	-2.237133
C	3.512400	-0.512007	-0.360600
H	4.477895	-0.166174	-0.729263
O	-0.442459	3.192282	-0.145330
H	-0.809686	3.071530	-1.027787
C	3.491152	-0.919668	1.082938
H	3.719882	-0.058270	1.721652
H	2.527943	-1.325480	1.400237
H	4.263038	-1.672176	1.280070

ts10-11-trans-OH-Crotyl.out

Zero-point correction=	0.225261
(Hartree/Particle)	
Thermal correction to Energy=	0.240067
Thermal correction to Enthalpy=	0.241011
Thermal correction to Gibbs Free Energy=	0.181632
Sum of electronic and zero-point Energies=	-540.208210
Sum of electronic and thermal Energies=	-540.193403
Sum of electronic and thermal Enthalpies=	-540.192459
Sum of electronic and thermal Free Energies=	-540.251838
E(U $\omega$ B97XD/6-311++G(3df,2p))=	-540.575540714

C	3.326324	-1.085740	0.659563
C	2.191637	-0.384026	0.781822
C	1.203682	-0.132486	-0.291267
C	0.479363	1.133448	-0.568108
O	0.417427	2.006912	-1.422773
C	-0.316377	0.103896	0.093589
C	-1.442615	-0.596035	-0.648592
H	1.949803	0.041296	1.753030
H	1.353210	-0.693231	-1.214765

C	3.867668	-1.753835	-0.569116
H	3.941706	-1.185884	1.552739
H	-0.448487	0.204527	1.168158
H	-1.159292	-0.690389	-1.704608
H	-1.551961	-1.609745	-0.252391
H	3.215453	-1.648232	-1.439301
H	4.846934	-1.335390	-0.829236
H	4.021696	-2.823502	-0.386186
C	-2.725866	0.184112	-0.550832
H	-2.694620	1.172113	-1.010422
C	-3.864357	-0.193050	0.043037
H	-4.695415	0.511694	0.020807
O	1.006473	2.583645	1.324225
H	1.122641	2.060548	2.124812
C	-4.147689	-1.486525	0.748162
H	-4.462798	-1.294783	1.780278
H	-4.974920	-2.014992	0.260150
H	-3.285772	-2.157040	0.775770

ts11-12-cis-OH-Crotyl.out

Zero-point correction=	0.226957
(Hartree/Particle)	
Thermal correction to Energy=	0.240891
Thermal correction to Enthalpy=	0.241836
Thermal correction to Gibbs Free Energy=	0.184780
Sum of electronic and zero-point Energies=	-540.234216
Sum of electronic and thermal Energies=	-540.220281
Sum of electronic and thermal Enthalpies=	-540.219337
Sum of electronic and thermal Free Energies=	-540.276393
E(UωB97XD/6-311++G(3df,2p))=	-540.604385869

C	-3.144375	-1.241369	0.511236
C	-1.845490	-0.950284	0.204182
C	-1.368163	0.106794	-0.621501
C	0.025530	1.196761	0.248092
O	0.345271	0.901959	1.438685
C	0.105879	0.338421	-0.936204
C	1.076532	-0.837663	-0.895873
H	-1.088628	-1.585683	0.668798
H	-2.075964	0.730218	-1.161096
C	-4.310328	-0.463452	-0.039649
H	-3.352884	-2.081834	1.169559
H	0.227257	0.911576	-1.858167
H	0.982870	-1.371475	0.052543
H	0.782223	-1.537106	-1.689041
H	-4.263495	0.603109	0.229011
H	-4.353782	-0.495577	-1.139601
H	-5.263498	-0.850451	0.333828
C	2.493289	-0.385576	-1.120842
H	2.689858	0.040361	-2.105555
C	3.509140	-0.422951	-0.249467
H	4.469973	-0.031759	-0.584240

