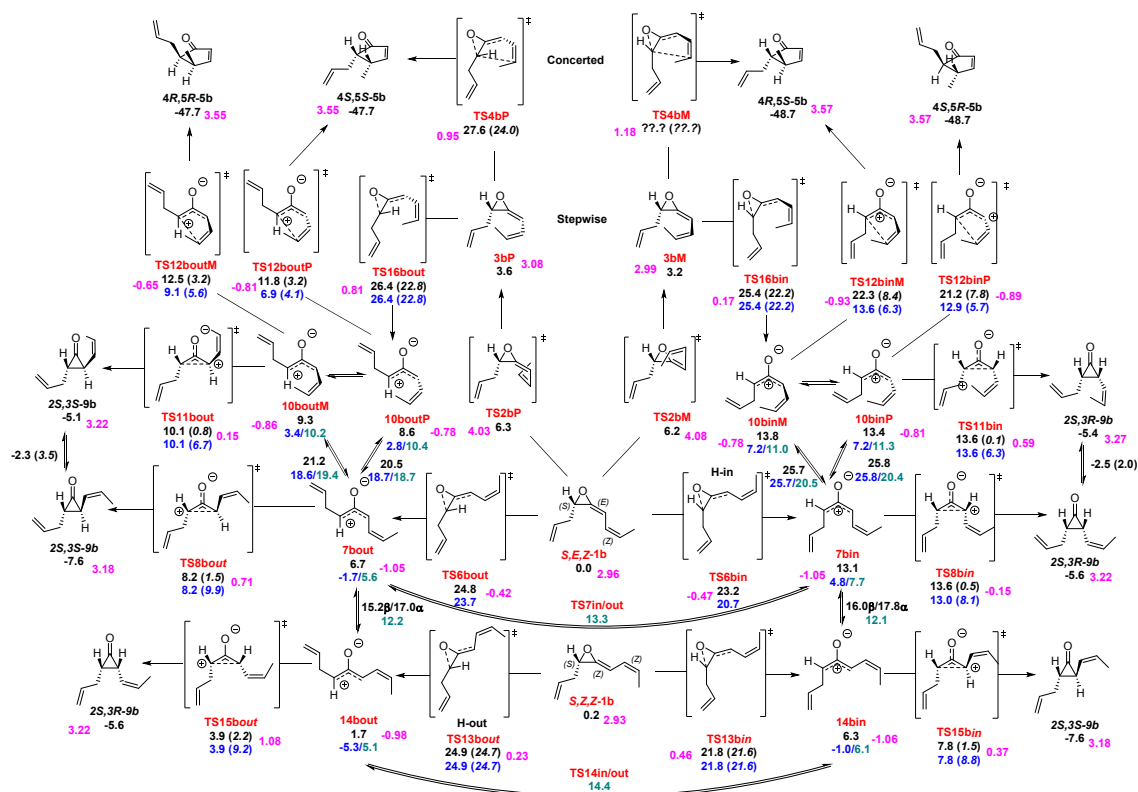


A Unifying Mechanism for the Rearrangement of Vinyl Allene Oxide Geometric Isomers to Cyclopentenones. A Correction and Further Computational Insights With Biologically Relevant Models

Supporting Information

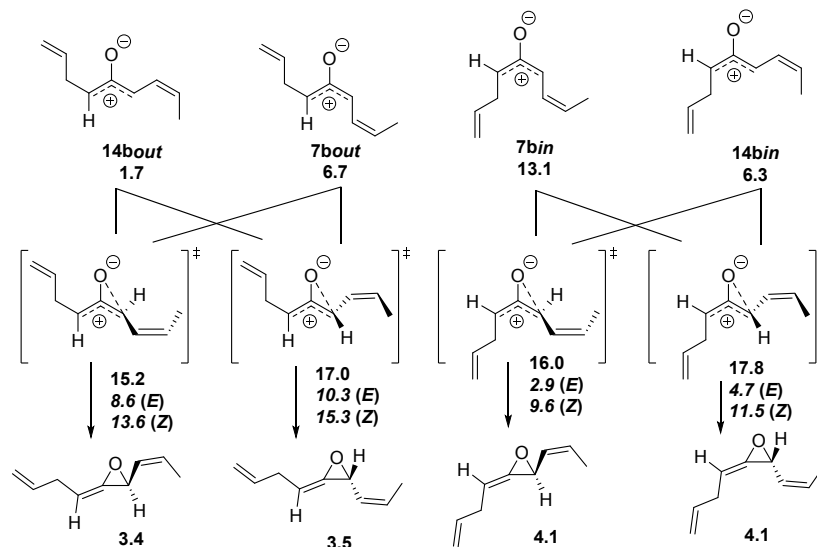
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S1. COMPLETE MANIFOLD FOR THE REARRANGEMENT OF *S,E,Z*-1 AND *S,Z,Z*-1.



Scheme S 1: Complete set for the stepwise and concerted path of the rearrangement of allene oxides to cyclopentenones through intermediates of diverse nature both electronic and chemistry. Energy values (in kcal/mol) have been computed at the (U)ωB97XD/6-311++G(3df,2p)(SMD,H₂O)/(U)ωB97XD/6-31++G(d,p)(SMD,H₂O) level of theory, in parenthesis activation barriers. Black indicate closed shell energies whereas, blue shows open shell singlet (by HOMO-LUMO mixing) structures and green were kept for the low lying triplet state. In mauve are the TDDFT energy gaps between the closed shell structure and the triplet state in eV. Several isomerization processes between the W, sickle and U conformers of the oxidopentadienyl geometry can only occur on the triplet state potential energy surface. Sickle-U isomerization can occur also in the closed shell an open shell singlet PES by anchimeric assistance of the allyl group during the rotation process.

S2. CLOSED-SHELL SICKEL-TRANS-W ISOMERIZATION TROUGH POSITIONAL EPOXIDE INTERCONVERSION.



Scheme S 2: W/sickel-trans isomerization for the closed-shell and open shell singlet calculations. Energy values (in kcal/mol; black for closed-shell, blue for open-shell singlet and green for triplet diradicals) have been computed at the (U)ωB97XD/6-311++G(3df,2p)(SMD,H₂O)//(U)ωB97XD/6-31++G(d,p)(SMD,H₂O) level of theory. Looking for the direct W/sickel-trans isomerization process by mere rotation of the C2-C3 bond we have found those four epoxide regioisomerization transition states leading to the respective allene oxide vinyl substituted regioisomers of the initial, energetically favored, allyl **S,E,Z-1b** and **S,Z,Z-1b**. Having lower energies than the determinant epoxide opening TS they are, indeed, feasible and competitive effective isomerization process.

S3. BIDIMENSIONAL RELAXED SCANS FOR THE CONCERTED REARRANGEMENT OF 3bM AND 3bP.

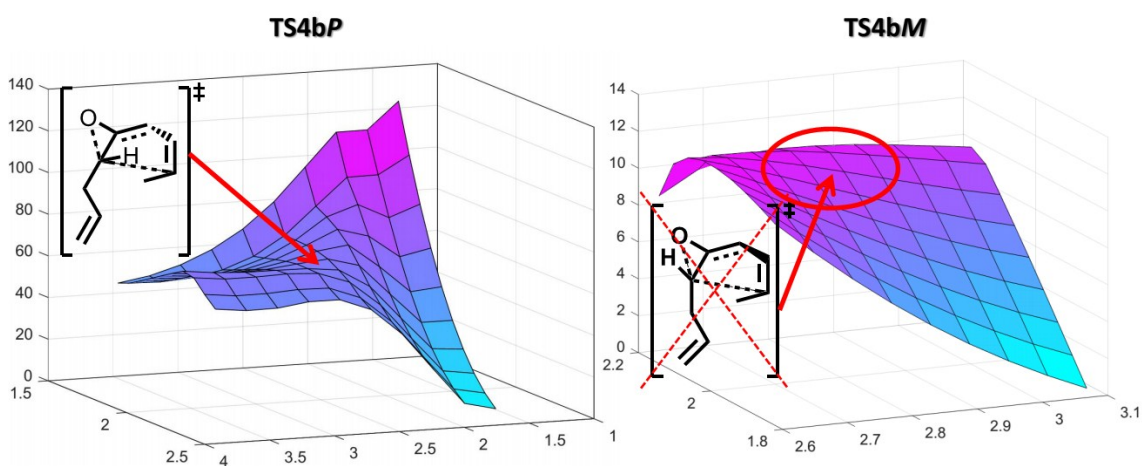


Figure S 1: Bidimensional relaxed scan of 2 bond distances, C-O epoxide cleavage and C-C cyclopentenone bond forming near 3bP and 3bM respectively passing through the possible concerted processes. The right one is a complete analysis of the space going from the initial epoxide 3bP to the final cis cyclopentenone and clearly shows a plateau region with a topology resembling a saddle point. Calculations from this geometry led to **TS4bP** location. On the contrary, no saddle point topology was found in the three different bidimensional relaxed scans carried out. Initially, the same procedure, parting from the 3bM, led to the terminal C3'-C4' double bond isomerization during the scan search. Then we have freeze the dihedral angle during the scan and finally a relaxed scan of geometries closer to the hypothetical **TS4bM** geometry corresponding. Solvent presence seems to inhibit the concerted transformation by stabilization of the separated charges forming during the stepwise rearrangement.

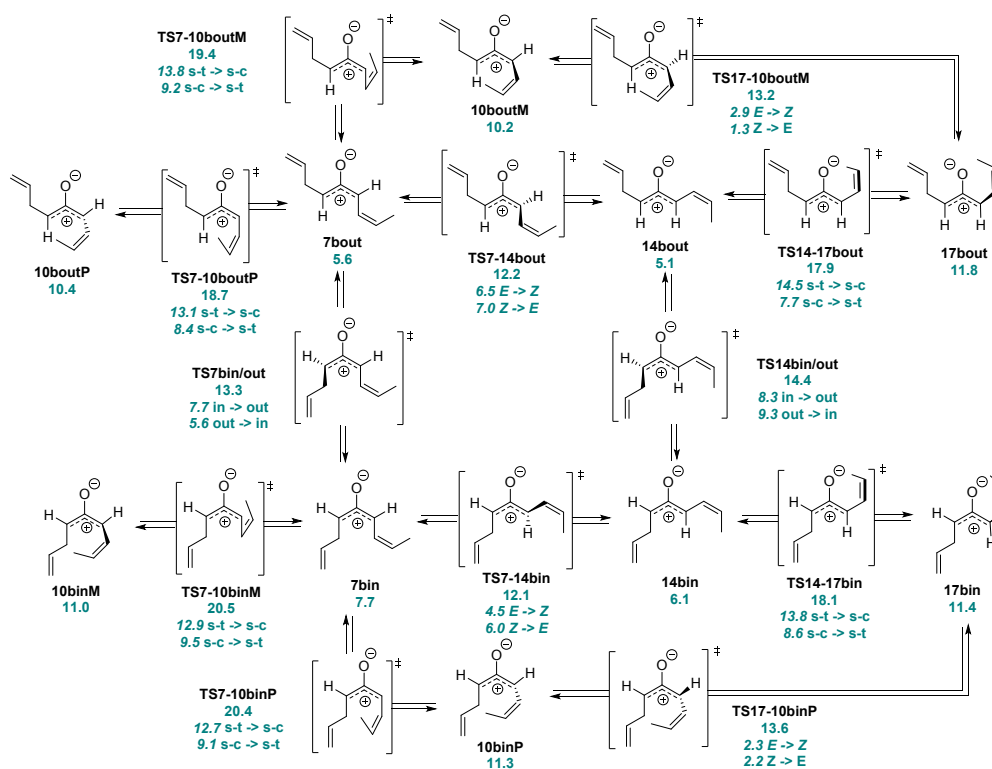
S4. SPIN CONTAMINATION OF THE OPEN SHELL SINGLET OPTIMIZATION PROCESS.

Table S 1: Spin contamination calculated for the open shell singlet structures that could be affected by a nearby low lying triplet state mixing both during the geometry optimization. Those with no spin contamination will have a pure closed shell nature while the ones with a triplet structure lower in energy nearby will stabilize an open shell singlet structure lower in energy that determine the diradical nature of the process in those.

	¹ <S ² >	¹ <S ² >after						
10binM	0.72	0.12	TS8bin	0.00	0.00	14din	0.69	0.09
10binP	0.72	0.12	TS8bout	0.00	0.00	14dout	0.56	0.06
10boutM	0.63	0.08	10ainM	0.75	0.13	14dout' _c3	0.00	0.00
10boutP	0.60	0.07	10ainP	0.75	0.13	7din	0.80	0.14
14bin	0.69	0.09	10aoutM	0.63	0.08	7dout	0.70	0.10
14bout	0.56	0.05	10aoutP	0.63	0.08	7dout' _c3	0.00	0.00
14bout'	0.57	0.06	14ain	0.73	0.11	TS13din	0.00	0.00
7bin	0.81	0.14	14aout	0.61	0.07	TS13dout	0.00	0.00
7bout	0.69	0.09	7ain	0.85	0.17	TS13dout'	0.00	0.00
7bout'	0.70	0.10	7aout	0.71	0.10	TS6din	0.00	0.00
TS11bin	0.00	0.00	TS12ainM	0.60	0.08	TS6dout	0.00	0.00
TS11bout	0.00	0.00	TS12ainP	0.60	0.08	TS6dout'	0.00	0.00
TS12binM	0.59	0.08	TS12aoutM	0.35	0.02	14ein	0.68	0.09
TS12binP	0.58	0.08	TS12aoutP	0.35	0.02	14eout	0.56	0.06
TS12boutM	0.23	0.01	TS13ain	0.00	0.00	14eout' _c3	0.00	0.00
TS12boutP	0.37	0.03	TS13aout	0.00	0.00	7ein	0.81	0.14
TS14bin	0.00	0.00	TS7-10ainM	0.70	0.02	7eout	0.69	0.09
TS14bout	0.00	0.00	TS7-10ainP	0.70	0.02	7eout' _c3	0.00	0.00
TS14bout'	0.00	0.00	TS7-10aoutM	0.58	0.01	TS13ein	0.00	0.00
TS15bin	0.00	0.00	TS7-10aoutP	0.59	0.01	TS13eout	0.00	0.00
TS15bout	0.00	0.00	TS7-14aint	0.00	0.00	TS13eout'	0.00	0.00
TS16bin	0.00	0.00	TS7-14aout	0.72	0.10	TS6ein	0.00	0.00
TS16bout	0.00	0.00	TS7ain-out	0.09	0.00	TS6eout	0.00	0.00
TS4bP	0.00	0.00	TS6ain	0.00	0.00	TS6eout'	0.00	0.00
TS6bin	0.27	0.01	TS6aout	0.00	0.00	10eoutM	0.60	0.07
TS6bout	0.30	0.01	14cin	0.71	0.10	10eoutP	0.60	0.07
TS6bout'	0.00	0.00	14cout	0.58	0.06	TS11eout	0.00	0.00
TS7-10binM	0.00	0.00	TS13cin	0.00	0.00	TS12eoutM	0.13	0.00
TS7-10binP	0.00	0.00	TS13cout	0.00	0.00	TS12eoutP	0.37	0.03
TS7-10boutM	0.00	0.00	7cin	0.81	0.14	TS7-10eoutM	0.00	0.00
TS7-10boutP	0.08	0.00	7cout	0.68	0.09	TS7-10eoutP	0.00	0.00
			TS6cin	0.00	0.00	TS8eout	0.00	0.00
			TS6cout	0.00	0.00			

S5. ISOMERIZATION PROCESS OF THE OXIDOPENTADIENYL CONFORMERS W-SICKEL-U IN THE TRIPLET STATE.

A considerable reduction of activation energies was computed compared to the closed shell zwitterions and singlet diradicals. In addition, pathways for the direct interconversion of the *in* and *out* configurational isomers that differ by the geometry of the bond containing the allyl substituents (**7bin**—**7bout** and **14bin**—**14bout**) were located (Scheme 4). As a consequence, structures **10boutP** and **10boutM** required for cyclization to the *cis*-cyclopentenone enantiomers can be easily obtained from any other of the oxidopentadienyl triplet diradical isomers as the energy barriers range from 4.5 kcal/mol to 13.8 kcal/mol (see Scheme 4). Scheme S3 provides an overall depiction of the rearrangement that includes all the isomerization pathways computed. Relevant for this discussion is the characterization of the **7bin** to **14bin** isomerization process, which is more favorable than the cyclization to (2*S*,3*R*)-**9b**, and drives the rearrangement of both *E*-**1b** and *Z*-**1b** to the same intermediate **14bin** on route to the *cis*-cyclopentenone **5b**.

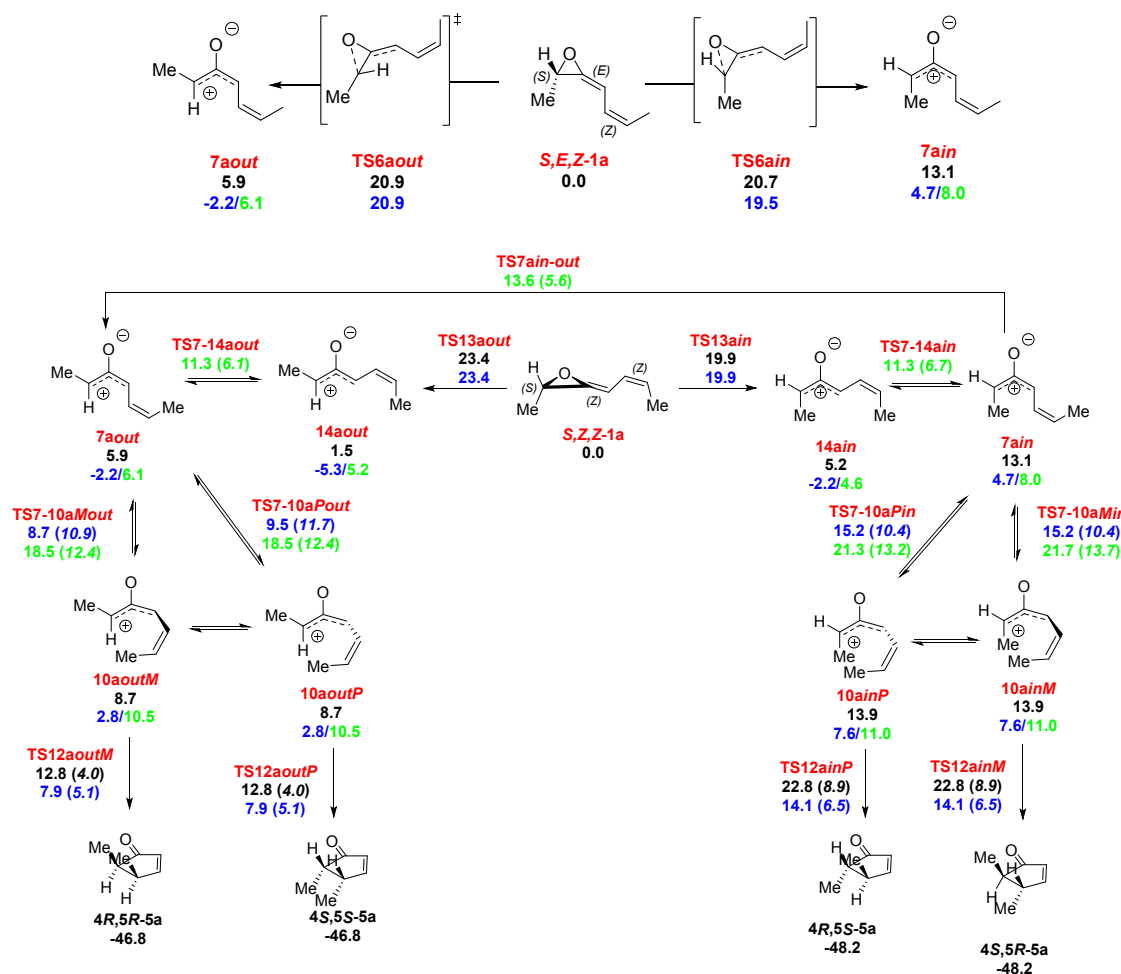


Scheme S 3: Triplet state isomerization processes by bond rotation computed at the UωB97XD/6-311++G(3df,2p)(SMD,H₂O)//UωB97XD/6-31++G(d,p)(SMD,H₂O) level of theory. The increasing order of activation barriers correspond to the increased double bond nature of rotating dihedral angle. Thus *Z/E* (W-sickel) isomerization corresponding to the bond with the less conjugation (1.46-1.47 Å) show the lower energy barriers, followed by the *in/out* isomerization (1.44 Å) and finally the highest energy barrier correspond to the *s-trans/s-cis* (sickle-U) isomerization process, rotating around the bond with the most double character (1.39-1.40 Å).

S6. EFFECT OF THE ALLYL ANCHIMERIC ASSISTANCE ON THE OXIRANE CLEAVAGE PROCESS.

In order to compare the effects of the different substituents on the allene oxide rearrangements (to explain the different behavior for the linoleic and linoleic acids in solution) we remake the already calculated methyl substituted system¹ (that was only carried out in the closed shell manifold and

without solvent reaction field on the optimization process, which changes considerably the mechanistic depiction) taking into account the solvent stabilizing effects and the possible diradical character during the rearrangement (Scheme S 4).



Scheme S 4: Rearrangement of the methyl substituted **S,E,Z-1a** and **S,Z,Z-1a** allene oxides with solvent reaction field during the optimization and open shell calculation to study the possible diradical character of the potential energy surface stationary points. Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-311++G(d,p)(SMD,H₂O) (black for closed-shell) and U ω B97XD/6-311++G(3df,2p)(SMD,H₂O)//U ω B97XD/6-311++G(d,p)(SMD,H₂O) (blue for open-shell singlet and green for triplet states) level of theory.

Oxirane cleavage of the initial *E* and *Z* allene oxide with methyl substituent leads to each oxidopentadienyl geometry from an in or out motion along the reaction coordinate. In rotation parting from the **S,Z,Z-1a** initial isomer results in the lower found energy barrier that should lead to the *trans*-cyclopentenones, but due to the low lying triplet state near an *E/Z* and *in/out* isomerization sequence in this triplet state surface will connect with the out branch that evolves easily to the final *cis*-cyclopentenones.

One important feature is that were not possible to locate none of the concerted transition states leading directly to the cyclopentenones by simple initial *s-trans/s-cis* conformational change of the **S,E,Z-1a** isomer. Relaxed bidimensional scans of both TS surroundings were carried out (Figure S 2) and no saddle point topology was found, so those TS could not be located due to, probably, the solvent stabilization of the oxidopentadienyl zwitterion leading TS, not only for the *s-trans* conformer, as shown in Scheme 3,

¹ Gonzalez-Perez, A. B.; Grechkin, A.; de Lera, A. R. *Org. Biomol. Chem.* **2014**, *12*, 7694.

but also for the *s-cis* one that would lead directly to the oxidopentadienyl U conformation intermediate of the concerted process.

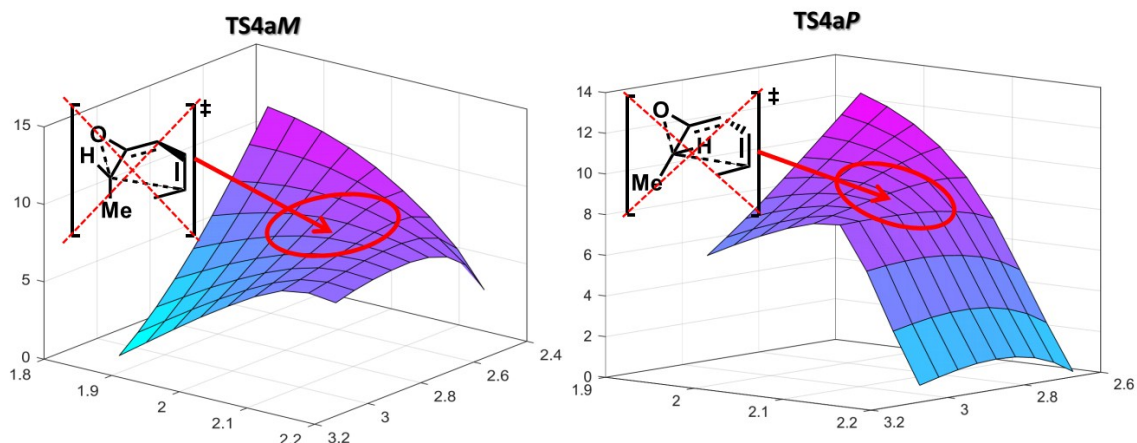
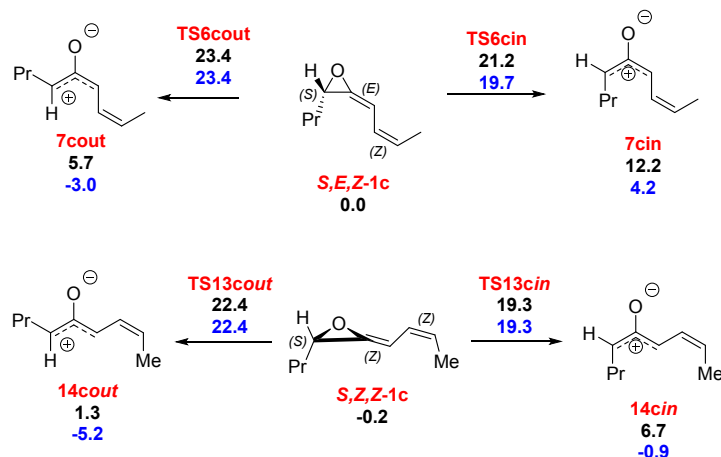


Figure S 2: Bidimensional relaxed scan of 2 bond distances, C-O epoxide cleavage and C-C cyclopentenone bond forming near 3aM and 3aP respectively passing through the possible concerted processes. Both surfaces show no saddle point topology in the geometry corresponding to the hypothetical TS. Solvent presence inhibits the concerted transformation by stabilization of the separated charges forming during the stepwise rearrangement.

Comparing the energies obtained of the allyl oxirane opening versus the values calculated for the methyl case, there are several important differences between them. Closed shell calculations show an energy barrier increase with respect to the Me substituted system. In order to determine the nature of this destabilization we carried out the propyl substituted opening process (Scheme S 5).



Scheme S 5: Propyl substituted allene oxide geometric isomers opening process. Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-31++G(d,p)(SMD,H₂O) (black for closed-shell) and U ω B97XD/6-311++G(3df,2p)(SMD,H₂O)//U ω B97XD/6-31++G(d,p)(SMD,H₂O) (blue for open-shell singlet) level of theory

The results found dismiss the steric effect as explanation for this feature, because the propyl substituent shows almost the same behavior as the methyl one except for the wavefunction instability found for TS6cin which has no homologue in the methyl opening process. Thus, if the steric hindrance is not the explanation, stereoelectronic effects must play a determinant role. Analysis of the orbitals involved (Figure S 3) lead us to the hypothesis of an extra stabilization of the initial allene oxide with allyl substituent. Both allyl and propyl HOMO's have similar features, but the allyl one presents more conjugation on the allene oxide, besides an electronic donation from the lone pair of the oxirane oxygen

and the σ_{C-O} bond to the homoallylic σ_{C-C} bond that continues the conjugation to the allyl substituent stabilizing the minima.

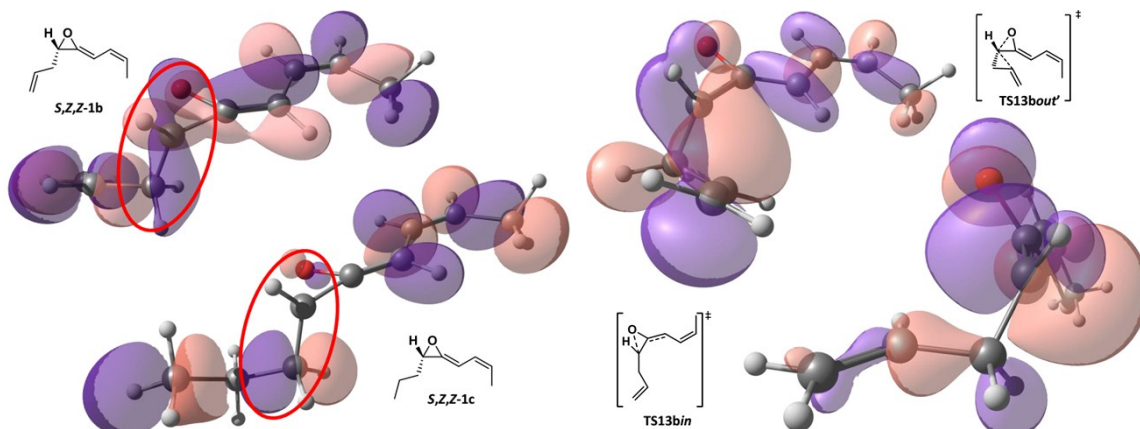
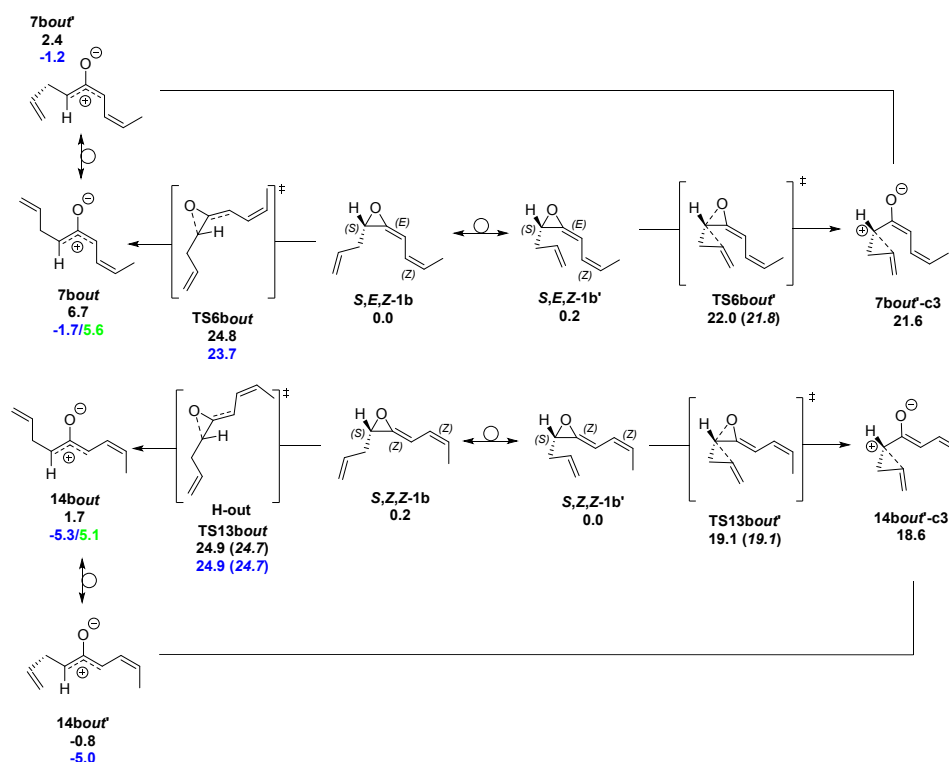


Figure S 3: Orbital depiction of the HOMO of the *Z,Z* initial allene oxide, both with an allyl and a propyl substituent. On the right hand it is the HOMO of the cleavage process with and without anchimeric assistance.

Curiously, we have found a TS stabilization only feasible with allylic substitution that is the formation of a vinyl cycloproponium cation during the oxirane opening process. Only out motion is possible when the allylic anchimeric assistance is set and takes to the high energy fleeting vinyl cycloproponium intermediate by an energy profit of ca. 2 kcal/mol for the *E* allene oxide and ca. 6 kcal/mol for the *Z* isomer (Figure S 3). Indeed, this stabilization seems to benefit enormously the oxirane opening process even counterbalancing the stabilization of the minima leading to an oxirane opening process of the **Z-1b** that is even more favorable than the methyl or propyl substituted. Comparing the HOMO of anchimeric assisted **TS13bout'** with the lower in energy of the **Z-1b** oxirane opening without the substituent stabilization **TS13bin** (Figure S 3) we have found a large component of donation from the allyl substituent to the incipient carbocation forming on the epoxide cleavage explaining the large stabilizing effect reflected on the activation barriers.

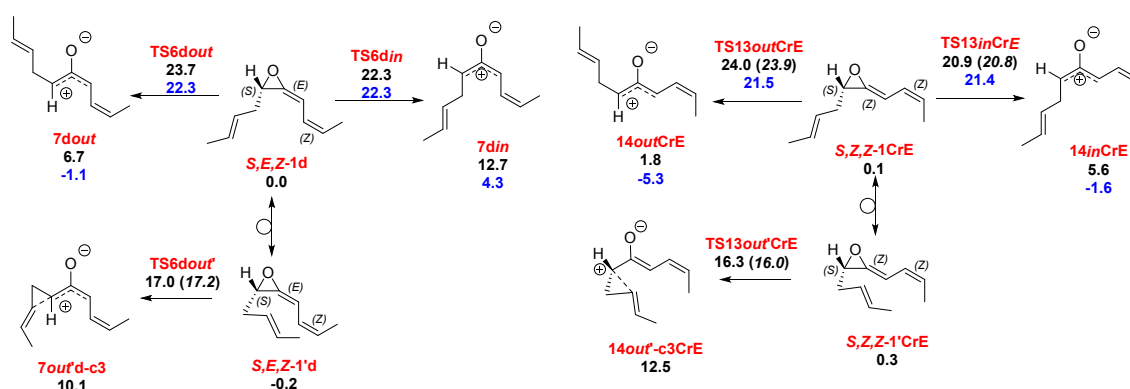
So it seems that the anchimeric assistance, as mentioned, benefits the overall process for the *Z* allene oxide but it is not the same with the *E* branch where (as shown in Table 1 of the main text) the diradical character of the TS6in opening (as for the methyl and propyl substitution) is the determinant effect explaining this preference. Indeed, we have also calculated the instabilities of the wavefunction only found in the **TS6in**, **a**, **b** and **c** processes being greater with the allyl substitution which could be the explanation for the **TS6outb** wavefunction instability also found that is not competitive with the anchimeric assisted opening **TS6out'b**.



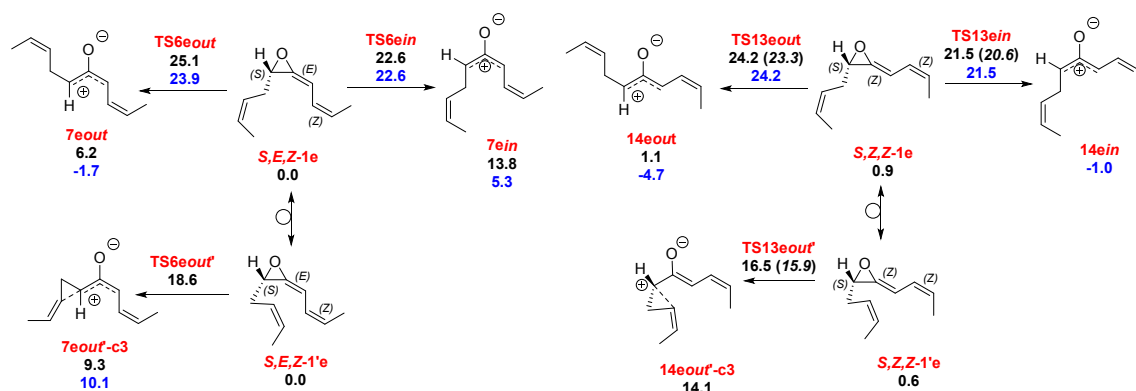
Scheme S 6: Oxirane opening assisted by the allyl substitution compared to the non-assisted cleavage out process. Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-31++G(d,p)(SMD,H₂O) (black for closed-shell) and $U\omega$ B97XD/6-311++G(3df,2p)(SMD,H₂O)// $U\omega$ B97XD/6-31++G(d,p)(SMD,H₂O) (blue for open-shell singlet and green for triplet states) level of theory.

S7. CROTYL SYSTEMS

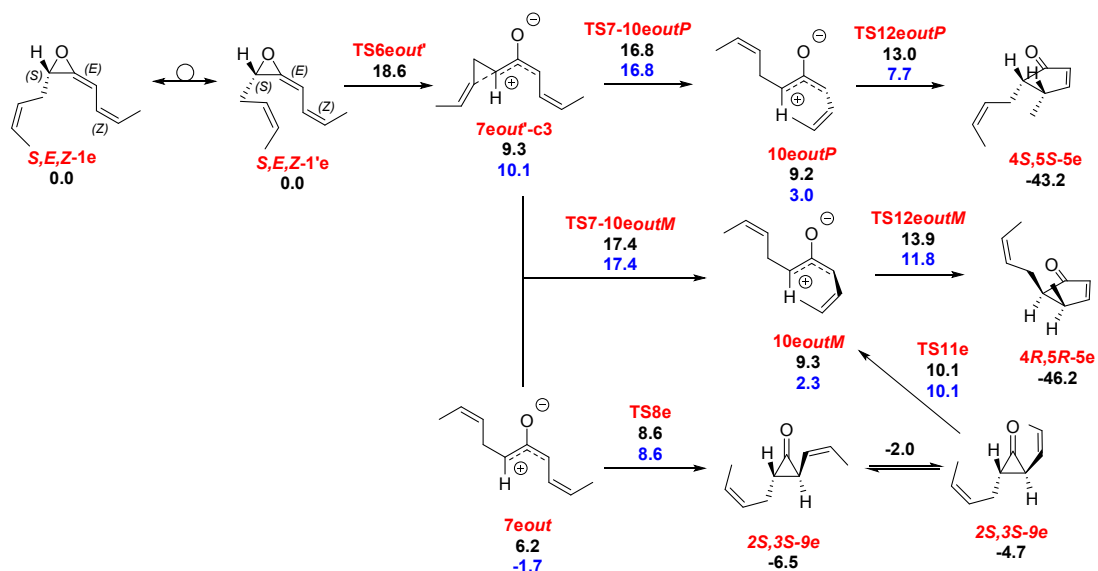
With all these summarized results we have decided to carry out the rearrangement mechanism calculations with a crotyl substituent, because the stabilization of the primary carbocation formed during the anchimeric assisted processes will be greatly stabilized by the presence of another donor adjacent substituent. Thus a crotyl substituent was chosen for the new model, Z in order to emulate the natural isomer, and E, to take into account possible isomerization processes due to the diradical character of some intermediates.



Scheme S 7: Crotyl E substituted epoxide opening different possibilities from **E-1d** or **Z-1d** respectively, both rotations and the anchimeric assisted process. Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-31++G(d,p)(SMD,H₂O) (black for closed-shell) and $U\omega$ B97XD/6-311++G(3df,2p)(SMD,H₂O)// $U\omega$ B97XD/6-31++G(d,p)(SMD,H₂O) (blue for open-shell singlet and green for triplet states) level of theory.



Scheme S 8: Crotyl Z substituted epoxide opening different possibilities from *E*-1e or *Z*-1e respectively, both rotations and the anchimeric assisted process. Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-31++G(d,p)(SMD,H₂O) (black for closed-shell) and U ω B97XD/6-311++G(3df,2p)(SMD,H₂O)//U ω B97XD/6-31++G(d,p)(SMD,H₂O) (blue for open-shell singlet and green for triplet states) level of theory.



Scheme S 9: Competing pathways for the rearrangement of Z crotyl substituted (natural product model) from the *E*-1e initial isomer (the only with an determinant reaction barrier high enough to identify the initial allene oxide). Crotyl assisted zwitterionic isomerization of P and M helicity versus the isomerization through the cyclopropanone intermediate which is the lower energy path. Because the initial energy barrier is the reaction determinant step with the higher energy, the molecule has the amount of energy enough to overcome the competing isomerization process without penalty, so cyclopropanone formation is one of the competing isomerization process (even in the triplet state). Energy values (kcal/mol) have been computed at the ω B97XD/6-311++G(3df,2p)(SMD,H₂O)// ω B97XD/6-31++G(d,p)(SMD,H₂O) (black for closed-shell) and U ω B97XD/6-311++G(3df,2p)(SMD,H₂O)//U ω B97XD/6-31++G(d,p)(SMD,H₂O) (blue for open-shell singlet and green for triplet states) level of theory.

