Investigation into 9*S*-HPODE-derived allene oxide to cyclopentenone cyclization mechanism via diradical oxyallyl intermediate

Sebastien Hebert, Jin K. Cha, and H. Bernhard Schlegel*

From the Department of Chemistry, Wayne State University, Detroit, Michigan, 48202

Supporting Information

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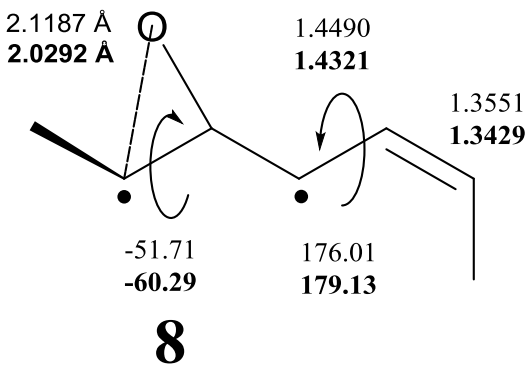
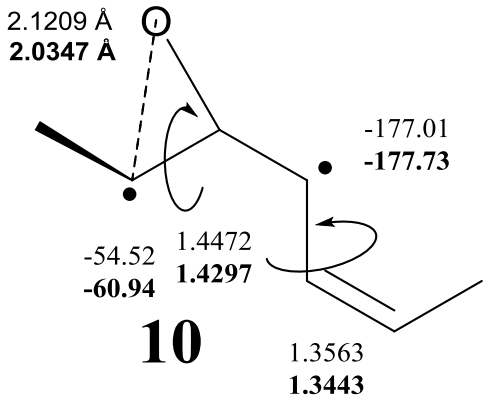
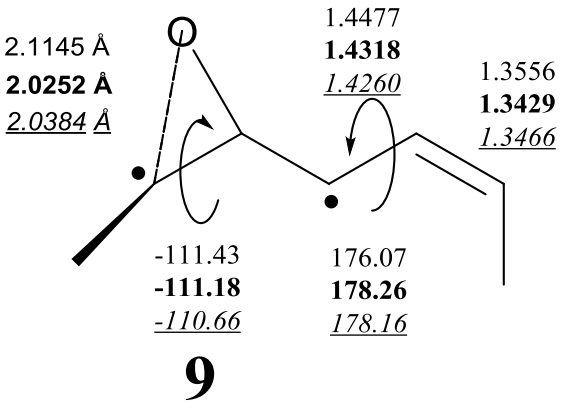
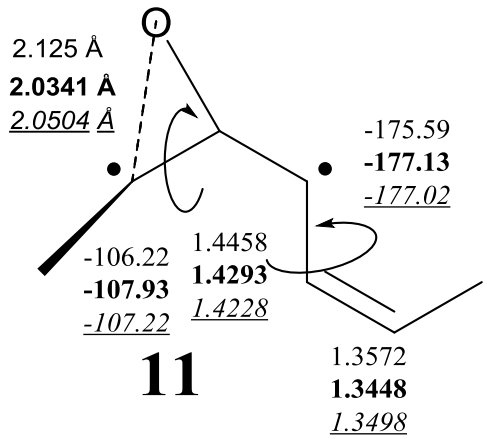
Full citation for reference 33:

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.









Scheme S1. Comparison of geometries of methyl vinyl substituted epoxide opening transition states optimized at CASSCF(10,8)/6-31++G(d,p) (plain), UωB97XD/cc-pVTZ (bold), and CCSD(T) from IRCmax (italics,underline) levels of theory.