O	-0.225534	2.534793	-0.047147
H	-0.423987	2.973180	0.791713
C	3.491037	-0.939295	1.159399
H	4.247501	-1.721832	1.290037
H	3.744492	-0.136139	1.861323
H	2.521863	-1.348925	1.452347

ts11-12-trans-OH-Crotyl.out

Zero-point correction=	0.226770
(Hartree/Particle)	
Thermal correction to Energy=	0.240727
Thermal correction to Enthalpy=	0.241671
Thermal correction to Gibbs Free Energy=	0.184372
Sum of electronic and zero-point Energies=	-540.235276
Sum of electronic and thermal Energies=	-540.221319
Sum of electronic and thermal Enthalpies=	-540.220375
Sum of electronic and thermal Free Energies=	-540.277675
E(UωB97XD/6-311++G(3df,2p))=	-540.605064405

C	-0.220779	0.091616	0.227653
C	0.310802	1.436076	-0.011562
C	1.190542	-0.323859	-0.150706
C	2.163606	-0.713488	0.813549
C	3.440770	-1.140185	0.585251
C	4.014618	-1.287634	-0.799167
O	0.242728	2.103578	-1.087845
H	1.849982	-0.638396	1.858562
H	1.378763	-0.462336	-1.213140
H	4.069125	-1.401340	1.433840
H	-0.427510	-0.090131	1.285923
C	-1.359969	-0.395761	-0.660683
H	5.053777	-1.629772	-0.769462
H	3.998479	-0.339589	-1.358587
H	3.451518	-2.008505	-1.412593
H	-1.444390	-1.480447	-0.543029
H	-1.086488	-0.208538	-1.707158
C	-2.654765	0.304757	-0.355623
H	-2.630618	1.387558	-0.485932
C	-3.802062	-0.241511	0.066070
H	-4.639709	0.431763	0.248382
O	0.731414	2.090326	1.139550
H	1.210895	2.880760	0.855741
C	-4.087949	-1.692609	0.320907
H	-4.400210	-1.843697	1.360810
H	-4.917571	-2.034831	-0.308737
H	-3.228065	-2.338146	0.127608

ts1-6-in-OH-Crotyl.out

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Zero-point correction=                                0.223407
(Hartree/Particle)
Thermal correction to Energy=                        0.239016
Thermal correction to Enthalpy=                     0.239960
Thermal correction to Gibbs Free Energy=            0.177781
Sum of electronic and zero-point Energies=          -540.169428
Sum of electronic and thermal Energies=              -540.153818
Sum of electronic and thermal Enthalpies=           -540.152874
Sum of electronic and thermal Free Energies=        -540.215053
E(UwB97XD/6-311++G(3df,2p))= -540.534670224

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C      0.411268   -0.049742   -0.533465
C     -0.591450    0.784572    0.088178
C     -1.939011    0.616255    0.151039
C     -2.627444   -0.524857   -0.424565
C     -3.955061   -0.753926   -0.405461
C     -5.018579    0.115926    0.192612
O      0.190561    1.693824    0.620410
H     -2.005025   -1.265664   -0.925762
H     -2.506307    1.394041    0.656425
H     -4.308530   -1.668578   -0.878641
H      1.063734    0.451266   -1.247400
C      0.793705   -1.393331   -0.089853
H     -4.622866    1.027205    0.646928
H     -5.573659   -0.432621    0.963079
H     -5.749458    0.407672   -0.570932
H      1.213570   -1.957575   -0.926354
H     -0.041647   -1.926307    0.366560
C      1.869161   -1.111940    0.965275
H      1.486183   -0.951944    1.968655
C      3.180760   -1.017266    0.724166
H      3.822971   -0.834195    1.584497
O      3.139654    2.549931   -0.512934
H      2.313430    2.182410   -0.176616
C      3.879680   -1.143538   -0.591113
H      4.454406   -0.233110   -0.793457
H      4.596954   -1.971504   -0.559584
H      3.196341   -1.304044   -1.428084