S8. CARTESIAN COORDINATES

CLOSED SHELL ALLYL SUBSTITUTION

s_E_Z-1b

SCF Energy: -425.189933105 H

Num. Imaginary Frequencies: 0

C	-2.188886	-0.635308	-0.319086
C	-1.404002	0.558204	-0.009074
C	-0.110586	0.623070	-0.299737
C	-3.493519	-0.821520	-0.059189
O	0.922923	1.510565	-0.162518
C	1.161165	0.165988	-0.774185
H	-1.642736	-1.441742	-0.806587
H	-1.863079	1.418678	0.468923
H	-3.927215	-1.774935	-0.356779
H	1.373067	0.238286	-1.839561
C	-4.437590	0.139181	0.598569
H	-4.882904	-0.312623	1.492557
H	-3.959868	1.075491	0.896555
H	-5.267691	0.381496	-0.075425
C	2.023103	-0.778655	0.021250
H	1.728219	-0.751188	1.074817
H	1.810024	-1.786149	-0.359506
C	3.486027	-0.474143	-0.137962
H	3.870207	-0.490675	-1.157917
C	4.308155	-0.192022	0.872658
H	3.954636	-0.166203	1.901485
H	5.360761	0.016280	0.702110

TS2bM

SCF Energy: -425.180826348 H

Num. Imaginary Frequencies: 1 (i53.1819)

C	-3.593134	-0.616517	1.067552
C	-3.261844	0.670115	0.376398
C	-2.312621	0.852808	-0.548783
C	-1.413044	-0.211965	-1.069718
C	-0.197144	-0.399990	-0.589114
C	0.947783	-0.160465	0.238297
C	1.888579	0.980381	-0.019602
O	0.881512	-1.218539	-0.817213
H	-2.194587	1.846523	-0.980098
H	-1.748354	-0.847930	-1.887281
H	-3.864103	1.532581	0.659755
H	0.956733	-0.587157	1.239834
H	-2.967605	-1.443371	0.721392
H	-4.643549	-0.880039	0.899190
H	-3.463222	-0.516290	2.151286
H	1.790967	1.308594	-1.061410
H	1.550957	1.825323	0.594572
C	3.332483	0.692130	0.288646
H	3.997719	1.548216	0.186069
C	3.841994	-0.484713	0.655139
H	3.230476	-1.377234	0.765288
H	4.904151	-0.591615	0.856219

TS2bP

SCF Energy: -425.181121209 H

Num. Imaginary Frequencies: 1 (i72.2678)

C	-3.087935	1.358864	-0.719478
C	-3.149317	0.511446	0.513666
C	-2.437583	-0.597747	0.745136
C	-1.474098	-1.198827	-0.216323
C	-0.170094	-1.020305	-0.107032
C	1.048662	-0.494686	0.431817
C	1.471427	0.924698	0.186628
O	0.976503	-1.386122	-0.768131
H	-2.582191	-1.121219	1.689565
H	-1.843324	-1.814323	-1.034817
H	-3.840159	0.842808	1.288036
H	1.495112	-1.001551	1.285445
H	-2.375902	0.970108	-1.452135
H	-2.794802	2.383953	-0.464607
H	-4.074783	1.423219	-1.192029
H	0.966296	1.308070	-0.708078
H	1.092231	1.523950	1.024770
C	2.955643	1.135435	0.061608
H	3.258412	2.177471	-0.029922
C	3.891861	0.185463	0.047286
H	3.652850	-0.872578	0.126676
H	4.942840	0.443023	-0.047701

3bM

SCF Energy: -425.187296303 H

Num. Imaginary Frequencies: 0

C	-2.039941	-1.643947	-0.711545
C	-2.922403	-0.817798	0.175996
C	-2.740543	0.469764	0.516002
C	-1.636532	1.360534	0.141600
C	-0.403223	0.975694	-0.167027
O	0.781182	1.585836	-0.490360
C	0.716484	0.099455	-0.337657
H	-3.501860	0.939726	1.135510
H	-1.825724	2.431368	0.156985
H	-3.805475	-1.312380	0.576052
H	0.826286	-0.411426	-1.292692
C	1.449942	-0.491027	0.830783
H	-1.598170	-1.040953	-1.512428
H	-1.210213	-2.094213	-0.151496
H	-2.606428	-2.461729	-1.165032
H	0.989499	-1.465760	1.039821
H	1.276627	0.121523	1.723646
C	2.927474	-0.677861	0.618814
H	3.441324	-1.190151	1.430828
C	3.630211	-0.273906	-0.440336
H	3.176707	0.249815	-1.278677
H	4.699161	-0.457953	-0.499414

3bP

SCF Energy: -425.186950371 H

Num. Imaginary Frequencies: 0

C	-1.950688	1.785179	-0.104776
C	-2.976547	0.752635	0.247792
C	-2.837860	-0.580254	0.157105
C	-1.658827	-1.347543	-0.261320
C	-0.387989	-1.020244	-0.056824
O	0.823048	-1.619278	-0.290457
C	0.763953	-0.317588	0.435675
H	-3.702497	-1.194643	0.401858
H	-1.834017	-2.312070	-0.733579
H	-3.936665	1.125577	0.599731
H	1.005584	-0.430863	1.491658
C	1.385598	0.853593	-0.267243
H	-1.275405	1.429483	-0.889797
H	-2.432546	2.704174	-0.450700
H	-1.332416	2.051612	0.761633
H	0.982922	1.766392	0.188951
H	1.063091	0.871084	-1.315080
C	2.888183	0.896818	-0.197820
H	3.333788	1.782542	-0.648217
C	3.686428	-0.024709	0.342999
H	3.305702	-0.934289	0.801451
H	4.764566	0.107919	0.342228

TS4bP

SCF Energy: -425.146394068 H

Num. Imaginary Frequencies: 1 (i496.7059)

C	0.190922	1.788134	1.219747
C	0.870166	1.924091	-0.112317
C	1.832056	1.133004	-0.641555
C	2.189648	-0.203905	-0.182815
C	1.186191	-1.103135	-0.048122
O	1.117332	-2.381889	0.215344
C	-0.196010	-0.887643	-0.429439
H	2.373647	1.515344	-1.507882
H	3.226835	-0.507190	-0.072659
H	0.651925	2.850043	-0.643658
H	-0.395405	-0.766569	-1.497669
C	-1.365455	-1.087896	0.444505
H	0.532412	0.912762	1.776746
H	0.405713	2.683440	1.815341
H	-0.897958	1.735076	1.121034
H	-1.101310	-0.955035	1.499181
H	-1.640885	-2.149226	0.335409
C	-2.588229	-0.285204	0.072465
H	-3.487008	-0.598528	0.598725
C	-2.655142	0.724780	-0.794116
H	-1.789589	1.099083	-1.335841
H	-3.601916	1.222551	-0.981597

4S_5S-5b

SCF Energy: -425.274877574 H

Num. Imaginary Frequencies: 0

C	0.005696	-0.343971	-0.315601
C	1.386017	-0.942885	-0.077269

C	2.383006	0.118911	-0.229458
C	1.751773	1.292674	-0.384614
C	0.252430	1.187709	-0.312787
O	1.613282	-2.127173	0.171034
H	2.244949	2.252381	-0.509431
H	3.451939	-0.055136	-0.198135
H	-0.189091	1.653177	-1.201044
C	-0.264280	1.940874	0.920235
H	-0.236360	-0.644308	-1.345963
C	-1.061769	-0.917079	0.611697
H	-0.932763	-2.006261	0.653763
H	-0.898660	-0.566930	1.638483
H	-1.354547	1.884966	0.981462
H	0.159650	1.530263	1.842147
H	0.017940	2.996290	0.859148
C	-2.487668	-0.637177	0.228430
H	-3.225857	-1.045189	0.918773
C	-2.918760	0.031498	-0.842763
H	-2.240380	0.471866	-1.569653
H	-3.981750	0.162939	-1.025042

TS16bin

SCF Energy: -425.150124301 H

Num. Imaginary Frequencies: 1 (i304.2684)

C	-0.471198	0.153868	0.603360
C	0.342146	1.291799	0.264848
C	1.515934	1.299064	-0.424631
C	2.200222	0.120386	-0.936960
C	2.352862	-1.099140	-0.377617
C	1.945736	-1.581391	0.981377
O	-0.416163	2.277538	0.685174
H	2.688172	0.271441	-1.899552
H	1.946782	2.270880	-0.658027
H	2.900717	-1.829385	-0.971578
H	-0.800754	0.098737	1.639712
C	-1.121857	-0.748448	-0.361288
H	1.665777	-0.764107	1.655011
H	2.773952	-2.132862	1.439401
H	1.101203	-2.279037	0.927735
H	-1.168777	-1.749184	0.083868
H	-0.582377	-0.769016	-1.310560
C	-2.540285	-0.230270	-0.564612
H	-2.621572	0.695814	-1.128326
C	-3.624044	-0.843966	-0.094169
H	-3.556162	-1.765995	0.478107
H	-4.614747	-0.439002	-0.279041

TS16bout

SCF Energy: -425.148723419 H

Num. Imaginary Frequencies: 1 (i489.2562)

C	0.384115	0.282749	-0.365671
C	-0.572290	1.266176	0.088438
C	-1.919002	1.207770	-0.065593
C	-2.517558	0.034653	-0.683878
C	-2.279177	-1.264226	-0.389696
C	-1.584338	-1.843516	0.806543
O	0.260795	2.209063	0.447315

H	-3.230476	0.234575	-1.484732
H	-2.524180	2.086042	0.142992
H	-2.759501	-2.000517	-1.033352
H	0.459682	0.101749	-1.441137
C	1.418635	-0.335873	0.479792
H	-1.247116	-1.080735	1.512882
H	-0.721945	-2.456693	0.521405
H	-2.278466	-2.514449	1.326130
H	1.262329	-1.418769	0.341525
H	1.262911	-0.088684	1.532404
C	2.821064	0.004844	0.027286
H	3.114361	1.042476	0.173928
C	3.667887	-0.869422	-0.512377
H	3.392230	-1.909735	-0.669996
H	4.667800	-0.566694	-0.809632

10boutP

SCF Energy: -425.176902036 H

Num. Imaginary Frequencies: 0

C	0.455477	-0.003288	0.146389
C	-0.368350	1.130223	0.115206
O	-0.094076	2.267254	0.645642
C	-1.343254	0.963719	-0.914985
C	-2.164741	-0.166252	-1.203280
C	-2.637147	-1.086163	-0.319124
C	-2.469374	-1.167731	1.157608
H	-2.528766	-0.232038	-2.225407
H	-1.475973	1.832889	-1.560297
H	-3.293787	-1.844901	-0.741798
H	0.082634	-0.945178	-0.239976
C	1.848825	0.045321	0.657680
H	-3.448882	-1.333082	1.618458
H	-1.854919	-2.038585	1.414297
H	-2.001793	-0.284473	1.595999
H	2.243919	1.065322	0.586145
H	1.787280	-0.176269	1.738091
C	2.763385	-0.950667	0.000686
H	2.438083	-1.990480	0.027045
C	3.914606	-0.631611	-0.589927
H	4.263417	0.398236	-0.634458
H	4.544834	-1.390788	-1.044751

10binM

SCF Energy: -425.170950076 H

Num. Imaginary Frequencies: 0

C	-0.464863	1.075156	0.160350
C	0.916461	1.345860	0.189600
C	1.638778	0.604263	-0.796856
C	1.703919	-0.779845	-1.099500
C	1.518775	-1.823926	-0.241220
C	1.220052	-1.797455	1.209914
O	1.401551	2.418489	0.699921
H	2.046473	-1.023177	-2.101978
H	2.243351	1.250056	-1.434647
H	1.675389	-2.816110	-0.660733
H	-1.065630	1.976579	0.299933
C	-1.236657	-0.182456	0.009560

H	1.229623	-0.795709	1.643341
H	1.940103	-2.433609	1.735727
H	0.233306	-2.244788	1.389876
H	-1.295128	-0.671348	0.995835
H	-0.699747	-0.902727	-0.626356
C	-2.624685	0.044795	-0.526008
H	-2.687591	0.560125	-1.484104
C	-3.739632	-0.352948	0.086232
H	-3.707359	-0.869454	1.043670
H	-4.718079	-0.178414	-0.352362

TS6bin

SCF Energy: -425.151955496 H

Num. Imaginary Frequencies: 1 (i329.9073)

C	1.117050	0.262087	-0.816495
C	0.058726	1.044040	-0.234319
C	-1.240578	0.699789	-0.007997
C	-1.793084	-0.605037	-0.312012
C	-3.063857	-0.999763	-0.096073
C	-4.182409	-0.190511	0.483363
O	0.714432	2.140405	0.069963
H	-1.119026	-1.329911	-0.766096
H	-1.880492	1.470169	0.415616
H	-3.320300	-2.020521	-0.374335
H	1.658938	0.743544	-1.628499
C	1.701231	-0.962475	-0.246152
H	-3.892278	0.833045	0.730878
H	-4.562015	-0.664901	1.396197
H	-5.024163	-0.145384	-0.217570
H	2.107231	-1.574589	-1.057627
H	0.968478	-1.518334	0.343605
C	2.846369	-0.504004	0.653307
H	2.545238	-0.028966	1.583551
C	4.131626	-0.652512	0.340413
H	4.443525	-1.115851	-0.592436
H	4.908952	-0.321230	1.022798

TS6bout

SCF Energy: -425.148973841 H

Num. Imaginary Frequencies: 1 (i541.5540)

C	0.980884	-0.091999	-0.247009
C	-0.078597	0.875560	-0.101871
C	-1.417134	0.630549	-0.039937
C	-1.964713	-0.704465	-0.173572
C	-3.265154	-1.051114	-0.101003
C	-4.427287	-0.147365	0.173689
O	0.595351	1.998354	-0.141312
H	-1.245799	-1.505452	-0.350752
H	-2.076123	1.483433	0.101258
H	-3.510266	-2.101150	-0.250682
H	1.027896	-0.708699	-1.148323
C	2.103615	-0.222114	0.691466
H	-4.132329	0.890964	0.341845
H	-4.978522	-0.490536	1.057110
H	-5.135374	-0.167801	-0.663452
H	2.017410	-1.270710	1.028964
H	1.978508	0.439429	1.550895

C	3.453099	-0.039214	0.032552
H	3.685356	0.981678	-0.264090
C	4.319796	-1.025626	-0.186771
H	4.100515	-2.051404	0.100742
H	5.278864	-0.831851	-0.658283

7bin

SCF Energy: -425.171027424 H

Num. Imaginary Frequencies: 0

C	1.145755	0.927614	0.086189
C	-0.106276	1.514114	-0.104036
C	-1.267010	0.677029	-0.046457
C	-1.416321	-0.659687	-0.468543
C	-2.561918	-1.379089	-0.265501
C	-3.793424	-0.977906	0.449282
O	-0.269456	2.808281	-0.137208
H	-0.620453	-1.141004	-1.022512
H	-2.147316	1.185264	0.344187
H	-2.576779	-2.387028	-0.676165
H	1.921261	1.647628	0.352602
C	1.594550	-0.499511	0.011608
H	-3.785367	0.040179	0.837723
H	-3.955435	-1.674721	1.281105
H	-4.650928	-1.108304	-0.221248
H	1.533420	-0.865458	-1.022904
H	0.920819	-1.140698	0.598073
C	2.998983	-0.675058	0.522425
H	3.183407	-0.327324	1.538901
C	3.990708	-1.223848	-0.178351
H	3.837843	-1.577843	-1.196179
H	4.984897	-1.338887	0.244380

7bout

SCF Energy: -425.180783160 H

Num. Imaginary Frequencies: 0

C	-4.105931	-0.419404	0.478984
C	-3.033312	-1.031058	-0.341623
C	-1.750608	-0.608096	-0.527715
C	-1.230965	0.567373	0.063094
C	0.083766	1.121488	-0.056109
C	1.081338	0.199083	-0.372601
C	2.522097	0.524128	-0.270052
O	0.302831	2.359564	0.266377
H	-1.121251	-1.196561	-1.187192
H	-1.909315	1.168001	0.667616
H	-3.323017	-1.937715	-0.869937
H	0.808498	-0.790760	-0.721853
H	-4.957806	-0.183192	-0.169929
H	-4.471268	-1.162613	1.197427
H	-3.809487	0.479903	1.018677
H	2.827958	0.964801	-1.234383
H	2.669232	1.338467	0.452592
C	3.441381	-0.624025	0.049524
H	4.497336	-0.424714	-0.124986
C	3.077094	-1.811699	0.535055
H	2.038988	-2.061673	0.743536
H	3.818336	-2.577190	0.746068

TS8bin

SCF Energy: -425.169426408 H

Num. Imaginary Frequencies: 1 (i167.2573)

C	0.950492	0.814058	-0.367583
C	-0.068788	1.635030	0.159036
O	-0.093490	2.903480	0.113165
C	-1.218164	0.795244	0.116178
C	-1.425432	-0.476357	0.740460
C	-2.439387	-1.316176	0.422555
C	-3.459171	-1.159040	-0.649068
H	-0.756740	-0.768910	1.542450
H	-2.034663	1.221025	-0.467361
H	-2.521873	-2.227380	1.012261
H	1.506125	1.298692	-1.173683
C	1.408507	-0.566115	-0.002641
H	-3.372563	-1.994677	-1.353590
H	-4.463436	-1.225632	-0.215767
H	-3.372685	-0.227170	-1.209922
H	1.380355	-0.721446	1.079762
H	0.723827	-1.310660	-0.442029
C	2.797704	-0.825326	-0.523480
H	2.938380	-0.691673	-1.596027
C	3.822130	-1.207528	0.237609
H	3.711948	-1.344533	1.311488
H	4.801894	-1.398218	-0.191298

TS8bout

SCF Energy: -425.178482554 H

Num. Imaginary Frequencies: 1 (i107.4289)

C	0.754091	-0.427378	0.081966
C	0.190707	0.813875	-0.256463
O	0.726583	1.960347	-0.205087
C	-1.189309	0.516067	-0.040255
C	-1.981619	-0.499512	-0.675859
C	-3.291673	-0.710547	-0.417711
C	-4.162174	-0.028685	0.581066
H	-1.510097	-1.096817	-1.451686
H	-1.685169	1.200521	0.647979
H	-3.786991	-1.471029	-1.018690
H	0.313942	-1.346992	-0.285122
C	1.995360	-0.534988	0.911031
H	-4.993375	0.467993	0.067363
H	-4.611169	-0.778181	1.242673
H	-3.641914	0.707592	1.195592
H	2.200278	0.413896	1.414343
H	1.863458	-1.320181	1.663390
C	3.147777	-0.898720	0.000815
H	3.108904	-1.891944	-0.443992
C	4.161039	-0.079943	-0.282554
H	4.219259	0.920377	0.141398
H	4.965015	-0.389031	-0.944775

2S_3R-9b

SCF Energy: -425.199829784 H

Num. Imaginary Frequencies: 0

C	2.709510	-0.780911	-0.468199
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C	1.586404	-1.140866	0.161514
C	0.738223	-0.235767	0.998367
C	0.006846	0.886489	0.400926
O	0.078403	1.928918	-0.214766
C	-0.837665	-0.216523	0.846381
C	-1.545441	-1.093932	-0.165381
H	1.247971	-2.173342	0.092731
H	1.052294	-0.097331	2.033297
C	3.336130	0.579711	-0.471759
H	3.239791	-1.550092	-1.028207
H	-1.354960	-0.078536	1.794706
H	-0.915121	-1.225555	-1.054267
H	-1.670520	-2.097409	0.259542
H	2.789676	1.294901	0.147807
H	4.366664	0.521438	-0.103274
H	3.388947	0.976546	-1.491939
C	-2.887731	-0.577035	-0.604910
H	-3.435388	-1.244907	-1.268974
C	-3.436962	0.590266	-0.265405
H	-2.937191	1.299639	0.390123
H	-4.415267	0.874717	-0.642614

2S_3S-9b

SCF Energy: -425.201449828 H

Num. Imaginary Frequencies: 0

C	-0.655127	0.060431	0.376319
C	-0.120727	1.322483	-0.113824
C	0.835195	0.204566	-0.145522
C	1.968370	0.137560	0.808803
C	3.161597	-0.425435	0.580674
C	3.628881	-1.106701	-0.669550
O	-0.301950	2.502727	-0.324422
H	1.785079	0.593086	1.780858
H	0.984852	-0.226324	-1.135032
H	3.885150	-0.393636	1.394008
H	-0.750766	-0.005028	1.461227
C	-1.655198	-0.758799	-0.425195
H	2.866077	-1.141894	-1.450830
H	3.937583	-2.134558	-0.447734
H	4.508506	-0.595218	-1.076819
H	-1.546587	-1.815312	-0.158926
H	-1.413856	-0.659129	-1.490677
C	-3.066124	-0.298710	-0.187553
H	-3.275216	0.741339	-0.438982
C	-4.040009	-1.067787	0.300376
H	-3.861240	-2.108632	0.563763
H	-5.045138	-0.682164	0.447347

TS7-10binM_c3

SCF Energy: -425.151149554 H

Num. Imaginary Frequencies: 1 (i72.1251)

C	0.902029	-0.025500	-0.651138
C	0.288997	1.149806	-0.003531
C	-0.895191	1.004322	0.674025
C	-1.630709	-0.226990	1.048692
C	-2.631555	-0.775716	0.348782
C	-3.141952	-0.302519	-0.977284

O	0.888079	2.289171	-0.236238
H	-1.365875	-0.685466	2.003115
H	-1.364616	1.944397	0.970675
H	-3.117824	-1.658152	0.763075
H	1.394418	0.201537	-1.593965
C	0.942061	-1.407747	-0.226970
H	-2.640372	0.612017	-1.305009
H	-4.220593	-0.113856	-0.932167
H	-2.988651	-1.070685	-1.744791
H	1.189626	-2.127375	-1.002225
H	0.203696	-1.744456	0.491293
C	2.166185	-0.817604	0.488137
H	2.010671	-0.523077	1.520434
C	3.350606	-0.612364	-0.123493
H	3.497752	-0.851127	-1.173140
H	4.194312	-0.211256	0.429285

TS7-10binP_c3

SCF Energy: -425.152006232 H

Num. Imaginary Frequencies: 1 (i80.2881)

C	-1.251994	0.402782	0.672902
C	-0.415335	1.354634	-0.083783
C	0.947496	1.364813	0.079141
C	1.827020	0.432964	0.823087
C	2.465167	-0.618976	0.295462
C	2.345765	-1.111762	-1.113892
O	-1.085072	2.214853	-0.809147
H	2.021288	0.671702	1.870484
H	1.451456	2.215334	-0.384032
H	3.127462	-1.188403	0.946527
H	-2.261717	0.769738	0.842308
C	-0.955846	-0.895948	1.241864
H	1.689930	-0.477420	-1.716668
H	1.948483	-2.133804	-1.129810
H	3.329942	-1.150528	-1.594591
H	-1.662825	-1.240674	1.991210
H	0.080814	-1.149865	1.429942
C	-1.354032	-1.250334	-0.195985
H	-0.533962	-1.381303	-0.893820
C	-2.637267	-1.329949	-0.606863
H	-3.464669	-1.147497	0.072995
H	-2.871470	-1.595444	-1.632961

TS7-10boutM_c3

SCF Energy: -425.159883095 H

Num. Imaginary Frequencies: 1 (i109.5241)

C	3.261694	-0.300808	0.991258
C	2.703022	-0.962099	-0.229939
C	1.722261	-0.481428	-1.002754
C	1.051413	0.825329	-0.822336
C	-0.172716	1.069529	-0.224039
C	-0.726169	-0.072978	0.467726
C	-1.942738	-0.017218	1.259560
O	-0.774513	2.222754	-0.184706
H	1.407450	-1.066546	-1.868564
H	1.561544	1.696608	-1.236917
H	3.135674	-1.924881	-0.497741

H	-0.204269	-1.023102	0.408824
H	3.122655	-0.940337	1.870621
H	4.340951	-0.144409	0.882747
H	2.788899	0.664700	1.190299
H	-2.045237	-0.804843	2.001704
H	-2.218356	0.975715	1.607688
C	-2.649344	-0.354946	-0.057189
H	-3.014312	0.489507	-0.632613
C	-2.756549	-1.611010	-0.519941
H	-2.354259	-2.456415	0.032166
H	-3.269879	-1.814260	-1.454643

TS7-10boutP_c3

SCF Energy: -425.159695114 H

Num. Imaginary Frequencies: 1 (i91.8663)

C	-2.656779	0.807621	-0.914132
C	-2.517244	0.372222	0.512272
C	-1.702324	-0.593441	0.957168
C	-0.848799	-1.423535	0.078341
C	0.517361	-1.302657	-0.080314
C	1.111208	-0.232355	0.707800
C	2.448863	0.283949	0.503699
O	1.257211	-2.000801	-0.893965
H	-1.668782	-0.790303	2.029046
H	-1.348076	-2.165528	-0.545866
H	-3.123637	0.906778	1.241981
H	0.513089	0.230255	1.485990
H	-3.682642	0.655756	-1.269648
H	-2.445653	1.878983	-1.007680
H	-1.976709	0.264769	-1.576862
H	2.871389	0.836556	1.338345
H	3.144873	-0.380712	-0.001066
C	1.702290	1.180737	-0.494246
H	1.688510	0.838789	-1.523796
C	1.024103	2.280921	-0.118023
H	0.990593	2.601409	0.919776
H	0.507294	2.888877	-0.853886

10boutM

SCF Energy: -425.176436865 H

Num. Imaginary Frequencies: 0

C	-0.366531	-0.350892	0.793362
C	0.205297	-1.110218	-0.234590
O	-0.441393	-1.834606	-1.080060
C	1.612162	-1.257263	-0.021311
C	2.566879	-0.278417	0.372572
C	2.529853	1.060870	0.122055
C	1.532886	1.871972	-0.626993
H	3.475178	-0.666737	0.826229
H	2.000614	-2.259616	-0.205223
H	3.398137	1.620353	0.466584
H	0.265842	0.285917	1.400478
C	-1.827567	-0.362585	1.078523
H	0.996535	2.528327	0.068601
H	2.060284	2.527732	-1.327407
H	0.792668	1.274677	-1.162142
H	-2.290126	-1.267055	0.673515

H	-2.003081	-0.312058	2.157678
C	-2.417718	0.862155	0.407447
H	-2.168282	1.820577	0.859687
C	-3.170524	0.818184	-0.692067
H	-3.425165	-0.125484	-1.169653
H	-3.559883	1.727385	-1.141867

10binP

SCF Energy: -425.171131779 H

Num. Imaginary Frequencies: 0

C	-0.394340	1.146693	-0.348072
C	0.959000	1.337324	-0.015511
C	1.402472	0.464818	1.026388
C	1.353565	-0.944473	1.178814
C	1.348039	-1.882689	0.188428
C	1.386881	-1.690053	-1.280054
O	1.590691	2.424179	-0.282365
H	1.447657	-1.307651	2.198987
H	1.864752	1.007653	1.851522
H	1.379178	-2.919680	0.517744
H	-0.905796	2.089279	-0.556257
C	-1.234136	-0.066807	-0.488438
H	1.548457	-0.654104	-1.584646
H	0.441623	-2.035978	-1.720431
H	2.168633	-2.326993	-1.706975
H	-0.889539	-0.892169	0.148192
H	-1.100145	-0.431433	-1.522862
C	-2.694877	0.212027	-0.256570
H	-3.126807	1.028543	-0.834789
C	-3.458016	-0.477991	0.590205
H	-3.052684	-1.296254	1.182009
H	-4.512380	-0.247739	0.715287

TS11bin

SCF Energy: -425.170715817 H

Num. Imaginary Frequencies: 1 (i134.1362)

C	0.455180	1.070724	0.061754
C	-0.926686	1.342169	0.207810
O	-1.407692	2.392190	0.725248
C	-1.539805	0.612127	-0.855935
C	-1.611439	-0.785122	-1.140599
C	-1.529295	-1.805137	-0.246870
C	-1.340845	-1.732665	1.225535
H	-1.842108	-1.040601	-2.171318
H	-2.057541	1.265512	-1.558999
H	-1.665118	-2.807701	-0.648465
H	1.047053	1.987705	0.012514
C	1.231594	-0.195712	0.057714
H	-2.089975	-2.358902	1.720880
H	-0.362067	-2.148802	1.496981
H	-1.399591	-0.716550	1.622566
H	1.281753	-0.573722	1.090937
H	0.699471	-0.981381	-0.501203
C	2.618372	-0.025979	-0.499790
H	2.678716	0.373287	-1.512113
C	3.735088	-0.343531	0.154051
H	3.705304	-0.741515	1.166632

H 4.712654 -0.216097 -0.302414

TS11bout

SCF Energy: -425.176107785 H

Num. Imaginary Frequencies: 1 (i56.8662)

C	0.404172	-0.257688	-0.635034
C	-0.222188	-1.000041	0.379592
O	0.337503	-1.700474	1.281533
C	-1.522886	-1.241908	-0.162332
C	-2.509704	-0.309802	-0.625927
C	-2.676997	0.970264	-0.209866
C	-1.897545	1.746668	0.795017
H	-3.246861	-0.713537	-1.314665
H	-1.799217	-2.296271	-0.203591
H	-3.525173	1.499911	-0.640267
H	-0.167942	0.462998	-1.206123
C	1.854032	-0.405841	-0.960217
H	-1.293657	2.509412	0.289469
H	-2.586618	2.280899	1.456759
H	-1.222870	1.130379	1.393051
H	2.269366	-1.293564	-0.476096
H	1.976452	-0.495615	-2.045671
C	2.574165	0.835085	-0.478714
H	2.308470	1.764909	-0.979533
C	3.475147	0.840897	0.503820
H	3.753571	-0.072267	1.025655
H	3.965274	1.760735	0.810716

2S_3R-9b_sc

SCF Energy: -425.198858988 H

Num. Imaginary Frequencies: 0

C	-2.507921	-0.795473	-0.032974
C	-1.994350	-0.035600	-1.008947
C	-0.857101	0.925881	-0.975448
C	0.027987	1.272485	0.141299
O	0.142454	1.819576	1.217969
C	0.674759	0.479922	-0.898468
C	1.036837	-0.965524	-0.627610
H	-2.442463	-0.123815	-1.996666
H	-0.973458	1.754080	-1.674898
C	-2.101840	-0.891933	1.405113
H	-3.335715	-1.444285	-0.316910
H	1.323339	1.006641	-1.596699
H	0.279946	-1.430794	0.015837
H	1.001162	-1.521089	-1.572627
H	-1.352447	-0.155682	1.697924
H	-2.977025	-0.764463	2.051625
H	-1.697073	-1.888692	1.616844
C	2.385908	-1.159098	0.007979
H	2.687589	-2.199725	0.122468
C	3.206619	-0.197813	0.434187
H	2.958799	0.857782	0.350085
H	4.162322	-0.443641	0.888480

2S_3S-9b_sc

SCF Energy: -425.198635237 H

Num. Imaginary Frequencies: 0

C	-0.443703	-0.195422	-0.140611
C	0.270680	1.068946	-0.267618
C	0.805785	-0.015072	-1.103721
C	2.089613	-0.750330	-0.927531
C	2.864877	-0.838419	0.161176
C	2.667789	-0.212558	1.508411
O	0.345753	2.239641	0.039889
H	2.406475	-1.291870	-1.815766
H	0.500599	0.094460	-2.145565
H	3.755841	-1.457993	0.069836
H	-0.212143	-0.749060	0.770641
C	-1.836571	-0.411864	-0.710333
H	1.876559	0.539767	1.534059
H	3.595247	0.264770	1.842030
H	2.420870	-0.979280	2.252006
H	-1.971283	-1.475773	-0.931668
H	-1.915397	0.138292	-1.655882
C	-2.899550	0.065219	0.239108
H	-2.874520	1.126736	0.486217
C	-3.833583	-0.715748	0.782644
H	-3.882051	-1.780195	0.560557
H	-4.578232	-0.315482	1.465278

TS12binM

SCF Energy: -425.157893481 H

Num. Imaginary Frequencies: 1 (i204.6563)

C	-1.926127	-1.143649	0.133446
C	-1.501122	-0.483295	1.282028
C	-0.902564	0.762738	1.238188
C	-0.256488	1.153173	0.008232
C	0.479928	0.151655	-0.660960
C	1.129174	-1.116173	-0.187710
O	-0.317770	2.368930	-0.426064
H	-0.882398	1.426791	2.098487
H	-1.614135	-1.000855	2.233582
H	-2.058846	-2.221644	0.231522
C	-2.550707	-0.575573	-1.091886
H	0.714841	-1.485844	0.754049
H	0.951814	-1.907983	-0.926472
H	0.911484	0.512675	-1.597630
H	-2.439974	0.503646	-1.191762
H	-2.178447	-1.075805	-1.989943
H	-3.621435	-0.817313	-1.031119
C	2.625214	-0.971816	-0.020339
H	3.165107	-1.914870	0.057764
C	3.302844	0.174615	0.061312
H	2.813037	1.143929	-0.004705
H	4.380195	0.175777	0.200877

TS12binP

SCF Energy: -425.160670395 H

Num. Imaginary Frequencies: 1 (i187.6646)

C	-0.188079	1.647757	0.417934
C	-0.948274	0.916344	1.327506
C	-1.702455	-0.177926	0.943239
C	-1.289359	-0.891670	-0.245543
C	0.096321	-1.112797	-0.379305

C	1.161983	-1.186821	0.671874
O	-2.156840	-1.333023	-1.095539
H	-2.563429	-0.518946	1.512693
H	-0.918631	1.219843	2.373011
H	0.596378	2.273048	0.844230
C	-0.542324	1.998202	-0.985199
H	0.814501	-0.830826	1.645801
H	1.377537	-2.258352	0.816819
H	0.368970	-1.613012	-1.311030
H	-1.311020	1.364437	-1.426671
H	-0.921365	3.030004	-0.951214
H	0.340921	2.022319	-1.627568
C	2.466270	-0.520476	0.338453
H	3.266881	-0.706309	1.053289
C	2.707707	0.249845	-0.724247
H	1.945295	0.456758	-1.470253
H	3.687941	0.690477	-0.883061

TS12boutM

SCF Energy: -425.173002286 H

Num. Imaginary Frequencies: 1 (i210.2746)

C	-1.439238	1.584533	-0.325828
C	-2.359067	0.553746	-0.492055
C	-2.123085	-0.734317	-0.038351
C	-0.756698	-1.155817	0.142661
O	-0.407475	-2.026880	1.020273
C	0.128241	-0.599673	-0.813363
C	1.592273	-0.890008	-0.775622
H	-3.268086	0.769066	-1.051451
H	-2.931762	-1.438671	0.140233
C	-0.579227	1.877894	0.856852
H	-1.554491	2.433699	-1.000165
H	-0.267213	-0.093505	-1.682801
H	2.046233	-0.706362	-1.752418
H	1.729645	-1.950434	-0.518759
H	-0.497479	1.049421	1.560489
H	0.420416	2.200253	0.551949
H	-1.037523	2.735307	1.369052
C	2.271896	-0.046560	0.279216
H	1.959045	-0.225089	1.306801
C	3.184071	0.888920	0.016743
H	3.507204	1.098815	-1.000992
H	3.638814	1.470227	0.814357

TS12boutP

SCF Energy: -425.173564429 H

Num. Imaginary Frequencies: 1 (i149.6379)

C	-1.522336	-1.659333	-0.218591
C	-2.242436	-0.651841	-0.835631
C	-2.112594	0.700150	-0.514535
C	-0.882353	1.174297	0.048974
O	-0.818252	2.184703	0.846740
C	0.255610	0.477315	-0.419003
C	1.602010	0.756059	0.136098
H	-2.931156	-0.940155	-1.627858
H	-2.928451	1.398977	-0.684888
C	-0.998815	-1.738645	1.179157

H	-1.531401	-2.621089	-0.731815
H	0.171603	-0.185494	-1.270686
H	1.601367	0.499769	1.207460
H	1.757052	1.847586	0.108188
H	-1.080751	-0.805439	1.736474
H	-1.576558	-2.516594	1.694889
H	0.042875	-2.074193	1.190888
C	2.714824	0.050207	-0.582382
H	2.797466	0.252535	-1.650228
C	3.575946	-0.784580	-0.000825
H	3.518401	-1.008098	1.062836
H	4.366425	-1.267204	-0.568747

4R_5R-5b

SCF Energy: -425.274877574 H

Num. Imaginary Frequencies: 0

C	-0.005696	-0.343971	-0.315601
C	-1.386017	-0.942885	-0.077269
C	-2.383006	0.118912	-0.229458
C	-1.751773	1.292674	-0.384614
C	-0.252430	1.187709	-0.312787
O	-1.613283	-2.127173	0.171033
H	-2.244948	2.252381	-0.509430
H	-3.451939	-0.055135	-0.198134
H	0.189092	1.653177	-1.201044
C	0.264281	1.940874	0.920235
H	0.236359	-0.644308	-1.345963
C	1.061768	-0.917080	0.611697
H	0.898660	-0.566930	1.638483
H	0.932763	-2.006261	0.653763
H	-0.017938	2.996290	0.859148
H	-0.159649	1.530263	1.842147
H	1.354548	1.884964	0.981462
C	2.487667	-0.637178	0.228430
H	3.225857	-1.045189	0.918773
C	2.918760	0.031498	-0.842763
H	2.240380	0.471866	-1.569653
H	3.981750	0.162938	-1.025042

4R_5S-5b

SCF Energy: -425.275483445 H

Num. Imaginary Frequencies: 0

C	-0.030575	-0.261903	-0.274204
C	1.342040	-0.924927	-0.292921
C	2.301718	-0.041207	0.369724
C	1.676149	1.089355	0.732172
C	0.227464	1.138502	0.328183
O	1.579318	-2.033975	-0.772484
H	2.148941	1.925388	1.239645
H	3.344011	-0.294642	0.522300
C	-0.019233	2.305238	-0.636101
H	-0.389764	1.291810	1.222490
H	-0.379411	-0.192732	-1.311481
C	-0.998090	-1.131865	0.540458
H	-0.913301	-2.173392	0.203385
H	-0.674553	-1.132326	1.589847
H	-1.079720	2.381908	-0.889083

H	0.290555	3.252511	-0.183851
H	0.548016	2.165881	-1.562558
C	-2.450230	-0.746214	0.488439
H	-3.076925	-1.274980	1.206520
C	-3.029290	0.127917	-0.336132
H	-2.472016	0.686529	-1.083233
H	-4.100094	0.306467	-0.291812

4S_5R-5b

SCF Energy: -425.275483445 H

Num. Imaginary Frequencies: 0

C	-0.227460	1.138502	0.328185
C	-1.676145	1.089360	0.732172
C	-2.301718	-0.041198	0.369723
C	-1.342043	-0.924924	-0.292920
C	0.030574	-0.261904	-0.274204
C	0.998087	-1.131871	0.540455
O	-1.579324	-2.033972	-0.772482
H	-3.344013	-0.294630	0.522297
H	-2.148934	1.925396	1.239644
H	0.389770	1.291808	1.222491
C	0.019243	2.305234	-0.636102
H	0.674553	-1.132334	1.589845
H	0.913293	-2.173397	0.203379
H	0.379409	-0.192733	-1.311481
H	-0.548010	2.165880	-1.562557
H	-0.290534	3.252510	-0.183853
H	1.079731	2.381893	-0.889086
C	2.450228	-0.746223	0.488433
H	3.076926	-1.275002	1.206503
C	3.029285	0.127920	-0.336126
H	2.472007	0.686545	-1.083215
H	4.100089	0.306467	-0.291809

S_Z_Z-1b

SCF Energy: -425.190184842 H

Num. Imaginary Frequencies: 0

C	-2.330332	0.745019	-0.021012
C	-1.379302	-0.345593	-0.225072
C	-0.101528	-0.128675	-0.513388
C	-3.633830	0.617518	0.278511
O	0.725734	0.949174	-0.701281
C	1.268274	-0.440939	-0.786796
H	-1.925824	1.750448	-0.124169
H	-1.692151	-1.381390	-0.143674
H	-4.207150	1.535071	0.400870
H	1.545979	-0.705429	-1.805732
C	-4.403433	-0.653985	0.468400
H	-5.254198	-0.693357	-0.221576
H	-3.798102	-1.549664	0.311253
H	-4.819898	-0.700440	1.481602
C	2.237299	-0.833840	0.297961
H	1.853769	-0.509252	1.270227
H	2.274706	-1.930912	0.301218
C	3.610470	-0.276478	0.047557
H	4.087490	-0.577396	-0.885224
C	4.247732	0.546972	0.879869

H	3.795908	0.866406	1.816901
H	5.241498	0.922533	0.652374

TS13bin

SCF Energy: -425.154337970 H

Num. Imaginary Frequencies: 1 (i350.5669)

C	-1.325998	0.579378	1.051348
C	-0.120482	0.855093	0.328347
C	1.051185	0.166214	0.324242
C	2.212674	0.609795	-0.420400
C	3.401338	-0.020132	-0.500516
C	3.780661	-1.322823	0.132458
O	-0.556022	1.886282	-0.360889
H	2.101157	1.550461	-0.957511
H	1.088362	-0.731982	0.933730
H	4.181482	0.460300	-1.088715
H	-1.724992	1.401603	1.640807
C	-2.117717	-0.651023	0.879681
H	2.956169	-1.794932	0.671669
H	4.609803	-1.178216	0.835577
H	4.137390	-2.027106	-0.628082
H	-2.955553	-0.678310	1.577446
H	-1.431194	-1.492044	1.068484
C	-2.611160	-0.766596	-0.554089
H	-1.838302	-0.828308	-1.317099
C	-3.901104	-0.803764	-0.876769
H	-4.681629	-0.738455	-0.122647
H	-4.210905	-0.910127	-1.912358

TS13bout

SCF Energy: -425.150009610 H

Num. Imaginary Frequencies: 1 (i556.2799)

C	1.174316	-0.407151	-0.308801
C	-0.049197	0.339419	-0.176360
C	-1.316815	-0.152391	-0.135221
C	-2.472682	0.688368	0.105015
C	-3.759092	0.288689	0.151473
C	-4.284189	-1.098579	-0.053807
O	0.427907	1.560263	-0.183736
H	-2.266062	1.744435	0.271393
H	-1.426943	-1.223804	-0.276600
H	-4.510476	1.048718	0.359330
H	1.365987	-0.974570	-1.223068
C	2.273791	-0.350697	0.667141
H	-3.500895	-1.824145	-0.284808
H	-5.014406	-1.113863	-0.871469
H	-4.813408	-1.443101	0.842775
H	2.410557	-1.407536	0.954549
H	1.987840	0.226115	1.549056
C	3.566502	0.154353	0.063729
H	3.577087	1.215231	-0.178393
C	4.632933	-0.607622	-0.169454
H	4.636682	-1.670157	0.062858
H	5.537373	-0.185760	-0.598028

14bin

SCF Energy: -425.181438577 H

Num. Imaginary Frequencies: 0

C	1.364423	1.036930	-0.345540
C	0.037943	1.406929	-0.100419
C	-0.901536	0.332544	-0.161094
C	-2.224767	0.450966	0.313327
C	-3.135878	-0.564935	0.280432
C	-2.963707	-1.941246	-0.238928
O	-0.302234	2.608420	0.263079
H	-2.529609	1.407263	0.726904
H	-0.575736	-0.619503	-0.562590
H	-4.123676	-0.345759	0.682328
H	2.109608	1.795008	-0.101820
C	1.931750	-0.255689	-0.836831
H	-1.972311	-2.155372	-0.638325
H	-3.711951	-2.121454	-1.020231
H	-3.190678	-2.652994	0.563870
H	2.752138	-0.024303	-1.525050
H	1.198640	-0.855561	-1.381682
C	2.474269	-1.048784	0.332623
H	1.721930	-1.432322	1.021345
C	3.768498	-1.271321	0.559657
H	4.536219	-0.888309	-0.109492
H	4.097326	-1.846422	1.420735

14bout

SCF Energy: -425.188370370 H

Num. Imaginary Frequencies: 0

C	-3.772268	1.499111	0.217803
C	-3.561207	0.097603	-0.214137
C	-2.396820	-0.610346	-0.255268
C	-1.140213	-0.079104	0.112214
C	0.069117	-0.837856	0.076533
C	1.185064	-0.042048	0.356314
C	2.569156	-0.562201	0.324254
O	0.112738	-2.098313	-0.218731
H	-2.428685	-1.642823	-0.590132
H	-1.072840	0.956260	0.430035
H	-4.461550	-0.425256	-0.532565
H	1.025056	0.990859	0.651730
H	-4.224232	2.061150	-0.608305
H	-4.510507	1.511344	1.028630
H	-2.869898	2.012760	0.549466
H	2.762410	-1.019672	1.310117
H	2.633296	-1.405874	-0.376096
C	3.660088	0.432604	0.031991
H	4.665649	0.077048	0.250094
C	3.502347	1.654955	-0.477683
H	2.525924	2.062107	-0.730566
H	4.361884	2.292291	-0.664677