RASSCF (RAS 3 Orbitals)

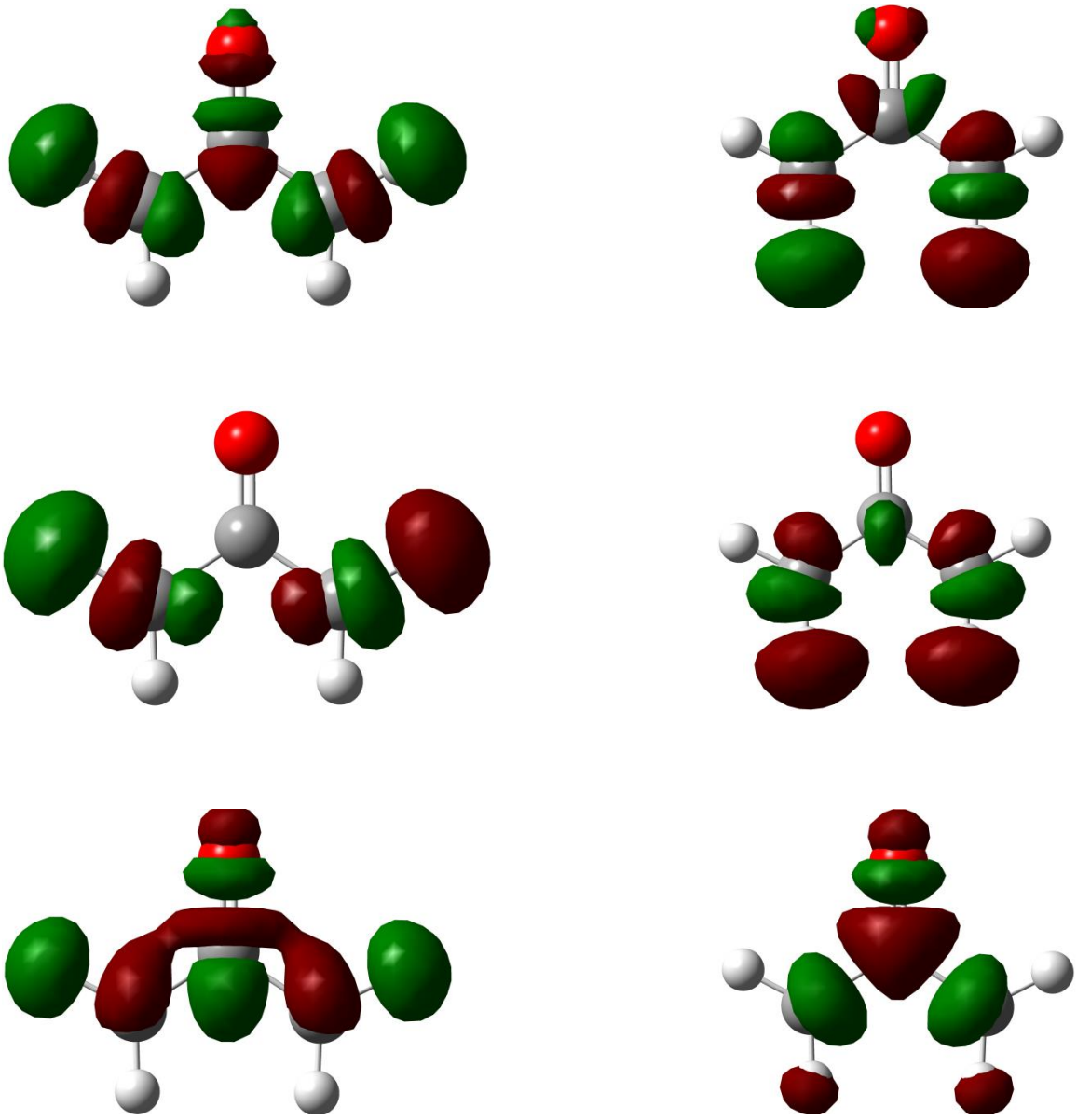
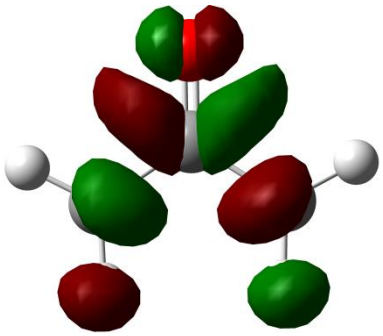
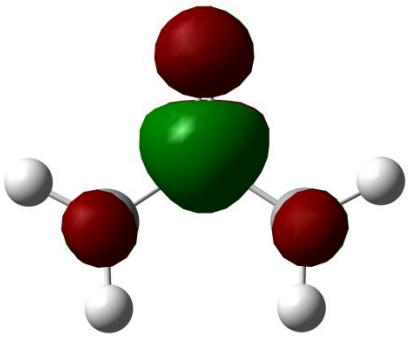
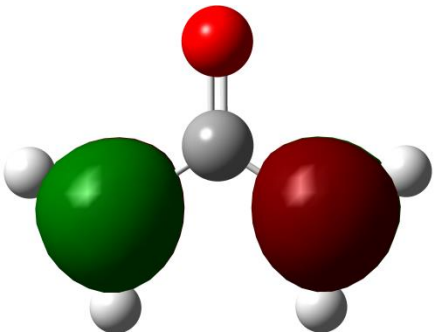