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ts1-6-out-OH-Crotyl.out

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Zero-point correction=                                0.222843
(Hartree/Particle)
Thermal correction to Energy=                        0.238554
Thermal correction to Enthalpy=                     0.239499
Thermal correction to Gibbs Free Energy=            0.177068
Sum of electronic and zero-point Energies=          -540.166466
Sum of electronic and thermal Energies=              -540.150755
Sum of electronic and thermal Enthalpies=           -540.149810
Sum of electronic and thermal Free Energies=        -540.212241
E(UwB97XD/6-311++G(3df,2p))= -540.530980338

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C	-0.431228	-0.046695	-0.104036
C	0.716653	0.713744	-0.543490
C	2.031392	0.416625	-0.361352
C	2.462981	-0.747301	0.388567
C	3.732441	-1.150298	0.592584
C	4.980110	-0.514929	0.058790
O	0.126498	1.763233	-1.059910
H	1.672397	-1.353121	0.833874
H	2.762495	1.098199	-0.788557
H	3.881572	-2.037292	1.205989
H	-0.608318	-0.190544	0.964502
C	-1.476053	-0.537313	-1.009921
H	4.781698	0.355019	-0.571680
H	5.555558	-1.237439	-0.532047
H	5.630611	-0.195718	0.882001
H	-1.475586	-1.624040	-0.820123
H	-1.208852	-0.363673	-2.053667
C	-2.837241	0.042563	-0.681245
H	-2.982246	1.058511	-1.041425
C	-3.816367	-0.557532	0.001337
H	-4.734879	0.011017	0.141290
O	-1.392326	2.567749	1.671547
H	-0.989589	2.496592	0.797565
C	-3.809504	-1.923525	0.613598
H	-3.907244	-1.845971	1.702563
H	-4.669869	-2.501983	0.259915
H	-2.900221	-2.489448	0.397705

ts6-10-cis-OH-Crotyl.out

Zero-point correction=	0.223996
(Hartree/Particle)	
Thermal correction to Energy=	0.239374
Thermal correction to Enthalpy=	0.240318
Thermal correction to Gibbs Free Energy=	0.179411
Sum of electronic and zero-point Energies=	-540.186148
Sum of electronic and thermal Energies=	-540.170771
Sum of electronic and thermal Enthalpies=	-540.169826
Sum of electronic and thermal Free Energies=	-540.230733
E(U $\omega$ B97XD/6-311++G(3df,2p))=	-540.551136741

C	-0.535529	0.932011	0.567728
C	0.433521	1.839746	0.091283
O	0.548949	3.052362	0.456768
C	1.516123	1.008682	-0.311979
C	1.517514	-0.063805	-1.259560
C	2.503092	-0.989047	-1.349852
C	3.698201	-1.142758	-0.477626
H	0.698044	-0.124332	-1.967640
H	2.452928	1.255056	0.188191
H	2.410433	-1.725210	-2.146317
H	-0.910897	1.198954	1.558223

C	-1.141119	-0.293719	-0.048080
H	3.643765	-2.111349	0.034175
H	4.604121	-1.167661	-1.093337
H	3.799086	-0.362787	0.278382
H	-1.347124	-0.127946	-1.108556
H	-0.417074	-1.124648	-0.008864
C	-2.381620	-0.707632	0.700360
H	-2.216517	-0.981034	1.742216
C	-3.627358	-0.770714	0.218686
H	-4.406252	-1.106093	0.902907
O	1.414318	-1.515817	2.403343
H	1.405967	-1.130860	1.519641
C	-4.098569	-0.434671	-1.164945
H	-4.519783	-1.322253	-1.651196
H	-4.901510	0.309551	-1.118819
H	-3.306862	-0.040306	-1.805980

ts6-10-trans-OH-Crotyl.out

Zero-point correction=	0.224029
(Hartree/Particle)	
Thermal correction to Energy=	0.239665
Thermal correction to Enthalpy=	0.240609
Thermal correction to Gibbs Free Energy=	0.178090
Sum of electronic and zero-point Energies=	-540.195224
Sum of electronic and thermal Energies=	-540.179589
Sum of electronic and thermal Enthalpies=	-540.178645
Sum of electronic and thermal Free Energies=	-540.241164
E(UωB97XD/6-311++G(3df,2p))=	-540.561087965