TS15bin

OPEN SHELL SINGLET ALLYL SUBSTITUTION

TS6bing

SCF Energy: -425.153356861 H

Num. Imaginary Frequencies: 1 (i331.8227)

SCF Energy: -425.178368978 H

Num. Imaginary Frequencies: 1 (i118.2607)

C	1.069825	0.583187	-0.641249
C	0.110892	1.224246	0.172752
O	-0.018665	2.475033	0.352457
C	-0.917733	0.247037	0.197127
H	1.472194	1.203391	-1.445597
C	1.696867	-0.769174	-0.502274
H	1.305362	-1.324003	0.353148
H	1.508960	-1.351447	-1.413487
C	3.189928	-0.585537	-0.345380
H	3.708511	-0.126069	-1.185653
C	3.871148	-0.950672	0.740175
H	3.376663	-1.407448	1.594998
H	4.946396	-0.808459	0.802658
C	-2.293404	0.592881	-0.015610
H	-2.521931	1.646986	-0.147481
C	-3.308671	-0.301218	-0.049871
H	-4.308997	0.099846	-0.204631
C	-3.239209	-1.779240	0.114038
H	-3.689918	-2.264469	-0.759236
H	-2.227047	-2.165248	0.244487
H	-3.842686	-2.079335	0.978697
H	-0.656038	-0.793066	0.344194

TS15bout

SCF Energy: -425.185645117 H

Num. Imaginary Frequencies: 1 (i58.9966)

C	0.857731	-0.610513	-0.202881
C	0.181442	0.596921	-0.464445
O	0.558363	1.783846	-0.239689
C	-1.141757	0.073361	-0.435766
H	0.585861	-1.510232	-0.744532
C	1.997054	-0.692340	0.762083
H	2.025732	0.199028	1.394808
H	1.872712	-1.578276	1.394436
C	3.283590	-0.813590	-0.024469
H	3.411262	-1.734398	-0.591582
C	4.224001	0.130454	-0.064011
H	4.117351	1.062497	0.486827
H	5.131482	-0.004893	-0.645843
C	-2.189941	0.703485	0.318388
H	-1.937256	1.627788	0.831305
C	-3.451373	0.227848	0.422505
H	-4.148788	0.814308	1.018449
C	-4.022088	-1.006094	-0.184831
H	-4.867434	-0.740303	-0.829994
H	-3.306472	-1.585606	-0.769727
H	-4.428286	-1.646307	0.606817
H	-1.355031	-0.831570	-0.992886

C	1.115484	0.655138	-0.638694
C	-0.063333	1.250992	-0.067593
C	-1.319798	0.731699	0.046646

C	-1.691968	-0.615942	-0.333013
C	-2.910201	-1.174193	-0.179834
C	-4.135793	-0.543476	0.404407
O	0.410475	2.397760	0.361720
H	-0.921456	-1.235553	-0.787618
H	-2.074963	1.398813	0.456369
H	-3.029892	-2.202147	-0.517794
H	1.644772	1.286913	-1.350704
C	1.733875	-0.615320	-0.258885
H	-4.485242	-1.122635	1.267517
H	-4.953040	-0.549032	-0.326413
H	-3.978240	0.486643	0.731121
H	1.390956	-1.262594	-1.098117
H	1.300862	-1.034487	0.652076
C	3.239241	-0.614212	-0.253177
H	3.723089	-0.197514	-1.134606
C	3.959963	-1.098466	0.755382
H	3.489109	-1.515334	1.642793
H	5.045433	-1.092484	0.720180

TS6boutg

SCF Energy: -425.148973841 H

Num. Imaginary Frequencies: 1 (i541.5519)

C	0.980884	-0.091992	-0.247002
C	-0.078598	0.875566	-0.101868
C	-1.417135	0.630553	-0.039944
C	-1.964708	-0.704464	-0.173569
C	-3.265147	-1.051119	-0.100998
C	-4.427284	-0.147373	0.173685
O	0.595347	1.998362	-0.141314
H	-1.245790	-1.505448	-0.350744
H	-2.076129	1.483436	0.101239
H	-3.510254	-2.101157	-0.250671
H	1.027897	-0.708692	-1.148317
C	2.103617	-0.222106	0.691470
H	-4.132331	0.890960	0.341829
H	-4.978516	-0.490536	1.057112
H	-5.135374	-0.167821	-0.663454
H	2.017405	-1.270701	1.028971
H	1.978513	0.439439	1.550898
C	3.453101	-0.039218	0.032555
H	3.685371	0.981674	-0.264080
C	4.319785	-1.025639	-0.186779
H	4.100492	-2.051417	0.100725
H	5.278854	-0.831872	-0.658292

7bing

SCF Energy: -425.179284175 H

Num. Imaginary Frequencies: 0

C	1.221149	0.911578	-0.089298
C	-0.101429	1.473209	-0.077946
C	-1.301735	0.668730	0.019197
C	-1.468656	-0.675923	-0.340412
C	-2.651122	-1.374452	-0.223216
C	-3.939707	-0.893624	0.343228
O	-0.219494	2.740726	-0.098785
H	-0.636786	-1.213561	-0.781801

H	-2.174074	1.235707	0.334765
H	-2.648072	-2.402219	-0.579615
H	2.007391	1.662877	-0.148652
C	1.657880	-0.510452	0.034629
H	-3.914982	0.141929	0.685893
H	-4.229186	-1.530297	1.188116
H	-4.734981	-0.997414	-0.404663
H	1.561197	-1.010906	-0.941285
H	0.995863	-1.049826	0.723425
C	3.080570	-0.625399	0.513848
H	3.295374	-0.172471	1.481379
C	4.053349	-1.238526	-0.159557
H	3.870199	-1.698752	-1.128670
H	5.062217	-1.301715	0.238559

7boutg

SCF Energy: -425.186573953 H

Num. Imaginary Frequencies: 0

C	4.250454	-0.312294	-0.264200
C	3.088080	-1.099044	0.227845
C	1.774172	-0.706570	0.310968
C	1.299194	0.561371	-0.068473
C	-0.057655	1.051026	-0.014277
C	-1.104984	0.137386	0.317445
C	-2.525999	0.550085	0.345446
O	-0.297653	2.272019	-0.286308
H	1.077517	-1.439509	0.706710
H	2.013683	1.293502	-0.437579
H	3.315890	-2.108822	0.562855
H	-0.862262	-0.879862	0.604732
H	5.002573	-0.236106	0.530311
H	4.732790	-0.847032	-1.091020
H	3.996536	0.693564	-0.601489
H	-2.733717	0.949949	1.353084
H	-2.682033	1.407047	-0.322139
C	-3.533843	-0.525629	0.039293
H	-4.560654	-0.271201	0.296381
C	-3.281683	-1.708094	-0.523795
H	-2.279766	-2.014474	-0.816354
H	-4.085747	-2.412622	-0.716530

TS8bing

SCF Energy: -425.169426216 H

Num. Imaginary Frequencies: 1 (i563.8528)

C	-0.949417	0.812098	0.369718
C	0.067518	1.634978	-0.159033
O	0.090545	2.903133	-0.113841
C	1.217389	0.795736	-0.115894
C	1.425889	-0.475400	-0.741017
C	2.440145	-1.314854	-0.423300
C	3.459371	-1.157767	0.648963
H	0.757724	-0.767722	-1.543549
H	2.033307	1.221772	0.468268
H	2.523478	-2.225563	-1.013646
H	-1.503075	1.294989	1.178211
C	-1.407455	-0.567786	0.003556
H	3.373003	-1.993809	1.353027

H	4.463933	-1.223316	0.216194
H	3.371961	-0.226260	1.210297
H	-1.378706	-0.722453	-1.078891
H	-0.723395	-1.312747	0.443153
C	-2.797144	-0.826555	0.523361
H	-2.938202	-0.694428	1.596045
C	-3.821572	-1.206552	-0.238826
H	-3.711005	-1.341957	-1.312865
H	-4.801725	-1.396957	0.189319

TS8boutg

SCF Energy: -425.178482554 H

Num. Imaginary Frequencies: 1 (i107.4303)

C	0.754091	-0.427378	0.081966
C	0.190707	0.813875	-0.256463
O	0.726583	1.960347	-0.205087
C	-1.189309	0.516067	-0.040255
C	-1.981619	-0.499512	-0.675859
C	-3.291673	-0.710547	-0.417711
C	-4.162174	-0.028685	0.581066
H	-1.510097	-1.096817	-1.451686
H	-1.685169	1.200521	0.647979
H	-3.786991	-1.471029	-1.018690
H	0.313942	-1.346992	-0.285122
C	1.995360	-0.534988	0.911031
H	-4.993375	0.467993	0.067363
H	-4.611169	-0.778181	1.242673
H	-3.641914	0.707592	1.195592
H	2.200278	0.413896	1.414343
H	1.863458	-1.320181	1.663390
C	3.147777	-0.898720	0.000815
H	3.108904	-1.891944	-0.443992
C	4.161039	-0.079943	-0.282554
H	4.219259	0.920377	0.141398
H	4.965015	-0.389031	-0.944775

TS7-10binMg

SCF Energy: -425.151149554 H

Num. Imaginary Frequencies: 1 (i72.1247)

C	0.902029	-0.025500	-0.651138
C	0.288997	1.149806	-0.003531
C	-0.895191	1.004322	0.674025
C	-1.630709	-0.226990	1.048692
C	-2.631555	-0.775716	0.348782
C	-3.141952	-0.302519	-0.977284
O	0.888079	2.289171	-0.236238
H	-1.365875	-0.685466	2.003115
H	-1.364616	1.944397	0.970675
H	-3.117824	-1.658152	0.763075
H	1.394418	0.201537	-1.593965
C	0.942061	-1.407747	-0.226970
H	-2.640372	0.612017	-1.305009
H	-4.220593	-0.113856	-0.932167
H	-2.988651	-1.070685	-1.744791
H	1.189626	-2.127375	-1.002225
H	0.203696	-1.744456	0.491293
C	2.166185	-0.817604	0.488137

H	2.010671	-0.523077	1.520434
C	3.350606	-0.612364	-0.123493
H	3.497752	-0.851127	-1.173140
H	4.194312	-0.211256	0.429285

TS7-10binPg

SCF Energy: -425.152006232 H

Num. Imaginary Frequencies: 1 (i80.2883)

C	-1.251994	0.402782	0.672902
C	-0.415335	1.354634	-0.083783
C	0.947496	1.364813	0.079141
C	1.827020	0.432964	0.823087
C	2.465167	-0.618976	0.295462
C	2.345765	-1.111762	-1.113892
O	-1.085072	2.214853	-0.809147
H	2.021288	0.671702	1.870484
H	1.451456	2.215334	-0.384032
H	3.127462	-1.188403	0.946527
H	-2.261717	0.769738	0.842308
C	-0.955846	-0.895948	1.241864
H	1.689930	-0.477420	-1.716668
H	1.948483	-2.133804	-1.129810
H	3.329942	-1.150528	-1.594591
H	-1.662825	-1.240674	1.991210
H	0.080814	-1.149865	1.429942
C	-1.354032	-1.250334	-0.195985
H	-0.533962	-1.381303	-0.893820
C	-2.637267	-1.329949	-0.606863
H	-3.464669	-1.147498	0.072995
H	-2.871470	-1.595444	-1.632961

TS7-10boutPg

SCF Energy: -425.159695114 H

Num. Imaginary Frequencies: 1 (i91.8657)

C	-2.656779	0.807621	-0.914132
C	-2.517244	0.372222	0.512272
C	-1.702324	-0.593441	0.957168
C	-0.848799	-1.423535	0.078341
C	0.517361	-1.302657	-0.080314
C	1.111208	-0.232355	0.707800
C	2.448863	0.283949	0.503699
O	1.257211	-2.000801	-0.893965
H	-1.668782	-0.790303	2.029046
H	-1.348076	-2.165528	-0.545866
H	-3.123637	0.906778	1.241981
H	0.513089	0.230255	1.485990
H	-3.682642	0.655756	-1.269648
H	-2.445653	1.878983	-1.007680
H	-1.976709	0.264769	-1.576862
H	2.871389	0.836556	1.338345
H	3.144873	-0.380712	-0.001066
C	1.702290	1.180737	-0.494246
H	1.688510	0.838789	-1.523796
C	1.024103	2.280921	-0.118023
H	0.990593	2.601409	0.919776
H	0.507294	2.888877	-0.853886

TS7-10boutMg

SCF Energy: -425.159946942 H

Num. Imaginary Frequencies: 1 (i302.4006)

C	3.261694	-0.300808	0.991258
C	2.703022	-0.962099	-0.229939
C	1.722261	-0.481428	-1.002754
C	1.051413	0.825329	-0.822336
C	-0.172716	1.069529	-0.224039
C	-0.726169	-0.072978	0.467726
C	-1.942738	-0.017218	1.259560
O	-0.774513	2.222754	-0.184706
H	1.407450	-1.066546	-1.868564
H	1.561544	1.696608	-1.236917
H	3.135674	-1.924881	-0.497741
H	-0.204269	-1.023102	0.408824
H	3.122655	-0.940337	1.870621
H	4.340951	-0.144409	0.882747
H	2.788899	0.664700	1.190299
H	-2.045237	-0.804843	2.001704
H	-2.218356	0.975715	1.607688
C	-2.649344	-0.354946	-0.057189
H	-3.014312	0.489507	-0.632613
C	-2.756549	-1.611010	-0.519941
H	-2.354259	-2.456415	0.032166
H	-3.269879	-1.814260	-1.454643

10binMg

SCF Energy: -425.174238827 H

Num. Imaginary Frequencies: 0

C	0.591438	0.876952	-0.459344
C	-0.712345	1.377744	-0.160438
C	-1.543029	0.759494	0.860761
C	-1.896729	-0.582479	1.092974
C	-1.850132	-1.661430	0.240391
C	-1.439503	-1.711341	-1.186864
O	-1.084570	2.487873	-0.656786
H	-2.368860	-0.765870	2.056066
H	-2.005239	1.492901	1.519433
H	-2.215485	-2.601199	0.649424
H	1.203230	1.570370	-1.035914
C	1.263622	-0.380173	-0.030627
H	-1.309718	-0.725525	-1.639552
H	-2.184080	-2.274472	-1.759553
H	-0.493846	-2.259313	-1.290926
H	1.393784	-1.019539	-0.916545
H	0.652667	-0.937750	0.684387
C	2.619746	-0.092359	0.567814
H	2.617169	0.493922	1.485971
C	3.775861	-0.505236	0.048878
H	3.810547	-1.090868	-0.867738
H	4.722825	-0.272666	0.527965

10binPg

SCF Energy: -425.174493276 H

Num. Imaginary Frequencies: 0

C	-0.549283	0.929458	-0.650067
C	0.635210	1.404629	-0.009889

C	1.255065	0.665300	1.077840
C	1.605539	-0.691519	1.205372
C	1.787083	-1.644393	0.229660
C	1.691556	-1.501168	-1.246094
O	1.053463	2.578866	-0.264487
H	1.868293	-0.997856	2.215895
H	1.535768	1.308655	1.910045
H	2.094911	-2.627362	0.580389
H	-1.050494	1.685324	-1.254590
C	-1.244585	-0.379808	-0.536431
H	1.628517	-0.463048	-1.581369
H	0.807259	-2.032706	-1.621920
H	2.557542	-1.979188	-1.716030
H	-0.806839	-1.019194	0.233338
H	-1.126571	-0.903361	-1.499363
C	-2.719381	-0.179000	-0.284168
H	-3.260242	0.394798	-1.036017
C	-3.362004	-0.651901	0.782932
H	-2.844082	-1.221580	1.551911
H	-4.426968	-0.484990	0.918672

10boutMg

SCF Energy: -425.179787005 H

Num. Imaginary Frequencies: 0

C	-0.354047	-0.397667	0.845158
C	0.288379	-1.220053	-0.125665
O	-0.347283	-2.028143	-0.875216
C	1.732891	-1.214197	-0.103959
C	2.615274	-0.150015	0.200608
C	2.418573	1.201464	0.080956
C	1.260850	1.949613	-0.487530
H	3.621318	-0.457831	0.479303
H	2.192410	-2.164549	-0.371189
H	3.262347	1.823403	0.374177
H	0.252909	0.264898	1.452901
C	-1.827546	-0.380829	1.037441
H	0.715523	2.475704	0.305119
H	1.634771	2.719488	-1.170851
H	0.550141	1.312601	-1.019069
H	-2.280908	-1.285922	0.624533
H	-2.060553	-0.313123	2.105660
C	-2.373945	0.841789	0.325800
H	-2.103788	1.804897	0.755798
C	-3.116735	0.788420	-0.779722
H	-3.391363	-0.160678	-1.234995
H	-3.476704	1.695103	-1.258182

10boutPg

SCF Energy: -425.179927488 H

Num. Imaginary Frequencies: 0

C	-0.458198	0.098271	0.017011
C	0.432644	1.201289	-0.114344
O	0.116636	2.267091	-0.736010
C	1.655630	1.121880	0.646335
C	2.435411	-0.014753	0.974179
C	2.558239	-1.204055	0.305642
C	1.981318	-1.625598	-1.002706

H	3.098758	0.119732	1.826396
H	2.022507	2.080885	1.009130
H	3.238621	-1.924359	0.756104
H	-0.128396	-0.782290	0.559376
C	-1.830999	0.124042	-0.542395
H	2.771727	-2.074744	-1.613380
H	1.222356	-2.403390	-0.856529
H	1.520268	-0.805559	-1.557919
H	-2.242768	1.139253	-0.481170
H	-1.737962	-0.087550	-1.622641
C	-2.753540	-0.883137	0.084418
H	-2.415412	-1.919036	0.064979
C	-3.926123	-0.580556	0.640516
H	-4.288793	0.444831	0.677674
H	-4.560289	-1.348799	1.074135

TS11bing

SCF Energy: -425.170715817 H

Num. Imaginary Frequencies: 1 (i134.1349)

C	0.455181	1.070724	0.061755
C	-0.926686	1.342169	0.207810
O	-1.407691	2.392191	0.725248
C	-1.539806	0.612128	-0.855934
C	-1.611440	-0.785121	-1.140599
C	-1.529295	-1.805137	-0.246870
C	-1.340846	-1.732665	1.225534
H	-1.842110	-1.040600	-2.171317
H	-2.057542	1.265513	-1.558998
H	-1.665120	-2.807700	-0.648465
H	1.047054	1.987704	0.012517
C	1.231594	-0.195713	0.057714
H	-2.089976	-2.358902	1.720879
H	-0.362068	-2.148803	1.496981
H	-1.399592	-0.716551	1.622566
H	1.281754	-0.573723	1.090936
H	0.699471	-0.981381	-0.501204
C	2.618372	-0.025980	-0.499791
H	2.678717	0.373287	-1.512113
C	3.735088	-0.343532	0.154050
H	3.705304	-0.741517	1.166631
H	4.712655	-0.216098	-0.302415

TS11boutg

SCF Energy: -425.176107785 H

Num. Imaginary Frequencies: 1 (i56.8659)

C	0.404172	-0.257688	-0.635034
C	-0.222188	-1.000041	0.379592
O	0.337503	-1.700474	1.281533
C	-1.522886	-1.241908	-0.162332
C	-2.509704	-0.309802	-0.625927
C	-2.676997	0.970264	-0.209866
C	-1.897545	1.746668	0.795017
H	-3.246861	-0.713537	-1.314665
H	-1.799217	-2.296271	-0.203591
H	-3.525173	1.499911	-0.640267
H	-0.167942	0.462998	-1.206123
C	1.854032	-0.405841	-0.960217

H	-1.293657	2.509412	0.289469
H	-2.586618	2.280899	1.456759
H	-1.222870	1.130379	1.393051
H	2.269366	-1.293564	-0.476096
H	1.976452	-0.495615	-2.045671
C	2.574165	0.835085	-0.478714
H	2.308470	1.764909	-0.979533
C	3.475147	0.840897	0.503820
H	3.753571	-0.072267	1.025655
H	3.965274	1.760735	0.810716

TS12binMg

SCF Energy: -425.162408924 H

Num. Imaginary Frequencies: 1 (i295.7133)

C	-1.994076	-1.054674	0.110790
C	-1.682888	-0.296632	1.251144
C	-0.985519	0.891904	1.196687
C	-0.179187	1.136742	0.016992
C	0.405442	-0.028014	-0.621266
C	1.089722	-1.180004	0.049009
O	0.026866	2.292816	-0.453084
H	-0.995978	1.615472	2.006346
H	-1.984270	-0.698243	2.218517
H	-2.188983	-2.113172	0.282765
C	-2.466804	-0.557431	-1.220649
H	0.704319	-1.352242	1.058462
H	0.896649	-2.097214	-0.520966
H	0.690944	0.133314	-1.661388
H	-2.306636	0.511636	-1.369425
H	-2.003187	-1.108024	-2.044222
H	-3.545663	-0.756163	-1.282538
C	2.588913	-0.998962	0.138836
H	3.130684	-1.891761	0.449091
C	3.267691	0.123171	-0.105044
H	2.778978	1.045495	-0.411972
H	4.348448	0.151781	0.001006

TS12binPg

SCF Energy: -425.164652013 H

Num. Imaginary Frequencies: 1 (i251.0238)

C	-0.214980	1.664275	0.396816
C	-1.034199	0.962879	1.291791
C	-1.771546	-0.146957	0.923749
C	-1.324460	-0.887950	-0.239967
C	0.107864	-0.933281	-0.457364
C	1.125618	-1.201508	0.602504
O	-2.113353	-1.490486	-1.025419
H	-2.635216	-0.489819	1.485962
H	-1.064411	1.308252	2.325018
H	0.561028	2.285675	0.842644
C	-0.519150	1.996790	-1.031962
H	0.757025	-0.920230	1.594348
H	1.244424	-2.298114	0.642952
H	0.407305	-1.182946	-1.475846
H	-1.315244	1.388919	-1.464342
H	-0.839301	3.047597	-1.060038
H	0.368627	1.928389	-1.666194

C	2.491530	-0.614062	0.385034
H	3.245022	-0.953592	1.094298
C	2.838131	0.253945	-0.566408
H	2.126955	0.623571	-1.300234
H	3.857759	0.621398	-0.640373

TS12boutMg

SCF Energy: -425.173460952 H

Num. Imaginary Frequencies: 1 (i272.3982)

C	-1.431716	1.572770	-0.339831
C	-2.384081	0.554258	-0.437961
C	-2.142918	-0.728591	0.015223
C	-0.767486	-1.155130	0.141047
O	-0.384878	-2.027794	0.990317
C	0.101896	-0.583442	-0.837239
C	1.572398	-0.841903	-0.814291
H	-3.320962	0.780700	-0.945269
H	-2.944985	-1.431465	0.223834
C	-0.547303	1.886925	0.822674
H	-1.549438	2.402899	-1.036742
H	-0.321680	-0.130184	-1.723226
H	2.016689	-0.601350	-1.783045
H	1.724025	-1.915404	-0.623885
H	-0.453363	1.068266	1.536997
H	0.447644	2.202328	0.497472
H	-0.995214	2.749812	1.335216
C	2.264407	-0.062597	0.280258
H	1.935134	-0.269299	1.297372
C	3.217311	0.843102	0.062782
H	3.559115	1.078833	-0.943147
H	3.687008	1.374866	0.885905

TS12boutPg

SCF Energy: -425.175015694 H

Num. Imaginary Frequencies: 1 (i226.6810)

C	1.198880	1.739212	-0.212498
C	2.191323	0.881756	-0.682286
C	2.254828	-0.469379	-0.365976
C	1.043691	-1.137108	0.040278
O	1.025766	-2.156684	0.805432
C	-0.150618	-0.583934	-0.524834
C	-1.488523	-0.949229	0.003402
H	2.935193	1.301590	-1.358366
H	3.182711	-1.031016	-0.432738
C	0.515316	1.745766	1.121011
H	1.079862	2.669686	-0.767567
H	-0.090520	-0.006283	-1.439729
H	-1.487404	-0.852451	1.098177
H	-1.646186	-2.023138	-0.195457
H	0.717038	0.856995	1.720753
H	0.874959	2.627627	1.667291
H	-0.567787	1.867816	1.017180
C	-2.601903	-0.146240	-0.606999
H	-2.696324	-0.205308	-1.691159
C	-3.445801	0.615028	0.089184
H	-3.374549	0.696727	1.172039
H	-4.236281	1.175991	-0.401578

TS16bing

SCF Energy: -425.150124301 H

Num. Imaginary Frequencies: 1 (i304.2676)

C	-0.471198	0.153868	0.603360
C	0.342146	1.291799	0.264848
C	1.515934	1.299064	-0.424631
C	2.200222	0.120386	-0.936960
C	2.352862	-1.099140	-0.377617
C	1.945736	-1.581391	0.981377
O	-0.416163	2.277538	0.685174
H	2.688172	0.271441	-1.899552
H	1.946782	2.270880	-0.658027
H	2.900717	-1.829385	-0.971578
H	-0.800754	0.098737	1.639712
C	-1.121857	-0.748448	-0.361288
H	1.665777	-0.764107	1.655011
H	2.773952	-2.132862	1.439401
H	1.101203	-2.279037	0.927735
H	-1.168777	-1.749184	0.083868
H	-0.582377	-0.769016	-1.310560
C	-2.540285	-0.230270	-0.564612
H	-2.621572	0.695814	-1.128326
C	-3.624044	-0.843966	-0.094169
H	-3.556162	-1.765995	0.478107
H	-4.614747	-0.439002	-0.279041

TS16boutg

SCF Energy: -425.148723421 H

Num. Imaginary Frequencies: 1 (i489.2551)

C	0.384115	0.282766	-0.365673
C	-0.572302	1.266179	0.088443
C	-1.919012	1.207759	-0.065595
C	-2.517545	0.034635	-0.683891
C	-2.279152	-1.264240	-0.389701
C	-1.584320	-1.843515	0.806549
O	0.260773	2.209068	0.447336
H	-3.230455	0.234546	-1.484755
H	-2.524205	2.086017	0.143002
H	-2.759462	-2.000540	-1.033357
H	0.459693	0.101784	-1.441141
C	1.418631	-0.335862	0.479789
H	-1.247106	-1.080727	1.512885
H	-0.721922	-2.456690	0.521422
H	-2.278448	-2.514449	1.326136
H	1.262319	-1.418757	0.341519
H	1.262906	-0.088676	1.532402
C	2.821062	0.004847	0.027286
H	3.114368	1.042476	0.173938
C	3.667877	-0.869421	-0.512386
H	3.392211	-1.909729	-0.670015
H	4.667792	-0.566698	-0.809641

TS13bing

SCF Energy: -425.154337970 H

Num. Imaginary Frequencies: 1 (i350.5671)

C	-1.325998	0.579378	1.051348
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C	-0.120482	0.855093	0.328347
C	1.051185	0.166214	0.324242
C	2.212674	0.609795	-0.420400
C	3.401338	-0.020132	-0.500516
C	3.780661	-1.322823	0.132458
O	-0.556022	1.886282	-0.360889
H	2.101157	1.550461	-0.957511
H	1.088362	-0.731982	0.933730
H	4.181482	0.460300	-1.088715
H	-1.724992	1.401603	1.640807
C	-2.117717	-0.651023	0.879681
H	2.956169	-1.794932	0.671669
H	4.609803	-1.178216	0.835577
H	4.137390	-2.027106	-0.628082
H	-2.955553	-0.678310	1.577446
H	-1.431194	-1.492044	1.068484
C	-2.611160	-0.766596	-0.554089
H	-1.838302	-0.828308	-1.317099
C	-3.901104	-0.803764	-0.876769
H	-4.681629	-0.738455	-0.122647
H	-4.210905	-0.910127	-1.912358

TS13boutg

SCF Energy: -425.150009610 H

Num. Imaginary Frequencies: 1 (i556.2801)

C	1.174316	-0.407151	-0.308801
C	-0.049197	0.339419	-0.176360
C	-1.316815	-0.152391	-0.135221
C	-2.472682	0.688368	0.105015
C	-3.759092	0.288689	0.151473
C	-4.284189	-1.098579	-0.053807
O	0.427907	1.560263	-0.183736
H	-2.266062	1.744435	0.271393
H	-1.426943	-1.223804	-0.276600
H	-4.510476	1.048718	0.359330
H	1.365987	-0.974570	-1.223068
C	2.273791	-0.350697	0.667141
H	-3.500895	-1.824145	-0.284808
H	-5.014406	-1.113863	-0.871469
H	-4.813408	-1.443101	0.842775
H	2.410557	-1.407536	0.954549
H	1.987840	0.226115	1.549056
C	3.566502	0.154353	0.063729
H	3.577087	1.215231	-0.178393
C	4.632933	-0.607622	-0.169454
H	4.636682	-1.670157	0.062858
H	5.537373	-0.185760	-0.598028

14bing

SCF Energy: -425.187194624 H

Num. Imaginary Frequencies: 0

C	-1.434490	1.087452	0.399280
C	-0.078709	1.393066	0.059749
C	0.880083	0.319073	0.136671
C	2.208335	0.467810	-0.295183
C	3.163284	-0.517539	-0.254079
C	3.010488	-1.906538	0.253987

O	0.238873	2.566212	-0.323223
H	2.497108	1.435964	-0.696187
H	0.549588	-0.637166	0.524935
H	4.151236	-0.262061	-0.631758
H	-2.148248	1.891090	0.226667
C	-1.993236	-0.214865	0.872557
H	2.012018	-2.133120	0.630947
H	3.736582	-2.084709	1.056293
H	3.255567	-2.618005	-0.543598
H	-2.870965	-0.015822	1.494521
H	-1.269513	-0.768722	1.478728
C	-2.402951	-1.058513	-0.317081
H	-1.586845	-1.393690	-0.956397
C	-3.661097	-1.384964	-0.610750
H	-4.493325	-1.055644	0.007816
H	-3.894432	-1.997699	-1.477085

14boutg

SCF Energy: -425.191637055 H

Num. Imaginary Frequencies: 0

C	-3.857959	1.459029	0.205294
C	-3.607437	0.048821	-0.191278
C	-2.408428	-0.611346	-0.232393
C	-1.163144	-0.042287	0.095982
C	0.067139	-0.784986	0.045332
C	1.215693	-0.004570	0.359690
C	2.584974	-0.563147	0.371252
O	0.128181	-2.022950	-0.255636
H	-2.412841	-1.652920	-0.543054
H	-1.103019	0.998408	0.397367
H	-4.490046	-0.518005	-0.481300
H	1.066850	1.030527	0.654922
H	-4.321691	1.995870	-0.631055
H	-4.587181	1.482285	1.023766
H	-2.963217	1.999535	0.517110
H	2.759114	-0.974091	1.380956
H	2.639696	-1.438129	-0.289110
C	3.701097	0.394473	0.047640
H	4.697141	0.021086	0.279231
C	3.573690	1.603848	-0.499978
H	2.607484	2.026115	-0.766913
H	4.448520	2.213906	-0.706077

TS15bing

SCF Energy: -425.178368977 H

Num. Imaginary Frequencies: 1 (i118.2569)

C	-1.069829	0.583187	0.641258
C	-0.110894	1.224244	-0.172744
O	0.018662	2.475031	-0.352451
C	0.917732	0.247036	-0.197121
H	-1.472202	1.203395	1.445601
C	-1.696871	-0.769173	0.502289
H	-1.305356	-1.324014	-0.353120
H	-1.508981	-1.351436	1.413512
C	-3.189928	-0.585529	0.345370
H	-3.708520	-0.126039	1.185626
C	-3.871137	-0.950683	-0.740185

H	-3.376643	-1.407481	-1.594992
H	-4.946383	-0.808464	-0.802686
C	2.293404	0.592882	0.015611
H	2.521930	1.646987	0.147484
C	3.308672	-0.301216	0.049867
H	4.308997	0.099848	0.204627
C	3.239212	-1.779238	-0.114052
H	3.689935	-2.264473	0.759211
H	2.227049	-2.165248	-0.244489
H	3.842676	-2.079323	-0.978724
H	0.656036	-0.793067	-0.344185

TS15boutg

SCF Energy: -425.185645117 H

Num. Imaginary Frequencies: 1 (i58.9963)

C	0.857731	-0.610513	-0.202881
C	0.181442	0.596921	-0.464445
O	0.558363	1.783846	-0.239689
C	-1.141757	0.073361	-0.435766

H	0.585861	-1.510232	-0.744532
C	1.997054	-0.692340	0.762083
H	2.025732	0.199028	1.394808
H	1.872712	-1.578276	1.394436
C	3.283590	-0.813590	-0.024469
H	3.411262	-1.734398	-0.591582
C	4.224001	0.130454	-0.064011
H	4.117351	1.062497	0.486827
H	5.131482	-0.004893	-0.645843
C	-2.189941	0.703485	0.318388
H	-1.937256	1.627788	0.831305
C	-3.451373	0.227848	0.422505
H	-4.148788	0.814308	1.018449
C	-4.022088	-1.006094	-0.184831
H	-4.867434	-0.740303	-0.829994
H	-3.306472	-1.585606	-0.769727
H	-4.428286	-1.646307	0.606817
H	-1.355031	-0.831570	-0.992886

OPEN SHELL TRIPLET ISOMERIZATION ALLYL SUBSTITUTION

7bint

SCF Energy: -425.176102390 H

Num. Imaginary Frequencies: 0

C	1.239584	0.875351	-0.261849
C	-0.073115	1.446725	-0.080664
C	-1.299650	0.675473	0.093182
C	-1.520208	-0.611112	-0.403568
C	-2.699019	-1.325656	-0.289650
C	-3.945035	-0.895061	0.405445
O	-0.160516	2.707775	-0.047171
H	-0.717305	-1.093995	-0.954496
H	-2.106416	1.223588	0.571852
H	-2.729443	-2.304739	-0.762213
H	2.003058	1.580899	-0.581988
C	1.656734	-0.528430	0.025730
H	-3.838158	0.044436	0.951227
H	-4.268711	-1.669222	1.110748
H	-4.759996	-0.779653	-0.320633
H	1.571190	-1.134422	-0.889810
H	0.974218	-0.976648	0.758626
C	3.073205	-0.601456	0.533232
H	3.276313	-0.063825	1.458978
C	4.056223	-1.267080	-0.072669
H	3.885970	-1.811324	-0.999727
H	5.061094	-1.289828	0.339678

TS7bin-outt

SCF Energy: -425.165318360 H

Num. Imaginary Frequencies: 1 (i182.3201)

C	1.380916	-0.598292	-0.277861
C	1.301839	0.766974	0.017085
C	0.071411	1.513493	-0.091361
C	2.514899	-1.380201	-0.188501
O	0.030511	2.721672	0.231224
C	-1.164012	0.845054	-0.569870

H	0.464882	-1.090875	-0.601638
H	2.170341	1.323914	0.358400
H	2.408643	-2.432036	-0.444461
C	3.877905	-0.945739	0.219581
H	3.950735	0.119250	0.445825
H	4.199840	-1.512639	1.101777
H	4.594659	-1.182823	-0.575849
H	-1.394285	0.886803	-1.631702
C	-2.164441	0.311125	0.407337
H	-1.652699	-0.075732	1.297700
H	-2.806480	1.138216	0.757371
C	-3.033584	-0.756387	-0.199264
H	-3.590447	-0.466750	-1.090612
C	-3.149828	-1.995626	0.277908
H	-2.603486	-2.316430	1.162871
H	-3.796417	-2.726690	-0.199792

7boutt

SCF Energy: -425.178304519 H

Num. Imaginary Frequencies: 0

C	4.282594	-0.192374	-0.298232
C	3.170609	-1.004418	0.270147
C	1.835197	-0.650522	0.345883
C	1.287426	0.550934	-0.107813
C	-0.120863	0.929651	-0.030496
C	-1.127234	0.071774	0.549330
C	-2.558019	0.453502	0.658378
O	-0.453317	2.055799	-0.494651
H	1.173508	-1.384039	0.800664
H	1.921129	1.303472	-0.568169
H	3.446300	-1.978147	0.668627
H	-0.836714	-0.900071	0.936064
H	5.046019	-0.012035	0.468672
H	4.781145	-0.746557	-1.102765
H	3.960972	0.772560	-0.694235

H	-2.820286	0.511113	1.726229
H	-2.724982	1.456906	0.253052
C	-3.518613	-0.510771	0.004371
H	-4.568312	-0.324909	0.226961
C	-3.190867	-1.521299	-0.802139
H	-2.157428	-1.743913	-1.059914
H	-3.956199	-2.159626	-1.234545

TS7-14bint

SCF Energy: -425.167887112 H

Num. Imaginary Frequencies: 1 (i101.2633)

C	1.973973	0.197615	0.662545
C	1.030889	0.420245	-0.327270
C	-0.160098	1.287281	-0.100902
C	3.122684	-0.572977	0.509612
O	-0.075301	2.522603	-0.308048
C	-1.396540	0.722830	0.342462
H	1.803053	0.655952	1.635991
H	1.130418	-0.021677	-1.316877
H	3.782533	-0.672188	1.367061
H	-2.220620	1.420637	0.478404
C	3.506493	-1.258752	-0.762261
H	4.424565	-1.836628	-0.638484
H	2.718556	-1.941400	-1.105881
H	3.668922	-0.536469	-1.573310
C	-1.607012	-0.705596	0.681072
H	-1.587382	-0.789868	1.780699
H	-0.768176	-1.320174	0.333150
C	-2.903263	-1.301217	0.193433
H	-3.138834	-2.276040	0.616928
C	-3.736814	-0.756327	-0.693459
H	-3.546834	0.210441	-1.154585
H	-4.645668	-1.272028	-0.990107

TS7-14boutt

SCF Energy: -425.167811032 H

Num. Imaginary Frequencies: 1 (i106.5339)

C	2.027952	-0.403378	0.657544
C	1.393866	0.421121	-0.256799
C	0.001359	0.909449	-0.045871
C	3.331606	-0.876981	0.537562
O	-0.199822	1.977740	0.575591
C	-1.082072	0.133591	-0.575511
H	1.464930	-0.706280	1.539790
H	1.893237	0.755912	-1.163975
H	3.712570	-1.512466	1.332251
H	-0.838127	-0.788622	-1.097252
C	4.240754	-0.550047	-0.603255
H	5.165388	-1.128621	-0.550291
H	3.765738	-0.752990	-1.571233
H	4.511439	0.514564	-0.604574
C	-2.516854	0.499565	-0.428062
H	-2.974192	0.535133	-1.425213
H	-2.607361	1.489685	0.028473
C	-3.242742	-0.526874	0.412074
H	-2.925184	-0.597306	1.451476
C	-4.208707	-1.324511	-0.043350

H	-4.544009	-1.277790	-1.077464
H	-4.696831	-2.044742	0.607286

14bint

SCF Energy: -425.179101959 H

Num. Imaginary Frequencies: 0

C	-1.493857	1.137354	0.374248
C	-0.115830	1.358749	0.006053
C	0.872233	0.286179	0.084533
C	2.221855	0.497551	-0.202016
C	3.214621	-0.462856	-0.161291
C	3.054586	-1.900631	0.196832
O	0.215331	2.511712	-0.389313
H	2.517699	1.505812	-0.483935
H	0.525725	-0.701219	0.370579
H	4.222811	-0.144965	-0.417542
H	-2.164769	1.975725	0.207697
C	-2.060634	-0.146677	0.884351
H	2.036374	-2.166563	0.487596
H	3.728688	-2.158995	1.022318
H	3.346932	-2.534339	-0.649749
H	-2.973810	0.058664	1.449860
H	-1.348977	-0.638984	1.559148
C	-2.381130	-1.077197	-0.267336
H	-1.528913	-1.424918	-0.850442
C	-3.613843	-1.460883	-0.599242
H	-4.484218	-1.125107	-0.039134
H	-3.788212	-2.128339	-1.438681

14boutt

SCF Energy: -425.178824973 H

Num. Imaginary Frequencies: 0

C	-4.045576	1.184871	0.294647
C	-3.596637	-0.084093	-0.345469
C	-2.309098	-0.590063	-0.373166
C	-1.183099	0.003254	0.194109
C	0.145253	-0.605569	0.116810
C	1.267759	0.091509	0.699984
C	2.648163	-0.453760	0.724516
O	0.317150	-1.716052	-0.451911
H	-2.162503	-1.537856	-0.887300
H	-1.256715	0.951857	0.717705
H	-4.368167	-0.665713	-0.845053
H	1.088671	1.070376	1.138232
H	-4.445352	1.869949	-0.463784
H	-4.868493	0.984228	0.991084
H	-3.252722	1.702583	0.838027
H	2.985516	-0.503978	1.770478
H	2.661895	-1.483086	0.349574
C	3.660313	0.363687	-0.043793
H	4.696517	0.067941	0.113650
C	3.385715	1.369914	-0.875015
H	2.366042	1.696405	-1.069326
H	4.181351	1.897207	-1.393738

TS14bin-outt

SCF Energy: -425.163251978 H

Num. Imaginary Frequencies: 1 (i186.1381)

C	2.450927	-0.494499	-0.186480
C	1.148363	-0.142644	0.189872
C	0.056968	-1.092481	0.189252
C	3.535208	0.355139	-0.210116
O	0.204590	-2.286384	-0.148276
C	-1.288163	-0.608948	0.593085
H	2.619682	-1.526950	-0.484163
H	0.911353	0.870220	0.501320
H	4.486621	-0.068986	-0.523858
C	3.556118	1.799723	0.146307
H	2.583268	2.193625	0.444994
H	4.266492	1.969148	0.964695
H	3.923984	2.385294	-0.704759
H	-1.602292	-0.779500	1.620488
C	-2.282387	-0.207194	-0.451464
H	-1.817882	0.478521	-1.173389
H	-2.569070	-1.102705	-1.030751
C	-3.521044	0.409998	0.135077
H	-4.050413	-0.197633	0.869435
C	-3.990509	1.616473	-0.182540
H	-3.484190	2.250453	-0.907953
H	-4.897158	2.006182	0.272192

TS7-10binMt

SCF Energy: -425.155068844 H

Num. Imaginary Frequencies: 1 (i141.9023)