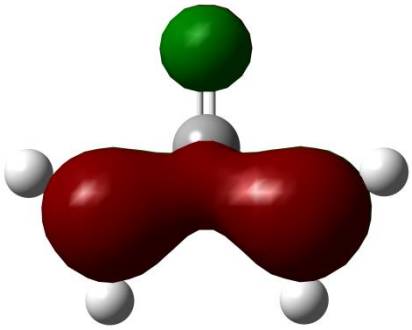
Figure S1. Orbitals selected for the 20,19 active space for RASSCF calculations of the unsubstituted allene oxide system.

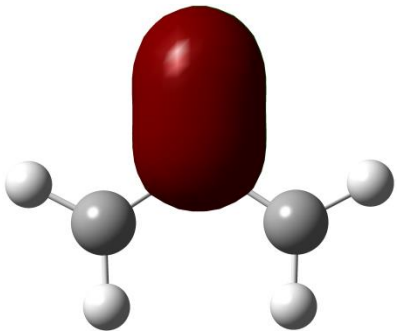
RASSCF (RAS 2 Orbitals)

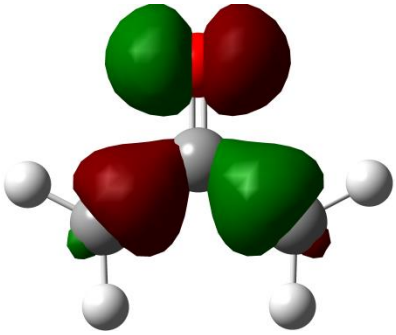




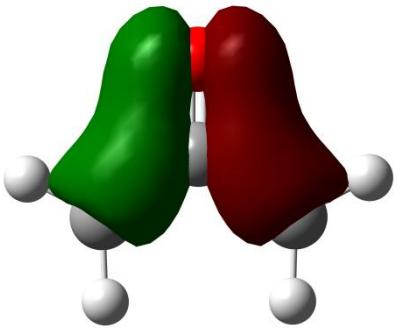


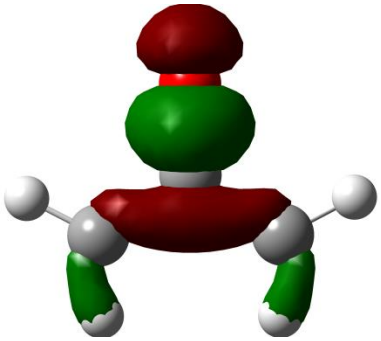


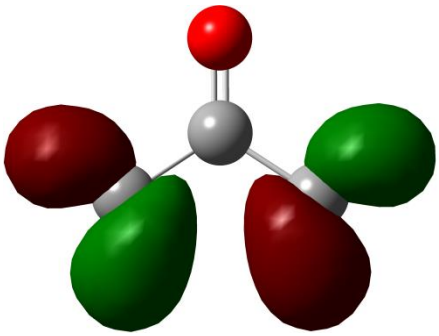


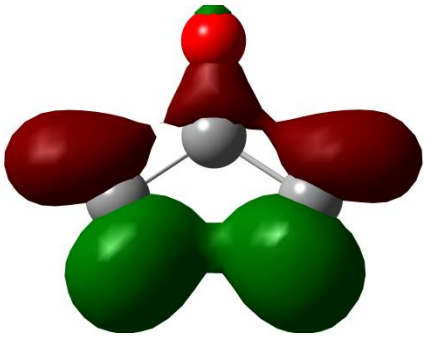


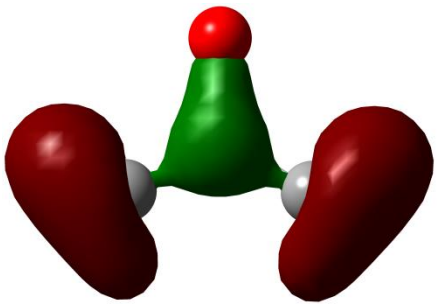
RASSCF (RAS 1 Orbitals)

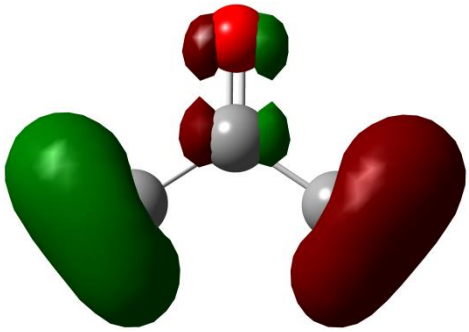












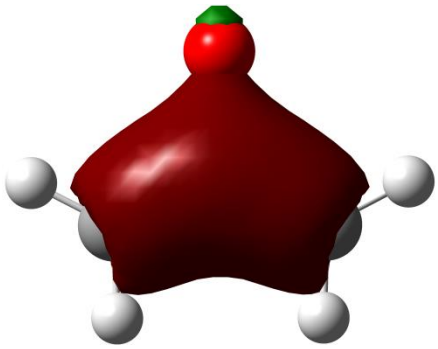


Table S1. Absolute enthalpies of optimized structures found along allene oxide cyclization pathways (Hartree/particle)

	CASSCF	UωB97xD[a]	UωB97xD[f]
1 [a,e]	-190.737604	-191.802824	
2 [a,d]	-190.694879	-191.747006	
3 [a,d]	-190.722911	-191.770957	
3 (triplet) [a,d]	-190.729432	-191.773183	
4 [a,d]	-190.723720	-191.768666	
5 [a,e]	-190.758202	-191.821173	
6 [c,e]	-345.609488	-347.749789	-347.760281
7 [c,e]	-345.608906	-347.749661	-347.760216
8[c,d]	-345.576227	-347.702281	-347.721600
9[c,d]	-345.571141	-347.707405	-347.727067
10[c,d]	-345.569944	-347.701893	-347.720740
11[c,d]	-345.574094	-347.750906	-347.724592
8[e]		-347.699213	
9[e]		-347.704398	-347.769400
10[e]		-347.697801	