C	-0.303031	0.503817	-0.266945
C	0.547897	1.193595	0.613971
C	1.791357	0.642064	0.187653
C	2.187168	-0.742136	0.193505
C	3.388907	-1.188658	-0.231079
C	4.502470	-0.408194	-0.843776
O	0.365922	2.320247	1.161725
H	1.491101	-1.461831	0.618005
H	2.531303	1.388081	-0.101452
H	3.582379	-2.252906	-0.109215
H	-0.191701	-0.563899	-0.413983
C	-1.438992	1.174648	-0.971632
H	4.270082	0.646276	-1.002450
H	4.768624	-0.852361	-1.809659
H	5.396060	-0.478756	-0.212782
H	-1.534261	0.781575	-1.986873
H	-1.271212	2.253430	-1.022613
C	-2.683533	0.890223	-0.150868
H	-2.911611	1.624013	0.618963
C	-3.461611	-0.193617	-0.261275
H	-4.314952	-0.267076	0.411749
O	-1.348693	-2.033217	2.033387
H	-1.671418	-1.346427	1.438640

C	-3.285138	-1.339725	-1.209860
H	-3.148077	-2.271585	-0.649103
H	-4.182042	-1.470643	-1.825886
H	-2.425071	-1.216238	-1.872403

### Favorskii rearrangement with H<sub>2</sub>O (R=Me)

m10-cis.out

Zero-point correction=	0.263939
(Hartree/Particle)	
Thermal correction to Energy=	0.282683
Thermal correction to Enthalpy=	0.283628
Thermal correction to Gibbs Free Energy=	0.214952
Sum of electronic and zero-point Energies=	-617.109894
Sum of electronic and thermal Energies=	-617.091150
Sum of electronic and thermal Enthalpies=	-617.090206
Sum of electronic and thermal Free Energies=	-617.158882
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.542472127

C	3.897961	-0.669323	-0.239579
C	2.563113	-0.668525	-0.349979
C	1.662657	0.456770	-0.000001
C	0.362838	0.597294	-0.661687
O	-0.209938	0.679110	-1.732068
C	0.258719	0.244120	0.742152
C	-0.250325	-1.131888	1.148932
H	2.078849	-1.563708	-0.735249
H	2.128089	1.388247	0.314013
C	4.780973	0.436365	0.251759
H	4.415268	-1.578865	-0.541733
H	0.057756	1.051487	1.443787
H	0.051385	-1.871061	0.403455
H	0.242383	-1.403900	2.089070
H	4.227180	1.321526	0.572693
H	5.387658	0.088277	1.095356
H	5.481185	0.740111	-0.534890
C	-1.742628	-1.142931	1.343249
H	-2.103406	-0.633676	2.236122
C	-2.645518	-1.704044	0.528633
H	-3.693980	-1.632199	0.818417
O	-2.078506	3.264637	0.740171
H	-2.357633	2.537574	0.147353
C	-2.387522	-2.415339	-0.766536
H	-2.751979	-3.447769	-0.717286
H	-2.936829	-1.925333	-1.578542
H	-1.330474	-2.437180	-1.040768
H	-1.434474	2.863566	1.333622
H	-2.026004	0.955071	-1.356943
O	-2.886739	1.187466	-0.960236
H	-3.035107	0.483139	-0.313070

m10-trans.out

Zero-point correction=	0.263288
(Hartree/Particle)	
Thermal correction to Energy=	0.282325
Thermal correction to Enthalpy=	0.283270
Thermal correction to Gibbs Free Energy=	0.213618
Sum of electronic and zero-point Energies=	-617.110443
Sum of electronic and thermal Energies=	-617.091406
Sum of electronic and thermal Enthalpies=	-617.090462
Sum of electronic and thermal Free Energies=	-617.160114
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.542469261