C	0.735533	1.231133	-0.013016
C	-0.661639	1.568465	-0.121586
C	-1.775595	0.724302	0.255381
C	-1.732499	-0.548968	0.993802
C	-1.737744	-1.765016	0.438367
C	-1.708392	-2.050229	-1.030798
O	-0.946704	2.711294	-0.602662
H	-1.730795	-0.465969	2.082549
H	-2.749307	1.149392	0.017217
H	-1.735690	-2.628719	1.100971
H	1.412241	2.036037	-0.289791
C	1.311359	-0.081953	0.397750
H	-1.742601	-1.134501	-1.628569
H	-2.551380	-2.687508	-1.320213
H	-0.794449	-2.596267	-1.294079
H	0.892997	-0.889127	-0.219111
H	0.992668	-0.306884	1.427229
C	2.812829	-0.099601	0.329031
H	3.326452	0.679119	0.892987
C	3.523456	-0.994076	-0.357547
H	3.040006	-1.781785	-0.932406
H	4.609650	-0.968478	-0.363791

TS7-10binPt

SCF Energy: -425.155058042 H

Num. Imaginary Frequencies: 1 (i135.3742)

C	-0.795565	1.121626	-0.194257
C	0.557489	1.576021	0.007216
C	1.660610	0.779688	0.500806
C	1.610179	-0.580258	1.063188

C	1.856144	-1.704182	0.382188
C	2.145329	-1.784904	-1.084197
O	0.810985	2.788627	-0.283426
H	1.384330	-0.646622	2.129364
H	2.614719	1.304129	0.503440
H	1.819087	-2.648030	0.923229
H	-1.481441	1.897767	-0.525131
C	-1.306711	-0.272142	-0.049417
H	2.168753	-0.796377	-1.552439
H	1.380447	-2.386084	-1.589920
H	3.106426	-2.279361	-1.264691
H	-1.150920	-0.635977	0.975157
H	-0.704772	-0.936667	-0.689012
C	-2.756716	-0.393215	-0.427291
H	-3.020284	-0.042519	-1.425271
C	-3.703198	-0.895826	0.365145
H	-3.474009	-1.251622	1.367857
H	-4.735576	-0.968494	0.034533

TS7-10boutMt

SCF Energy: -425.156964314 H

Num. Imaginary Frequencies: 1 (i111.9818)

C	3.225479	-0.557109	1.138197
C	2.750731	-1.119921	-0.165399
C	1.919953	-0.509799	-1.018469
C	1.350282	0.832848	-0.826072
C	0.055469	1.083503	-0.226364
C	-0.735921	0.012970	0.328025
C	-2.063622	0.217855	0.960437
O	-0.368258	2.277330	-0.191099
H	1.622842	-1.031104	-1.931300
H	1.888322	1.711180	-1.176121
H	3.110180	-2.114543	-0.423880
H	-0.328223	-0.993668	0.291852
H	2.936352	-1.215202	1.965550
H	4.319232	-0.491126	1.154910
H	2.814708	0.438551	1.330076
H	-1.985671	-0.043951	2.027143
H	-2.346134	1.275901	0.933084
C	-3.181216	-0.607598	0.369101
H	-4.114090	-0.574585	0.930094
C	-3.117443	-1.334808	-0.747182
H	-2.212020	-1.396654	-1.347326
H	-3.981705	-1.891084	-1.098927

TS7-10boutPt

SCF Energy: -425.157651817 H

Num. Imaginary Frequencies: 1 (i113.7677)

C	2.417462	-1.544540	-0.656410
C	2.632266	-0.707511	0.566755
C	2.151628	0.526521	0.758784
C	1.343148	1.269105	-0.220197
C	-0.104504	1.265566	-0.229862
C	-0.859148	0.536203	0.760971
C	-2.329116	0.336735	0.673705
O	-0.703405	1.899824	-1.148448
H	2.348255	1.029299	1.708167

H	1.824155	1.860030	-0.996575
H	3.218731	-1.157953	1.365669
H	-0.312046	0.034016	1.553670
H	3.376543	-1.822810	-1.107703
H	1.909519	-2.479667	-0.394130
H	1.816848	-1.026468	-1.410007
H	-2.766355	0.416046	1.677093
H	-2.793074	1.121541	0.065686
C	-2.720843	-1.008404	0.099149
H	-3.787628	-1.224686	0.136012
C	-1.886909	-1.902937	-0.433612
H	-0.813846	-1.728419	-0.496053
H	-2.257763	-2.843941	-0.829950

10binMt

SCF Energy: -425.171353920 H

Num. Imaginary Frequencies: 0

C	0.124613	1.292703	-0.222389
C	-1.292795	1.078090	-0.112492
C	-1.886590	0.042898	0.750381
C	-1.547579	-1.308434	0.853881
C	-0.745529	-2.081631	0.029746
C	-0.133316	-1.684345	-1.272045
O	-2.069243	1.865768	-0.717560
H	-2.027187	-1.838315	1.675187
H	-2.712775	0.402103	1.359870
H	-0.583428	-3.109670	0.344778
H	0.431055	2.000818	-0.989706
C	1.156482	0.774476	0.719274
H	-0.713239	-0.915366	-1.790416
H	-0.054439	-2.555545	-1.928820
H	0.887089	-1.297785	-1.139546
H	0.884769	-0.207917	1.117841
H	1.168165	1.457854	1.587034
C	2.534449	0.741147	0.116592
H	2.895725	1.677631	-0.307767
C	3.307656	-0.343634	0.082393
H	2.972020	-1.293214	0.494757
H	4.301839	-0.314364	-0.354782

10binPt

SCF Energy: -425.170358299 H

Num. Imaginary Frequencies: 0

C	-0.551524	0.673783	-0.641621
C	0.591260	1.334857	-0.070331
C	1.332678	0.764118	1.065187
C	1.810649	-0.544039	1.205150
C	1.985814	-1.521689	0.242041
C	1.856116	-1.380634	-1.238650
O	0.914833	2.474969	-0.497991
H	2.143841	-0.805860	2.208278
H	1.517167	1.462577	1.878342
H	2.324591	-2.492217	0.597456
H	-0.925036	1.089027	-1.575247
C	-1.291075	-0.450717	-0.002333
H	1.873870	-0.340720	-1.572933
H	0.931643	-1.841908	-1.610120

H	2.680665	-1.908920	-1.729031
H	-1.147352	-0.435092	1.084069
H	-0.857270	-1.403764	-0.348447
C	-2.756197	-0.437376	-0.348203
H	-2.997271	-0.452212	-1.410933
C	-3.737045	-0.414536	0.553677
H	-3.526885	-0.396058	1.621265
H	-4.780682	-0.417206	0.251725

10boutMt

SCF Energy: -425.172149319 H

Num. Imaginary Frequencies: 0

C	-0.343179	-0.647498	0.692272
C	0.706160	-1.273082	-0.068057
O	0.451680	-2.259354	-0.808871
C	2.102900	-0.839459	0.067471
C	2.605131	0.453414	0.255834
C	1.998456	1.685741	0.079280
C	0.651270	1.973896	-0.494644
H	3.657686	0.491192	0.532857
H	2.821663	-1.654997	0.032460
H	2.596766	2.553567	0.347221
H	-0.061781	0.027651	1.495986
C	-1.789616	-0.893227	0.442256
H	-0.099691	2.112830	0.295481
H	0.682774	2.909199	-1.062422
H	0.293833	1.182773	-1.159062
H	-1.935160	-1.398542	-0.516792
H	-2.164274	-1.571906	1.225766
C	-2.580889	0.389522	0.498714
H	-2.536518	0.937696	1.439409
C	-3.295095	0.872590	-0.517200
H	-3.351903	0.350362	-1.470173
H	-3.847659	1.803631	-0.425320

10boutPt

SCF Energy: -425.172207120 H

Num. Imaginary Frequencies: 0

C	-0.408277	0.579702	0.511579
C	0.739784	1.264959	-0.024664
O	0.590996	2.310846	-0.710351
C	2.103945	0.825073	0.294810
C	2.587024	-0.475738	0.482886
C	2.037916	-1.693521	0.120248
C	0.822327	-1.939193	-0.709003
H	3.576727	-0.528594	0.934353
H	2.807553	1.643745	0.427631
H	2.588600	-2.578314	0.431340
H	-0.243684	-0.181153	1.269501
C	-1.810283	0.883174	0.111897
H	0.976414	-2.822080	-1.337443
H	-0.054227	-2.151224	-0.081010
H	0.573723	-1.095457	-1.358062
H	-2.329452	1.346113	0.963281
H	-1.812713	1.607086	-0.709200
C	-2.552285	-0.367196	-0.294857
H	-2.171237	-0.878402	-1.178082

C	-3.607868	-0.861726	0.352001
H	-4.008901	-0.375390	1.239139
H	-4.104475	-1.766305	0.011970

TS14-17bint

SCF Energy: -425.156172051 H

Num. Imaginary Frequencies: 1 (i138.8574)

C	-1.190900	0.962022	0.567800
C	0.102706	0.926023	-0.070672
C	0.725330	-0.311653	-0.492904
C	2.074914	-0.352156	-1.079849
C	3.201272	-0.565634	-0.391145
C	3.292481	-0.771816	1.089440
O	0.710042	2.022944	-0.259684
H	2.134238	-0.213219	-2.160979
H	0.158198	-1.236493	-0.418791
H	4.139480	-0.592934	-0.942753
H	-1.593138	1.951983	0.763726
C	-2.015685	-0.235959	0.905867
H	2.313493	-0.710998	1.574205
H	3.948018	-0.019011	1.541525
H	3.731679	-1.750043	1.315706
H	-2.692085	0.008500	1.729855
H	-1.370940	-1.062316	1.232340
C	-2.825131	-0.682382	-0.293684
H	-2.252137	-1.016220	-1.158227
C	-4.157150	-0.669730	-0.345583
H	-4.755814	-0.337145	0.500026
H	-4.688362	-0.997940	-1.234784

TS14-17bount

SCF Energy: -425.155585556 H

Num. Imaginary Frequencies: 1 (i142.2408)

C	-3.636745	-0.987243	0.338595
C	-3.433273	0.389065	-0.215817
C	-2.312626	1.112183	-0.111564
C	-1.095075	0.677456	0.591780
C	-0.002874	0.001862	-0.081946
C	1.177590	-0.386206	0.654689
C	2.332601	-1.087783	0.036935
O	-0.089971	-0.247648	-1.318727
H	-2.281224	2.105160	-0.564252
H	-0.984335	0.887811	1.653874
H	-4.275491	0.824935	-0.750728
H	1.230784	-0.120105	1.707342
H	-4.493379	-1.005105	1.021726
H	-3.860102	-1.695853	-0.467040
H	-2.755638	-1.347202	0.878016
H	2.586273	-1.962692	0.651736
H	2.063952	-1.473857	-0.952738
C	3.579764	-0.242521	-0.095372
H	4.470145	-0.791921	-0.398053
C	3.660691	1.072449	0.111993
H	2.796905	1.664026	0.409017
H	4.601568	1.600425	-0.014839

TS17-10binPt

SCF Energy: -425.167276125 H

Num. Imaginary Frequencies: 1 (i67.5588)

C	1.857297	-0.751690	1.166443
C	0.820608	0.166668	1.250930
C	0.353717	1.089382	0.175276
C	2.616434	-1.103302	0.053761
O	0.924333	2.194782	0.017285
C	-0.771245	0.738877	-0.637027
H	2.094688	-1.273376	2.091658
H	0.293203	0.274900	2.196580
H	3.395260	-1.844428	0.213046
C	2.451017	-0.572662	-1.335389
H	3.129527	-1.078240	-2.025661
H	1.427941	-0.717491	-1.705701
H	2.658617	0.503317	-1.390206
C	-1.502068	-0.556845	-0.551437
H	-0.841906	-1.336381	-0.154565
H	-1.834017	-0.854750	-1.551016
H	-1.122966	1.496025	-1.334356
C	-2.705325	-0.408918	0.357016
H	-2.484117	-0.201946	1.403297
C	-3.970119	-0.505818	-0.051912
H	-4.216823	-0.707753	-1.092181
H	-4.795965	-0.392289	0.644859

TS17-10boutMt

SCF Energy: -425.167624702 H

Num. Imaginary Frequencies: 1 (i69.9318)

C	-2.663799	-0.152922	-0.290374
C	-1.771004	-1.204848	-0.140765
C	-0.347051	-1.089672	0.287098
C	-2.419369	1.215298	-0.196880
O	-0.069754	-0.986069	1.502687
C	0.680042	-1.128579	-0.714155
H	-3.687357	-0.438839	-0.525376
H	-2.122118	-2.221524	-0.304315
H	-3.277002	1.869167	-0.331919
H	0.374132	-1.183509	-1.755574
C	-1.093829	1.867762	0.044839
H	-0.687160	1.623897	1.034346
H	-0.344952	1.545832	-0.689406
H	-1.180706	2.954414	-0.021443
C	2.122245	-0.959746	-0.385420
H	2.724905	-1.575720	-1.061169
H	2.317854	-1.263147	0.646366
C	2.486953	0.500634	-0.569195
H	2.516900	0.860248	-1.596415
C	2.719864	1.339664	0.439928
H	2.680513	1.008334	1.475452
H	2.958716	2.383848	0.257505

17bint

SCF Energy: -425.170502169 H

Num. Imaginary Frequencies: 0

C	-1.038027	-0.972137	-0.092965
C	0.240174	-0.558677	0.425220
C	0.642002	0.850857	0.357366

C	1.938935	1.369562	0.257441
C	3.116129	0.765965	-0.147495
C	3.309934	-0.600682	-0.713475
O	0.973157	-1.415721	0.986334
H	2.018390	2.431468	0.485446
H	-0.165287	1.570933	0.470207
H	4.008305	1.386060	-0.090787
H	-1.345486	-1.987915	0.142912
C	-1.969820	-0.102371	-0.867815
H	3.624709	-1.310027	0.062560
H	4.104229	-0.578432	-1.465917
H	2.402334	-0.997511	-1.173911
H	-2.491082	-0.705927	-1.617815
H	-1.410901	0.685726	-1.386796
C	-2.987083	0.530313	0.058718
H	-2.589217	1.230849	0.792135
C	-4.293250	0.265534	0.031669
H	-4.716511	-0.434682	-0.685671
H	-4.978707	0.745030	0.724980

17boutt

SCF Energy: -425.169917266 H

Num. Imaginary Frequencies: 0

C	3.170770	-1.202566	-0.172350
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C	3.355245	0.261658	0.045917
C	2.405160	1.267544	-0.000864
C	1.014429	1.204232	-0.142919
C	0.126755	0.056023	0.077477
C	-1.117504	0.012669	-0.651766
C	-2.193950	-0.974743	-0.388537
O	0.402085	-0.831142	0.924055
H	2.805833	2.279994	0.025427
H	0.503643	2.130153	-0.398348
H	4.379113	0.588624	0.214766
H	-1.280093	0.760997	-1.423825
H	4.043540	-1.609612	-0.692393
H	3.091052	-1.737900	0.782613
H	2.275934	-1.432515	-0.754657
H	-2.364784	-1.558961	-1.305239
H	-1.880239	-1.693773	0.375924
C	-3.513867	-0.362376	0.018939
H	-4.348303	-1.061346	0.050748
C	-3.717703	0.915464	0.341990
H	-2.914654	1.649721	0.332040
H	-4.703724	1.266324	0.633186

CLOSED SHELL ALLYL SUBSTITUTION ANCHIMERIC ASSISTANCE

S_E_Z-1b'

SCF Energy: -425.190079257 H

Num. Imaginary Frequencies: 0

C	-1.375123	-0.986000	-0.449683
C	0.022720	-1.119223	-0.164993
C	1.282402	-0.732050	-0.008758
C	1.687283	0.645380	-0.284749
C	2.925749	1.150740	-0.161228
C	4.162152	0.427424	0.279767
O	-0.726201	-2.254755	-0.004567
H	0.891406	1.309711	-0.618985
H	2.005135	-1.467759	0.331834
H	3.060072	2.203571	-0.404387
H	-1.698674	-1.032667	-1.487720
C	-2.329579	-0.340744	0.523503
H	4.934399	0.481202	-0.496473
H	3.985364	-0.626589	0.506303
H	4.584697	0.899530	1.174414
H	-1.961817	-0.521154	1.539975
H	-3.318172	-0.799302	0.421864
C	-2.405840	1.139500	0.261910
H	-1.477965	1.694564	0.400050
C	-3.509434	1.780210	-0.123008
H	-4.449550	1.252663	-0.271261
H	-3.507267	2.852850	-0.295643

TS6bout'

SCF Energy: -425.156909088 H

Num. Imaginary Frequencies: 1 (i149.3313)

C	1.639475	0.451886	-0.349955
C	0.385510	1.240554	-0.193940

C	-0.911515	0.847123	-0.115875
C	-1.399357	-0.517333	-0.247211
C	-2.668632	-0.942802	-0.089291
C	-3.860513	-0.114761	0.293371
O	0.885608	2.446129	-0.204796
H	-0.666918	-1.269824	-0.530713
H	-1.631581	1.653395	0.008453
H	-2.865142	-2.000634	-0.257993
H	2.032711	0.362167	-1.359413
C	2.522843	0.115352	0.751710
H	-4.606283	-0.104660	-0.511286
H	-3.601817	0.922186	0.522792
H	-4.358607	-0.537374	1.174288
H	2.282917	0.567514	1.710035
H	3.582753	0.071622	0.516412
C	1.781670	-1.202688	0.554037
H	0.943925	-1.393252	1.214846
C	2.076922	-2.048374	-0.455199
H	2.895501	-1.850471	-1.141762
H	1.509264	-2.963436	-0.593177

7bout'_c3

SCF Energy: -425.156973621 H

Num. Imaginary Frequencies: 0

C	1.645939	0.368921	-0.382548
C	0.425252	1.228190	-0.195649
C	-0.877326	0.836824	-0.111014
C	-1.394192	-0.514658	-0.253212
C	-2.672156	-0.915150	-0.092300
C	-3.845220	-0.065727	0.302314
O	0.893605	2.442178	-0.187241

H	-0.684066	-1.283926	-0.546859
H	-1.586257	1.649424	0.036414
H	-2.891604	-1.967322	-0.268044
H	1.985134	0.227648	-1.405395
C	2.596972	0.106815	0.682378
H	-4.595791	-0.036007	-0.497481
H	-3.564897	0.964628	0.535935
H	-4.346567	-0.482761	1.184169
H	2.429440	0.627658	1.620335
H	3.635999	-0.014731	0.391160
C	1.753606	-1.157973	0.583862
H	0.939022	-1.269700	1.289557
C	1.946643	-2.064284	-0.404464
H	2.745836	-1.951468	-1.131763
H	1.307804	-2.938611	-0.486293

7bout'g

SCF Energy: -425.186635124 H

Num. Imaginary Frequencies: 0

C	-0.982177	-0.114187	0.583915
C	-0.053535	0.856564	0.094188
C	1.338497	0.490419	-0.021067
C	1.911841	-0.778200	0.172742
C	3.251431	-1.052893	0.038179
C	4.346918	-0.111511	-0.316539
O	-0.423772	2.034173	-0.217334
H	1.272263	-1.614096	0.440132
H	1.985854	1.315401	-0.309589
H	3.557240	-2.082836	0.209353
H	-0.652269	-1.127525	0.784632
C	-2.427108	0.188510	0.769564
H	5.111307	-0.127121	0.469342
H	4.018250	0.918141	-0.463107
H	4.842350	-0.454940	-1.232752
H	-2.562818	1.258795	0.958787
H	-2.819214	-0.379589	1.618486
C	-3.183586	-0.195367	-0.485764
H	-2.923573	0.363639	-1.383498
C	-4.107945	-1.154408	-0.539764
H	-4.382948	-1.729277	0.342199
H	-4.622286	-1.387538	-1.468030

S_Z_Z-1b'

SCF Energy: -425.189900058 H

Num. Imaginary Frequencies: 0

C	-1.394442	-0.835991	-0.480798
C	0.009037	-0.623303	-0.293809
C	1.156536	0.042677	-0.244391
C	2.411077	-0.584565	0.166046
C	3.611392	0.014025	0.244117
C	3.939022	1.442449	-0.068397
O	-0.441169	-1.893460	-0.035235
H	2.347627	-1.638492	0.431149
H	1.121960	1.089595	-0.527440
H	4.451058	-0.597771	0.570167
H	-1.760511	-1.012541	-1.490601
C	-2.416496	-0.384010	0.532621

H	4.360187	1.939647	0.813234
H	3.073358	2.020014	-0.400618
H	4.703533	1.494769	-0.852290
H	-1.953795	-0.408476	1.525871
H	-3.264977	-1.075507	0.525417
C	-2.874615	1.014005	0.215996
H	-2.104487	1.784666	0.245879
C	-4.128555	1.344740	-0.091512
H	-4.919264	0.598182	-0.130440
H	-4.403073	2.373438	-0.307688

TS13bout'

SCF Energy: -425.159809730 H

Num. Imaginary Frequencies: 1 (i259.9242)

C	-1.696390	-0.612552	-0.260239
C	-0.266406	-0.947184	-0.191463
C	0.826411	-0.152838	-0.102917
C	2.174601	-0.695925	-0.038486
C	3.327611	-0.004500	0.043818
C	3.481927	1.487168	0.091425
O	-0.421991	-2.246299	-0.229165
H	2.245545	-1.783119	-0.062721
H	0.664243	0.919952	-0.090569
H	4.254864	-0.574637	0.077861
H	-2.191868	-0.793006	-1.210359
C	-2.514773	-0.271627	0.889919
H	4.028809	1.792795	0.991542
H	2.524489	2.014345	0.086658
H	4.066197	1.845067	-0.765189
H	-2.059422	-0.458309	1.859400
H	-3.562887	-0.552817	0.822116
C	-2.232444	1.153457	0.405930
H	-1.410682	1.673333	0.886076
C	-2.902250	1.709062	-0.618438
H	-3.701122	1.179132	-1.130536
H	-2.671963	2.717293	-0.948251

14bout'_c3

SCF Energy: -425.160680746 H

Num. Imaginary Frequencies: 0

C	1.758541	0.484788	-0.263280
C	0.341647	0.978172	-0.186030
C	-0.759306	0.181199	-0.071568
C	-2.104431	0.728776	-0.016805
C	-3.266270	0.048588	0.057980
C	-3.437200	-1.442310	0.098137
O	0.427869	2.270660	-0.278650
H	-2.169483	1.816447	-0.039849
H	-0.615594	-0.892937	-0.037830
H	-4.187861	0.628159	0.091175
H	2.248797	0.638645	-1.220826
C	2.606759	0.234879	0.886606
H	-3.965099	-1.751737	1.008578
H	-2.486267	-1.980435	0.064962
H	-4.045650	-1.787565	-0.746906
H	2.202697	0.501630	1.858609
H	3.673149	0.391452	0.755187

C	2.095296	-1.132161	0.432139	H	1.238869	-1.682823	-0.261622
H	1.260884	-1.554195	0.978151	H	1.994251	1.319685	-0.006461
C	2.604179	-1.766235	-0.651857	H	3.551159	-2.078522	-0.230686
H	3.430987	-1.349679	-1.220333	H	-0.565506	-1.166076	0.609923
H	2.195195	-2.719237	-0.973648	C	-2.337639	0.133211	0.844119

14bout'

SCF Energy: -425.180664165 H

Num. Imaginary Frequencies: 0

C	-0.921317	-0.150286	0.478397
C	-0.071281	0.829054	-0.033778
C	1.316065	0.468026	-0.041471
C	1.886909	-0.821375	-0.136792
C	3.232761	-1.043383	-0.121146
C	4.335908	-0.064834	0.025108
O	-0.431593	2.041690	-0.321158

H	4.937346	-0.341080	0.899601
H	4.014289	0.971135	0.130902
H	5.005364	-0.147426	-0.839102
H	-2.438106	1.187399	1.128646
H	-2.648252	-0.499021	1.680704
C	-3.220177	-0.141364	-0.355275
H	-3.056548	0.501964	-1.218518
C	-4.140178	-1.105186	-0.404633
H	-4.319509	-1.764907	0.441782
H	-4.746930	-1.257024	-1.293080

CLOSED SHELL ALLYL SUBSTITUTION, EPOXIDE ISOMERIZATION

R_E_Z-1br

SCF Energy: -425.293366474 H

Num. Imaginary Frequencies: 0

C	-1.420553	1.061692	0.185357
C	-0.106857	1.149322	0.082618
C	1.252686	0.696597	0.199585
C	1.834991	-0.247583	-0.772594
C	2.902844	-1.024454	-0.549594
C	3.735763	-1.118696	0.690338
O	0.837750	2.031141	-0.375187
H	1.321574	-0.305130	-1.730092
H	1.742847	0.814025	1.161709
H	3.205146	-1.685870	-1.360116
H	-2.031781	1.889936	-0.165312
C	-2.103959	-0.156922	0.753619
H	3.450537	-0.404818	1.465594
H	4.790634	-0.957461	0.443105
H	3.663018	-2.127735	1.111779
H	-2.733824	0.130057	1.603860
H	-1.341340	-0.849910	1.129402
C	-2.948121	-0.858156	-0.278301
H	-2.415398	-1.218319	-1.158976
C	-4.264554	-1.047934	-0.181337
H	-4.825201	-0.695829	0.682765
H	-4.821653	-1.561278	-0.960366

R_Z_Z-1br

SCF Energy: -425.293835633 H

Num. Imaginary Frequencies: 0

C	-4.239931	0.077783	0.440904
C	-3.191221	0.942686	-0.185224
C	-1.892886	0.669532	-0.367279
C	-1.220327	-0.580578	0.034617
C	0.207136	-0.643385	0.188903
C	1.376421	-0.456667	0.773621
C	2.689306	-0.851658	0.159659
O	-0.271749	-1.150927	-0.992918
H	-1.250583	1.413875	-0.833491
H	-1.814655	-1.360369	0.502548

H	-3.538068	1.918437	-0.521852
H	1.371106	0.011758	1.753703
H	-4.634491	0.561768	1.341393
H	-5.083660	-0.040577	-0.247531
H	-3.879872	-0.914924	0.717514
H	3.207151	-1.554786	0.825311
H	2.519016	-1.401199	-0.774474
C	3.626385	0.295491	-0.122609
H	4.618615	-0.000507	-0.462191
C	3.345227	1.593564	0.000978
H	2.369807	1.942759	0.332585
H	4.088967	2.350570	-0.231591

S_E_Z-1br

SCF Energy: -425.293319992 H

Num. Imaginary Frequencies: 0

C	-1.401921	0.916678	0.231205
C	-0.131383	0.989163	-0.122112
C	1.192205	0.490150	-0.380034
C	2.121620	0.175570	0.721480
C	3.191374	-0.624647	0.627267
C	3.693448	-1.364382	-0.573018
O	0.787308	1.942811	-0.477409
H	1.881059	0.635532	1.677726
H	1.389900	0.067154	-1.360837
H	3.772722	-0.772926	1.536030
H	-1.990976	1.830448	0.259088
C	-2.073906	-0.389587	0.573958
H	3.127542	-1.159635	-1.483711
H	3.661259	-2.443795	-0.386252
H	4.743439	-1.109941	-0.753891
H	-2.493354	-0.337424	1.585552
H	-1.323446	-1.189304	0.569136
C	-3.168599	-0.726921	-0.404346
H	-2.853401	-0.853102	-1.440527
C	-4.457024	-0.861240	-0.087608
H	-4.805007	-0.736432	0.936278
H	-5.203084	-1.101768	-0.840073

S_Z_Z-1br

SCF Energy: -425.293750661 H

Num. Imaginary Frequencies: 0

C	4.146492	1.006752	0.052568
C	3.526919	-0.262646	-0.442285
C	2.251400	-0.657777	-0.339252
C	1.170170	0.115160	0.300947
C	-0.213483	-0.165018	0.031042
C	-1.343234	-0.168545	-0.653166
C	-2.590475	-0.869659	-0.195393
O	0.265866	-0.686329	1.206719
H	1.952801	-1.614891	-0.761840
H	1.415124	1.079822	0.736436
H	4.208235	-0.938716	-0.956578
H	-1.353250	0.367096	-1.598189
H	4.998222	0.774734	0.701257
H	4.542287	1.583630	-0.790784
H	3.454997	1.643612	0.607655
H	-2.876064	-1.625396	-0.939520
H	-2.391742	-1.427410	0.728043
C	-3.781451	0.026344	0.030565
H	-4.704982	-0.499359	0.271732
C	-3.793927	1.358326	-0.038629
H	-2.899672	1.931795	-0.272490
H	-4.707360	1.918097	0.142135

TS1bR_E

SCF Energy: -425.269764880 H

Num. Imaginary Frequencies: 1 (i136.0697)

C	-1.392822	1.134087	0.300079
C	-0.087780	1.398582	0.079169
C	1.012094	0.435024	0.276046
C	1.745602	-0.084814	-0.786985
C	2.820047	-0.923393	-0.601022
C	3.468381	-1.329435	0.657035
O	0.523116	2.502272	-0.292830
H	1.418655	0.129798	-1.799807
H	1.314731	0.205760	1.297339
H	3.251567	-1.357998	-1.501176
H	-2.123631	1.913120	0.090423
C	-1.897359	-0.204130	0.779009
H	3.074628	-0.856488	1.555668
H	4.541558	-1.119795	0.569645
H	3.391193	-2.420527	0.748160
H	-2.597637	-0.071498	1.612802
H	-1.056908	-0.803076	1.158987
C	-2.577913	-0.983109	-0.317887
H	-1.949009	-1.237339	-1.172238
C	-3.862399	-1.344043	-0.316673
H	-4.518592	-1.099356	0.516941
H	-4.298603	-1.893394	-1.146734

TS1bR_Z

SCF Energy: -425.270044161 H

Num. Imaginary Frequencies: 1 (i310.4385)

C	-4.176708	0.350595	0.624284
C	-3.248482	0.763057	-0.441665

C	-1.933011	0.410302	-0.629253
C	-1.221262	-0.357875	0.289208
C	0.167336	-0.780938	0.039018
C	1.250004	-0.299853	0.683912
C	2.659407	-0.707996	0.371253
O	0.040614	-1.698895	-0.895738
H	-1.407869	0.796640	-1.497683
H	-1.724302	-0.740229	1.176856
H	-3.668848	1.449933	-1.174522
H	1.080867	0.429317	1.473597
H	-4.525967	1.250702	1.145805
H	-5.069163	-0.075530	0.149152
H	-3.771908	-0.358303	1.344807
H	3.106937	-1.229273	1.230562
H	2.663880	-1.446096	-0.441463
C	3.592903	0.414603	-0.008402
H	4.633695	0.118454	-0.141321
C	3.261456	1.694483	-0.188910
H	2.238365	2.044829	-0.071156
H	4.009546	2.432447	-0.465411

TS1bS_E

SCF Energy: -425.273248997 H

Num. Imaginary Frequencies: 1 (i262.6045)

C	-1.325435	1.010422	0.296340
C	-0.061000	1.331028	-0.047741
C	1.076578	0.435608	-0.260378
C	1.713940	-0.284922	0.753817
C	2.865605	-1.002611	0.543797
C	3.669181	-1.116957	-0.685231
O	0.513348	2.502134	-0.246723
H	1.258976	-0.302504	1.739425
H	1.505684	0.471678	-1.258376
H	3.238415	-1.575434	1.391501
H	-2.048689	1.820537	0.378193
C	-1.819961	-0.392482	0.540852
H	3.312853	-0.526861	-1.528419
H	3.712389	-2.176141	-0.968775
H	4.702489	-0.836456	-0.446441
H	-2.280805	-0.465648	1.534056
H	-0.976773	-1.094599	0.524319
C	-2.824495	-0.824466	-0.497401
H	-2.458246	-0.854682	-1.524339
C	-4.095096	-1.142656	-0.243785
H	-4.493705	-1.115896	0.768906
H	-4.775271	-1.438849	-1.037897

TS1bS_Z

SCF Energy: -425.274215872 H

Num. Imaginary Frequencies: 1 (i171.8539)

C	-4.154469	0.697241	-0.561856
C	-3.431843	0.288055	0.656902
C	-2.116253	-0.068840	0.794503
C	-1.199178	-0.022059	-0.265079
C	0.164076	-0.531286	-0.181174
C	1.219416	-0.035530	0.489401
C	2.580513	-0.664801	0.489895

O	-0.008857	-1.619707	-0.910671	H	2.821785	-1.046302	1.493003
H	-1.752851	-0.365925	1.773709	H	2.583328	-1.551388	-0.158056
H	-1.519797	0.286784	-1.256579	C	3.712372	0.237060	0.065220
H	-4.032004	0.278144	1.565345	H	4.706930	-0.196178	0.172598
H	1.059395	0.870068	1.069675	C	3.599594	1.476508	-0.416090
H	-5.003670	0.016106	-0.698928	H	2.632155	1.956636	-0.545627
H	-4.594890	1.686856	-0.390210	H	4.478874	2.048525	-0.699759
H	-3.553768	0.716245	-1.470133				

CLOSED SHELL METHYL SUBSTITUTION

10ainM

SCF Energy: -347.905968486 H

Num. Imaginary Frequencies: 0

C	1.249570	1.018519	-0.181336
C	1.260741	-0.341826	0.179647
C	0.362207	-1.127462	-0.605091
C	-1.022241	-1.002042	-0.892155
C	-1.979533	-0.422473	-0.113080
C	-1.837982	0.227178	1.211015
O	2.245448	-0.885890	0.802540
H	-1.364908	-1.532135	-1.777183
H	0.856469	-1.984861	-1.063380
H	-3.000583	-0.496549	-0.483150
H	2.249918	1.454595	-0.161750
C	0.162604	1.946120	-0.553165
H	-0.843578	0.120727	1.649009
H	-2.588454	-0.180460	1.896417
H	-2.060604	1.298989	1.118659
H	-0.264068	2.392696	0.358308
H	-0.674182	1.462412	-1.070253
H	0.554207	2.763622	-1.162010

10ainP

SCF Energy: -347.905968495 H

Num. Imaginary Frequencies: 0

C	-1.249571	1.018518	-0.181335
C	-1.260741	-0.341827	0.179648
C	-0.362207	-1.127461	-0.605092
C	1.022241	-1.002038	-0.892157
C	1.979534	-0.422471	-0.113082
C	1.837984	0.227175	1.211015
O	-2.245448	-0.885893	0.802540
H	1.364907	-1.532128	-1.777187
H	-0.856469	-1.984860	-1.063381
H	3.000583	-0.496544	-0.483154
H	-2.249920	1.454593	-0.161752
C	-0.162607	1.946122	-0.553161
H	0.843579	0.120728	1.649008
H	2.060616	1.298985	1.118666
H	2.588453	-0.180472	1.896416
H	0.674182	1.462415	-1.070246
H	0.264061	2.392700	0.358312
H	-0.554211	2.763620	-1.162008

10aoutM

SCF Energy: -347.912094805 H

Num. Imaginary Frequencies: 0

C	1.053981	0.568686	-0.462867
C	0.806443	-0.613215	0.251293
O	1.630085	-1.183214	1.057477
C	-0.301351	-1.294401	-0.336240
C	-1.562651	-0.778461	-0.761146
C	-2.241030	0.278017	-0.238271
C	-1.893676	1.166740	0.904304
H	-2.075324	-1.367241	-1.517671
H	-0.156159	-2.367392	-0.468168
H	-3.219024	0.467651	-0.677790
H	0.249383	1.015373	-1.034684
C	2.382991	1.214356	-0.502403
H	-1.684876	2.178394	0.537256
H	-2.760285	1.249802	1.568425
H	-1.024889	0.828987	1.472299
H	3.183263	0.513247	-0.249967
H	2.573858	1.682201	-1.471198
H	2.405129	2.014364	0.253665

10aoutP

SCF Energy: -347.912094804 H

Num. Imaginary Frequencies: 0

C	-1.053979	0.568684	-0.462869
C	-0.806443	-0.613216	0.251292
O	-1.630085	-1.183214	1.057476
C	0.301352	-1.294403	-0.336239
C	1.562652	-0.778462	-0.761144
C	2.241028	0.278018	-0.238270
C	1.893670	1.166742	0.904303
H	2.075328	-1.367243	-1.517666
H	0.156162	-2.367395	-0.468164
H	3.219023	0.467653	-0.677786
H	-0.249382	1.015370	-1.034687
C	-2.382988	1.214357	-0.502404
H	2.760276	1.249802	1.568428
H	1.684876	2.178397	0.537253
H	1.024879	0.828992	1.472294
H	-3.183261	0.513249	-0.249966
H	-2.405123	2.014364	0.253665
H	-2.573855	1.682202	-1.471198

14ain

SCF Energy: -347.916357559 H

Num. Imaginary Frequencies: 0

C	-2.254922	0.251700	0.000001
C	-1.185970	-0.653806	0.000000
C	0.115348	-0.074792	-0.000003

C	1.293896	-0.854324	-0.000003
C	2.552801	-0.330127	-0.000001
C	2.955924	1.095722	0.000003
O	-1.372717	-1.945094	0.000002
H	1.181427	-1.934128	-0.000003
H	0.205953	1.004379	-0.000005
H	3.377909	-1.040561	-0.000001
H	-3.240096	-0.216444	0.000004
C	-2.282952	1.732199	-0.000001
H	2.125224	1.801359	0.000002
H	3.588575	1.286695	-0.875110
H	3.588570	1.286691	0.875120
H	-2.850462	2.075952	-0.874467
H	-1.309656	2.221415	-0.000003
H	-2.850459	2.075956	0.874466

14aout

SCF Energy: -347.924666612 H

Num. Imaginary Frequencies: 0

C	3.291269	-0.957986	0.013529
C	2.720053	0.409201	-0.036605
C	1.409041	0.779628	-0.028011
C	0.328102	-0.131589	0.023831
C	-1.036624	0.278929	0.032867
C	-1.911781	-0.813846	0.005986
C	-3.377776	-0.651275	-0.046258
O	-1.417163	1.518134	0.037070
H	1.169507	1.838358	-0.063675
H	0.529490	-1.197584	0.054035
H	3.453588	1.212492	-0.082578
H	-1.493438	-1.815232	0.040038
H	3.935143	-1.108064	-0.861136
H	3.947685	-1.036228	0.888556
H	2.549538	-1.755789	0.052416
H	-3.744403	-0.327548	0.939804
H	-3.656913	0.145428	-0.745680
H	-3.886592	-1.579285	-0.310369

4R-5R-5a

SCF Energy: -348.008948368 H

Num. Imaginary Frequencies: 0

C	-0.124480	0.646660	0.567265
C	-1.232735	-0.220336	-0.012476
C	-0.730281	-1.590400	-0.143053
C	0.577979	-1.606466	0.156065
C	1.137972	-0.250791	0.491658
O	-2.364149	0.172020	-0.301701
H	1.210157	-2.489542	0.131158
H	-1.344087	-2.427272	-0.454546
H	1.638408	-0.294980	1.465776
C	2.180595	0.166365	-0.553604
H	-0.392862	0.759618	1.626915
C	-0.049257	2.036843	-0.054345
H	0.164542	1.989891	-1.126062
H	-0.999076	2.561872	0.079745
H	3.002200	-0.556163	-0.573560
H	1.742587	0.210989	-1.555810

H	2.599097	1.148007	-0.315207
H	0.733466	2.630174	0.426148

4R-5S-5a

SCF Energy: -348.010669207 H

Num. Imaginary Frequencies: 0

C	0.123494	0.714626	0.238389
C	1.191214	-0.368838	0.193791
C	0.558077	-1.633642	-0.188468
C	-0.736115	-1.409296	-0.466529
C	-1.143786	0.030417	-0.314827
O	2.385925	-0.195426	0.439848
H	-1.445217	-2.170160	-0.780486
H	1.089047	-2.576559	-0.244639
C	-2.387859	0.210162	0.555522
H	-1.363743	0.423986	-1.317003
H	-0.029673	0.938926	1.303179
C	0.537411	1.992878	-0.485008
H	1.442421	2.419825	-0.043816
H	0.729711	1.794603	-1.544610
H	-2.634080	1.272136	0.650626
H	-3.250197	-0.302301	0.117942
H	-2.220879	-0.194137	1.559726
H	-0.259417	2.739250	-0.416920

4S-5R-5a

SCF Energy: -348.010669207 H

Num. Imaginary Frequencies: 0

C	1.143786	0.030417	-0.314827
C	0.736115	-1.409296	-0.466529
C	-0.558077	-1.633642	-0.188468
C	-1.191214	-0.368838	0.193791
C	-0.123494	0.714626	0.238389
C	-0.537411	1.992878	-0.485008
O	-2.385925	-0.195426	0.439848
H	-1.089047	-2.576559	-0.244639
H	1.445217	-2.170160	-0.780486
H	1.363743	0.423986	-1.317003
C	2.387859	0.210162	0.555522
H	-0.729711	1.794603	-1.544610
H	-1.442421	2.419825	-0.043816
H	0.029673	0.938926	1.303179
H	2.220879	-0.194137	1.559726
H	3.250197	-0.302301	0.117942
H	2.634080	1.272136	0.650626
H	0.259417	2.739250	-0.416920

4S-5S-5a

SCF Energy: -348.008948368 H

Num. Imaginary Frequencies: 0

C	0.124480	0.646660	0.567265
C	1.232735	-0.220336	-0.012476
C	0.730281	-1.590400	-0.143053
C	-0.577979	-1.606466	0.156065
C	-1.137972	-0.250791	0.491658
O	2.364149	0.172020	-0.301701
H	-1.210157	-2.489542	0.131158

H	1.344087	-2.427272	-0.454546
H	-1.638408	-0.294980	1.465776
C	-2.180595	0.166365	-0.553604
H	0.392862	0.759618	1.626915
C	0.049257	2.036843	-0.054345
H	0.999076	2.561872	0.079745
H	-0.164542	1.989891	-1.126062
H	-2.599097	1.148007	-0.315207
H	-1.742587	0.210989	-1.555810
H	-3.002200	-0.556163	-0.573560
H	-0.733466	2.630174	0.426148