11[e]		-347.700243	-347.765603
12[c,d]	-345.603252	-347.741974	-347.758988
13 [c,d]	-345.596781	-347.736158	-347.753602
14[b,d]	-345.596965	-347.737265	-347.753790
15 [c,d]	-345.592755	-347.729618	-347.746191
16 [c,d]	-345.596782	-347.732970	-347.753079
17 [c,d]	-345.592681	-347.726060	-347.745753
18 [c,d]	-345.592488	-347.726813	-347.745860
19 [c,d]	-345.589486	-347.718129	-347.736613
20 [b,e]	-345.612287	-347.757200	-347.770343
21 [b,e]	-345.610938	-347.756152	-347.769503
22 [b,e]	-345.612162	-347.757062	-347.768801
23 [b,e]	-345.611252	-347.756843	-347.768732
24 [b,d]	-345.586771	-347.757062	-347.739898
25 [b,d]	-345.590749	-347.725414	-347.743262
26 [b,d]	-345.592034	-347.730104	-347.747791
27 [c,d]	-345.585781	-347.719508	-347.736846
28 [c,d]	-345.58879	-347.727933	-347.743436
29 [c,d]	-345.591797	-347.730213	-347.746424
30 [c,d]	-345.593669	-347.734054	-347.749203
31 [c,d]	-345.588048	-347.730434	-347.741163
32 [c,d]	-345.570284	-347.712117	-347.727249
33 [c,d]	-345.585583	-347.723713	-347.740575
34 [c,d]	-345.573554	-347.716975	-347.732096
35 [c,d]	-345.578409	-347.713918	-347.729901
36 [c,e]	-345.654476	-347.796246	-347.806368
37 [c,e]	-345.679924	-347.823549	-347.837237
38 [c,e]	-345.656872	-347.798277	-347.807998
39 [c,e]	-345.683066	-347.825547	-347.839187
40[e]		-347.715314	-347.779852