C	-3.252982	-1.544693	-0.160669
C	-1.965520	-1.686820	-0.499330
C	-0.830973	-0.935023	0.087575
C	0.540414	-1.456710	0.113197
O	1.320361	-2.251649	0.599724
C	0.329710	-0.376091	-0.834689
C	0.838099	1.037840	-0.589974
H	-1.704481	-2.392842	-1.285827
H	-1.053947	-0.272325	0.923847
C	-3.829907	-0.628168	0.875608
H	-3.975900	-2.154374	-0.700734
H	0.263966	-0.689307	-1.877801
H	0.939214	1.195887	0.488509
H	1.839415	1.127449	-1.024779
H	-3.070081	-0.078471	1.436136
H	-4.498498	0.102315	0.405201
H	-4.436003	-1.195786	1.590506
C	-0.087584	2.049716	-1.210568
H	0.028615	2.192759	-2.284267
C	-1.050530	2.737838	-0.585663
H	-1.651171	3.416873	-1.190422
O	4.008865	1.009303	1.221553
H	3.901022	0.238032	0.628695
C	-1.421103	2.684023	0.866891
H	-1.396921	3.687888	1.305860
H	-2.447211	2.314549	0.979739
H	-0.765233	2.036130	1.453506
H	3.194986	1.514450	1.118734
H	2.985468	-1.687635	-0.079840
O	3.765516	-1.228457	-0.442385
H	3.471093	-0.880649	-1.292464

m11-cis.out

Zero-point correction=	0.268503
(Hartree/Particle)	
Thermal correction to Energy=	0.285464

Thermal correction to Enthalpy=	0.286408
Thermal correction to Gibbs Free Energy=	0.223251
Sum of electronic and zero-point Energies=	-617.128561
Sum of electronic and thermal Energies=	-617.111601
Sum of electronic and thermal Enthalpies=	-617.110657
Sum of electronic and thermal Free Energies=	-617.173813
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.563553887

C	3.405244	-1.108742	-0.732759
C	2.146130	-0.657013	-0.651199
C	1.617482	0.282139	0.364225
C	0.478012	1.200491	0.048568
O	-0.037369	1.168836	-1.242658
C	0.217086	0.069433	0.991395
C	-0.645499	-1.120689	0.622128
H	1.436994	-1.006435	-1.398138
H	2.343644	0.701283	1.053544
C	4.561821	-0.781095	0.164253
H	3.631148	-1.798129	-1.545533
H	0.165425	0.355629	2.039771
H	-0.663944	-1.259639	-0.461050
H	-0.184821	-2.023357	1.046962
H	4.300308	-0.091655	0.970178
H	4.963418	-1.695209	0.616826
H	5.378144	-0.333133	-0.414243
C	-2.041184	-0.991759	1.171759
H	-2.100059	-0.687401	2.217125
C	-3.193073	-1.236545	0.531606
H	-4.115049	-1.114896	1.099458
O	0.579233	2.496387	0.578530
H	-2.604712	2.492037	-0.130326
C	-3.371728	-1.675850	-0.892175
H	-3.767633	-2.697682	-0.927618
H	-4.102546	-1.036699	-1.399311
H	-2.441918	-1.654518	-1.465304
H	-0.299068	2.762328	0.882029
H	-1.002869	1.329240	-1.168446
O	-2.689689	1.697918	-0.671668
H	-2.799615	0.970896	-0.036365

m11-trans.out

Zero-point correction=	0.267433
(Hartree/Particle)	
Thermal correction to Energy=	0.285071
Thermal correction to Enthalpy=	0.286015
Thermal correction to Gibbs Free Energy=	0.219823
Sum of electronic and zero-point Energies=	-617.128798
Sum of electronic and thermal Energies=	-617.111161
Sum of electronic and thermal Enthalpies=	-617.110217
Sum of electronic and thermal Free Energies=	-617.176409
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.562825678