7ain

SCF Energy: -347.905790934 H

Num. Imaginary Frequencies: 0

C	-2.065398	0.365382	0.210211
C	-1.280811	-0.756094	-0.071661
C	0.140620	-0.602136	-0.060252
C	0.910360	0.510995	-0.463649
C	2.261877	0.589812	-0.279485
C	3.159973	-0.367025	0.406262
O	-1.787554	-1.957457	-0.135487
H	0.430493	1.330336	-0.984160
H	0.673392	-1.494060	0.266565
H	2.752545	1.477011	-0.675828
H	-3.081357	0.107210	0.510146
C	-1.749495	1.820716	0.199650
H	2.668544	-1.264560	0.781528
H	3.644163	0.147831	1.245290
H	3.968767	-0.650004	-0.277440
H	-1.628315	2.197836	-0.824711
H	-0.823666	2.061072	0.734667
H	-2.566896	2.377082	0.661393

7aout

SCF Energy: -347.916378838 H

Num. Imaginary Frequencies: 0

C	-3.434871	0.388977	0.279054
C	-2.545301	-0.728498	-0.121578
C	-1.189366	-0.742328	-0.255416
C	-0.374412	0.395612	-0.037461
C	1.048312	0.505994	-0.115679
C	1.751242	-0.692134	0.034445
C	3.213911	-0.722244	0.239482
O	1.615184	1.674329	-0.174100
H	-0.731402	-1.676104	-0.564817
H	-0.878182	1.333564	0.192922
H	-3.057964	-1.665143	-0.333604
H	1.219451	-1.636215	0.008526
H	-4.196653	0.537015	-0.495125
H	-3.978191	0.098266	1.186399
H	-2.924924	1.334733	0.462497
H	3.718826	-0.633460	-0.734870
H	3.547991	0.135766	0.833306
H	3.542483	-1.655332	0.700478

TS12ainM

SCF Energy: -347.891379785 H

Num. Imaginary Frequencies: 1 (i238.1230)

C	1.710713	0.113982	0.109515
C	0.984372	-0.190672	1.252544
C	-0.288249	-0.739991	1.199819
C	-1.069070	-0.502814	0.016336
C	-0.949326	0.779843	-0.572975
C	-0.606530	2.116664	0.002565
O	-1.869867	-1.400609	-0.462141
H	-0.700534	-1.323889	2.018815
H	1.431513	0.051883	2.215750
H	2.530547	0.819867	0.247443
C	1.771282	-0.617166	-1.188697
H	-0.170203	2.077341	1.000389
H	0.070465	2.666397	-0.659851
H	-1.488412	0.853428	-1.520052
H	0.976655	-1.349806	-1.326895
H	1.782217	0.079959	-2.031213
H	2.739142	-1.136972	-1.210436
H	-1.531600	2.707583	0.048536

TS12ainP

SCF Energy: -347.891379781 H

Num. Imaginary Frequencies: 1 (i238.1318)

C	-1.710715	0.114030	0.109510
C	-0.984381	-0.190626	1.252544
C	0.288226	-0.739979	1.199827
C	1.069055	-0.502839	0.016340
C	0.949354	0.779814	-0.572986
C	0.606608	2.116652	0.002544
O	1.869820	-1.400670	-0.462126
H	0.700493	-1.323879	2.018829
H	-1.431516	0.051954	2.215746
H	-2.530529	0.819940	0.247426
C	-1.771306	-0.617145	-1.188686
H	0.170271	2.077354	1.000365
H	1.531702	2.707533	0.048520
H	1.488444	0.853371	-1.520063
H	-0.976686	-1.349792	-1.326880
H	-2.739170	-1.136946	-1.210398
H	-1.782252	0.079963	-2.031216
H	-0.070358	2.666411	-0.659881

TS12aoutM

SCF Energy: -347.907797336 H

Num. Imaginary Frequencies: 1 (i180.9692)

C	1.838452	-0.516781	-0.240363
C	1.609714	0.808865	-0.570133
C	0.466232	1.509222	-0.188055
C	-0.737921	0.780895	0.086056
O	-1.631733	1.197492	0.916469
C	-0.880358	-0.391568	-0.697407
C	-1.973088	-1.352540	-0.454275
H	2.356524	1.311041	-1.182998
H	0.473947	2.592361	-0.090260
C	1.430407	-1.275852	0.980795

H	2.616506	-1.015200	-0.819230
H	-0.239937	-0.538472	-1.556568
H	-2.176858	-1.983757	-1.320412
H	-2.887003	-0.837093	-0.136805
H	0.735169	-0.736548	1.624479
H	0.996666	-2.246164	0.717172
H	2.346121	-1.494198	1.545425
H	-1.687894	-2.005345	0.387733

TS12aoutP

SCF Energy: -347.907797319 H

Num. Imaginary Frequencies: 1 (i180.9634)

C	1.838459	0.516775	-0.240360
C	1.609713	-0.808868	-0.570132
C	0.466228	-1.509222	-0.188053
C	-0.737924	-0.780895	0.086056
O	-1.631742	-1.197494	0.916463
C	-0.880357	0.391571	-0.697403
C	-1.973083	1.352547	-0.454275
H	2.356520	-1.311047	-1.182998
H	0.473941	-2.592361	-0.090256
C	1.430409	1.275851	0.980793
H	2.616520	1.015188	-0.819223
H	-0.239931	0.538477	-1.556561
H	-1.687897	2.005334	0.387750
H	-2.887009	0.837105	-0.136831
H	0.735179	0.736542	1.624482
H	2.346121	1.494214	1.545419
H	0.996652	2.246155	0.717165
H	-2.176832	1.983782	-1.320404

S_Z_Z-1a

SCF Energy: -347.928629147 H

Num. Imaginary Frequencies: 0

C	-1.430870	0.704944	0.166473
C	-0.399299	-0.248425	-0.236887
C	0.888921	0.071446	-0.283230
C	-2.749809	0.461280	0.246355
O	1.668948	1.168908	-0.024645
C	2.295990	-0.114489	-0.476916
H	-1.078823	1.702261	0.424603
H	-0.659014	-1.263731	-0.518138
H	-3.388879	1.282259	0.567730
H	2.683642	-0.032724	-1.490386
C	-3.456090	-0.825874	-0.052746
H	-4.236372	-0.667688	-0.806157
H	-2.787942	-1.609236	-0.417950
H	-3.961132	-1.201338	0.845198
C	3.168330	-0.811070	0.521368
H	2.704295	-0.824100	1.510449
H	3.325821	-1.843385	0.194060
H	4.143786	-0.320459	0.581253

TS13ain

SCF Energy: -347.893978938 H

Num. Imaginary Frequencies: 1 (i326.9450)

C	-2.259867	0.212255	-0.450260
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C	-1.019415	-0.452485	-0.163858
C	0.243829	0.046670	-0.180236
C	1.408991	-0.777126	0.076969
C	2.690393	-0.363287	0.124484
C	3.196998	1.035228	-0.048194
O	-1.517918	-1.616863	0.186149
H	1.213833	-1.835818	0.241913
H	0.347352	1.102205	-0.413901
H	3.451793	-1.118170	0.314028
H	-2.885459	-0.265619	-1.200615
C	-2.794286	1.321594	0.329851
H	2.400993	1.760055	-0.234094
H	3.905229	1.085167	-0.883815
H	3.745960	1.355558	0.845307
H	-3.590274	1.848317	-0.199391
H	-1.996889	1.986293	0.675791
H	-3.249054	0.879820	1.233046

TS13aout

SCF Energy: -347.888771357 H

Num. Imaginary Frequencies: 1 (i543.8598)

C	2.124951	-0.596560	-0.418767
C	0.959507	0.232653	-0.223031
C	-0.336746	-0.173261	-0.161614
C	-1.425085	0.734604	0.147117
C	-2.734536	0.424267	0.219486
C	-3.359866	-0.915680	-0.019178
O	1.519823	1.417094	-0.196082
H	-1.139573	1.766395	0.346577
H	-0.524875	-1.228920	-0.335494
H	-3.424903	1.225111	0.479610
H	2.248759	-1.126697	-1.365842
C	3.228227	-0.685914	0.529031
H	-2.635154	-1.682365	-0.302868
H	-4.114235	-0.851738	-0.812266
H	-3.883199	-1.259804	0.881079
H	3.336136	-1.763415	0.738038
H	3.064374	-0.129626	1.450272
H	4.175368	-0.406352	0.051292

TS7-10ainM

SCF Energy: -347.826476115 H

Num. Imaginary Frequencies: 0

C	-1.571288	0.473774	0.098316
C	-0.952455	-0.824912	0.339344
C	-0.352213	0.266046	1.112875
C	0.988753	0.883846	0.922446
C	1.981953	0.510722	0.105357
C	2.016532	-0.658266	-0.840025
O	-0.920889	-2.003576	0.051279
H	1.153803	1.756148	1.551847
H	-0.703590	0.297773	2.144316
H	2.886195	1.116060	0.142370
H	-2.516260	0.665138	0.603591
C	-1.374348	1.183221	-1.223183
H	1.075965	-0.800067	-1.377365
H	2.232598	-1.589890	-0.303086

H	2.804542	-0.521719	-1.584699
H	-0.402333	0.948452	-1.665017
H	-1.433126	2.266098	-1.081793
H	-2.152292	0.884026	-1.931175

TS7-10ainP

SCF Energy: -347.936873924 H

Num. Imaginary Frequencies: 1 (i131.7299)

C	1.394472	0.490498	0.701242
C	1.295437	-0.855733	0.166475
C	-0.009731	-0.226565	0.410192
C	-0.878693	0.159658	-0.726142
C	-2.215109	0.221522	-0.669863
C	-3.058546	-0.087659	0.538405
O	1.870759	-1.775450	-0.379027
H	-0.377597	0.407414	-1.659618
H	-0.510319	-0.505468	1.335146
H	-2.739857	0.526840	-1.572890
H	1.565733	0.573687	1.772671
C	1.928356	1.624568	-0.145823
H	-2.860263	-1.092866	0.926063
H	-4.122031	-0.027490	0.297054
H	-2.862763	0.616781	1.355314
H	1.425719	2.560153	0.115832
H	1.777475	1.437770	-1.212434
H	3.000725	1.749049	0.028164

TS7-10outaM

SCF Energy: -347.902037447 H

Num. Imaginary Frequencies: 1 (i210.7406)

C	2.183723	-1.116628	0.473368
C	2.287913	0.191706	-0.248383
C	1.374079	1.168885	-0.315859
C	0.039603	1.246749	0.293036
C	-1.193576	0.679700	-0.094241
C	-0.854151	-0.642712	-0.444566
C	-1.669122	-1.812131	-0.071773
O	-2.346511	1.106418	0.245311
H	1.659154	2.104379	-0.801452
H	-0.039580	1.934018	1.140703
H	3.234969	0.379048	-0.750670
H	0.044904	-0.808854	-1.026749
H	2.114318	-1.949123	-0.237099
H	3.089119	-1.280844	1.066352
H	1.317903	-1.163930	1.138923
H	-2.386324	-1.582194	0.718899
H	-2.236167	-2.116837	-0.964807
H	-1.037020	-2.660424	0.203925

TS7-10aoutP

SCF Energy: -347.935709785 H

Num. Imaginary Frequencies: 1 (i31.8243)

C	-2.685682	-0.703337	0.114691
C	-2.249494	0.697941	-0.183173
C	-1.009103	1.177611	-0.041765
C	0.137056	0.358827	0.459425
C	1.514993	0.585361	0.022241

C	0.918132	-0.646983	-0.483603
C	1.304922	-2.015871	0.030083
O	2.476919	1.325274	0.043625
H	-0.805111	2.215771	-0.295056
H	0.053768	-0.015595	1.482329
H	-3.019844	1.374022	-0.551281
H	0.612332	-0.596780	-1.529365
H	-3.084735	-1.179388	-0.788518
H	-1.868312	-1.322341	0.493655
H	-3.493819	-0.705207	0.854913
H	2.135787	-2.424685	-0.551969
H	1.613242	-1.967582	1.078527
H	0.456398	-2.701699	-0.049630

TS7-14ain

SCF Energy: -347.895339013 H

Num. Imaginary Frequencies: 1 (i298.8587)

C	-1.096103	-0.378417	0.713344
C	-0.134139	-0.138288	-0.267615
C	1.250973	-0.623182	-0.147982
C	-2.405076	0.015170	0.578174
O	1.116434	-1.926387	-0.306455
C	2.340243	0.149798	0.031414
H	-0.782856	-0.839411	1.645126
H	-0.433096	0.334765	-1.202867
H	-3.043989	-0.137077	1.446526
H	3.306301	-0.343339	0.124722
C	-3.071337	0.632700	-0.582027
H	-3.935147	0.011295	-0.849332
H	-3.489983	1.597039	-0.268299
H	-2.439248	0.775136	-1.457382
C	2.290365	1.649924	0.110756
H	2.524683	2.018459	1.117502
H	1.298170	2.039486	-0.147871
H	3.014139	2.108523	-0.572868

TS7-14aout

SCF Energy: -347.919780608 H

Num. Imaginary Frequencies: 1 (i150.0210)

C	1.253425	0.386879	-0.673446
C	0.317172	-0.315064	0.225181
C	-1.092406	-0.034898	0.212939
C	2.576889	0.479393	-0.489425
O	-0.717364	-1.168729	-0.468307
C	-2.211669	0.620288	0.464536
H	0.798401	0.871480	-1.534796
H	0.723273	-0.816340	1.099326
H	3.135627	1.050018	-1.229722
H	-2.125227	1.526511	1.055818
C	3.399065	-0.092137	0.623362
H	2.833003	-0.733660	1.301394
H	4.229687	-0.673974	0.209862
H	3.845742	0.717558	1.211633
C	-3.565028	0.166024	-0.018818
H	-4.340827	0.859303	0.312348
H	-3.817774	-0.827661	0.366722
H	-3.607685	0.113690	-1.112100

TS7ain-out

SCF Energy: -347.891670698 H

Num. Imaginary Frequencies: 1 (i321.2045)

C	1.014339	-0.591475	-0.209047
C	0.284258	0.646689	-0.020189
C	-1.073351	0.743278	-0.095160
C	2.350218	-0.750167	-0.121942
O	-1.869665	1.757818	0.150199
C	-2.033478	-0.285369	-0.400424
H	0.426343	-1.475610	-0.451484
H	0.826214	1.565405	0.191141
H	2.741862	-1.752899	-0.284658
C	3.375802	0.300824	0.171500
H	2.947598	1.295965	0.311069
H	3.937967	0.043254	1.077069
H	4.107320	0.356705	-0.643311
H	-2.748054	-0.030089	-1.180363
C	-2.270876	-1.501345	0.365466
H	-1.479243	-1.737605	1.075115
H	-3.226994	-1.376226	0.898448
H	-2.457165	-2.326052	-0.335849

3aM

SCF Energy: -347.907809867 H

Num. Imaginary Frequencies: 0

C	1.681494	1.396693	-0.599200
C	2.297526	0.309849	0.230534
C	1.770084	-0.897976	0.494607
C	0.470463	-1.434842	0.076322
C	-0.609441	-0.716177	-0.211364
O	-1.910268	-0.975802	-0.563176
C	-1.457517	0.432160	-0.337168
H	2.369763	-1.591010	1.081536
H	0.362014	-2.516348	0.038137
H	3.277402	0.521590	0.654279
H	-1.416119	0.994592	-1.267533
C	-2.040457	1.136355	0.848830
H	1.103923	0.987628	-1.435281
H	0.996471	2.018195	-0.008290
H	2.452809	2.058483	-1.002424
H	-1.420613	2.008092	1.080889
H	-2.064587	0.482158	1.723723
H	-3.051832	1.486658	0.624998

3aP

SCF Energy: -347.907884646 H

Num. Imaginary Frequencies: 0

C	-1.483890	1.574655	-0.089765
C	-2.323107	0.351252	0.119001
C	-1.904510	-0.922997	0.038011
C	-0.553115	-1.424547	-0.231873
C	0.596556	-0.809556	0.027909
O	1.922709	-1.146757	-0.086517
C	1.535694	0.159618	0.521669
H	-2.647751	-1.706729	0.171262

H	-0.471314	-2.429696	-0.640381
H	-3.374897	0.512312	0.347365
H	1.717501	0.172647	1.594782
C	1.960749	1.379829	-0.236358
H	-0.733393	1.412230	-0.871317
H	-2.103908	2.427812	-0.377798
H	-0.943495	1.857487	0.822516
H	1.426369	2.252235	0.150033
H	1.746986	1.278778	-1.303142
H	3.031971	1.547453	-0.092752

S_E_Z-1a

SCF Energy: -347.910502018 H

Num. Imaginary Frequencies: 0

C	1.259842	0.657730	-0.267409
C	0.431969	-0.514030	0.012376
C	-0.885481	-0.478531	-0.148534
C	2.595671	0.736708	-0.150165
O	-1.952133	-1.320763	0.011493
C	-2.166780	0.089327	-0.450685
H	0.721251	1.543393	-0.601786
H	0.879380	-1.440687	0.360389
H	3.061016	1.689281	-0.398649
H	-2.473806	0.124008	-1.493816
C	3.536076	-0.345966	0.285963
H	4.103492	-0.027900	1.168468
H	3.029053	-1.282292	0.530999
H	4.271083	-0.554811	-0.500254
C	-2.895039	0.992181	0.496631
H	-2.531517	0.866981	1.519342
H	-2.730648	2.030281	0.191742
H	-3.969782	0.793335	0.462553

TS2aM

SCF Energy: -347.901644595 H

Num. Imaginary Frequencies: 1 (i69.4618)

C	-2.879698	-0.480687	0.849295
C	-2.450553	0.687931	0.016680
C	-1.368377	0.745584	-0.768198
C	-0.400189	-0.367322	-0.964027
C	0.731330	-0.444379	-0.286263
C	1.750132	-0.048752	0.641807
C	2.738162	1.036370	0.340780
O	1.827967	-1.271089	-0.218382
H	-1.184815	1.659697	-1.332208
H	-0.613105	-1.140581	-1.700386
H	-3.092462	1.567066	0.060492
H	1.610755	-0.304228	1.690299
H	-2.200804	-1.331063	0.744399
H	-3.888028	-0.803266	0.565530
H	-2.923880	-0.203116	1.908736
H	2.828030	1.201082	-0.735655
H	2.397330	1.964696	0.809689
H	3.718394	0.785958	0.755711

TS2aP

SCF Energy: -347.901889775 H

Num. Imaginary Frequencies: 1 (i63.0900)

C	-2.518934	1.003173	-0.706627
C	-2.411516	0.115123	0.494568
C	-1.480054	-0.821889	0.706361
C	-0.388576	-1.164319	-0.245176
C	0.841169	-0.703863	-0.100369
C	1.908671	0.064339	0.469775
C	2.037064	1.541646	0.256975
O	2.050469	-0.794341	-0.748208
H	-1.528694	-1.401423	1.627766
H	-0.595827	-1.825643	-1.084869
H	-3.171920	0.255320	1.261997
H	2.442474	-0.355614	1.319731
H	-1.720426	0.815895	-1.429416
H	-2.474483	2.057171	-0.409142
H	-3.483206	0.858525	-1.207214
H	1.492028	1.859307	-0.635386
H	1.620073	2.061481	1.125118
H	3.089285	1.824447	0.164039

TS6ain

SCF Energy: -347.874776629 H

Num. Imaginary Frequencies: 1 (i321.2049)

C	2.033480	-0.285368	-0.400424
C	1.073351	0.743278	-0.095158
C	-0.284258	0.646686	-0.020188
C	-1.014339	-0.591478	-0.209043
C	-2.350219	-0.750167	-0.121941
C	-3.375802	0.300825	0.171497
O	1.869661	1.757821	0.150199
H	-0.426344	-1.475614	-0.451476
H	-0.826215	1.565402	0.191142
H	-2.741863	-1.752900	-0.284655

H	2.748055	-0.030085	-1.180362
C	2.270879	-1.501344	0.365464
H	-2.947599	1.295969	0.311049
H	-3.937958	0.043265	1.077075
H	-4.107329	0.356692	-0.643308
H	2.457155	-2.326052	-0.335855
H	1.479252	-1.737601	1.075121
H	3.227005	-1.376232	0.898435

TS6aout

SCF Energy: -347.870560527 H

Num. Imaginary Frequencies: 1 (i527.1952)

C	1.851895	-0.526752	-0.378621
C	0.975982	0.595318	-0.123933
C	-0.381400	0.576528	-0.024360
C	-1.157728	-0.631398	-0.230094
C	-2.493845	-0.762745	-0.113562
C	-3.476062	0.292093	0.296189
O	1.832537	1.586059	-0.110572
H	-0.596643	-1.523594	-0.512467
H	-0.877034	1.516234	0.205843
H	-2.919110	-1.740639	-0.332987
H	1.767986	-1.061233	-1.327854
C	2.942497	-0.925581	0.499158
H	-3.003828	1.245336	0.545031
H	-4.050473	-0.038082	1.169756
H	-4.202845	0.474074	-0.504725
H	2.756151	-1.991920	0.712447
H	3.000436	-0.352099	1.422359
H	3.897034	-0.921325	-0.041491

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10ainMg

SCF Energy: -347.910228232 H

Num. Imaginary Frequencies: 0

C	1.274611	1.028080	-0.037545
C	1.246173	-0.388759	0.136348
C	0.294668	-1.221692	-0.582401
C	-1.096382	-1.111695	-0.766026
C	-2.022949	-0.387802	-0.051516
C	-1.817855	0.470879	1.143759
O	2.180960	-0.957674	0.787032
H	-1.505480	-1.779294	-1.521938
H	0.757207	-2.114983	-0.998967
H	-3.056958	-0.497151	-0.372253
H	2.172293	1.495298	0.365071
C	0.331148	1.921823	-0.742235
H	-0.828695	0.359270	1.594883
H	-2.582991	0.242200	1.893008
H	-1.950744	1.528618	0.880753
H	-0.159563	2.586613	-0.016951
H	-0.441512	1.397398	-1.305090
H	0.892280	2.578425	-1.417076

10ainPg

SCF Energy: -347.910228239 H

Num. Imaginary Frequencies: 0

C	-1.274618	1.028069	-0.037552
C	-1.246163	-0.388768	0.136347
C	-0.294657	-1.221692	-0.582414
C	1.096391	-1.111681	-0.766040
C	2.022947	-0.387786	-0.051515
C	1.817837	0.470875	1.143771
O	-2.180939	-0.957691	0.787040
H	1.505497	-1.779266	-1.521958
H	-0.757194	-2.114978	-0.998994
H	3.056958	-0.497117	-0.372252
H	-2.172310	1.495274	0.365058
C	-0.331163	1.921831	-0.742227
H	0.828675	0.359253	1.594886
H	1.950721	1.528618	0.880780
H	2.582970	0.242192	1.893022
H	0.441516	1.397419	-1.305070
H	0.159526	2.586629	-0.016936
H	-0.892295	2.578421	-1.417080

10aoutMg

SCF Energy: -347.915485246 H

Num. Imaginary Frequencies: 0

C	1.038738	0.550784	-0.508087
C	0.824661	-0.701876	0.135846
O	1.709349	-1.260937	0.862125
C	-0.387729	-1.398189	-0.221290
C	-1.660501	-0.871365	-0.554904
C	-2.237175	0.311584	-0.175184
C	-1.739128	1.355170	0.765747
H	-2.300068	-1.550365	-1.115731
H	-0.297416	-2.483442	-0.227770
H	-3.241879	0.485071	-0.556371
H	0.236149	0.967984	-1.106635
C	2.311753	1.291572	-0.411614
H	-1.480960	2.272261	0.222772
H	-2.542386	1.621283	1.460983
H	-0.860355	1.042842	1.334700
H	3.153595	0.626366	-0.199976
H	2.505197	1.873185	-1.316043
H	2.249617	2.006227	0.423981

10aoutPg

SCF Energy: -347.915485239 H

Num. Imaginary Frequencies: 0

C	-1.038745	0.550785	-0.508082
C	-0.824663	-0.701875	0.135847
O	-1.709346	-1.260944	0.862129
C	0.387727	-1.398185	-0.221298
C	1.660503	-0.871365	-0.554904
C	2.237180	0.311582	-0.175182
C	1.739134	1.355171	0.765744
H	2.300069	-1.550368	-1.115727
H	0.297412	-2.483438	-0.227783
H	3.241886	0.485063	-0.556365
H	-0.236155	0.967994	-1.106622
C	-2.311761	1.291572	-0.411612
H	2.542389	1.621277	1.460988
H	1.480981	2.272266	0.222767
H	0.860354	1.042853	1.334689
H	-3.153593	0.626382	-0.199887
H	-2.249585	2.006300	0.423918
H	-2.505243	1.873114	-1.316080

14aing

SCF Energy: -347.923212246 H

Num. Imaginary Frequencies: 0

C	-2.309677	0.217110	-0.000003
C	-1.175331	-0.652532	-0.000002
C	0.135193	-0.053575	0.000000
C	1.308289	-0.828138	0.000004
C	2.586009	-0.327867	0.000004
C	3.001979	1.099879	-0.000004
O	-1.345501	-1.917876	-0.000002
H	1.189570	-1.908627	0.000007
H	0.208682	1.026958	-0.000001
H	3.398319	-1.051997	0.000007

H	-3.269230	-0.297858	-0.000009
C	-2.367024	1.696205	0.000003
H	2.169109	1.804433	0.000011
H	3.629940	1.299504	-0.876558
H	3.629974	1.299506	0.876526
H	-2.935896	2.035754	-0.875363
H	-1.397181	2.193102	0.000014
H	-2.935907	2.035745	0.875367

14aoutg

SCF Energy: -347.928547262 H

Num. Imaginary Frequencies: 0

C	3.326699	-0.943293	0.009623
C	2.740237	0.422437	-0.018765
C	1.414565	0.764176	-0.015386
C	0.344547	-0.151984	0.007991
C	-1.031506	0.261406	0.012554
C	-1.959148	-0.819374	-0.002575
C	-3.419624	-0.603032	-0.023109
O	-1.401767	1.482830	0.022985
H	1.162777	1.821468	-0.033820
H	0.543030	-1.218995	0.021008
H	3.458920	1.239365	-0.042483
H	-1.569612	-1.832756	0.023409
H	3.973949	-1.081325	-0.864568
H	3.975055	-1.042698	0.888414
H	2.585831	-1.743625	0.028201
H	-3.760343	-0.280775	0.972638
H	-3.687992	0.206620	-0.711190
H	-3.962101	-1.511934	-0.287498

7aing

SCF Energy: -347.915513524 H

Num. Imaginary Frequencies: 0

C	-2.182760	0.282528	-0.001701
C	-1.228423	-0.790467	-0.030149
C	0.203233	-0.579446	0.030921
C	0.918080	0.588017	-0.272671
C	2.289851	0.703447	-0.203920
C	3.269073	-0.328867	0.231565
O	-1.663985	-1.987241	-0.073648
H	0.380360	1.463404	-0.619195
H	0.760207	-1.482897	0.266996
H	2.714170	1.662863	-0.491945
H	-3.211586	-0.057052	-0.102464
C	-1.970170	1.736522	0.205226
H	2.824683	-1.305316	0.430806
H	3.778001	0.010009	1.142785
H	4.048996	-0.446647	-0.529419
H	-1.737706	2.236763	-0.746656
H	-1.151750	1.953520	0.896625
H	-2.886797	2.192890	0.586029

7aoutg

SCF Energy: -347.923303697 H

Num. Imaginary Frequencies: 0

C	-3.489595	0.400393	0.083832
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C	-2.568287	-0.761302	-0.041401
C	-1.195304	-0.753260	-0.077248
C	-0.403994	0.407915	-0.010583
C	1.035688	0.496528	-0.024144
C	1.806812	-0.705557	0.030176
C	3.284223	-0.669393	0.063355
O	1.598691	1.639604	-0.058439
H	-0.709614	-1.720471	-0.167049
H	-0.902104	1.373328	0.041289
H	-3.051255	-1.733786	-0.110376
H	1.305998	-1.666887	0.036429
H	-4.164854	0.428392	-0.779792
H	-4.126489	0.267176	0.966414
H	-2.984650	1.363987	0.163311
H	3.674091	-0.318803	-0.903726
H	3.643341	0.051112	0.808373
H	3.708753	-1.652821	0.268720

TS12ainMg

SCF Energy: -347.897318931 H

Num. Imaginary Frequencies: 1 (i314.6248)

C	1.696539	0.151231	0.159752
C	0.975917	-0.366068	1.246732
C	-0.286557	-0.910146	1.119514
C	-1.057955	-0.525772	-0.044015
C	-0.810176	0.803241	-0.572687
C	-0.714687	2.071370	0.207494
O	-1.916765	-1.279395	-0.590684
H	-0.717750	-1.573176	1.863729
H	1.432707	-0.294126	2.233816
H	2.472798	0.876096	0.404681
C	1.817174	-0.426216	-1.218151
H	-0.441032	1.914484	1.251809
H	-0.008167	2.767676	-0.254576
H	-1.080477	0.921578	-1.622276
H	1.073418	-1.195378	-1.433102
H	1.764623	0.348691	-1.988451
H	2.814489	-0.879279	-1.302011
H	-1.698008	2.562754	0.180016

TS12ainPg

SCF Energy: -347.897319020 H

Num. Imaginary Frequencies: 1 (i314.6271)

C	-1.696534	0.151241	0.159747
C	-0.975914	-0.366035	1.246739
C	0.286558	-0.910121	1.119532
C	1.057953	-0.525776	-0.044009
C	0.810179	0.803230	-0.572702
C	0.714693	2.071368	0.207463
O	1.916753	-1.279412	-0.590669
H	0.717752	-1.573131	1.863764
H	-1.432703	-0.294068	2.233822
H	-2.472787	0.876120	0.404658
C	-1.817175	-0.426242	-1.218140
H	0.441031	1.914496	1.251778
H	1.698016	2.562748	0.179986
H	1.080477	0.921551	-1.622294

H	-1.073428	-1.195420	-1.433068
H	-2.814496	-0.879295	-1.301989
H	-1.764613	0.348642	-1.988463
H	0.008178	2.767672	-0.254619

TS12aoutMg

SCF Energy: -347.909285013 H

Num. Imaginary Frequencies: 1 (i246.8807)

C	1.778365	-0.554240	-0.245574
C	1.631403	0.805813	-0.518758
C	0.507370	1.533496	-0.158077
C	-0.723091	0.816108	0.068335
O	-1.629108	1.224683	0.868833
C	-0.863862	-0.370487	-0.721944
C	-1.915460	-1.365941	-0.433726
H	2.429014	1.296739	-1.074908
H	0.528429	2.615272	-0.056675
C	1.348347	-1.312434	0.971505
H	2.517568	-1.080345	-0.849896
H	-0.270476	-0.476018	-1.621064
H	-2.847721	-0.874979	-0.130258
H	-1.604426	-1.981155	0.426437
H	0.691568	-0.742901	1.630719
H	0.857733	-2.255307	0.706693
H	2.255907	-1.583380	1.526808
H	-2.103168	-2.029280	-1.279086

TS12aoutPg

SCF Energy: -347.909285022 H

Num. Imaginary Frequencies: 1 (i246.8833)

C	1.778364	0.554240	-0.245570
C	1.631406	-0.805814	-0.518752
C	0.507371	-1.533498	-0.158076
C	-0.723091	-0.816111	0.068333
O	-1.629111	-1.224690	0.868825
C	-0.863859	0.370487	-0.721944
C	-1.915452	1.365944	-0.433725
H	2.429021	-1.296741	-1.074895
H	0.528431	-2.615273	-0.056673
C	1.348335	1.312439	0.971503
H	2.517570	1.080344	-0.849889
H	-0.270466	0.476023	-1.621058
H	-1.604384	1.981201	0.426396
H	-2.847696	0.874989	-0.130197
H	0.691569	0.742899	1.630724
H	2.255891	1.583409	1.526801
H	0.857701	2.255298	0.706682
H	-2.103198	2.029249	-1.279105

TS13aing

SCF Energy: -347.893978938 H

Num. Imaginary Frequencies: 1 (i326.9449)

C	-2.259867	0.212255	-0.450260
C	-1.019415	-0.452485	-0.163858
C	0.243829	0.046670	-0.180236
C	1.408991	-0.777126	0.076969
C	2.690393	-0.363287	0.124484

C	3.196998	1.035228	-0.048194
O	-1.517918	-1.616863	0.186149
H	1.213833	-1.835818	0.241913
H	0.347352	1.102205	-0.413901
H	3.451793	-1.118170	0.314028
H	-2.885459	-0.265619	-1.200615
C	-2.794286	1.321594	0.329851
H	2.400993	1.760055	-0.234095
H	3.905229	1.085167	-0.883816
H	3.745960	1.355558	0.845307
H	-3.590274	1.848318	-0.199391
H	-1.996889	1.986293	0.675791
H	-3.249055	0.879820	1.233046

TS13aoutg

SCF Energy: -347.888771357 H

Num. Imaginary Frequencies: 1 (i543.8600)

C	2.124951	-0.596560	-0.418767
C	0.959507	0.232653	-0.223031
C	-0.336746	-0.173261	-0.161614
C	-1.425085	0.734604	0.147117
C	-2.734536	0.424267	0.219486
C	-3.359866	-0.915680	-0.019178
O	1.519823	1.417094	-0.196083
H	-1.139573	1.766395	0.346577
H	-0.524875	-1.228920	-0.335494
H	-3.424903	1.225111	0.479610
H	2.248759	-1.126697	-1.365842
C	3.228227	-0.685914	0.529031
H	-2.635154	-1.682365	-0.302868
H	-4.114235	-0.851738	-0.812267
H	-3.883199	-1.259804	0.881078
H	3.336136	-1.763415	0.738038
H	3.064374	-0.129626	1.450272
H	4.175368	-0.406352	0.051292

TS7-10ainMg

SCF Energy: -347.896300325 H

Num. Imaginary Frequencies: 1 (i171.0549)

C	-1.552743	0.856079	-0.308011
C	-1.331146	-0.529228	-0.006148
C	-0.120499	-0.970137	0.628406
C	1.034790	-0.177416	1.071538
C	2.127087	0.064616	0.340539
C	2.336454	-0.350423	-1.082333
O	-2.222338	-1.386170	-0.326284
H	0.986313	0.193169	2.097496
H	-0.077815	-2.046070	0.800852
H	2.930567	0.633970	0.803805
H	-2.480234	1.034515	-0.848935
C	-0.716044	2.036471	0.006131
H	1.502077	-0.943684	-1.467768
H	3.256228	-0.936976	-1.182785
H	2.452800	0.533112	-1.720854
H	0.166578	2.066548	-0.648061
H	-0.338439	2.022616	1.032608
H	-1.286759	2.952388	-0.156825

TS7-10ainPg

SCF Energy: -347.896300332 H

Num. Imaginary Frequencies: 1 (i171.0548)

C	1.552737	0.856078	-0.308022
C	1.331147	-0.529228	-0.006150
C	0.120499	-0.970138	0.628403
C	-1.034788	-0.177417	1.071537
C	-2.127087	0.064616	0.340540
C	-2.336458	-0.350424	-1.082331
O	2.222344	-1.386167	-0.326278
H	-0.986311	0.193167	2.097495
H	0.077815	-2.046072	0.800846
H	-2.930566	0.633970	0.803808
H	2.480217	1.034514	-0.848965
C	0.716046	2.036471	0.006139
H	-1.502087	-0.943693	-1.467766
H	-2.452797	0.533112	-1.720854
H	-3.256238	-0.936967	-1.182782
H	0.338429	2.022597	1.032610
H	-0.166567	2.066573	-0.648066
H	1.286772	2.952386	-0.156793

TS7-10aoutMg

SCF Energy: -347.903995455 H

Num. Imaginary Frequencies: 1 (i167.1269)

C	2.552452	-0.549064	1.064075
C	2.366971	-0.372718	-0.410588
C	1.389211	0.325466	-0.997356
C	0.351103	1.087061	-0.282644
C	-0.971658	0.642053	0.025774
C	-1.269301	-0.717608	-0.299426
C	-2.576167	-1.319895	0.012278
O	-1.825851	1.411541	0.579668
H	1.350018	0.380741	-2.086038
H	0.585913	2.108466	0.019001
H	3.089314	-0.871379	-1.054039
H	-0.507613	-1.306674	-0.800935
H	2.453962	-1.606020	1.337130
H	3.559525	-0.238265	1.362934
H	1.824029	0.022634	1.646259
H	-2.876037	-1.086792	1.041329
H	-3.348009	-0.868388	-0.629552
H	-2.579958	-2.398429	-0.146105

TS7-10aoutPg

SCF Energy: -347.903999717 H

Num. Imaginary Frequencies: 1 (i170.2656)

C	-2.558201	-0.498439	1.083792
C	-2.366059	-0.399723	-0.397294
C	-1.387097	0.268977	-1.015523
C	-0.354452	1.067990	-0.334429
C	0.964028	0.638873	0.011756
C	1.283744	-0.721504	-0.289714
C	2.600551	-1.294044	0.036860
O	1.799657	1.424991	0.570528
H	-1.343093	0.267947	-2.105368

H	-0.593142	2.102470	-0.084945
H	-3.084676	-0.933389	-1.016392
H	0.525242	-1.337748	-0.762640
H	-3.568961	-0.179205	1.360387
H	-2.454082	-1.538834	1.413036
H	-1.837064	0.108522	1.638733
H	2.702226	-2.321573	-0.311908
H	3.400762	-0.676311	-0.392265
H	2.760448	-1.264591	1.124443

TS7-14out_Met

SCF Energy: -347.816494100 H

Num. Imaginary Frequencies: 1 (i298.8589)

C	1.200126	-0.789261	-0.049725
C	0.419630	0.378384	-0.022406
C	-1.019648	0.487254	-0.012307
C	2.574887	-0.779771	-0.024335
O	-1.565779	1.637649	-0.024375
C	-1.810874	-0.703627	0.021773
H	0.716942	-1.761038	-0.086642
H	0.933594	1.337496	-0.010149
H	3.073527	-1.745845	-0.034230
H	-1.324984	-1.671736	0.059364
C	3.445679	0.430568	0.047538
H	4.479912	0.178237	-0.194184
H	3.111553	1.222371	-0.630148
H	3.435925	0.849146	1.062321

C	-3.287558	-0.641132	0.026979
H	-3.643959	-0.120663	0.927723
H	-3.734890	-1.634947	-0.003065
H	-3.654837	-0.048699	-0.821090

TS7ain-outg

SCF Energy: -347.780497747 H

Num. Imaginary Frequencies: 1

C	1.163686	-0.641799	-0.218421
C	0.386767	0.565810	-0.010176
C	-0.970956	0.587605	-0.112217
C	2.500668	-0.765165	-0.112567
O	-1.824290	1.581380	-0.130178
C	-1.849617	-0.530587	-0.364946
H	0.604240	-1.534808	-0.501795
H	0.884823	1.505521	0.215854
H	2.932324	-1.737470	-0.343426
C	3.476670	0.299507	0.288558
H	4.137860	-0.068580	1.081246
H	4.123510	0.574827	-0.553626
H	2.989837	1.208640	0.650456
H	-1.751813	-1.078343	-1.305367
C	-2.966331	-0.906991	0.490653
H	-3.015599	-0.350046	1.424419
H	-3.909425	-0.834493	-0.066959
H	-2.846764	-1.986565	0.675325

OPEN SHELL TRIPLET ISOMERIZATION METHYL SUBSTITUTION

10ainMt

SCF Energy: -347.906529241 H

Num. Imaginary Frequencies: 0

C	1.265421	0.938716	0.193725
C	1.143105	-0.492369	0.132765
C	0.176869	-1.158785	-0.756946
C	-1.186713	-0.882800	-0.901621
C	-2.026276	-0.146107	-0.083877
C	-1.724559	0.421552	1.263769
O	1.939962	-1.204092	0.801809
H	-1.663948	-1.364102	-1.753954
H	0.600559	-1.958199	-1.360769
H	-3.048603	-0.020172	-0.433267
H	1.881340	1.322314	1.003582
C	0.696893	1.892085	-0.788273
H	-0.856185	-0.041339	1.738892
H	-2.587647	0.277430	1.922147
H	-1.547963	1.504032	1.218087
H	-0.192859	2.393600	-0.381716
H	0.404100	1.402929	-1.720402
H	1.423069	2.682493	-1.004322

10ainPt

SCF Energy: -347.906529247 H

Num. Imaginary Frequencies: 0

C	-1.265420	0.938718	0.193723
C	-1.143106	-0.492368	0.132765
C	-0.176870	-1.158788	-0.756941

C	1.186713	-0.882805	-0.901617
C	2.026277	-0.146110	-0.083877
C	1.724560	0.421556	1.263766
O	-1.939966	-1.204088	0.801809
H	1.663948	-1.364113	-1.753947
H	-0.600561	-1.958204	-1.360760
H	3.048604	-0.020179	-0.433266
H	-1.881342	1.322318	1.003577
C	-0.696890	1.892084	-0.788276
H	0.856176	-0.041318	1.738886
H	1.547983	1.504039	1.218081
H	2.587643	0.277422	1.922150
H	-0.404087	1.402924	-1.720400
H	0.192857	2.393605	-0.381715
H	-1.423068	2.682488	-1.004334

10aoutMt

SCF Energy: -347.907866964 H

Num. Imaginary Frequencies: 0

C	1.103890	0.465579	-0.596455
C	0.770047	-0.778907	0.043588
O	1.616281	-1.374063	0.763013
C	-0.524429	-1.433355	-0.197244
C	-1.783158	-0.849319	-0.378496
C	-2.225283	0.431528	-0.091645
C	-1.492264	1.515130	0.626469
H	-2.546179	-1.530007	-0.753648
H	-0.461634	-2.517182	-0.263591

H	-3.249419	0.658139	-0.379044
H	0.437417	0.828368	-1.373485
C	2.309185	1.258896	-0.268795
H	-1.007912	2.206993	-0.076587
H	-2.196041	2.110964	1.215927
H	-0.722115	1.130541	1.300554
H	2.866586	0.836476	0.569261
H	2.975468	1.319557	-1.139576
H	2.025643	2.291341	-0.028448

10aoutPt

SCF Energy: -347.907866984 H

Num. Imaginary Frequencies: 0

C	-1.103890	0.465584	-0.596452
C	-0.770051	-0.778905	0.043587
O	-1.616289	-1.374064	0.763005
C	0.524425	-1.433356	-0.197242
C	1.783157	-0.849325	-0.378489
C	2.225288	0.431521	-0.091643
C	1.492273	1.515133	0.626460
H	2.546177	-1.530018	-0.753634
H	0.461626	-2.517182	-0.263593
H	3.249426	0.658124	-0.379040
H	-0.437414	0.828377	-1.373476
C	-2.309186	1.258900	-0.268790
H	2.196049	2.110950	1.215937
H	1.007954	2.207009	-0.076606
H	0.722101	1.130558	1.300525
H	-2.866580	0.836485	0.569273
H	-2.025644	2.291348	-0.028451
H	-2.975476	1.319553	-1.139565