C	-1.744375	-2.501835	-0.687921
C	-0.538586	-1.917618	-0.679136
C	-0.123390	-0.788741	0.180896
C	1.310650	-0.542708	0.537867
O	2.274620	-1.428617	0.059397
C	0.658627	0.395538	-0.423006
C	0.266255	1.813010	-0.056123
H	0.212052	-2.277946	-1.380595
H	-0.817897	-0.489437	0.961132
C	-2.930052	-2.161373	0.166365
H	-1.900347	-3.311082	-1.400230
H	0.959907	0.249689	-1.459176
H	0.042904	1.861382	1.013307
H	1.120819	2.476394	-0.236210
H	-2.712862	-1.398070	0.917172
H	-3.756116	-1.795685	-0.455362
H	-3.297930	-3.054072	0.684835
C	-0.909539	2.276156	-0.877458
H	-0.674069	2.610911	-1.887472
C	-2.196035	2.267532	-0.507698
H	-2.929601	2.613142	-1.235942
O	1.542289	-0.129534	1.856965
H	4.244929	0.970282	0.143320
C	-2.765744	1.821493	0.806855
H	-3.367142	2.619849	1.256734
H	-3.436877	0.967505	0.657048
H	-1.998430	1.522474	1.525009
H	2.245027	0.534497	1.843885
H	3.020167	-0.877636	-0.258491
O	4.105957	0.522428	-0.700258
H	3.495673	1.094851	-1.181646

ts10-11-cis.out

Zero-point correction=	0.263247
(Hartree/Particle)	
Thermal correction to Energy=	0.278652
Thermal correction to Enthalpy=	0.279596
Thermal correction to Gibbs Free Energy=	0.219189
Sum of electronic and zero-point Energies=	-617.082986
Sum of electronic and thermal Energies=	-617.067581
Sum of electronic and thermal Enthalpies=	-617.066637
Sum of electronic and thermal Free Energies=	-617.127043
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.511742227

C	-3.498199	-0.812969	0.752841
C	-2.186415	-0.541809	0.703105
C	-1.498760	0.295185	-0.304119
C	-0.170593	0.916838	0.030140
O	0.424885	0.873669	1.212059
C	-0.174575	-0.178750	-0.982811

C	0.497424	-1.500130	-0.664362
H	-1.551974	-0.971465	1.476212
H	-2.135594	0.863489	-0.976260
C	-4.566106	-0.348092	-0.192326
H	-3.843947	-1.446041	1.569314
H	-0.109946	0.114349	-2.029516
H	0.427265	-1.708513	0.405757
H	-0.030182	-2.307331	-1.187219
H	-4.179371	0.273935	-1.002965
H	-5.078023	-1.207792	-0.640370
H	-5.330051	0.227095	0.343714
C	1.933970	-1.460717	-1.116586
H	2.075440	-1.444246	-2.197669
C	3.028216	-1.396166	-0.347881
H	3.991366	-1.339119	-0.855115
O	0.044315	2.301900	-0.559175
H	1.195594	2.443150	-0.322567
C	3.097919	-1.381558	1.150710
H	3.792294	-2.150240	1.508218
H	3.484704	-0.417992	1.504471
H	2.128568	-1.547866	1.625261
H	-0.098868	2.305143	-1.518394
H	1.750972	1.558663	0.866083
O	2.262275	2.254557	0.288055
H	2.882659	1.762775	-0.268736

ts10-11-trans.out

Zero-point correction=	0.263081
(Hartree/Particle)	
Thermal correction to Energy=	0.278602
Thermal correction to Enthalpy=	0.279546
Thermal correction to Gibbs Free Energy=	0.218773
Sum of electronic and zero-point Energies=	-617.081915
Sum of electronic and thermal Energies=	-617.066395
Sum of electronic and thermal Enthalpies=	-617.065450
Sum of electronic and thermal Free Energies=	-617.126224
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.510326946

C	3.637259	-1.074435	-0.585322
C	2.426297	-0.569291	-0.858261
C	1.366073	-0.228961	0.114049
C	0.478567	0.963776	-0.131088
O	0.608322	1.842654	-1.115163
C	-0.129788	-0.394068	-0.267389
C	-1.119322	-1.017498	0.700560
H	2.176676	-0.379992	-1.901693
H	1.568046	-0.446395	1.160502
C	4.206045	-1.411525	0.761280
H	4.296642	-1.268837	-1.430442
H	-0.301705	-0.660405	-1.309716
H	-1.126191	-2.100738	0.548150
H	-0.784904	-0.864551	1.735407

H	3.516015	-1.202543	1.582204
H	4.477776	-2.472584	0.807714
H	5.126707	-0.843948	0.940240
C	-2.493130	-0.423848	0.527779
H	-2.586544	0.614991	0.846729
C	-3.573685	-1.014123	0.003408
H	-4.486694	-0.422030	-0.057174
O	0.120764	1.720848	1.136334
H	-0.652794	2.512773	0.725587
C	-3.687396	-2.413620	-0.525044
H	-4.436562	-2.978587	0.041842
H	-4.028342	-2.397706	-1.566545
H	-2.744667	-2.964283	-0.486611
H	-0.293564	1.156695	1.807136
H	-0.575006	2.810076	-0.820888
O	-1.193508	3.245358	-0.117811
H	-2.095031	2.938752	-0.289152

ts11-12-cis.out

Zero-point correction=	0.264618
(Hartree/Particle)	
Thermal correction to Energy=	0.280770
Thermal correction to Enthalpy=	0.281714
Thermal correction to Gibbs Free Energy=	0.220694
Sum of electronic and zero-point Energies=	-617.073208
Sum of electronic and thermal Energies=	-617.057056
Sum of electronic and thermal Enthalpies=	-617.056112
Sum of electronic and thermal Free Energies=	-617.117132
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.508210460

C	-2.832235	-1.874206	0.626277
C	-1.644192	-1.212961	0.472644
C	-1.331217	-0.206220	-0.484394
C	0.369084	1.015687	0.576206
O	1.029063	0.416048	1.518443
C	0.097543	0.273618	-0.685376
C	1.173237	-0.779885	-1.018299
H	-0.853264	-1.468675	1.184073
H	-1.981143	-0.074854	-1.349213
C	-4.016150	-1.594699	-0.259000
H	-2.938924	-2.601837	1.427413
H	0.089055	1.032012	-1.475938
H	1.205770	-1.533247	-0.226962
H	0.817173	-1.283115	-1.924768
H	-3.822161	-1.833023	-1.317198
H	-4.896521	-2.169859	0.045019
H	-4.297682	-0.527815	-0.242754
C	2.523288	-0.171147	-1.277891
H	2.562480	0.505597	-2.132296
C	3.648375	-0.347825	-0.574399
H	4.535110	0.193297	-0.904412
O	-0.023781	2.214549	0.831795



H	-2.227303	1.698704	-0.533685
C	3.844785	-1.209883	0.637290
H	2.951978	-1.777693	0.907912
H	4.663761	-1.919084	0.471684
H	4.130512	-0.594921	1.498946
H	-0.756456	2.534739	0.188804
H	1.052167	0.947420	2.333500
O	-2.066965	2.672830	-0.598701
H	-2.736193	3.090067	-0.040775

ts11-12-trans.out

Zero-point correction=	0.264516
(Hartree/Particle)	
Thermal correction to Energy=	0.280878
Thermal correction to Enthalpy=	0.281822
Thermal correction to Gibbs Free Energy=	0.219557
Sum of electronic and zero-point Energies=	-617.071912
Sum of electronic and thermal Energies=	-617.055550
Sum of electronic and thermal Enthalpies=	-617.054606
Sum of electronic and thermal Free Energies=	-617.116871
E( $\omega$ B97XD/6-311++G(3df,2p))=	-617.507078786