14aint

SCF Energy: -347.916015336 H

Num. Imaginary Frequencies: 0

C	-2.371609	0.209871	-0.000002
C	-1.200836	-0.631668	0.000000
C	0.137202	-0.043859	0.000001
C	1.293755	-0.825280	0.000002
C	2.591787	-0.351262	0.000001
C	3.026470	1.074229	-0.000002
O	-1.357598	-1.885403	-0.000001
H	1.162389	-1.905264	0.000002
H	0.208301	1.038688	0.000001
H	3.388779	-1.091602	0.000001
H	-3.324066	-0.312456	-0.000005
C	-2.334160	1.693031	0.000001
H	2.196924	1.783865	0.000012
H	3.652993	1.276649	-0.877302
H	3.653019	1.276646	0.877280
H	-3.340722	2.113568	-0.000001
H	-1.796245	2.076383	-0.878396
H	-1.796252	2.076379	0.878404

14aoutt

SCF Energy: -347.915975615 H

Num. Imaginary Frequencies: 0

C	3.385266	-0.921816	-0.005067
C	2.773217	0.437298	0.005877
C	1.421969	0.737784	0.006079
C	0.379054	-0.185493	-0.000884
C	-1.029505	0.218224	-0.002433
C	-2.047540	-0.805413	0.002240
C	-3.499724	-0.520637	0.001076
O	-1.352927	1.435778	-0.007772
H	1.151133	1.791632	0.012516
H	0.581939	-1.252425	-0.005018
H	3.467657	1.274488	0.012938
H	-1.720768	-1.841958	0.013689
H	4.028521	-1.038221	-0.886023
H	4.035307	-1.050129	0.869122
H	2.650781	-1.729552	-0.007914
H	-3.969643	-0.928137	0.906344
H	-3.710264	0.549332	-0.049615
H	-3.987666	-1.020937	-0.845202

7aint

SCF Energy: -347.912687759 H

Num. Imaginary Frequencies: 0

C	-2.195164	0.304158	-0.084205
C	-1.235928	-0.770575	-0.032201
C	0.208429	-0.591525	0.092539
C	0.924822	0.521178	-0.353739
C	2.298480	0.672808	-0.291229
C	3.282689	-0.284390	0.288465
O	-1.678690	-1.955134	-0.074336
H	0.372646	1.335984	-0.815018
H	0.732084	-1.458498	0.485885
H	2.711688	1.592397	-0.699434
H	-3.193982	0.002931	-0.389849
C	-1.970369	1.719255	0.301309
H	2.834767	-1.219829	0.629061
H	3.800366	0.177029	1.138892
H	4.057151	-0.520220	-0.450997
H	-1.752361	2.338303	-0.581881
H	-1.134603	1.835477	0.996788
H	-2.875983	2.132038	0.755604

7aoutt

SCF Energy: -347.915196148 H

Num. Imaginary Frequencies: 0

C	-3.526538	0.370136	-0.039582
C	-2.583754	-0.781271	0.035825
C	-1.200766	-0.727797	0.045124
C	-0.430871	0.434914	-0.006965
C	1.030261	0.491473	-0.000161
C	1.856277	-0.691246	-0.043257
C	3.336354	-0.652007	-0.004199
O	1.571800	1.631739	0.035664
H	-0.688980	-1.685729	0.098848
H	-0.909672	1.409256	-0.045484
H	-3.038233	-1.768474	0.078187
H	1.379556	-1.661675	-0.137083
H	-4.092520	0.331959	-0.979188

H	-4.265629	0.305088	0.767371
H	-3.033387	1.342150	0.021991
H	3.749886	-0.974941	-0.970023
H	3.721949	0.344310	0.218617
H	3.716849	-1.361079	0.740737

TS7-10ainMt

SCF Energy: -347.891217490 H

Num. Imaginary Frequencies: 1 (i114.0338)

C	-1.740916	0.524429	-0.490745
C	-1.171476	-0.675724	0.067894
C	0.047138	-0.738832	0.848836
C	1.056064	0.325007	0.989140
C	2.133939	0.452116	0.206841
C	2.474760	-0.423229	-0.959316
O	-1.775008	-1.773316	-0.148884
H	0.910095	1.035070	1.804493
H	0.236542	-1.706299	1.310613
H	2.824866	1.266326	0.419208
H	-2.560890	0.353726	-1.182855
C	-1.341311	1.918788	-0.173464
H	1.747719	-1.228733	-1.098191
H	3.467162	-0.869349	-0.829165
H	2.512696	0.167037	-1.882189
H	-0.431148	2.207464	-0.718290
H	-1.123572	2.050522	0.891629
H	-2.132596	2.615427	-0.459301

TS7-10ainPt

SCF Energy: -347.891058403 H

Num. Imaginary Frequencies: 1 (i135.5510)

C	1.641790	0.872847	-0.209722
C	1.327215	-0.521674	-0.026612
C	0.087228	-1.054437	0.498274
C	-1.050347	-0.306056	1.058706
C	-2.148162	0.044472	0.381055
C	-2.381313	-0.192307	-1.078679
O	2.214093	-1.368895	-0.367622
H	-0.982100	-0.056293	2.119317
H	0.044553	-2.142342	0.509033
H	-2.934769	0.570199	0.919558
H	2.639594	1.051641	-0.600609
C	0.750167	2.032020	0.048623
H	-1.555685	-0.739579	-1.543260
H	-2.497909	0.762491	-1.605014
H	-3.307146	-0.756127	-1.238297
H	0.406235	2.057911	1.089557
H	-0.154533	1.986470	-0.571972
H	1.269549	2.967596	-0.167204

TS7-10aoutMt

SCF Energy: -347.893680756 H

Num. Imaginary Frequencies: 1 (i114.3948)

C	2.530184	-0.601914	1.061389
C	2.361770	-0.417569	-0.414881
C	1.421555	0.332214	-1.001419
C	0.405326	1.119410	-0.285877

C	-0.924954	0.634011	0.028256
C	-1.328420	-0.714345	-0.284647
C	-2.680295	-1.252515	-0.008078
O	-1.730751	1.428792	0.598877
H	1.385210	0.375576	-2.092299
H	0.617918	2.143876	0.011997
H	3.064719	-0.949513	-1.053775
H	-0.591782	-1.369184	-0.741419
H	2.467687	-1.663913	1.324151
H	3.518526	-0.254871	1.383868
H	1.769552	-0.060687	1.632051
H	-2.618552	-2.099626	0.688101
H	-3.348687	-0.500849	0.416273
H	-3.129575	-1.646889	-0.928421

TS7-10aoutPt

SCF Energy: -347.893680754 H

Num. Imaginary Frequencies: 1 (i114.3951)

C	-2.530186	-0.601910	1.061390
C	-2.361770	-0.417571	-0.414880
C	-1.421554	0.332209	-1.001421
C	-0.405326	1.119408	-0.285881
C	0.924954	0.634011	0.028256
C	1.328421	-0.714346	-0.284644
C	2.680297	-1.252513	-0.008076
O	1.730749	1.428793	0.598876
H	-1.385208	0.375567	-2.092301
H	-0.617919	2.143875	0.011990
H	-3.064718	-0.949518	-1.053773
H	0.591783	-1.369187	-0.741413
H	-3.518527	-0.254863	1.383867
H	-2.467691	-1.663907	1.324156
H	-1.769553	-0.060682	1.632051
H	3.129576	-1.646889	-0.928419
H	3.348690	-0.500844	0.416270
H	2.618558	-2.099621	0.688106

TS7-14aint

SCF Energy: -347.904895408 H

Num. Imaginary Frequencies: 1 (i117.1958)

C	-1.049974	-0.194245	0.756704
C	-0.185612	-0.333269	-0.316642
C	1.250734	-0.687155	-0.134734
C	-2.406244	0.100057	0.653774
O	1.589698	-1.897113	-0.109371
C	2.240733	0.334128	0.000309
H	-0.638200	-0.319869	1.757483
H	-0.529831	-0.208264	-1.341489
H	-2.974674	0.194467	1.574868
H	3.264046	-0.011091	0.132105
C	-3.121185	0.306233	-0.643239
H	-4.195309	0.426231	-0.487831
H	-2.755002	1.202576	-1.161945
H	-2.966924	-0.536476	-1.328792
C	1.981558	1.789650	-0.019642
H	2.270240	2.232556	0.943348
H	0.935166	2.030970	-0.216457

H 2.612848 2.273411 -0.775504

TS7-14aoutt

SCF Energy: -347.904974850 H

Num. Imaginary Frequencies: 1 (i119.3781)

C	1.280646	-0.009893	0.746172
C	0.427293	0.165432	-0.330924
C	-1.035811	0.389210	-0.149718
C	2.656404	-0.202237	0.657684
O	-1.476158	1.555264	-0.016614
C	-1.907614	-0.747684	-0.142223
H	0.842510	0.005535	1.743627
H	0.794393	0.159355	-1.355378
H	3.211165	-0.307857	1.586032
H	-1.455341	-1.726139	-0.281793
C	3.421754	-0.239933	-0.625694
H	4.422324	-0.651936	-0.475826
H	2.913109	-0.840982	-1.388285
H	3.539580	0.768844	-1.045588
C	-3.372600	-0.663046	0.033028
H	-3.878246	-1.056594	-0.858813
H	-3.712572	0.358327	0.211605
H	-3.688095	-1.301763	0.867373

TS7ain-outt

SCF Energy: -347.900782293 H

Num. Imaginary Frequencies: 1 (i226.2513)

C	1.005833	-0.598609	-0.238672
C	0.328633	0.604716	-0.014545
C	-1.103524	0.729479	-0.145442
C	2.368161	-0.791357	-0.127052
O	-1.666292	1.823092	0.087199
C	-1.929296	-0.440051	-0.540803
H	0.406240	-1.461507	-0.524283
H	0.860885	1.504650	0.281969
H	2.741584	-1.793011	-0.327992
C	3.391946	0.222675	0.244853
H	2.984480	1.224203	0.392261
H	3.900610	-0.085728	1.166700
H	4.165710	0.270369	-0.530513
H	-2.174186	-0.551412	-1.593517
C	-2.598164	-1.268200	0.501746
H	-1.896260	-1.551019	1.296314
H	-3.416156	-0.715688	0.989709
H	-3.024102	-2.177507	0.071254

CLOSED SHELL PROPYL SUBSTITUTION EPOXIDE OPENING COMPETITION

14cin

SCF Energy: -426.549548199 H

Num. Imaginary Frequencies: 0

C	-1.370637	0.961961	0.434554
C	-0.071570	1.419525	0.173672
C	0.914460	0.391748	0.218453
C	2.202063	0.536334	-0.348006
C	3.139082	-0.453534	-0.363031
C	3.030414	-1.832517	0.170561
O	0.187415	2.628284	-0.228916
H	2.451727	1.493699	-0.795210
H	0.651575	-0.554165	0.677242
H	4.094799	-0.214275	-0.826401
H	-2.163928	1.643651	0.125335
C	-1.824096	-0.320824	1.041439
H	3.824612	-1.994904	0.909000
H	3.225386	-2.542369	-0.642265
H	2.067508	-2.067980	0.624356
H	-2.706230	-0.093903	1.652837
H	-1.071211	-0.749828	1.707006
C	-2.227206	-1.380293	-0.009679
H	-1.328974	-1.662105	-0.571971
H	-2.561685	-2.270631	0.533588
C	-3.320734	-0.921352	-0.969489
H	-4.215791	-0.603602	-0.423039
H	-2.989595	-0.080568	-1.588294
H	-3.608170	-1.735584	-1.641701

14cout

SCF Energy: -426.557705081 H

Num. Imaginary Frequencies: 0

C	4.254597	-1.132945	0.153772
C	3.783528	0.270987	0.217938
C	2.509649	0.743034	0.112870
C	1.375017	-0.076726	-0.089553
C	0.050845	0.442004	-0.204725
C	-0.875003	-0.564634	-0.508904
C	-2.314470	-0.307987	-0.730379
O	-0.237701	1.699321	-0.077628
H	2.346657	1.814358	0.185732
H	1.500542	-1.151743	-0.169158
H	4.567027	1.011807	0.368342
H	-0.526147	-1.593033	-0.542053
H	4.986181	-1.224867	-0.658072
H	4.797051	-1.370300	1.076727
H	3.464222	-1.868772	0.005438
H	-2.458841	0.704272	-1.124148
H	-2.716241	-1.028901	-1.450350
C	-3.105217	-0.439103	0.594299
H	-2.959468	-1.445456	1.001985
H	-2.693769	0.267059	1.323705
C	-4.592731	-0.169442	0.387644
H	-4.757140	0.839201	-0.006547
H	-5.027059	-0.883328	-0.320622
H	-5.138692	-0.255989	1.332274

S_Z_Z-1c

SCF Energy: -426.561789146 H

Num. Imaginary Frequencies: 0

C	-2.507297	0.701278	0.151661
C	-1.470112	-0.239184	-0.267326
C	-0.183598	0.089219	-0.303195

C	-3.823630	0.445875	0.237538
O	0.586889	1.185124	-0.017816
C	1.224373	-0.087092	-0.495338
H	-2.162055	1.699142	0.416847
H	-1.723783	-1.250255	-0.568539
H	-4.467807	1.258521	0.569705
H	1.612119	0.020039	-1.506673
C	-4.520077	-0.845565	-0.066228
H	-5.307637	-0.689716	-0.812497
H	-3.847077	-1.619851	-0.441780
H	-5.014689	-1.232188	0.832827
C	2.095633	-0.800333	0.500267
H	1.550468	-0.899413	1.444510
H	2.258374	-1.813232	0.110100
C	3.443879	-0.111266	0.737372
H	3.973362	-0.670694	1.516193
H	3.266428	0.892155	1.142441
C	4.324207	-0.018152	-0.507677
H	5.300166	0.410593	-0.260153
H	4.492911	-1.009483	-0.943505
H	3.873832	0.614708	-1.279382

TS13cin

SCF Energy: -426.528054556 H

Num. Imaginary Frequencies: 1 (i285.4637)

C	1.211693	0.258629	-0.469747
C	-0.107035	0.749295	-0.176782
C	-1.277100	0.057125	-0.166673
C	-2.556972	0.692966	0.077526
C	-3.758399	0.085549	0.138022
C	-4.042490	-1.377842	-0.004980
O	0.198821	1.989735	0.126023
H	-2.529688	1.772264	0.220691
H	-1.215118	-1.007072	-0.374000
H	-4.627776	0.716545	0.315821
H	1.746728	0.797076	-1.251569
C	1.888585	-0.775337	0.307832
H	-3.142516	-1.977658	-0.159144
H	-4.719036	-1.556045	-0.849406
H	-4.553831	-1.755356	0.888412
H	1.209991	-1.647248	0.283526
H	1.846794	-0.460674	1.363958
C	3.315416	-1.110334	-0.118315
H	3.323192	-1.352072	-1.186864
H	3.625263	-2.014723	0.413978
C	4.294183	0.023430	0.175037
H	5.305838	-0.239974	-0.146842
H	4.007385	0.943808	-0.346205
H	4.324918	0.242365	1.247934

TS13cout

SCF Energy: -426.522842634 H

Num. Imaginary Frequencies: 1 (i528.3637)

C	0.999022	-0.398625	-0.598792
C	-0.193571	0.353496	-0.286832
C	-1.460631	-0.132039	-0.189469
C	-2.578952	0.682362	0.245532

C	-3.864197	0.291574	0.354587
C	-4.429446	-1.057997	0.033374
O	0.297846	1.564630	-0.201206
H	-2.340222	1.709988	0.515700
H	-1.599165	-1.181649	-0.433301
H	-4.581185	1.027267	0.715478
H	1.100056	-0.854702	-1.587475
C	2.156542	-0.490569	0.284485
H	-4.870195	-1.512157	0.929147
H	-3.684550	-1.751022	-0.364924
H	-5.238348	-0.970071	-0.701426
H	2.232955	-1.582666	0.451180
H	1.974222	-0.005832	1.245669
C	3.483418	-0.031384	-0.350691
H	3.612526	-0.527011	-1.318720
H	3.415405	1.044435	-0.541422
C	4.667655	-0.331915	0.561058
H	4.554571	0.165223	1.530170
H	4.762480	-1.407945	0.741256
H	5.599641	0.019686	0.108803

S_E_Z-1c

SCF Energy: -426.540174255 H

Num. Imaginary Frequencies: 0

C	-2.257818	-0.607676	-0.440905
C	-1.577634	0.560570	0.114907
C	-0.292343	0.787295	-0.129251
C	-3.545385	-0.943725	-0.257250
O	0.655155	1.716710	0.198229
C	1.016027	0.537022	-0.657962
H	-1.642428	-1.256957	-1.062181
H	-2.111969	1.270474	0.739944
H	-3.896499	-1.850994	-0.746255
H	1.219373	0.838305	-1.684607
C	-4.570075	-0.208915	0.553227
H	-4.977194	-0.859560	1.336128
H	-4.173908	0.689276	1.032935
H	-5.416660	0.088848	-0.076605
C	1.963458	-0.455186	-0.048593
H	1.652923	-0.668486	0.980551
H	1.861604	-1.387798	-0.618293
C	3.416473	0.020851	-0.085781
H	3.694238	0.247608	-1.122376
H	3.501896	0.957666	0.477465
C	4.376809	-1.015529	0.491128
H	5.410038	-0.656142	0.460517
H	4.130767	-1.241557	1.534674
H	4.329516	-1.952609	-0.074849

TS6cin

SCF Energy: -426.504295006 H

Num. Imaginary Frequencies: 1 (i293.6295)

C	1.002522	1.019559	-0.409928
C	-0.317010	1.466640	-0.045220
C	-1.469779	0.744286	0.040152
C	-1.547713	-0.682694	-0.206785
C	-2.658735	-1.443458	-0.147636

C	-4.052816	-0.998622	0.171511
O	-0.081766	2.730127	0.221514
H	-0.619180	-1.183242	-0.478204
H	-2.371375	1.298228	0.291050
H	-2.544173	-2.505480	-0.358303
H	1.477025	1.586144	-1.210801
C	1.820851	0.073324	0.340316
H	-4.129795	0.072448	0.371501
H	-4.431875	-1.535596	1.049200
H	-4.729590	-1.238376	-0.657202
H	1.198630	-0.618323	0.917832
H	2.323263	0.717383	1.090098
C	2.895646	-0.635325	-0.495001
H	2.405935	-1.223877	-1.277695
H	3.514604	0.117891	-0.993869
C	3.761816	-1.543387	0.370881
H	3.157589	-2.318377	0.854313
H	4.525204	-2.040257	-0.234934
H	4.269168	-0.971522	1.155167

TS6cout

SCF Energy: -426.500476715 H

Num. Imaginary Frequencies: 1 (i498.9675)

C	0.810187	-0.044812	-0.475754
C	-0.221367	0.897809	-0.100089
C	-1.552278	0.638291	0.031657
C	-2.119967	-0.661862	-0.268004
C	-3.409927	-1.029790	-0.137992
C	-4.538443	-0.197833	0.390044
O	0.451207	2.017562	-0.016646
H	-1.425844	-1.415992	-0.642212
H	-2.191130	1.455357	0.357474
H	-3.672784	-2.041885	-0.440876
H	0.774454	-0.506021	-1.466758
C	1.981685	-0.340625	0.336959
H	-4.215697	0.780961	0.752893
H	-5.043823	-0.714635	1.214130
H	-5.295501	-0.036498	-0.387268
H	1.838725	-1.423431	0.531728
H	1.962831	0.184282	1.293775
C	3.329305	-0.182440	-0.391521
H	3.276230	-0.690653	-1.360191
H	3.485182	0.882790	-0.590262
C	4.481469	-0.740141	0.436376
H	4.351233	-1.812081	0.618530
H	5.432857	-0.597341	-0.084392
H	4.549618	-0.236929	1.406542

7cin

SCF Energy: -426.518862923 H

Num. Imaginary Frequencies: 0

C	-0.972732	1.181374	-0.010442
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C	0.343455	1.643273	0.076717
C	1.396610	0.678271	0.032217
C	1.416769	-0.631076	0.561764
C	2.432560	-1.513490	0.325551
C	3.620506	-1.343802	-0.542061
O	0.639718	2.911571	-0.014859
H	0.622211	-0.952479	1.223819
H	2.305388	1.044152	-0.443569
H	2.361359	-2.477699	0.825616
H	-1.676615	1.962353	-0.306437
C	-1.574690	-0.169219	0.187900
H	3.702272	-0.364361	-1.013813
H	3.591528	-2.111083	-1.325838
H	4.524248	-1.546635	0.043965
H	-1.539184	-0.435583	1.255692
H	-0.982081	-0.940794	-0.322619
C	-3.024726	-0.237616	-0.298834
H	-3.620081	0.513272	0.234092
H	-3.057856	0.029272	-1.361920
C	-3.634073	-1.620817	-0.094130
H	-4.668773	-1.652019	-0.448966
H	-3.068754	-2.384924	-0.639411
H	-3.633476	-1.897428	0.966180

7cout

SCF Energy: -426.529089586 H

Num. Imaginary Frequencies: 0

C	-4.461186	-0.271396	0.434002
C	-3.370541	-1.086635	-0.155244
C	-2.061743	-0.758019	-0.343438
C	-1.522585	0.504978	0.003684
C	-0.181272	0.976822	-0.134306
C	0.795607	-0.016322	-0.244325
C	2.243828	0.272094	-0.156650
O	0.081558	2.246157	-0.024895
H	-1.422606	-1.504143	-0.804031
H	-2.212784	1.247128	0.402732
H	-3.668507	-2.081995	-0.479899
H	0.496336	-1.048999	-0.394516
H	-5.276611	-0.183822	-0.293586
H	-4.879007	-0.808113	1.294099
H	-4.161250	0.726684	0.753660
H	2.557310	0.676825	-1.135064
H	2.408076	1.097910	0.549883
C	3.106732	-0.938781	0.198971
H	2.797573	-1.322903	1.178252
H	2.921904	-1.739860	-0.526785
C	4.593760	-0.599123	0.224480
H	4.803944	0.192476	0.952396
H	5.194296	-1.472803	0.495962
H	4.933269	-0.249345	-0.756980

OPEN SHELL SINGLET PROPYL SUBSTITUTION EPOXIDE OPENING COMPETITION

14aing

SCF Energy: -426.556029542 H

Num. Imaginary Frequencies: 0

C	-1.445631	0.943072	0.559232
C	-0.136179	1.346475	0.147068
C	0.901534	0.346016	0.180921

C	2.191136	0.580777	-0.325383
C	3.209634	-0.339291	-0.341786
C	3.176662	-1.737290	0.164361
O	0.073580	2.536014	-0.261979
H	2.392759	1.564050	-0.742582
H	0.660142	-0.625868	0.595912
H	4.154907	-0.019862	-0.775872
H	-2.217094	1.699400	0.425668
C	-1.869459	-0.389973	1.071562
H	2.226160	-2.021958	0.618002
H	3.974881	-1.880459	0.902272
H	3.393767	-2.429494	-0.658294
H	-2.767578	-0.250415	1.682614
H	-1.101360	-0.831233	1.713854
C	-2.200395	-1.389860	-0.062096
H	-1.283213	-1.596165	-0.625880
H	-2.508971	-2.330202	0.407114
C	-3.292234	-0.899836	-1.008472
H	-4.208244	-0.654470	-0.459433
H	-2.977639	-0.002824	-1.552972
H	-3.537562	-1.669157	-1.747012

14aoutg

SCF Energy: -426.561527259 H

Num. Imaginary Frequencies: 0

C	4.314630	-1.080044	0.171051
C	3.797693	0.311152	0.254917
C	2.501541	0.733529	0.127697
C	1.396588	-0.106464	-0.112022
C	0.056963	0.397213	-0.251166
C	-0.909770	-0.609902	-0.537444
C	-2.347600	-0.317633	-0.725000
O	-0.242317	1.632702	-0.140545
H	2.304735	1.799140	0.214230
H	1.538338	-1.178630	-0.203557
H	4.548374	1.077947	0.435859
H	-0.577906	-1.644328	-0.567931
H	5.059520	-1.143055	-0.631345
H	4.842888	-1.331497	1.098455
H	3.543436	-1.830538	-0.007792
H	-2.475571	0.692622	-1.129244
H	-2.782153	-1.035466	-1.429045
C	-3.116578	-0.413417	0.614627
H	-2.983469	-1.416348	1.035110
H	-2.678977	0.295044	1.326554
C	-4.601978	-0.117859	0.429942
H	-4.754452	0.889567	0.027737
H	-5.060570	-0.830696	-0.263998
H	-5.134593	-0.184828	1.383711

TSa13ing

SCF Energy: -426.528054556 H

Num. Imaginary Frequencies: 1 (i285.4637)

C	1.211693	0.258629	-0.469747
C	-0.107035	0.749295	-0.176782
C	-1.277100	0.057125	-0.166673
C	-2.556972	0.692966	0.077526

C	-3.758399	0.085549	0.138022
C	-4.042490	-1.377842	-0.004980
O	0.198821	1.989735	0.126023
H	-2.529688	1.772264	0.220691
H	-1.215118	-1.007072	-0.374000
H	-4.627776	0.716545	0.315821
H	1.746728	0.797075	-1.251569
C	1.888585	-0.775337	0.307832
H	-3.142516	-1.977658	-0.159144
H	-4.719036	-1.556045	-0.849406
H	-4.553831	-1.755356	0.888412
H	1.209991	-1.647248	0.283526
H	1.846794	-0.460674	1.363958
C	3.315415	-1.110334	-0.118315
H	3.323192	-1.352072	-1.186864
H	3.625263	-2.014723	0.413978
C	4.294183	0.023430	0.175037
H	5.305838	-0.239974	-0.146842
H	4.007385	0.943808	-0.346205
H	4.324918	0.242365	1.247933

TS13aoutg

SCF Energy: -426.522842630 H

Num. Imaginary Frequencies: 1 (i528.3640)

C	0.999022	-0.398612	-0.598800
C	-0.193571	0.353504	-0.286835
C	-1.460630	-0.132034	-0.189477
C	-2.578953	0.682360	0.245531
C	-3.864197	0.291567	0.354590
C	-4.429441	-1.058005	0.033376
O	0.297844	1.564639	-0.201196
H	-2.340227	1.709987	0.515702
H	-1.599162	-1.181642	-0.433320
H	-4.581186	1.027258	0.715485
H	1.100059	-0.854680	-1.587487
C	2.156539	-0.490566	0.284480
H	-4.870204	-1.512158	0.929146
H	-3.684540	-1.751034	-0.364906
H	-5.238332	-0.970084	-0.701436
H	2.232944	-1.582664	0.451171
H	1.974220	-0.005833	1.245665
C	3.483421	-0.031389	-0.350690
H	3.612531	-0.527016	-1.318719
H	3.415415	1.044431	-0.541421
C	4.667653	-0.331926	0.561064
H	4.554566	0.165212	1.530176
H	4.762471	-1.407956	0.741262
H	5.599643	0.019671	0.108813

TS6cing

SCF Energy: -426.504320769 H

Num. Imaginary Frequencies: 1 (i1906.7794)

C	1.003186	1.015444	-0.413185
C	-0.315934	1.461439	-0.046756
C	-1.472192	0.744833	0.041968
C	-1.555234	-0.680648	-0.209541
C	-2.668049	-1.439101	-0.149715

C	-4.060167	-0.991599	0.174199
O	-0.070885	2.722409	0.222583
H	-0.628352	-1.182362	-0.484775
H	-2.369883	1.301498	0.300440
H	-2.556610	-2.500761	-0.363819
H	1.475056	1.578907	-1.217647
C	1.823576	0.072115	0.340301
H	-4.134077	0.079354	0.375992
H	-4.438085	-1.529048	1.052100
H	-4.739767	-1.228484	-0.653026
H	1.200419	-0.622583	0.913387
H	2.322212	0.714395	1.093514
C	2.901238	-0.633442	-0.493736
H	2.414630	-1.220654	-1.279415
H	3.520834	0.121633	-0.989059
C	3.766277	-1.542718	0.372044
H	3.161633	-2.319321	0.852391
H	4.531561	-2.037598	-0.233024
H	4.271301	-0.972177	1.158806

TS6coutg

SCF Energy: -426.500476713 H

Num. Imaginary Frequencies: 1 (i498.9670)

C	0.810188	-0.044811	-0.475758
C	-0.221367	0.897809	-0.100091
C	-1.552277	0.638290	0.031656
C	-2.119967	-0.661862	-0.268007
C	-3.409927	-1.029790	-0.137993
C	-4.538442	-0.197833	0.390048
O	0.451207	2.017562	-0.016644
H	-1.425846	-1.415992	-0.642217
H	-2.191129	1.455356	0.357475
H	-3.672786	-2.041883	-0.440878
H	0.774456	-0.506019	-1.466763
C	1.981684	-0.340627	0.336956
H	-4.215695	0.780963	0.752891
H	-5.043814	-0.714633	1.214139
H	-5.295506	-0.036503	-0.387259
H	1.838724	-1.423434	0.531722
H	1.962827	0.184278	1.293774
C	3.329306	-0.182438	-0.391519
H	3.276235	-0.690648	-1.360191
H	3.485183	0.882793	-0.590255
C	4.481468	-0.740142	0.436379
H	4.351232	-1.812082	0.618528
H	5.432857	-0.597339	-0.084387
H	4.549615	-0.236934	1.406547

7cing

SCF Energy: -426.527370589 H

Num. Imaginary Frequencies: 0

C	-1.062522	1.143860	0.184637
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C	0.298737	1.574231	0.028839
C	1.416395	0.657299	-0.055268
C	1.474920	-0.678716	0.367201
C	2.586723	-1.485162	0.253583
C	3.899091	-1.146969	-0.360003
O	0.529198	2.823300	-0.082150
H	0.611547	-1.121140	0.850721
H	2.325236	1.123885	-0.427320
H	2.501809	-2.493054	0.654209
H	-1.765941	1.972662	0.263100
C	-1.648178	-0.223030	0.174984
H	3.959884	-0.129362	-0.748601
H	4.110346	-1.843864	-1.180223
H	4.699416	-1.289715	0.376057
H	-1.520286	-0.677668	1.171346
H	-1.107032	-0.873324	-0.522915
C	-3.140732	-0.214947	-0.171089
H	-3.674631	0.404504	0.559262
H	-3.279427	0.258675	-1.150016
C	-3.731831	-1.620898	-0.190174
H	-4.798821	-1.596192	-0.431855
H	-3.232339	-2.247354	-0.937544
H	-3.618966	-2.108465	0.784716

7coutg

SCF Energy: -426.535017676 H

Num. Imaginary Frequencies: 0

C	-4.582929	-0.180527	0.073865
C	-3.424700	-1.108704	-0.028869
C	-2.088063	-0.795743	-0.059308
C	-1.575390	0.513097	0.000805
C	-0.192493	0.922897	-0.018379
C	0.827821	-0.077118	-0.039554
C	2.265669	0.274911	-0.041656
O	0.099731	2.164308	-0.004616
H	-1.400424	-1.632597	-0.136565
H	-2.277056	1.341863	0.062334
H	-3.677734	-2.165467	-0.082765
H	0.554444	-1.127404	-0.058327
H	-5.261024	-0.345208	-0.771803
H	-5.159402	-0.412933	0.977491
H	-4.308319	0.874832	0.099578
H	2.479406	0.853975	-0.955355
H	2.459221	0.982912	0.779094
C	3.204515	-0.926913	0.053228
H	2.987472	-1.479901	0.974836
H	2.999452	-1.610041	-0.779771
C	4.673636	-0.516417	0.033596
H	4.905052	0.155313	0.867902
H	5.328427	-1.389620	0.113912
H	4.924234	0.006905	-0.896006

CLOSED SHELL CROTYL E SUBSTITUTION EPOXIDE OPENING COMPETITION

S_E_Z-1d

SCF Energy: -464.619530144 H

Num. Imaginary Frequencies: 0

C	-2.795359	-0.651927	-0.223281
C	-1.974059	0.545701	-0.057331
C	-0.692318	0.554693	-0.402173

C	-4.093163	-0.777338	0.099935
O	0.359095	1.431407	-0.389304
C	0.552440	0.030671	-0.880165
H	-2.286766	-1.515119	-0.650338
H	-2.398129	1.457389	0.353681
H	-4.561491	-1.742224	-0.087896
H	0.721671	0.000484	-1.955198
C	-4.986503	0.268301	0.696018
H	-5.411336	-0.085300	1.642711
H	-4.473713	1.213664	0.888663
H	-5.833359	0.472196	0.030124
C	1.437422	-0.847613	-0.034769
H	1.176048	-0.723491	1.020979
H	1.203507	-1.883068	-0.314764
C	2.895567	-0.563407	-0.265653
H	3.261456	-0.709244	-1.283393
C	3.737516	-0.142689	0.681113
H	3.356336	0.001493	1.693287
C	5.192625	0.147385	0.469927
H	5.814579	-0.486738	1.112248
H	5.489188	-0.019914	-0.569953
H	5.424235	1.185953	0.732552

TS6din

SCF Energy: -464.581165495 H

Num. Imaginary Frequencies: 1 (i319.9178)

C	0.530391	0.154990	-1.020316
C	-0.452438	0.981684	-0.362934
C	-1.736850	0.691971	-0.018813
C	-2.361103	-0.596507	-0.252952
C	-3.623390	-0.943343	0.067220
C	-4.665960	-0.086772	0.718158
O	0.272753	2.053890	-0.140610
H	-1.748739	-1.353288	-0.741588
H	-2.306695	1.492194	0.447399
H	-3.934442	-1.958871	-0.171879
H	0.995160	0.595264	-1.900534
C	1.147170	-1.055080	-0.460455
H	-4.322677	0.929840	0.922646
H	-4.987602	-0.532415	1.667104
H	-5.559228	-0.022640	0.085700
H	1.538237	-1.677373	-1.269636
H	0.450988	-1.610185	0.172043
C	2.307753	-0.518728	0.377665
H	2.033881	-0.091099	1.339651
C	3.577200	-0.533549	-0.034430
H	3.807721	-0.950274	-1.014990
C	4.731596	-0.023671	0.768106
H	4.408944	0.369175	1.736290
H	5.463726	-0.820369	0.940303
H	5.252474	0.772959	0.224877

TS6dout

SCF Energy: -464.577534212 H

Num. Imaginary Frequencies: 1 (i533.0103)

C	0.417132	-0.052459	-0.120035
C	-0.677491	0.886965	-0.092198

C	-2.010364	0.607910	-0.080923
C	-2.518494	-0.746907	-0.165324
C	-3.811883	-1.124170	-0.131729
C	-5.006806	-0.238389	0.044263
O	-0.032097	2.024554	-0.169391
H	-1.773370	-1.536459	-0.270728
H	-2.696768	1.449090	-0.025237
H	-4.024512	-2.186463	-0.238867
H	0.532894	-0.719355	-0.978455
C	1.500650	-0.076701	0.871947
H	-4.743284	0.809885	0.203215
H	-5.607595	-0.569576	0.899260
H	-5.659500	-0.293222	-0.835483
H	1.480029	-1.115577	1.244637
H	1.292940	0.604346	1.699679
C	2.856027	0.182371	0.249444
H	3.017645	1.200836	-0.101363
C	3.809982	-0.740852	0.116892
H	3.615765	-1.752712	0.474176
C	5.156014	-0.492279	-0.488784
H	5.950941	-0.701472	0.235860
H	5.322407	-1.159932	-1.341675
H	5.260584	0.541242	-0.831213

7din

SCF Energy: -464.597430184 H

Num. Imaginary Frequencies: 0

C	0.468901	1.129466	0.045979
C	-0.843208	1.587003	-0.094404
C	-1.899835	0.623671	-0.041798
C	-1.912268	-0.699550	-0.531778
C	-2.936333	-1.572036	-0.289321
C	-4.140870	-1.373248	0.547296
O	-1.142916	2.856125	-0.057864
H	-1.105285	-1.043466	-1.166947
H	-2.814947	1.005497	0.408417
H	-2.857260	-2.551717	-0.757119
H	1.165941	1.916003	0.340205
C	1.070992	-0.233733	-0.102070
H	-4.231001	-0.379713	0.986706
H	-4.129378	-2.116490	1.354391
H	-5.032337	-1.594042	-0.051002
H	1.054250	-0.540204	-1.157926
H	0.460747	-0.976808	0.431037
C	2.483450	-0.287462	0.415636
H	2.622431	-0.005402	1.460661
C	3.539141	-0.659949	-0.310729
H	3.383987	-0.936507	-1.355017
C	4.947459	-0.737541	0.196314
H	5.015074	-0.429281	1.243979
H	5.335827	-1.759110	0.111423
H	5.610700	-0.097470	-0.396645

7dout

SCF Energy: -464.607607617 H

Num. Imaginary Frequencies: 0

C	-4.361038	-1.079796	0.515257
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C	-3.245317	-1.356102	-0.422066
C	-2.086859	-0.661358	-0.605326
C	-1.770735	0.517692	0.111206
C	-0.599717	1.335480	0.026270
C	0.538343	0.681525	-0.449074
C	1.893844	1.267847	-0.351325
O	-0.606408	2.538069	0.516555
H	-1.398276	-1.030558	-1.358399
H	-2.517150	0.893007	0.809801
H	-3.382556	-2.236424	-1.047483
H	0.440951	-0.289094	-0.922946
H	-5.289984	-0.975204	-0.057530
H	-4.502360	-1.953562	1.162566
H	-4.225109	-0.196694	1.139506
H	2.056424	1.848576	-1.275893
H	1.913625	2.022429	0.446516
C	3.032467	0.295487	-0.183924
H	4.020388	0.704818	-0.395144
C	2.933429	-0.973312	0.220775
H	1.951567	-1.388789	0.451360
C	4.097728	-1.901430	0.399400
H	4.155671	-2.259622	1.433699
H	3.991243	-2.788234	-0.235952
H	5.043952	-1.411399	0.150311

S_E_Z-1d'

SCF Energy: -464.619647270 H

Num. Imaginary Frequencies: 0

C	0.696029	1.506591	-0.454625
C	-0.701861	1.326793	-0.197986
C	-1.840061	0.662440	-0.040348
C	-1.900568	-0.783117	-0.250994
C	-2.986267	-1.562927	-0.118966
C	-4.370503	-1.136304	0.265653
O	-0.241102	2.611184	-0.084477
H	-0.961930	-1.254019	-0.540402
H	-2.724945	1.221505	0.249816
H	-2.860404	-2.627100	-0.312166
H	1.025941	1.579815	-1.489240
C	1.747590	1.140984	0.562431
H	-5.082847	-1.387828	-0.528917
H	-4.450114	-0.064619	0.462892
H	-4.700501	-1.671964	1.163430
H	1.323775	1.281148	1.563430
H	2.605733	1.811666	0.451793
C	2.170696	-0.291541	0.372341
H	1.399284	-1.045235	0.538950
C	3.399596	-0.673786	0.017342
H	4.158232	0.092846	-0.147618
C	3.836914	-2.094757	-0.168085
H	3.016007	-2.794978	0.013567
H	4.212589	-2.256821	-1.184833
H	4.658614	-2.340142	0.514543

TS6dout'

SCF Energy: -464.591534587 H

Num. Imaginary Frequencies: 1 (i400.1952)

C	1.231091	1.179758	-0.312958
C	-0.186711	1.560044	-0.273024
C	-1.355977	0.889721	-0.173113
C	-1.477307	-0.560856	-0.132380
C	-2.607206	-1.273750	0.039204
C	-3.991608	-0.736259	0.254301
O	0.072520	2.839255	-0.416532
H	-0.557735	-1.124807	-0.277593
H	-2.254217	1.503090	-0.164603
H	-2.520474	-2.359171	0.021123
H	1.694908	1.132439	-1.294619
C	2.095591	1.089367	0.856699
H	-4.672890	-1.084096	-0.531711
H	-4.025530	0.356097	0.267746
H	-4.404113	-1.094521	1.205416
H	1.676429	1.496198	1.773734
H	3.131399	1.373773	0.684861
C	1.832861	-0.404102	0.731150
H	1.048016	-0.810655	1.361367
C	2.443488	-1.180744	-0.188126
H	3.200892	-0.735349	-0.832768
C	2.153911	-2.625062	-0.386734
H	3.074921	-3.209873	-0.287376
H	1.411492	-2.996176	0.323505
H	1.787942	-2.789700	-1.406931

7dout'_c3

SCF Energy: -464.603609843 H

Num. Imaginary Frequencies: 0

C	-0.873931	-0.671464	-0.731035
C	0.129342	-1.220409	0.212843
C	1.385783	-0.645605	0.225933
C	1.833478	0.539372	-0.477204
C	3.081188	1.056991	-0.454152
C	4.279382	0.525170	0.272661
O	-0.223095	-2.234514	0.944488
H	1.104252	1.088816	-1.068611
H	2.107635	-1.147379	0.867664
H	3.250098	1.968567	-1.025341
H	-0.569734	0.078190	-1.449654
C	-2.186171	-1.255552	-0.913665
H	5.099105	0.331289	-0.429776
H	4.078777	-0.401007	0.816216
H	4.655412	1.263125	0.991811
H	-2.350344	-2.241279	-0.490566
H	-2.690557	-1.050324	-1.852238
C	-2.330607	-0.155864	0.140406
H	-2.300316	-0.458916	1.181289
C	-2.531143	1.152131	-0.195892
H	-2.531886	1.422201	-1.251295
C	-2.737200	2.240571	0.777530
H	-1.940721	2.985559	0.656114
H	-3.673778	2.761350	0.545572
H	-2.753911	1.883871	1.808359