C	-3.332872	1.375738	-0.610437
C	-2.017912	1.023816	-0.783612
C	-1.117015	0.521561	0.186623
C	0.348682	-0.967872	-0.970162
O	0.598520	-0.820603	-2.238466
C	0.340254	0.272338	-0.138479
H	-1.612356	1.132034	-1.795059
H	-1.370891	0.544637	1.246216
C	-4.013440	1.239797	0.723907
H	-3.903449	1.750776	-1.456629
H	-3.578515	1.895941	1.496193
H	-5.080500	1.477614	0.664213
H	-3.925971	0.215056	1.125870
O	0.105389	-2.165530	-0.578062
H	-1.667026	-1.331893	1.256482
H	-0.353782	-2.229564	0.343616
H	0.490389	-1.656501	-2.725681
O	-1.308854	-2.211145	1.510546
H	-2.020586	-2.845024	1.351628
C	1.227376	0.119112	1.110903
H	0.776222	-0.616887	1.783734
H	1.191534	1.084601	1.625812
C	2.644591	-0.284712	0.788924
H	2.874973	-1.345620	0.877226
C	3.614656	0.537286	0.371102
H	4.589514	0.102727	0.152040
C	3.502959	2.017208	0.156192
H	4.289242	2.546548	0.706011
H	3.643585	2.257994	-0.904264
H	2.534858	2.418677	0.466404

H 0.778640 1.051470 -0.775725

Vm.out

Zero-point correction= 0.268813  
(Hartree/Particle)  
Thermal correction to Energy= 0.285950  
Thermal correction to Enthalpy= 0.286895  
Thermal correction to Gibbs Free Energy= 0.222654  
Sum of electronic and zero-point Energies= -617.177363  
Sum of electronic and thermal Energies= -617.160226  
Sum of electronic and thermal Enthalpies= -617.159282  
Sum of electronic and thermal Free Energies= -617.223522  
E( $\omega$ B97XD/6-311++G(3df,2p))= -617.614482392

C -0.414164 -3.016816 0.667881  
C -1.099561 -1.872677 0.778358  
C -1.483632 -0.940386 -0.339029  
C -0.579764 1.112880 0.753305  
O 0.391740 0.864404 1.627188  
C -0.535741 0.279872 -0.505398  
C 0.880549 -0.130564 -0.932690  
H -1.407828 -1.561954 1.776304  
H -1.495951 -1.457805 -1.302385  
C 0.139535 -3.629846 -0.583626  
H -0.215337 -3.572408 1.584081  
H -0.973152 0.913881 -1.283567  
H 1.334209 -0.765854 -0.168265  
H 0.765956 -0.748907 -1.831307  
H -0.150656 -3.090024 -1.487807  
H 1.235209 -3.647897 -0.541261  
H -0.189561 -4.670484 -0.680719  
C 1.744688 1.054752 -1.262376  
H 1.371593 1.683067 -2.071799  
C 2.890848 1.414579 -0.672787  
H 3.382220 2.313973 -1.043543  
O -1.460379 1.933065 0.991736  
H -2.497210 -0.564393 -0.162867  
C 3.595732 0.725420 0.457699  
H 3.093957 -0.188923 0.781940  
H 4.620592 0.467675 0.166958  
H 3.672938 1.395806 1.321739  
H -2.857869 2.026285 -0.231470  
H 0.265687 1.420883 2.413165  
O -3.593885 2.054179 -0.870846  
H -3.485534 1.250610 -1.391850

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