S_Z_Z-1d

SCF Energy: -464.619624044 H

Num. Imaginary Frequencies: 0

C	-2.867329	0.796844	-0.116229
C	-1.978865	-0.362762	-0.148227
C	-0.699691	-0.274548	-0.493263
C	-4.170491	0.787655	0.210658
O	0.182979	0.701977	-0.878806
C	0.638739	-0.716418	-0.740620
H	-2.413784	1.749103	-0.385763
H	-2.344780	-1.350418	0.112765
H	-4.696914	1.740420	0.185072
H	0.864443	-1.163492	-1.707474
C	-4.998859	-0.395673	0.609049
H	-5.834981	-0.527900	-0.087753
H	-4.430205	-1.328163	0.635651
H	-5.439521	-0.238316	1.600344
C	1.619770	-0.988775	0.369641
H	1.296782	-0.470898	1.278516
H	1.572246	-2.067735	0.567215
C	3.019928	-0.592866	-0.008636
H	3.445464	-1.095688	-0.878741
C	3.744089	0.320982	0.641447
H	3.304403	0.817400	1.507913
C	5.140976	0.725949	0.279883
H	5.831208	0.526203	1.107681
H	5.498278	0.189587	-0.604427
H	5.193929	1.801753	0.077234

TS13din

SCF Energy: -464.583024013 H

Num. Imaginary Frequencies: 1 (i348.6517)

C	-0.670619	0.032175	1.347387
C	0.460413	0.589509	0.662027
C	1.650292	0.016887	0.347684
C	2.711869	0.740987	-0.324652
C	3.913626	0.251345	-0.687487
C	4.416147	-1.147522	-0.504588
O	-0.085183	1.749819	0.368670
H	2.505700	1.787322	-0.545249
H	1.782016	-1.019889	0.642944
H	4.606310	0.938286	-1.170996
H	-1.039054	0.598754	2.199646
C	-1.471146	-1.092974	0.837129
H	3.684157	-1.810209	-0.037327
H	5.321676	-1.151001	0.114022
H	4.698748	-1.581023	-1.471146
H	-2.092585	-1.502105	1.636591
H	-0.801425	-1.856885	0.425075
C	-2.356386	-0.542147	-0.275989
H	-1.843089	-0.269071	-1.195983
C	-3.674222	-0.380528	-0.149106
H	-4.150171	-0.651952	0.793358
C	-4.570727	0.144498	-1.226489
H	-4.013295	0.384805	-2.136219
H	-5.346534	-0.588418	-1.473965
H	-5.086474	1.049450	-0.885607

TS13dout

SCF Energy: -464.578416788 H

Num. Imaginary Frequencies: 1 (i546.1649)

C	0.590549	-0.399520	-0.193446
C	-0.640634	0.344182	-0.118983
C	-1.906280	-0.154066	-0.122927
C	-3.076062	0.682855	0.058279
C	-4.361668	0.278080	0.051456
C	-4.871866	-1.113760	-0.162313
O	-0.169878	1.567499	-0.122814
H	-2.881698	1.741618	0.222758
H	-2.005398	-1.227899	-0.253903
H	-5.124399	1.036816	0.218997
H	0.819983	-0.974274	-1.094440
C	1.651864	-0.328479	0.821533
H	-4.077264	-1.835524	-0.365482
H	-5.576838	-1.138525	-1.001522
H	-5.425372	-1.457427	0.719940
H	1.780367	-1.382324	1.124337
H	1.329602	0.253276	1.687703
C	2.962868	0.173156	0.256157
H	2.977643	1.228635	-0.012936
C	4.045657	-0.586489	0.081409
H	3.998811	-1.640823	0.356080
C	5.348731	-0.096500	-0.468508
H	6.158648	-0.262284	0.250752
H	5.615811	-0.647975	-1.377176
H	5.310170	0.969957	-0.708544

14din

SCF Energy: -464.608434501 H

Num. Imaginary Frequencies: 0

C	-0.625770	1.421730	0.423649
C	0.705555	1.515660	0.000880
C	1.459893	0.312040	0.134140
C	2.739181	0.140903	-0.437831
C	3.453597	-1.018826	-0.357007
C	3.076565	-2.287962	0.308188
O	1.190577	2.585196	-0.560130
H	3.170533	0.980320	-0.974331
H	1.019788	-0.515364	0.676996
H	4.427178	-1.027391	-0.844064
H	-1.256492	2.271168	0.158055
C	-1.341656	0.319606	1.132771
H	2.112395	-2.265942	0.816279
H	3.857434	-2.557417	1.029040
H	3.069373	-3.089434	-0.440745
H	-1.992351	0.774240	1.888628
H	-0.661861	-0.362727	1.648535
C	-2.192221	-0.446562	0.142237
H	-1.640207	-1.030105	-0.595730
C	-3.526910	-0.427998	0.116829
H	-4.056741	0.171740	0.858255
C	-4.374173	-1.180492	-0.862827
H	-3.763394	-1.760530	-1.561033
H	-5.053206	-1.866610	-0.344077
H	-5.001427	-0.492105	-1.440940

14dout

SCF Energy: -464.614495378 H

Num. Imaginary Frequencies: 0

C	4.013666	1.594858	-0.481574
C	3.890318	0.289716	0.210677
C	2.780546	-0.486405	0.359011
C	1.503548	-0.142818	-0.143559
C	0.353918	-0.968448	0.019424
C	-0.798812	-0.362754	-0.495790
C	-2.137059	-0.991665	-0.389700
O	0.373871	-2.126973	0.599260
H	2.871936	-1.425732	0.896441
H	1.374252	0.794416	-0.674807
H	4.811762	-0.085956	0.652289
H	-0.711119	0.601192	-0.989527
H	4.380142	2.342603	0.232112
H	4.784328	1.515902	-1.257550
H	3.089506	1.955021	-0.933705
H	-2.124890	-1.905274	-1.002827
H	-2.251163	-1.365816	0.639739
C	-3.291360	-0.105824	-0.788640
H	-3.843225	-0.396149	-1.679799
C	-3.665714	0.998678	-0.133728
H	-4.510881	1.563100	-0.525600
C	-3.026408	1.553927	1.103909
H	-2.273381	0.884159	1.528608
H	-2.541109	2.513385	0.888540
H	-3.782992	1.749332	1.871832

S_Z_Z-1d'

SCF Energy: -464.619438738 H

Num. Imaginary Frequencies: 0

C	-0.754954	-1.229210	-0.481584
C	0.597517	-0.797153	-0.298141
C	1.618886	0.047583	-0.218877
C	2.972015	-0.385973	0.122388
C	4.059830	0.397861	0.208314
C	4.137500	1.875671	-0.027068
O	0.375238	-2.140670	-0.130457
H	3.091089	-1.449169	0.324112
H	1.402210	1.091166	-0.422240
H	4.998667	-0.083031	0.478501
H	-1.110730	-1.391173	-1.497622
C	-1.815020	-1.030202	0.573111
H	4.488478	2.389089	0.875765
H	3.181037	2.316543	-0.317144
H	4.865607	2.097371	-0.815988
H	-1.334427	-1.060493	1.557616
H	-2.537455	-1.850763	0.514221
C	-2.503388	0.293344	0.369280
H	-1.884221	1.181224	0.506452
C	-3.787297	0.433023	0.030787
H	-4.393041	-0.464107	-0.105894
C	-4.482654	1.744591	-0.172742
H	-4.890761	1.815065	-1.187589
H	-5.329202	1.848369	0.515570
H	-3.803758	2.588062	-0.014915

TS13dout'

SCF Energy: -464.592994819 H

Num. Imaginary Frequencies: 1 (i405.9606)

C	-1.159797	-1.214901	-0.269354
C	0.296733	-1.165717	-0.266488
C	1.203086	-0.177718	-0.109935
C	2.636234	-0.431590	-0.138145
C	3.625614	0.469368	0.010684
C	3.475094	1.943366	0.246394
O	0.385378	-2.464355	-0.451786
H	2.925740	-1.469512	-0.300973
H	0.818765	0.826842	0.034540
H	4.650224	0.104235	-0.043245
H	-1.647855	-1.353912	-1.229763
C	-1.979208	-1.227628	0.935846
H	3.969697	2.239490	1.179363
H	2.430994	2.261041	0.304946
H	3.956178	2.515494	-0.556234
H	-1.437787	-1.438443	1.855579
H	-2.916416	-1.773304	0.848430
C	-2.122547	0.273127	0.697073
H	-1.417710	0.916886	1.215595
C	-3.005385	0.786563	-0.181170
H	-3.669294	0.105501	-0.713476
C	-3.156137	2.237554	-0.473019
H	-2.472009	2.847696	0.121350
H	-2.969694	2.423110	-1.537065
H	-4.185986	2.555175	-0.276079

14dout'_c3

SCF Energy: -464.599081343 H

Num. Imaginary Frequencies: 0

C	-1.414735	-1.001522	-0.272893
C	0.069035	-1.300772	-0.257702
C	1.007305	-0.319112	-0.082490
C	2.433732	-0.591970	-0.106458
C	3.443990	0.288994	0.047359
C	3.320002	1.766823	0.284063
O	0.250919	-2.565158	-0.479573
H	2.709593	-1.633817	-0.269850
H	0.663759	0.699870	0.062566
H	4.462049	-0.095034	-0.004068
H	-1.873337	-1.044506	-1.257365
C	-2.299245	-1.188871	0.866733
H	3.823830	2.058707	1.213827
H	2.280918	2.100274	0.350351
H	3.801617	2.335063	-0.521593
H	-1.864338	-1.591936	1.775864
H	-3.330681	-1.460120	0.666644
C	-1.948055	0.285786	0.686036
H	-1.178841	0.703362	1.324158
C	-2.585655	1.086786	-0.228476
H	-3.366125	0.648641	-0.849571
C	-2.270721	2.505156	-0.447823
H	-2.021012	2.658566	-1.504323
H	-3.183798	3.088940	-0.272318

H -1.464901 2.865472 0.192176

OPEN SHELL SINGLET CROTYL E SUBSTITUTION EPOXIDE OPENING COMPETITION

TS6ding

SCF Energy: -464.581165508 H

Num. Imaginary Frequencies: 1 (i319.9175)

C	0.530392	0.154979	-1.020314
C	-0.452435	0.981678	-0.362936
C	-1.736848	0.691971	-0.018815
C	-2.361104	-0.596507	-0.252948
C	-3.623392	-0.943339	0.067223
C	-4.665962	-0.086762	0.718154
O	0.272758	2.053883	-0.140617
H	-1.748741	-1.353292	-0.741579
H	-2.306692	1.492197	0.447394
H	-3.934447	-1.958867	-0.171871
H	0.995160	0.595248	-1.900536
C	1.147170	-1.055088	-0.460448
H	-4.322682	0.929855	0.922624
H	-4.987596	-0.532391	1.667109
H	-5.559235	-0.022643	0.085700
H	1.538237	-1.677386	-1.269624
H	0.450987	-1.610188	0.172054
C	2.307752	-0.518729	0.377668
H	2.033881	-0.091097	1.339653
C	3.577199	-0.533547	-0.034428
H	3.807719	-0.950274	-1.014987
C	4.731595	-0.023661	0.768102
H	4.408943	0.369189	1.736285
H	5.463728	-0.820355	0.940300
H	5.252467	0.772969	0.224868

TS6doutg

SCF Energy: -464.577586803 H

Num. Imaginary Frequencies: 1 (i3356.7171)

C	0.420549	-0.043328	-0.139595
C	-0.681351	0.886011	-0.092845
C	-2.015269	0.608206	-0.074753
C	-2.521872	-0.745863	-0.161522
C	-3.815505	-1.124634	-0.129147
C	-5.011166	-0.239867	0.045685
O	-0.035453	2.023246	-0.163945
H	-1.775564	-1.534214	-0.267283
H	-2.700834	1.449437	-0.011571
H	-4.026982	-2.187094	-0.236721
H	0.544242	-0.687368	-1.014022
C	1.500009	-0.083917	0.858109
H	-4.748686	0.808495	0.205715
H	-5.613058	-0.572222	0.899449
H	-5.662422	-0.294667	-0.835145
H	1.473092	-1.127394	1.217580
H	1.286853	0.584401	1.694967
C	2.860726	0.180835	0.251807
H	3.027818	1.203241	-0.085021
C	3.814444	-0.742145	0.115541
H	3.615580	-1.758023	0.458739
C	5.165578	-0.489181	-0.477089

H	5.954846	-0.708172	0.250841
H	5.337251	-1.147134	-1.336440
H	5.274636	0.548056	-0.806680

7ding

SCF Energy: -464.605893528 H

Num. Imaginary Frequencies: 0

C	0.560291	1.099190	-0.067062
C	-0.814044	1.519361	-0.068195
C	-1.932260	0.602983	0.007492
C	-1.955387	-0.775263	-0.250145
C	-3.079787	-1.566246	-0.151223
C	-4.448203	-1.160037	0.266223
O	-1.058846	2.769847	-0.098089
H	-1.051318	-1.273436	-0.579563
H	-2.871536	1.100511	0.236058
H	-2.960158	-2.617236	-0.405535
H	1.260572	1.931211	-0.126263
C	1.154136	-0.264211	0.054815
H	-4.547111	-0.098508	0.497970
H	-4.749386	-1.736777	1.149290
H	-5.164371	-1.414169	-0.524285
H	1.044423	-0.798912	-0.901370
H	0.594626	-0.849273	0.796497
C	2.610119	-0.218686	0.435162
H	2.844934	0.275873	1.378847
C	3.595913	-0.741532	-0.296905
H	3.344922	-1.231530	-1.239200
C	5.047672	-0.713914	0.073021
H	5.209862	-0.201738	1.026276
H	5.448717	-1.730671	0.155394
H	5.635887	-0.203982	-0.698510

7doutg

SCF Energy: -464.613338598 H

Num. Imaginary Frequencies: 0

C	4.554061	-0.851446	-0.343562
C	3.340157	-1.321846	0.376217
C	2.112588	-0.709339	0.452032
C	1.796964	0.513359	-0.165831
C	0.536494	1.217885	-0.139279
C	-0.568569	0.610677	0.532384
C	-1.912957	1.227098	0.603193
O	0.434003	2.346983	-0.719513
H	1.352023	-1.220810	1.034522
H	2.571561	1.020537	-0.736210
H	3.447842	-2.264566	0.908488
H	-0.427119	-0.336314	1.042706
H	5.371081	-0.704340	0.373399
H	4.893105	-1.628253	-1.038838
H	4.409855	0.075626	-0.900236
H	-2.034092	1.628535	1.623248
H	-1.970946	2.096290	-0.061360
C	-3.060032	0.283633	0.331170

H	-4.040817	0.653490	0.629960
C	-2.966463	-0.915498	-0.249267
H	-1.988106	-1.284269	-0.561071
C	-4.128167	-1.822509	-0.523370
H	-4.209217	-2.037781	-1.595063
H	-4.000170	-2.786084	-0.016790
H	-5.071472	-1.380015	-0.188765

TS6dout'g

SCF Energy: -464.591534591 H

Num. Imaginary Frequencies: 1 (i400.1991)

C	1.231094	1.179756	-0.312967
C	-0.186705	1.560048	-0.273017
C	-1.355973	0.889728	-0.173101
C	-1.477307	-0.560849	-0.132384
C	-2.607208	-1.273742	0.039195
C	-3.991608	-0.736249	0.254305
O	0.072531	2.839258	-0.416523
H	-0.557737	-1.124801	-0.277609
H	-2.254211	1.503100	-0.164582
H	-2.520480	-2.359163	0.021094
H	1.694899	1.132429	-1.294633
C	2.095609	1.089365	0.856680
H	-4.025516	0.356107	0.267823
H	-4.404133	-1.094571	1.205387
H	-4.672880	-1.084022	-0.531744
H	1.676462	1.496206	1.773717
H	3.131416	1.373761	0.684826
C	1.832866	-0.404103	0.731146
H	1.048023	-0.810644	1.361374
C	2.443475	-1.180758	-0.188129
H	3.200876	-0.735376	-0.832784
C	2.153884	-2.625077	-0.386719
H	3.074888	-3.209896	-0.287347
H	1.411457	-2.996172	0.323521
H	1.787919	-2.789725	-1.406916

7dout'_c3g

SCF Energy: -464.603609829 H

Num. Imaginary Frequencies: 0

C	0.873930	-0.671465	0.731033
C	-0.129345	-1.220412	-0.212841
C	-1.385786	-0.645606	-0.225930
C	-1.833479	0.539374	0.477204
C	-3.081187	1.056996	0.454150
C	-4.279383	0.525175	-0.272661
O	0.223090	-2.234517	-0.944485
H	-1.104252	1.088816	1.068611
H	-2.107640	-1.147381	-0.867658
H	-3.250095	1.968572	1.025338
H	0.569734	0.078190	1.449652
C	2.186170	-1.255554	0.913663
H	-5.099101	0.331283	0.429778
H	-4.078776	-0.400995	-0.816228
H	-4.655421	1.263137	-0.991802
H	2.350341	-2.241281	0.490564
H	2.690559	-1.050325	1.852234

C	2.330603	-0.155865	-0.140409
H	2.300309	-0.458917	-1.181293
C	2.531149	1.152128	0.195890
H	2.531894	1.422195	1.251294
C	2.737209	2.240572	-0.777527
H	1.940735	2.985565	-0.656103
H	3.673792	2.761343	-0.545573
H	2.753911	1.883876	-1.808358

TS13ding

SCF Energy: -464.583028515 H

Num. Imaginary Frequencies: 1 (i349.0960)

C	-0.676973	1.139745	0.953982
C	0.444458	0.995230	0.071329
C	1.607555	0.319637	0.256647
C	2.660451	0.292285	-0.739966
C	3.812855	-0.402427	-0.671521
C	4.252594	-1.323592	0.424097
O	-0.082436	1.608786	-0.965755
H	2.489506	0.902536	-1.625713
H	1.723119	-0.195243	1.205832
H	4.508210	-0.297795	-1.502857
H	-1.014311	2.158005	1.133107
C	-1.494641	0.009016	1.424826
H	3.519438	-1.417050	1.228601
H	5.196136	-0.975777	0.861402
H	4.445621	-2.325616	0.023074
H	-2.188134	0.335000	2.201673
H	-0.816929	-0.767424	1.805508
C	-2.261837	-0.549677	0.232732
H	-1.658824	-1.037937	-0.530864
C	-3.585461	-0.451898	0.104877
H	-4.154882	0.055601	0.883694
C	-4.366545	-1.006391	-1.045704
H	-3.716806	-1.497847	-1.775365
H	-5.109836	-1.731160	-0.695610
H	-4.917554	-0.207150	-1.554230

TS13doutg

SCF Energy: -464.582365918 H

Num. Imaginary Frequencies: 1 (i546.1648)

C	0.842897	-0.015927	-0.858140
C	-0.392892	0.555277	-0.398475
C	-1.623055	-0.006907	-0.292591
C	-2.783047	0.736586	0.162154
C	-4.035306	0.261423	0.307618
C	-4.507235	-1.137550	0.054878
O	0.097554	1.722454	-0.041906
H	-2.609963	1.785261	0.399638
H	-1.706740	-1.050361	-0.581902
H	-4.797563	0.959665	0.649599
H	1.351560	0.525832	-1.652535
C	1.558757	-1.109971	-0.187749
H	-3.718149	-1.796434	-0.315048
H	-5.323216	-1.138528	-0.677245
H	-4.912958	-1.576963	0.974071
H	2.215258	-1.607721	-0.905207

H	0.851044	-1.817599	0.252329
C	2.377775	-0.451713	0.923925
H	1.839619	-0.302590	1.855512
C	3.643566	-0.038889	0.810942
H	4.096284	0.397081	1.700558
C	4.523017	-0.100689	-0.397082
H	4.814905	0.912420	-0.696356
H	5.448523	-0.639483	-0.166755
H	4.044104	-0.580050	-1.254283

14ding

SCF Energy: -464.614113432 H

Num. Imaginary Frequencies: 0

C	-0.679549	1.558401	0.442316
C	0.657528	1.526399	-0.064761
C	1.403341	0.306060	0.115788
C	2.684309	0.120008	-0.430848
C	3.426979	-1.029004	-0.319667
C	3.050354	-2.288638	0.375369
O	1.137326	2.537112	-0.676223
H	3.115133	0.948287	-0.987385
H	0.943069	-0.497751	0.678174
H	4.404156	-1.032218	-0.798257
H	-1.248846	2.451719	0.190643
C	-1.408482	0.490684	1.189620
H	2.081975	-2.247020	0.876203
H	3.818472	-2.543524	1.114875
H	3.035986	-3.113595	-0.347448
H	-2.141072	0.964197	1.850378
H	-0.732523	-0.104481	1.810672
C	-2.127152	-0.409010	0.204614
H	-1.484276	-1.013909	-0.436156
C	-3.454136	-0.481655	0.077221
H	-4.078409	0.139405	0.721074
C	-4.170731	-1.369170	-0.894072
H	-3.470267	-1.957384	-1.494346
H	-4.841806	-2.058830	-0.369638
H	-4.794958	-0.776246	-1.572486

14doutg

SCF Energy: -464.618222383 H

Num. Imaginary Frequencies: 0

C	-4.131007	1.772141	0.339124
C	-4.038648	0.421082	-0.273544
C	-2.935849	-0.385569	-0.367025
C	-1.655518	-0.065963	0.124116
C	-0.531940	-0.954270	-0.009306
C	0.674603	-0.436733	0.542537
C	1.951897	-1.182889	0.551367
O	-0.607746	-2.098675	-0.567301
H	-3.053454	-1.349492	-0.855468
H	-1.487592	0.880296	0.628491
H	-4.964777	0.036507	-0.696249
H	0.644860	0.538671	1.021129
H	-4.508847	2.484297	-0.404029
H	-4.871222	1.754840	1.148213
H	-3.185973	2.146537	0.734983

H	2.039596	-1.651128	1.546852
H	1.904617	-2.021868	-0.152854
C	3.192291	-0.359986	0.307656
H	4.126997	-0.845826	0.587376
C	3.232193	0.862456	-0.228259
H	2.301934	1.349701	-0.523555
C	4.488181	1.644993	-0.468356
H	4.466590	2.595584	0.076881
H	5.375611	1.088013	-0.152380
H	4.596407	1.891701	-1.530844

TS13dout'pg

SCF Energy: -464.592994835 H

Num. Imaginary Frequencies: 1 (i405.9606)

C	-1.159797	-1.214901	-0.269354
C	0.296733	-1.165717	-0.266488
C	1.203086	-0.177718	-0.109935
C	2.636234	-0.431590	-0.138145
C	3.625614	0.469368	0.010684
C	3.475094	1.943366	0.246394
O	0.385378	-2.464355	-0.451786
H	2.925740	-1.469512	-0.300973
H	0.818765	0.826842	0.034539
H	4.650224	0.104235	-0.043245
H	-1.647855	-1.353912	-1.229763
C	-1.979208	-1.227628	0.935846
H	3.969697	2.239490	1.179363
H	2.430994	2.261041	0.304946
H	3.956178	2.515494	-0.556234
H	-1.437787	-1.438443	1.855579
H	-2.916416	-1.773304	0.848430
C	-2.122546	0.273127	0.697073
H	-1.417709	0.916886	1.215595
C	-3.005385	0.786563	-0.181170
H	-3.669294	0.105501	-0.713476
C	-3.156137	2.237554	-0.473019
H	-2.472008	2.847696	0.121350
H	-2.969694	2.423110	-1.537065
H	-4.185986	2.555175	-0.276079

14dout'_c3g

SCF Energy: -464.599081336 H

Num. Imaginary Frequencies: 0

C	-1.414735	-1.001521	-0.272893
C	0.069034	-1.300772	-0.257702
C	1.007305	-0.319112	-0.082490
C	2.433732	-0.591971	-0.106458
C	3.443990	0.288993	0.047359
C	3.320002	1.766822	0.284063
O	0.250918	-2.565158	-0.479573
H	2.709592	-1.633818	-0.269850
H	0.663759	0.699869	0.062566
H	4.462049	-0.095035	-0.004068
H	-1.873337	-1.044505	-1.257365
C	-2.299246	-1.188870	0.866733
H	3.823831	2.058706	1.213827
H	2.280918	2.100273	0.350351

H	3.801617	2.335062	-0.521593	H	-3.366124	0.648642	-0.849571
H	-1.864339	-1.591936	1.775864	C	-2.270719	2.505156	-0.447823
H	-3.330682	-1.460119	0.666644	H	-2.021008	2.658566	-1.504323
C	-1.948055	0.285786	0.686036	H	-3.183796	3.088941	-0.272319
H	-1.178841	0.703362	1.324158	H	-1.464899	2.865472	0.192177
C	-2.585654	1.086787	-0.228476				

CLOSED SHELL CROTYL Z SUBSTITUTION EPOXIDE OPENING COMPETITION

S_E_Z-1e

SCF Energy: -464.618130674 H

Num. Imaginary Frequencies: 0

C	2.635740	-0.532192	-0.433692
C	1.776856	0.178942	0.511413
C	0.518718	-0.193828	0.711665
C	3.913898	-0.238712	-0.724520
O	-0.554124	0.204903	1.462448
C	-0.681582	-0.953248	0.523551
H	2.174820	-1.377476	-0.942745
H	2.151465	1.030934	1.071509
H	4.414816	-0.870229	-1.456522
H	-0.787405	-1.895784	1.057821
C	4.743356	0.871695	-0.154386
H	5.104117	1.529118	-0.954113
H	4.200611	1.486142	0.567744
H	5.632706	0.469565	0.344929
C	-1.592036	-0.739000	-0.657922
H	-1.366074	0.227533	-1.114730
H	-1.338844	-1.513541	-1.392438
C	-3.040609	-0.864874	-0.268672
H	-3.363661	-1.869923	0.000363
C	-3.939403	0.124218	-0.205618
H	-4.951390	-0.141829	0.098581
C	-3.728449	1.577993	-0.507670
H	-2.694208	1.819281	-0.762810
H	-4.369206	1.893507	-1.339242
H	-4.013693	2.187528	0.357178

TS6ein

SCF Energy: -464.580890261 H

Num. Imaginary Frequencies: 1 (i327.4994)

C	0.706366	0.123032	-0.653209
C	-0.380702	0.980865	-0.243636
C	-1.696437	0.688094	-0.067544
C	-2.250320	-0.639755	-0.259241
C	-3.539908	-0.998563	-0.105606
C	-4.687401	-0.115697	0.279627
O	0.293788	2.088192	-0.033440
H	-1.552195	-1.418382	-0.564890
H	-2.345932	1.510063	0.223562
H	-3.790263	-2.043162	-0.282777
H	1.281534	0.471914	-1.509310
C	1.255186	-0.991587	0.125907
H	-4.393870	0.924129	0.441125
H	-5.159203	-0.480846	1.199776
H	-5.461927	-0.133294	-0.496236
H	1.718462	-1.719755	-0.545074
H	0.497642	-1.462000	0.754288

C	2.314579	-0.317643	1.004503
H	1.946626	0.039742	1.961483
C	3.589540	-0.113925	0.657297
H	4.226922	0.367445	1.397632
C	4.249536	-0.468165	-0.636785
H	5.163008	-1.043324	-0.452649
H	3.604256	-1.043200	-1.305249
H	4.552005	0.445187	-1.162040

TS6eout

SCF Energy: -464.576866050 H

Num. Imaginary Frequencies: 1 (i516.4537)

C	0.599200	0.132972	-0.088031
C	-0.554959	0.998040	-0.155368
C	-1.866132	0.634205	-0.119407
C	-2.283120	-0.753294	-0.062362
C	-3.548883	-1.211362	0.002689
C	-4.803333	-0.395495	0.069708
O	0.017564	2.161635	-0.341768
H	-1.485592	-1.497601	-0.075142
H	-2.606610	1.429403	-0.150883
H	-3.689109	-2.290932	0.014183
H	0.769403	-0.600678	-0.880463
C	1.675102	0.274061	0.900399
H	-4.615616	0.680781	0.071654
H	-5.374036	-0.641122	0.973113
H	-5.455020	-0.624755	-0.782063
H	1.755147	-0.728953	1.349509
H	1.413426	0.992492	1.677782
C	2.983590	0.640822	0.221124
H	3.131829	1.710194	0.092380
C	3.897563	-0.213876	-0.247234
H	4.780670	0.217808	-0.716218
C	3.848481	-1.709865	-0.216419
H	3.768778	-2.103955	-1.236288
H	4.775063	-2.112631	0.206110
H	3.006096	-2.100387	0.359874

7ein

SCF Energy: -464.596069784 H

Num. Imaginary Frequencies: 0

C	0.563429	1.178328	0.174919
C	-0.719801	1.596483	-0.185523
C	-1.775223	0.631895	-0.138930
C	-1.728031	-0.742295	-0.458280
C	-2.773727	-1.594038	-0.236766
C	-4.069337	-1.314041	0.421424
O	-1.017174	2.855398	-0.349998
H	-0.850565	-1.147805	-0.946835

H	-2.737966	1.053564	0.146470
H	-2.642047	-2.620085	-0.575732
H	1.218045	2.004689	0.457280
C	1.179554	-0.183543	0.265908
H	-4.190454	-0.288370	0.769583
H	-4.180208	-1.992886	1.275855
H	-4.882553	-1.566533	-0.269400
H	1.278533	-0.612064	-0.739505
H	0.511634	-0.867201	0.809256
C	2.510038	-0.144224	0.970630
H	2.475438	0.236675	1.991050
C	3.695365	-0.522914	0.480485
H	4.556717	-0.431358	1.141555
C	3.998379	-1.067467	-0.883864
H	4.769564	-0.459511	-1.370162
H	4.401146	-2.084156	-0.808253
H	3.126235	-1.097254	-1.541197

7eout

SCF Energy: -464.606578257 H

Num. Imaginary Frequencies: 0

C	-4.530065	-0.558270	0.153201
C	-3.297127	-1.219443	-0.339310
C	-2.020045	-0.742887	-0.371374
C	-1.663875	0.539564	0.109187
C	-0.384063	1.173587	0.142948
C	0.685893	0.447177	-0.385012
C	2.064660	0.994305	-0.406578
O	-0.260794	2.369064	0.645126
H	-1.257825	-1.396474	-0.782204
H	-2.464383	1.151323	0.522160
H	-3.444993	-2.224454	-0.730609
H	0.523829	-0.543342	-0.795511
H	-5.260890	-0.521632	-0.663478
H	-4.980549	-1.183280	0.933420
H	-4.384938	0.448641	0.544276
H	2.064455	1.886650	-1.050339
H	2.281441	1.394383	0.596638
C	3.126826	0.020831	-0.854399
H	3.604309	0.226245	-1.809939
C	3.503564	-1.065493	-0.170944
H	4.275811	-1.699250	-0.605113
C	2.958373	-1.513952	1.152153
H	2.422629	-2.464492	1.043867
H	3.773314	-1.690664	1.862841
H	2.269294	-0.788682	1.593753

S_E_Z-1'e

SCF Energy: -464.618339726 H

Num. Imaginary Frequencies: 0

C	0.838675	1.146489	-0.361220
C	-0.581015	1.184970	-0.174507
C	-1.813969	0.705686	-0.065814
C	-2.087371	-0.717692	-0.256669
C	-3.284538	-1.319566	-0.161620
C	-4.602602	-0.680336	0.155903
O	0.062326	2.388307	-0.057830

H	-1.220875	-1.332688	-0.496501
H	-2.614919	1.400753	0.168979
H	-3.314677	-2.394417	-0.332987
H	1.226144	1.144538	-1.378384
C	1.774703	0.651521	0.712842
H	-5.315027	-0.848081	-0.660411
H	-4.529178	0.396636	0.324365
H	-5.042171	-1.132735	1.052555
H	1.321383	0.849806	1.689848
H	2.712719	1.209375	0.652321
C	1.989444	-0.831451	0.544199
H	1.144102	-1.454088	0.834418
C	3.082789	-1.434068	0.062950
H	3.067203	-2.522160	0.007059
C	4.349190	-0.790057	-0.415236
H	4.556943	-1.089945	-1.448576
H	4.316923	0.301267	-0.381360
H	5.200992	-1.127695	0.186346

TS6eout'

SCF Energy: -464.589767931 H

Num. Imaginary Frequencies: 1 (i382.8274)

C	1.139966	0.912327	-0.176087
C	-0.253290	1.383400	-0.232619
C	-1.462231	0.777909	-0.199072
C	-1.675687	-0.661622	-0.156600
C	-2.857974	-1.298426	-0.048524
C	-4.213498	-0.668928	0.084788
O	0.070843	2.646260	-0.376920
H	-0.787798	-1.284310	-0.246698
H	-2.322189	1.441980	-0.253227
H	-2.843089	-2.387278	-0.060030
H	1.661010	0.822904	-1.126371
C	1.919181	0.807143	1.045549
H	-4.723245	-1.034766	0.984218
H	-4.854325	-0.932078	-0.765904
H	-4.170266	0.421494	0.145616
H	1.450200	1.224496	1.933061
H	2.975571	1.049320	0.953241
C	1.595861	-0.675638	0.894250
H	0.738398	-1.026924	1.456333
C	2.252673	-1.533319	0.080187
H	1.894447	-2.561229	0.071081
C	3.424872	-1.253750	-0.790557
H	3.806251	-0.234209	-0.708648
H	4.228997	-1.954146	-0.539400
H	3.160059	-1.449895	-1.835797

7eout'_c3

SCF Energy: -464.602349738 H

Num. Imaginary Frequencies: 0

C	0.940123	0.447426	-0.580919
C	-0.157025	1.276450	-0.043707
C	-1.413826	0.703190	0.028611
C	-1.776596	-0.676689	-0.214991
C	-3.021996	-1.195909	-0.144081
C	-4.297199	-0.478208	0.178052

O	0.112663	2.502917	0.290614
H	-0.982038	-1.378693	-0.458263
H	-2.207942	1.382858	0.331594
H	-3.125936	-2.261691	-0.341778
H	0.712541	-0.523406	-1.003728
C	2.285171	0.944927	-0.763350
H	-5.007723	-0.567880	-0.652698
H	-4.155535	0.585101	0.384274
H	-4.782644	-0.930079	1.051477
H	2.424904	2.018150	-0.682131
H	2.904012	0.446541	-1.502726
C	2.269029	0.278406	0.617446
H	2.101931	0.935208	1.462656
C	2.503200	-1.049445	0.835895
H	2.526054	-1.372339	1.874965
C	2.726256	-2.105514	-0.173652
H	3.639613	-2.652935	0.084697
H	1.909066	-2.835284	-0.111542
H	2.799575	-1.736693	-1.197521

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SCF Energy: -464.618384224 H

Num. Imaginary Frequencies: 0

C	-2.632061	0.622342	-0.455413
C	-1.778971	-0.472337	0.001890
C	-0.509346	-0.593342	-0.367624
C	-3.920553	0.813651	-0.126084
O	0.389827	0.083637	-1.150447
C	0.810923	-1.144632	-0.407601
H	-2.161574	1.343424	-1.121589
H	-2.163181	-1.232698	0.673932
H	-4.418023	1.685747	-0.547536
H	1.005307	-1.977782	-1.080832
C	-4.767172	-0.042143	0.766222
H	-5.663421	-0.378344	0.232094
H	-4.243418	-0.925773	1.138146
H	-5.116391	0.534425	1.630998
C	1.807969	-0.925705	0.701174
H	1.500964	-0.057579	1.290233
H	1.748276	-1.802570	1.357116
C	3.209016	-0.788437	0.166446
H	3.669932	-1.713478	-0.177562
C	3.910870	0.345153	0.054883
H	4.915273	0.270698	-0.361196
C	3.479395	1.730589	0.432781
H	2.466207	1.768913	0.839142
H	4.164858	2.157213	1.174092
H	3.516156	2.387880	-0.443506

TS13ein

SCF Energy: -464.582426644 H

Num. Imaginary Frequencies: 1 (i348.7915)

C	0.850126	-0.040452	-0.834269
C	-0.386869	0.543242	-0.392188
C	-1.620595	-0.011459	-0.290304
C	-2.780117	0.740511	0.151741
C	-4.035392	0.272393	0.293789

C	-4.514037	-1.125443	0.047801
O	0.107644	1.710953	-0.043214
H	-2.604060	1.790461	0.381401
H	-1.707486	-1.056700	-0.572298
H	-4.796770	0.977654	0.623125
H	1.369731	0.486240	-1.631901
C	1.555873	-1.126018	-0.140177
H	-4.991339	-1.530239	0.947957
H	-3.713113	-1.807475	-0.247012
H	-5.276439	-1.135305	-0.740407
H	2.203823	-1.650020	-0.847152
H	0.845146	-1.813761	0.324478
C	2.389667	-0.439279	0.943378
H	1.868862	-0.275691	1.882280
C	3.647770	-0.015230	0.792590
H	4.117796	0.444604	1.660823
C	4.496529	-0.098229	-0.436170
H	4.774356	0.909329	-0.765936
H	5.431029	-0.626427	-0.217387
H	3.999576	-0.600514	-1.269401

TS13eout

SCF Energy: -464.577577174 H

Num. Imaginary Frequencies: 1 (i534.7190)

C	-0.765265	0.198611	-0.099065
C	0.525209	-0.441535	-0.143399
C	1.747349	0.147799	-0.057681
C	2.979161	-0.616152	-0.011431
C	4.231944	-0.120832	0.025462
C	4.635985	1.321020	-0.001615
O	0.152236	-1.680719	-0.353786
H	2.864249	-1.699131	0.001305
H	1.761401	1.232811	-0.007644
H	5.051218	-0.836296	0.075899
H	-1.054610	0.887081	-0.897105
C	-1.810921	-0.130534	0.879575
H	3.786773	2.004111	-0.077102
H	5.303701	1.515050	-0.849380
H	5.199501	1.579283	0.903074
H	-2.075762	0.843028	1.321741
H	-1.430248	-0.785132	1.664643
C	-3.025647	-0.732892	0.195927
H	-2.965231	-1.809287	0.054302
C	-4.093091	-0.067939	-0.255322
H	-4.878897	-0.659252	-0.723530
C	-4.342268	1.407321	-0.203180
H	-3.555704	1.959933	0.316280
H	-4.421575	1.810023	-1.219506
H	-5.297446	1.614327	0.291690

14ein

SCF Energy: -464.607465896 H

Num. Imaginary Frequencies: 0

C	-0.873438	0.948884	0.411531
C	0.435271	1.351834	0.115105
C	1.407496	0.310401	0.147219
C	2.730565	0.483980	-0.316670

C	3.675697	-0.499220	-0.298014
C	3.548400	-1.889515	0.199632
O	0.726661	2.570321	-0.240368
H	3.003084	1.458359	-0.710521
H	1.112534	-0.662373	0.521018
H	4.656667	-0.240849	-0.693264
H	-1.641329	1.703133	0.233088
C	-1.405462	-0.366770	0.869962
H	2.568712	-2.136758	0.609021
H	4.310979	-2.063602	0.968127
H	3.781744	-2.581983	-0.618166
H	-2.153105	-0.175652	1.646448
H	-0.640957	-1.012242	1.305110
C	-2.042729	-1.058027	-0.321257
H	-1.348605	-1.621894	-0.942241
C	-3.328318	-0.989502	-0.684154
H	-3.624315	-1.538500	-1.577457
C	-4.424206	-0.226462	-0.005201
H	-4.835758	0.527311	-0.686364
H	-5.250989	-0.895833	0.257840
H	-4.091616	0.284706	0.901392

14eout

SCF Energy: -464.614495378 H

Num. Imaginary Frequencies: 0

C	4.013666	1.594858	-0.481574
C	3.890318	0.289716	0.210677
C	2.780546	-0.486405	0.359011
C	1.503548	-0.142818	-0.143559
C	0.353918	-0.968448	0.019424
C	-0.798812	-0.362754	-0.495790
C	-2.137059	-0.991665	-0.389700
O	0.373871	-2.126973	0.599260
H	2.871936	-1.425732	0.896441
H	1.374252	0.794416	-0.674807
H	4.811762	-0.085956	0.652289
H	-0.711119	0.601192	-0.989527
H	4.380142	2.342603	0.232112
H	4.784328	1.515902	-1.257550
H	3.089506	1.955021	-0.933705
H	-2.124890	-1.905274	-1.002827
H	-2.251163	-1.365816	0.639739
C	-3.291360	-0.105824	-0.788640
H	-3.843225	-0.396149	-1.679799
C	-3.665714	0.998678	-0.133728
H	-4.510881	1.563100	-0.525600
C	-3.026408	1.553927	1.103909
H	-2.273381	0.884159	1.528608
H	-2.541109	2.513385	0.888540
H	-3.782992	1.749332	1.871832

S_Z_Z-1'e

SCF Energy: -464.618123348 H

Num. Imaginary Frequencies: 0

C	0.853019	-0.889702	0.421930
C	-0.549686	-0.645533	0.272737
C	-1.680725	0.049229	0.239103

C	-2.962150	-0.554981	-0.119511
C	-4.148400	0.072576	-0.184565
C	-4.431648	1.517885	0.092276
O	-0.142004	-1.933753	0.033453
H	-2.933742	-1.617679	-0.354085
H	-1.611193	1.101981	0.492795
H	-5.011549	-0.526946	-0.469605
H	1.245632	-1.051084	1.424364
C	1.855282	-0.490574	-0.632530
H	-4.875224	1.995836	-0.788985
H	-3.541106	2.085486	0.371927
H	-5.163920	1.614910	0.902370
H	1.357032	-0.505621	-1.608288
H	2.661918	-1.227823	-0.650553
C	2.367294	0.897124	-0.345465
H	1.623910	1.687913	-0.440920
C	3.609020	1.241126	0.014800
H	3.800760	2.300868	0.180900
C	4.792865	0.343448	0.215984
H	5.187826	0.460332	1.231533
H	4.564315	-0.713414	0.061236
H	5.602151	0.621677	-0.468860

TS13eout'

SCF Energy: -464.592101546 H

Num. Imaginary Frequencies: 1 (i390.4252)

C	1.186762	0.846138	-0.113650
C	-0.262967	0.996444	-0.166021
C	-1.293711	0.128043	-0.084559
C	-2.680661	0.563780	-0.155040
C	-3.780979	-0.210730	-0.105737
C	-3.827004	-1.703491	0.035758
O	-0.179552	2.300712	-0.303249
H	-2.830245	1.637850	-0.262153
H	-1.046619	-0.922330	0.030747
H	-4.747877	0.285423	-0.176097
H	1.726650	0.962488	-1.049561
C	1.948409	0.696096	1.116965
H	-4.379122	-1.992062	0.938492
H	-2.833803	-2.156157	0.092293
H	-4.355681	-2.157304	-0.811225
H	1.393060	0.906752	2.028139
H	2.945250	1.131786	1.107832
C	1.915754	-0.795417	0.783029
H	1.106825	-1.359787	1.234144
C	2.763539	-1.412041	-0.066979
H	2.612497	-2.479880	-0.214983
C	3.902491	-0.811805	-0.814324
H	3.730763	-0.917526	-1.891557
H	4.067559	0.243392	-0.588060
H	4.817356	-1.370438	-0.588660

14eout'_c3

SCF Energy: -464.597038651 H

Num. Imaginary Frequencies: 0

C	1.271864	0.758398	-0.065424
C	-0.194852	1.113045	-0.173013

C	-1.196994	0.185674	-0.072643	H	-4.156692	-2.281809	-0.710508
C	-2.599184	0.546233	-0.189637	H	1.455224	0.973159	2.088295
C	-3.670923	-0.269982	-0.115474	H	3.052544	1.039171	1.171052
C	-3.657590	-1.754448	0.111889	C	1.700333	-0.681332	0.687070
O	-0.296694	2.387871	-0.391240	H	0.869782	-1.187688	1.159528
H	-2.798288	1.604403	-0.359211	C	2.560414	-1.411303	-0.099122
H	-0.930125	-0.852938	0.086684	H	2.317124	-2.464820	-0.230205
H	-4.656276	0.180212	-0.229411	C	3.772748	-0.949113	-0.787186
H	1.838465	0.928754	-0.977095	H	4.602234	-1.585165	-0.451776
C	2.004592	0.758304	1.176982	H	3.666193	-1.151290	-1.860174
H	-4.203819	-2.017610	1.026369	H	4.020794	0.099461	-0.625491
H	-2.646046	-2.159673	0.201215				

OPEN SHELL SINGLET CROTYL Z SUBSTITUTION EPOXIDE OPENING COMPETITION

TS6eing

SCF Energy: -464.580890272 H

Num. Imaginary Frequencies: 1 (i327.5000)

C	0.706366	0.123032	-0.653209
C	-0.380702	0.980865	-0.243636
C	-1.696437	0.688094	-0.067544
C	-2.250320	-0.639755	-0.259241
C	-3.539908	-0.998563	-0.105606
C	-4.687401	-0.115697	0.279627
O	0.293788	2.088192	-0.033440
H	-1.552195	-1.418382	-0.564890
H	-2.345932	1.510063	0.223562
H	-3.790263	-2.043162	-0.282777
H	1.281534	0.471914	-1.509310
C	1.255186	-0.991587	0.125907
H	-4.393870	0.924129	0.441125
H	-5.159203	-0.480846	1.199776
H	-5.461927	-0.133294	-0.496236
H	1.718462	-1.719755	-0.545074
H	0.497642	-1.462000	0.754288
C	2.314579	-0.317643	1.004503
H	1.946626	0.039742	1.961483
C	3.589540	-0.113925	0.657297
H	4.226922	0.367445	1.397632
C	4.249536	-0.468165	-0.636785
H	5.163008	-1.043324	-0.452649
H	3.604256	-1.043200	-1.305249
H	4.552005	0.445187	-1.162040

TS6eoutg

SCF Energy: -464.576875709 H

Num. Imaginary Frequencies: 1 (i3456.4380)

C	0.599550	0.133450	-0.092958
C	-0.556347	0.996163	-0.155488
C	-1.868122	0.633627	-0.118031
C	-2.285628	-0.753349	-0.060947
C	-3.551808	-1.210913	0.003519
C	-4.805882	-0.394452	0.069132
O	0.016925	2.159418	-0.340980
H	-1.488348	-1.497906	-0.073096
H	-2.607867	1.429521	-0.148456
H	-3.692494	-2.290412	0.015559

H	0.771637	-0.594679	-0.890008
C	1.674659	0.270829	0.897533
H	-4.617719	0.681742	0.070471
H	-5.377293	-0.639270	0.972310
H	-5.457083	-0.624058	-0.782918
H	1.753506	-0.733947	1.342972
H	1.410987	0.985527	1.677755
C	2.984724	0.640840	0.223733
H	3.132521	1.710731	0.098546
C	3.901398	-0.211298	-0.244032
H	4.785394	0.222788	-0.709125
C	3.854410	-1.707492	-0.217427
H	3.780441	-2.098978	-1.238727
H	4.779440	-2.110035	0.208736
H	3.009756	-2.100803	0.353617

7eing

SCF Energy: -464.604600207 H

Num. Imaginary Frequencies: 0

C	0.669179	1.174658	-0.013579
C	-0.707627	1.554641	-0.171917
C	-1.808672	0.620411	-0.065803
C	-1.776057	-0.775604	-0.191361
C	-2.879684	-1.594444	-0.084481
C	-4.280960	-1.201740	0.223714
O	-0.972406	2.784008	-0.375780
H	-0.838557	-1.266714	-0.425968
H	-2.772745	1.108919	0.051411
H	-2.715011	-2.657847	-0.244592
H	1.361683	2.004907	-0.143790
C	1.264607	-0.141274	0.362774
H	-4.412140	-0.136934	0.422461
H	-4.635208	-1.763410	1.096256
H	-4.935621	-1.485229	-0.609587
H	1.267433	-0.800173	-0.516871
H	0.630324	-0.639676	1.106551
C	2.656928	0.013615	0.917621
H	2.720481	0.584425	1.843187
C	3.790169	-0.467995	0.395223
H	4.712252	-0.262703	0.938293
C	3.959092	-1.268182	-0.861733
H	4.667365	-0.770751	-1.533812

H	4.382654	-2.252851	-0.632873
H	3.024484	-1.418551	-1.407172

7eoutg

SCF Energy: -464.612605364 H

Num. Imaginary Frequencies: 0

C	-4.497596	-0.489608	0.297115
C	-3.354527	-1.049783	-0.472886
C	-2.064737	-0.581684	-0.534030
C	-1.595538	0.549268	0.158439
C	-0.263659	1.104717	0.145966
C	0.740619	0.458838	-0.638549
C	2.147955	0.928945	-0.684825
O	-0.008080	2.150134	0.828630
H	-1.378490	-1.141244	-1.162984
H	-2.292140	1.096990	0.788892
H	-3.577392	-1.939537	-1.058047
H	0.480584	-0.404516	-1.241190
H	-5.319026	-0.251194	-0.389088
H	-4.885740	-1.250007	0.985375
H	-4.253412	0.405493	0.870872
H	2.241184	1.633761	-1.524528
H	2.364727	1.515106	0.216128
C	3.138905	-0.200584	-0.864046
H	3.706644	-0.214953	-1.791439
C	3.344166	-1.172131	0.032375
H	4.077517	-1.940928	-0.207466
C	2.651453	-1.315516	1.354893
H	1.965605	-2.171142	1.340787
H	3.379155	-1.506488	2.150938
H	2.073185	-0.427185	1.625993

TS6eout'g

SCF Energy: -464.589767931 H

Num. Imaginary Frequencies: 1 (i382.8273)

C	1.139965	0.912327	-0.176088
C	-0.253290	1.383399	-0.232619
C	-1.462232	0.777908	-0.199070
C	-1.675687	-0.661623	-0.156597
C	-2.857975	-1.298427	-0.048522
C	-4.213499	-0.668928	0.084785
O	0.070841	2.646260	-0.376919
H	-0.787798	-1.284311	-0.246692
H	-2.322189	1.441979	-0.253225
H	-2.843089	-2.387279	-0.060026
H	1.661008	0.822904	-1.126372
C	1.919183	0.807144	1.045547
H	-4.723253	-1.034773	0.984209
H	-4.854320	-0.932071	-0.765914
H	-4.170266	0.421494	0.145622
H	1.450204	1.224497	1.933059
H	2.975572	1.049321	0.953236
C	1.595863	-0.675637	0.894249
H	0.738400	-1.026922	1.456334
C	2.252674	-1.533319	0.080188
H	1.894448	-2.561229	0.071083
C	3.424873	-1.253750	-0.790558

H	3.806248	-0.234208	-0.708654
H	4.229001	-1.954142	-0.539396
H	3.160061	-1.449903	-1.835796

7eout' _c3g

SCF Energy: -464.602315503 H

Num. Imaginary Frequencies: 0

C	0.937374	0.450367	-0.578073
C	-0.155808	1.282227	-0.036547
C	-1.411214	0.707048	0.044663
C	-1.765790	-0.679115	-0.176204
C	-3.011293	-1.199941	-0.124105
C	-4.297029	-0.476347	0.138299
O	0.114708	2.510791	0.288660
H	-0.962987	-1.385213	-0.377954
H	-2.207417	1.386384	0.343163
H	-3.106617	-2.271971	-0.289599
H	0.703599	-0.519581	-0.999578
C	2.283016	0.943246	-0.767938
H	-5.011930	-0.667207	-0.670862
H	-4.173969	0.605228	0.229517
H	-4.765313	-0.843150	1.060056
H	2.427311	2.015862	-0.686717
H	2.896231	0.443064	-1.510776
C	2.270995	0.275438	0.612334
H	2.111557	0.932006	1.459225
C	2.498978	-1.054153	0.827507
H	2.525322	-1.379026	1.865875
C	2.710167	-2.109669	-0.185008
H	3.620668	-2.664150	0.068129
H	1.887910	-2.833576	-0.120763
H	2.781590	-1.739611	-1.208552

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SCF Energy: -464.582426633 H

Num. Imaginary Frequencies: 1 (i348.7901)

C	0.850124	-0.040449	-0.834278
C	-0.386872	0.543244	-0.392194
C	-1.620596	-0.011459	-0.290306
C	-2.780120	0.740510	0.151737
C	-4.035393	0.272389	0.293790
C	-4.514035	-1.125450	0.047814
O	0.107641	1.710956	-0.043223
H	-2.604065	1.790462	0.381389
H	-1.707486	-1.056700	-0.572301
H	-4.796772	0.977650	0.623124
H	1.369723	0.486241	-1.631916
C	1.555876	-1.126010	-0.140185
H	-3.713113	-1.807478	-0.247015
H	-5.276453	-1.135317	-0.740378
H	-4.991315	-1.530248	0.947980
H	2.203834	-1.650007	-0.847156
H	0.845153	-1.813759	0.324467
C	2.389659	-0.439261	0.943372
H	1.868842	-0.275656	1.882265
C	3.647768	-0.015225	0.792594
H	4.117787	0.444615	1.660827

C	4.496542	-0.098249	-0.436152
H	4.774400	0.909301	-0.765916
H	5.431025	-0.626470	-0.217353
H	3.999590	-0.600523	-1.269390

TS13eoutg

SCF Energy: -464.577577180 H

Num. Imaginary Frequencies: 1 (i534.7179)

C	-0.765265	0.198609	-0.099060
C	0.525208	-0.441538	-0.143401
C	1.747349	0.147796	-0.057684
C	2.979161	-0.616154	-0.011438
C	4.231944	-0.120831	0.025458
C	4.635978	1.321023	-0.001609
O	0.152233	-1.680720	-0.353791
H	2.864252	-1.699133	0.001294
H	1.761400	1.232808	-0.007641
H	5.051220	-0.836293	0.075894
H	-1.054612	0.887082	-0.897098
C	-1.810918	-0.130535	0.879582
H	3.786770	2.004106	-0.077211
H	5.303790	1.515036	-0.849302
H	5.199388	1.579315	0.903139
H	-2.075758	0.843026	1.321749
H	-1.430244	-0.785134	1.664649
C	-3.025646	-0.732891	0.195935
H	-2.965235	-1.809287	0.054315
C	-4.093088	-0.067937	-0.255318
H	-4.878895	-0.659252	-0.723522
C	-4.342262	1.407323	-0.203190
H	-3.555714	1.959936	0.316293
H	-4.421533	1.810021	-1.219520
H	-5.297456	1.614334	0.291646

14eing

SCF Energy: -464.613046706 H

Num. Imaginary Frequencies: 0

C	-0.922317	1.069834	0.475055
C	0.419796	1.376520	0.089155
C	1.384107	0.307070	0.144636
C	2.699468	0.457960	-0.326508
C	3.658155	-0.523938	-0.310593
C	3.522679	-1.913751	0.201316
O	0.720664	2.548725	-0.313608
H	2.973812	1.426203	-0.737422
H	1.068413	-0.649114	0.544802
H	4.634255	-0.266701	-0.716850
H	-1.647517	1.864604	0.306849
C	-1.465331	-0.224027	0.982054
H	2.539378	-2.138654	0.617279
H	4.279631	-2.096521	0.973305
H	3.732983	-2.624298	-0.607155
H	-2.287814	-0.011699	1.670018
H	-0.716600	-0.801302	1.529543
C	-1.953599	-1.027621	-0.210344
H	-1.176379	-1.581603	-0.734275
C	-3.204880	-1.068437	-0.681813

H	-3.386664	-1.691694	-1.556738
C	-4.402819	-0.344431	-0.147884
H	-4.814162	0.320804	-0.915722
H	-5.196931	-1.054226	0.109941
H	-4.179265	0.259337	0.734851

14eoutg

SCF Energy: -464.617813195 H

Num. Imaginary Frequencies: 0

C	-4.179772	1.676532	-0.000960
C	-4.021337	0.222332	-0.266176
C	-2.872979	-0.520820	-0.203641
C	-1.602974	-0.016939	0.138816
C	-0.425884	-0.840703	0.185277
C	0.739100	-0.143652	0.616765
C	2.076945	-0.775876	0.737216
O	-0.421944	-2.081232	-0.113819
H	-2.941226	-1.580853	-0.434629
H	-1.483785	1.033235	0.385130
H	-4.933193	-0.303485	-0.542643
H	0.665076	0.924169	0.805445
H	-4.606862	2.165058	-0.884806
H	-4.904526	1.823185	0.808928
H	-3.251410	2.183915	0.264988
H	2.613348	-0.348185	1.588469
H	1.980482	-1.854676	0.884731
C	2.820470	-0.504798	-0.560867
H	2.614261	-1.205956	-1.366662
C	3.641589	0.525441	-0.796159
H	4.090915	0.588340	-1.786689
C	4.017682	1.621791	0.153227
H	3.699706	2.591818	-0.246106
H	3.569710	1.501842	1.142643
H	5.106020	1.671600	0.270766

TS13eout'g

SCF Energy: -464.592101567 H

Num. Imaginary Frequencies: 1 (i390.4249)

C	1.186762	0.846138	-0.113650
C	-0.262967	0.996444	-0.166021
C	-1.293711	0.128043	-0.084560
C	-2.680661	0.563780	-0.155041
C	-3.780979	-0.210730	-0.105737
C	-3.827004	-1.703491	0.035758
O	-0.179553	2.300712	-0.303249
H	-2.830245	1.637850	-0.262153
H	-1.046619	-0.922330	0.030747
H	-4.747877	0.285423	-0.176097
H	1.726650	0.962489	-1.049561
C	1.948409	0.696096	1.116965
H	-4.379123	-1.992062	0.938492
H	-2.833803	-2.156157	0.092293
H	-4.355681	-2.157304	-0.811225
H	1.393060	0.906751	2.028139
H	2.945250	1.131786	1.107832
C	1.915754	-0.795417	0.783028
H	1.106825	-1.359787	1.234143

C	2.763540	-1.412041	-0.066979	H	-0.930125	-0.852938	0.086684
H	2.612498	-2.479880	-0.214983	H	-4.656276	0.180212	-0.229411
C	3.902492	-0.811805	-0.814323	H	1.838465	0.928754	-0.977095
H	3.730767	-0.917531	-1.891556	C	2.004592	0.758304	1.176982
H	4.067557	0.243393	-0.588064	H	-4.203818	-2.017610	1.026370
H	4.817358	-1.370435	-0.588654	H	-2.646046	-2.159673	0.201214

14out'_c3g

SCF Energy: -464.597038632 H

Num. Imaginary Frequencies: 0

C	1.271864	0.758398	-0.065424
C	-0.194852	1.113045	-0.173013
C	-1.196994	0.185674	-0.072643
C	-2.599184	0.546233	-0.189637
C	-3.670923	-0.269982	-0.115474
C	-3.657590	-1.754448	0.111889
O	-0.296694	2.387871	-0.391240
H	-2.798288	1.604403	-0.359211

H	1.455224	0.973160	2.088295
H	3.052544	1.039171	1.171051
C	1.700333	-0.681332	0.687070
H	0.869782	-1.187687	1.159528
C	2.560413	-1.411303	-0.099122
H	2.317123	-2.464820	-0.230205
C	3.772748	-0.949113	-0.787186
H	4.602233	-1.585165	-0.451775
H	3.666193	-1.151290	-1.860174
H	4.020794	0.099461	-0.625491

CLOSED SHELL CROTYL Z SUBSTITUTION FROM OXIRANE OPENED INTERMEDIATE

TS7-10eoutM

SCF Energy: -464.592220979 H

Num. Imaginary Frequencies: 1 (i76.9045)

C	3.308538	-0.799613	1.001095
C	2.610734	-1.284553	-0.232382
C	1.783574	-0.565784	-1.002674
C	1.444388	0.866347	-0.810728
C	0.319687	1.364012	-0.203007
C	-0.540618	0.357555	0.461394
C	-1.694316	0.694928	1.259922
O	-0.018815	2.621333	-0.122879
H	1.339940	-1.064400	-1.867577
H	2.135186	1.599044	-1.230419
H	2.790947	-2.323332	-0.507413
H	-0.191475	-0.668932	0.480455
H	2.971683	-1.362797	1.879806
H	4.390243	-0.957146	0.922913
H	3.122454	0.262081	1.184465
H	-2.015939	-0.022393	2.008003
H	-1.817439	1.739666	1.527969
C	-2.213304	0.423422	-0.159935
H	-2.350809	1.291928	-0.792613
C	-2.562386	-0.810123	-0.631299
H	-2.982914	-0.840353	-1.634885
C	-2.446625	-2.114237	0.053997
H	-1.797315	-2.770667	-0.537798
H	-2.067909	-2.054720	1.074933
H	-3.434166	-2.590368	0.056904

TS7-10eoutP

SCF Energy: -464.593308607 H

Num. Imaginary Frequencies: 1 (i86.2752)

C	-2.610784	-0.957178	1.065518
C	-2.374684	-0.874824	-0.412157
C	-1.778645	0.140123	-1.054129
C	-1.298332	1.382849	-0.402632
C	0.015034	1.665072	-0.127703

C	0.981234	0.622152	-0.562020
C	2.363991	0.577587	-0.159511
O	0.474714	2.707817	0.504612
H	-1.643976	0.043610	-2.133401
H	-2.045986	2.095327	-0.053866
H	-2.712007	-1.727145	-1.001219
H	0.659176	-0.068463	-1.333940
H	-2.124422	-0.136419	1.600684
H	-3.682550	-0.929699	1.296348
H	-2.228925	-1.904864	1.461914
H	3.055253	0.022531	-0.785342
H	2.769730	1.459982	0.324905
C	1.561365	-0.281134	0.836627
H	1.280460	0.206743	1.762412
C	1.237899	-1.596655	0.652348
H	0.722367	-2.084782	1.477594
C	1.493204	-2.439685	-0.533385
H	0.530384	-2.757265	-0.953448
H	2.084449	-1.955710	-1.311639
H	1.996645	-3.356234	-0.205642

TS8eout

SCF Energy: -464.605969021 H

Num. Imaginary Frequencies: 1 (i101.2399)

C	0.290026	-0.587650	0.117338
C	-0.171550	0.695462	-0.220846
O	0.449625	1.797927	-0.149630
C	-1.574238	0.506749	-0.038135
C	-2.429912	-0.449378	-0.685573
C	-3.754899	-0.565773	-0.445363
C	-4.586785	0.175410	0.544702
H	-1.991546	-1.081419	-1.453443
H	-2.032086	1.232368	0.634068
H	-4.295380	-1.289939	-1.052266
H	-0.216799	-1.466216	-0.264253
C	1.506333	-0.806702	0.960698
H	-5.379596	0.725155	0.024494

H	-5.089281	-0.541439	1.204082
H	-4.023644	0.876460	1.162748
H	1.775630	0.112662	1.484566
H	1.301693	-1.588502	1.699175
C	2.615620	-1.270180	0.039216
H	2.516924	-2.292160	-0.322288
C	3.655902	-0.542837	-0.385393
H	4.356877	-1.032816	-1.060661
C	3.985506	0.878395	-0.044724
H	3.302643	1.315411	0.686421
H	5.005157	0.946797	0.350789
H	3.956389	1.499248	-0.947918

TS9est-sc

SCF Energy: -464.623210947 H

Num. Imaginary Frequencies: 1 (i63.7843)

C	2.287183	-1.968610	-0.909577
C	3.092903	-1.170605	0.081268
C	2.703378	-0.125841	0.822839
C	1.391460	0.576736	0.869905
C	0.888516	1.405623	-0.239460
C	0.069727	0.241850	0.066174
C	-1.262116	0.357642	0.796501
O	1.110351	2.340747	-0.978504
H	3.441047	0.314616	1.491120
H	1.152567	0.997500	1.848275
H	4.125365	-1.487698	0.216984
H	0.117689	-0.553523	-0.674413
H	1.903234	-1.343688	-1.723704
H	2.905783	-2.749104	-1.358332
H	1.429098	-2.458189	-0.437635
H	-1.440780	-0.574034	1.339447
H	-1.184024	1.157881	1.542655
C	-2.379535	0.678107	-0.158002
H	-2.269795	1.624147	-0.688151
C	-3.461937	-0.063712	-0.420405
H	-4.171795	0.333131	-1.145852
C	-3.835348	-1.391172	0.169596
H	-4.789252	-1.315179	0.704384
H	-3.979488	-2.132306	-0.624784
H	-3.087844	-1.779633	0.865003

2S-3S-9e

SCF Energy: -464.628781491 H

Num. Imaginary Frequencies: 0

C	-0.245588	0.268668	0.280516
C	0.530993	1.476691	0.049556
C	1.283111	0.224089	-0.134960
C	2.303274	-0.204513	0.852792
C	3.444162	-0.851624	0.584610
C	3.959771	-1.281913	-0.754835
O	0.571637	2.688459	0.037247
H	2.076161	0.041274	1.889231
H	1.441939	-0.053751	-1.176691
H	4.081366	-1.099025	1.432464
H	-0.431663	0.038645	1.330810
C	-1.313444	-0.206833	-0.694671

H	3.276445	-1.045837	-1.573960
H	4.142349	-2.362460	-0.762784
H	4.921358	-0.799855	-0.965977
H	-1.378038	-1.296354	-0.634433
H	-0.992720	0.042032	-1.713245
C	-2.638012	0.450528	-0.417185
H	-2.662894	1.525325	-0.595965
C	-3.753552	-0.137786	0.030276
H	-4.627212	0.496990	0.176110
C	-3.958179	-1.586632	0.360383
H	-4.335489	-1.691774	1.383787
H	-4.714875	-2.027055	-0.299501
H	-3.045030	-2.179879	0.273282

2S-3S-9e_sc

SCF Energy: -464.625882578 H

Num. Imaginary Frequencies: 0

C	0.035828	0.140180	0.231640
C	-0.878891	1.220987	-0.111180
C	-1.301392	0.412936	1.042753
C	-2.440095	-0.545726	1.105441
C	-3.058919	-1.181478	0.101796
C	-2.788428	-1.097356	-1.370433
O	-1.124284	2.173468	-0.820897
H	-2.782046	-0.751013	2.117136
H	-1.102623	0.923861	1.986045
H	-3.857292	-1.866218	0.383819
H	-0.020221	-0.723217	-0.432728
C	1.393575	0.382450	0.874625
H	-2.168183	-0.244496	-1.656745
H	-3.730411	-1.026655	-1.923818
H	-2.283280	-2.006071	-1.718735
H	1.661029	-0.499534	1.462649
H	1.303550	1.223275	1.572321
C	2.437049	0.704049	-0.160921
H	2.323792	1.675150	-0.642147
C	3.449577	-0.077279	-0.554731
H	4.110812	0.314887	-1.327113
C	3.792409	-1.451567	-0.061710
H	3.095720	-1.824049	0.692800
H	3.797949	-2.161451	-0.896801
H	4.801203	-1.465401	0.366817

TS11eout

SCF Energy: -464.603542127 H

Num. Imaginary Frequencies: 1 (i61.5112)

C	0.027623	-0.302655	0.811768
C	0.522725	-1.015388	-0.295424
O	-0.138121	-1.712805	-1.126637
C	1.881211	-1.239962	0.082395
C	2.903889	-0.291219	0.428033
C	2.998547	0.992070	0.002832
C	2.088613	1.758260	-0.895910
H	3.724580	-0.684983	1.021551
H	2.179979	-2.288897	0.073237
H	3.883218	1.535259	0.330908
H	0.657898	0.426710	1.305475

C	-1.359172	-0.478504	1.336032
H	1.543717	2.515614	-0.319872
H	2.681201	2.297850	-1.641669
H	1.350791	1.132518	-1.402839
H	-1.838054	-1.344133	0.874545
H	-1.328222	-0.625378	2.420494
C	-2.102649	0.807036	1.029587
H	-1.886966	1.636587	1.700147
C	-2.942059	1.014680	0.007805
H	-3.382511	2.007925	-0.075022
C	-3.359450	0.038971	-1.049563
H	-3.048840	0.399222	-2.037314
H	-2.936026	-0.957038	-0.905782
H	-4.451456	-0.048545	-1.076096

10eoutM

SCF Energy: -464.604634916 H

Num. Imaginary Frequencies: 0

C	0.004685	-0.755371	-0.794087
C	-0.746788	-1.240692	0.288207
O	-0.317673	-2.069751	1.180389
C	-2.132698	-0.935353	0.131456
C	-2.710748	0.262299	-0.372027
C	-2.205372	1.526098	-0.273970
C	-0.985485	2.018672	0.422082
H	-3.712764	0.167091	-0.783740
H	-2.826455	-1.710678	0.457175
H	-2.830778	2.309803	-0.698715
H	-0.462791	-0.069995	-1.491261
C	1.418317	-1.122091	-1.062121
H	-0.237966	2.347572	-0.310784
H	-1.246345	2.899286	1.018102
H	-0.516582	1.265934	1.057987
H	1.800632	-1.784052	-0.281612
H	1.496218	-1.640814	-2.024001
C	2.200848	0.179051	-1.139924
H	2.416759	0.546578	-2.140426
C	2.583406	0.914622	-0.088992
H	3.131184	1.833631	-0.295034
C	2.348526	0.610611	1.358403
H	1.786509	1.426371	1.828065
H	1.793119	-0.317642	1.513742
H	3.302499	0.537845	1.893217

10eoutP

SCF Energy: -464.602758524 H

Num. Imaginary Frequencies: 0

C	0.014257	-0.065433	-0.218634
C	0.777534	1.110174	-0.227283
O	0.474626	2.188388	-0.860503
C	1.719015	1.080443	0.845089
C	2.567874	0.016910	1.271398
C	3.108006	-0.967125	0.501876
C	2.999386	-1.206309	-0.963144
H	2.897706	0.068796	2.305909
H	1.801136	2.012200	1.406022
H	3.777283	-1.650387	1.022240

H	0.403639	-0.949753	0.273842
C	-1.336846	-0.135989	-0.829068
H	4.000202	-1.380199	-1.371801
H	2.425032	-2.121724	-1.147417
H	2.516152	-0.391303	-1.504996
H	-1.781479	0.864064	-0.855549
H	-1.178493	-0.407098	-1.888380
C	-2.227052	-1.163966	-0.185947
H	-1.834128	-2.180233	-0.188605
C	-3.422860	-0.950874	0.373709
H	-3.936569	-1.816797	0.790380
C	-4.161163	0.348403	0.500755
H	-5.111087	0.303146	-0.044378
H	-4.409884	0.541274	1.550346
H	-3.595418	1.203505	0.123905

TS12eoutM

SCF Energy: -464.599548207 H

Num. Imaginary Frequencies: 1 (i227.4525)

C	-0.982713	1.802639	-0.097734
C	-2.160035	1.234616	-0.586712
C	-2.481661	-0.086141	-0.334289
C	-1.397094	-0.986570	-0.023754
O	-1.527679	-1.998047	0.753592
C	-0.219917	-0.703219	-0.765176
C	1.015793	-1.527942	-0.613174
H	-2.793071	1.839401	-1.234010
H	-3.496420	-0.467231	-0.414937
C	-0.401736	1.642768	1.265137
H	-0.620704	2.684422	-0.627703
H	-0.263050	-0.009252	-1.592441
H	1.588263	-1.514552	-1.544404
H	0.731580	-2.564317	-0.400093
H	-0.774736	0.771169	1.803976
H	0.690644	1.615035	1.236535
H	-0.674335	2.547708	1.826314
C	1.856258	-1.004711	0.539422
H	1.767711	-1.540554	1.481680
C	2.641677	0.076565	0.484866
H	3.181844	0.355525	1.389044
C	2.833456	0.979767	-0.695678
H	2.375905	1.958196	-0.499667
H	3.897816	1.160319	-0.880264
H	2.385817	0.581875	-1.610216

TS12eoutP

SCF Energy: -464.599987452 H

Num. Imaginary Frequencies: 1 (i222.9862)

C	1.511497	1.619597	-0.385369
C	2.571804	0.716436	-0.345140
C	2.434141	-0.547114	0.202171
C	1.110363	-1.115378	0.260906
O	0.747116	-1.943024	1.172413
C	0.308001	-0.758899	-0.855762
C	-1.102797	-1.219517	-1.002205
H	3.508325	1.005413	-0.819579
H	3.287555	-1.130363	0.538577

C	0.502724	1.902529	0.676125
H	1.593324	2.412852	-1.129413
H	0.768588	-0.304147	-1.722237
H	-1.396014	-1.817281	-0.136722
H	-1.182088	-1.852983	-1.894248
H	0.433417	1.125699	1.437997
H	0.807497	2.843846	1.154238
H	-0.485239	2.081237	0.242686
C	-2.016632	-0.021789	-1.178179
H	-2.108820	0.357858	-2.193916
C	-2.673335	0.606235	-0.196552
H	-3.298416	1.454734	-0.473701
C	-2.641696	0.276471	1.265677
H	-1.926738	-0.514080	1.506527
H	-2.369511	1.165374	1.845767
H	-3.633230	-0.035398	1.614695

4R_5R-5e

SCF Energy: -464.699326029 H

Num. Imaginary Frequencies: 0

C	-0.231445	-0.168334	-0.139041
C	-1.271433	-1.239436	0.156240
C	-2.552076	-0.798650	-0.403940
C	-2.428025	0.468169	-0.829252
C	-1.070444	1.063176	-0.564800
O	-1.054683	-2.302940	0.737710
H	-3.224986	1.054132	-1.277850
H	-3.440943	-1.417773	-0.429977
H	-0.673602	1.509011	-1.483287
C	-1.194615	2.172332	0.490046
H	0.281919	-0.542750	-1.036980
C	0.823387	-0.002212	0.961097
H	0.356476	0.412489	1.859718
H	1.181173	-1.002559	1.226993
H	-1.893536	2.940421	0.144932
H	-1.569240	1.774103	1.438526
H	-0.230048	2.653536	0.670622
C	1.980199	0.869766	0.536937

H	1.947733	1.910362	0.854889
C	3.018576	0.476841	-0.210520
H	3.778643	1.218267	-0.455047
C	3.250685	-0.896092	-0.768800
H	4.239007	-1.269337	-0.477190
H	2.500425	-1.619569	-0.439848
H	3.235589	-0.870169	-1.864980

4S_5S-5e

SCF Energy: -464.695437559 H

Num. Imaginary Frequencies: 0

C	0.325551	-0.359805	-0.285368
C	1.783834	-0.811169	-0.252393
C	2.642864	0.372937	-0.280682
C	1.875256	1.471264	-0.218435
C	0.403754	1.180383	-0.111232
O	2.160696	-1.983208	-0.230220
H	2.248706	2.491308	-0.213296
H	3.724211	0.327342	-0.331002
H	-0.115319	1.684397	-0.933644
C	-0.153667	1.740184	1.203403
H	0.003198	-0.585581	-1.309780
C	-0.525610	-1.171814	0.692732
H	-0.287669	-2.230885	0.529804
H	-0.187265	-0.962501	1.716074
H	-1.226890	1.549427	1.284617
H	0.344727	1.293296	2.069444
H	0.004324	2.822229	1.243573
C	-2.028447	-1.052465	0.688617
H	-2.472077	-1.646717	1.488449
C	-2.898687	-0.379833	-0.075814
H	-3.946775	-0.494297	0.200777
C	-2.671502	0.546025	-1.238959
H	-1.767080	0.326730	-1.806302
H	-3.517566	0.489141	-1.930354
H	-2.610167	1.587529	-0.897823

OPEN SHELL SINGLET CROTYL Z SUBSTITUTION FROM OXIRANE OPENED

INTERMEDIATE

TS7-10eoutMg

SCF Energy: -464.592220979 H

Num. Imaginary Frequencies: 1 (i76.9059)

C	3.308542	-0.799615	1.001093
C	2.610734	-1.284552	-0.232383
C	1.783575	-0.565781	-1.002674
C	1.444388	0.866349	-0.810726
C	0.319686	1.364013	-0.203006
C	-0.540619	0.357556	0.461395
C	-1.694318	0.694927	1.259921
O	-0.018818	2.621335	-0.122879
H	1.339939	-1.064396	-1.867577
H	2.135186	1.599047	-1.230416
H	2.790946	-2.323331	-0.507415
H	-0.191474	-0.668931	0.480456

H	2.971700	-1.362808	1.879802
H	4.390249	-0.957137	0.922901
H	3.122450	0.262077	1.184472
H	-2.015940	-0.022393	2.008002
H	-1.817442	1.739666	1.527967
C	-2.213306	0.423420	-0.159936
H	-2.350814	1.291925	-0.792614
C	-2.562386	-0.810125	-0.631299
H	-2.982916	-0.840356	-1.634883
C	-2.446622	-2.114239	0.053997
H	-1.797323	-2.770673	-0.537807
H	-2.067893	-2.054723	1.074928
H	-3.434166	-2.590365	0.056917

TS7-10eoutPg

SCF Energy: -464.593308615 H

Num. Imaginary Frequencies: 1 (i86.2695)

C	-2.610797	-0.957182	1.065515
C	-2.374698	-0.874822	-0.412161
C	-1.778652	0.140124	-1.054127
C	-1.298336	1.382847	-0.402623
C	0.015031	1.665068	-0.127696
C	0.981228	0.622151	-0.562023
C	2.363992	0.577593	-0.159534
O	0.474713	2.707810	0.504620
H	-1.643980	0.043615	-2.133399
H	-2.045989	2.095324	-0.053856
H	-2.712021	-1.727139	-1.001227
H	0.659161	-0.068470	-1.333935
H	-3.682563	-0.929729	1.296343
H	-2.228913	-1.904858	1.461910
H	-2.124456	-0.136411	1.600681
H	3.055247	0.022538	-0.785375
H	2.769735	1.459992	0.324870
C	1.561389	-0.281128	0.836622
H	1.280499	0.206753	1.762410
C	1.237921	-1.596649	0.652356
H	0.722404	-2.084772	1.477613
C	1.493206	-2.439688	-0.533377
H	0.530378	-2.757270	-0.953421
H	2.084435	-1.955717	-1.311646
H	1.996652	-3.356233	-0.205638

TS8eoutg

SCF Energy: -464.605969038 H

Num. Imaginary Frequencies: 1 (i101.2417)

C	0.290024	-0.587646	0.117336
C	-0.171549	0.695466	-0.220851
O	0.449626	1.797931	-0.149636
C	-1.574236	0.506751	-0.038135
C	-2.429911	-0.449374	-0.685575
C	-3.754897	-0.565773	-0.445363
C	-4.586783	0.175404	0.544708
H	-1.991546	-1.081410	-1.453449
H	-2.032083	1.232368	0.634072
H	-4.295378	-1.289937	-1.052267
H	-0.216801	-1.466211	-0.264256
C	1.506331	-0.806700	0.960697
H	-5.379605	0.725138	0.024505
H	-5.089265	-0.541449	1.204094
H	-4.023645	0.876462	1.162746
H	1.775630	0.112665	1.484563
H	1.301688	-1.588498	1.699174
C	2.615615	-1.270182	0.039215
H	2.516915	-2.292160	-0.322293
C	3.655899	-0.542841	-0.385393
H	4.356873	-1.032819	-1.060662
C	3.985507	0.878388	-0.044716
H	3.302647	1.315402	0.686434
H	5.005159	0.946785	0.350795
H	3.956391	1.499247	-0.947907

TS11eoutg

SCF Energy: -464.603542137 H

Num. Imaginary Frequencies: 1 (i61.5112)

C	0.027620	-0.302659	0.811765
C	0.522726	-1.015392	-0.295425
O	-0.138117	-1.712813	-1.126637
C	1.881212	-1.239959	0.082394
C	2.903886	-0.291212	0.428032
C	2.998538	0.992078	0.002833
C	2.088597	1.758265	-0.895905
H	3.724580	-0.684973	1.021548
H	2.179985	-2.288893	0.073238
H	3.883207	1.535271	0.330908
H	0.657892	0.426709	1.305471
C	-1.359173	-0.478514	1.336032
H	1.543696	2.515612	-0.319863
H	2.681181	2.297863	-1.641662
H	1.350780	1.132520	-1.402836
H	-1.838055	-1.344141	0.874541
H	-1.328219	-0.625393	2.420493
C	-2.102654	0.807027	1.029597
H	-1.886981	1.636571	1.700169
C	-2.942053	1.014679	0.007808
H	-3.382509	2.007924	-0.075012
C	-3.359430	0.038980	-1.049574
H	-3.048804	0.399239	-2.037318
H	-2.936008	-0.957030	-0.905795
H	-4.451435	-0.048535	-1.076124

10eoutMg

SCF Energy: -464.607590836 H

Num. Imaginary Frequencies: 0

C	0.011428	-0.740415	-0.822421
C	-0.803320	-1.279454	0.215428
O	-0.387855	-2.160684	1.035975
C	-2.195672	-0.900054	0.172349
C	-2.767436	0.322935	-0.255786
C	-2.220192	1.579694	-0.248645
C	-0.913086	2.038827	0.301859
H	-3.816655	0.264105	-0.539347
H	-2.887101	-1.665864	0.520408
H	-2.863028	2.373206	-0.625303
H	-0.433161	-0.032785	-1.514746
C	1.435362	-1.103530	-1.033487
H	-0.224920	2.314422	-0.506471
H	-1.072781	2.943104	0.898551
H	-0.418916	1.283915	0.917056
H	1.778328	-1.774681	-0.242055
H	1.535770	-1.633839	-1.988480
C	2.262831	0.169269	-1.091955
H	2.525000	0.526836	-2.085098
C	2.646418	0.885583	-0.029029
H	3.233878	1.784237	-0.214101
C	2.357092	0.583699	1.409694
H	1.826123	1.423448	1.873008
H	1.749321	-0.315204	1.540831
H	3.290438	0.455251	1.969914

10eoutPg

SCF Energy: -464.605326262 H

Num. Imaginary Frequencies: 0

C	0.003648	0.044788	-0.071101
C	0.845057	1.187585	-0.190396
O	0.513814	2.213346	-0.869798
C	2.022702	1.197868	0.641893
C	2.829646	0.112122	1.064412
C	3.043912	-1.096326	0.456123
C	2.567894	-1.594978	-0.865822
H	3.433206	0.310942	1.947960
H	2.324659	2.186949	0.983272
H	3.724759	-1.767410	0.976538
H	0.340311	-0.793483	0.530574
C	-1.328203	-0.025857	-0.718735
H	3.412245	-2.035861	-1.406235
H	1.831674	-2.396714	-0.733239
H	2.111335	-0.818370	-1.483835
H	-1.792526	0.966531	-0.708066
H	-1.149068	-0.238297	-1.788051
C	-2.214802	-1.095974	-0.143278
H	-1.795554	-2.101467	-0.165856
C	-3.437091	-0.934375	0.374746
H	-3.942987	-1.827442	0.740562
C	-4.215380	0.339717	0.515761
H	-5.137466	0.292394	-0.075233
H	-4.518882	0.484459	1.558648
H	-3.656521	1.223574	0.199730

TS12eoutMg

SCF Energy: -464.599691270 H

Num. Imaginary Frequencies: 1 (i283.0484)

C	-0.973461	1.792689	-0.107577
C	-2.171177	1.238152	-0.573127
C	-2.496834	-0.078657	-0.319952
C	-1.407923	-0.983455	-0.023569
O	-1.528996	-1.993529	0.749575
C	-0.228600	-0.698630	-0.771310
C	1.010392	-1.518778	-0.616842
H	-2.813741	1.852983	-1.201582
H	-3.512142	-0.458787	-0.394585
C	-0.389815	1.642927	1.256718
H	-0.603491	2.662549	-0.651329
H	-0.284138	-0.020810	-1.611602

H	1.582607	-1.501177	-1.548132
H	0.726114	-2.556837	-0.411002
H	-0.763743	0.775348	1.801849
H	0.702162	1.612736	1.228214
H	-0.662227	2.550469	1.813958
C	1.854900	-1.007209	0.537758
H	1.763354	-1.547152	1.477411
C	2.651213	0.065990	0.486846
H	3.195304	0.335762	1.391461
C	2.849450	0.973391	-0.689505
H	3.915198	1.140814	-0.878570
H	2.391643	0.587184	-1.604008
H	2.406205	1.956634	-0.485316

TS12eoutPg

SCF Energy: -464.601380511 H

Num. Imaginary Frequencies: 1 (i225.6889)

C	1.284253	1.787504	-0.360929
C	2.466571	1.074392	-0.549180
C	2.672435	-0.211854	-0.068153
C	1.522168	-1.039178	0.194402
O	1.515211	-1.982291	1.052815
C	0.385740	-0.747090	-0.627669
C	-0.958759	-1.292967	-0.309925
H	3.251412	1.552538	-1.134117
H	3.670263	-0.612159	0.090398
C	0.378603	1.806162	0.832547
H	1.129062	2.628404	-1.037015
H	0.530220	-0.255457	-1.582715
H	-1.107745	-1.287205	0.774916
H	-0.963933	-2.357292	-0.601326
H	0.579719	1.009572	1.550050
H	0.519048	2.773599	1.332988
H	-0.673518	1.762411	0.535239
C	-2.055330	-0.571049	-1.047283
H	-2.034092	-0.680865	-2.130950
C	-3.016533	0.186300	-0.507312
H	-3.732972	0.641520	-1.190588
C	-3.237782	0.494309	0.943856
H	-2.481331	0.054091	1.597382
H	-3.235364	1.578535	1.104768
H	-4.220664	0.131465	1.266331