41[e]		-347.696944	-347.762272
14 → 15 [c,d]	-345.591235	-347.721749	
12 → 30 [b,d]	-345.584097		
29 → 30 [c,d]	-345.590739	-347.725450	
13 → 15 [c,d]	-345.592602	-347.725249	-347.739247
28 → 31 [c,d]		-347.724394	

[a]CASSCF(4,4)/6-311++G(d,p) optimized geometry used [b]CASSCF(8,7)/6-31++G(d,p) optimized geometry used [c]CASSCF(10,8)/6-31++G(d,p) optimized geometry used [d]UωB97xD/cc-pVTZ optimized geometry used [e]RωB97xD/cc-pVTZ optimized geometry used [f]UωB97xD/cc-pVTZ solvent optimized geometry used

Table S2. Absolute energies of optimized structures found along allene oxide cyclization pathways (Hartree/particle)

	CASSCF [f]	ωB97xD [b,f]	CCSD(T) [b,f]	ωB97xD [d,f]	ωB97xD [d,f,h]	CCSD(T) [d,f]
1 [a]	-190.82681291	-191.86927668	-191.5469687	-191.86991204		-191.5470017
2 [a]	-190.77653976	-191.80926217	-191.4849015	-191.80889007		-191.4905044
3 [a]	-190.8055114	-191.83336963	-191.5087958	-191.83423742		-191.5098589
3 (Triplet) [a]	-190.8112065	-191.8354716	-191.5104575	-191.83603291		-191.5110584
4 [a]	-190.80536693	-191.83220223	-191.5073177	-191.83134465		-191.5078044
5 [a]	-190.84520821	-191.8868299	-191.5628335	-191.8900636		-191.5634003
6 [b]	-345.8767772	-347.9109042	-347.2924804	-347.9126045	-347.92254953	-347.2930016
7 [b]	-345.8762897	-347.9107695	-347.2920827	-347.9124291	-347.92240022	-347.292579
8 [b]	-345.8308975	-347.8646768	-347.2379105	-347.8609594	-347.87954664	-347.2341148
9 [b]	-345.8358695	-347.8683531	-347.2379129	-347.8660734	-347.88469655	-347.2398456
10 [b]	-345.8294755	-347.8635535	-347.2368058	-347.8604462	-347.87842675	-347.2322888
11 [b]	-345.8333538	-347.8668759	-347.2398993	-347.8647308	-347.88240611	-347.2371898
12 [b]	-345.8653365	-347.9001814	-347.2744559	-347.9021006	-347.91914641	-347.2756891
13 [b]	-345.8581761	-347.8942716	-347.2686632	-347.8961849	-347.91378868	-347.2697709
14 [c]	-345.8602185	-347.895362	-347.2695554	-347.8973017	-347.91394696	-347.271112
15 [b]	-345.85317	-347.8869715	-347.2613056	-347.8894392	-347.90634978	-347.2632392
16 [c]	-345.8596618	-347.8902305	-347.2681828	-347.8927407	-347.91308717	-347.2693297
17 [c]	-345.8545162	-347.8825763	-347.2533424 [g]	-347.8858495	-347.90576019	-347.262482
18 [c]	-345.8543517	-347.8831745	-347.2601704	-347.8864065	-347.90568488	-347.2628962
19 [b]	-345.8492823	-347.8738091	-347.249685	-347.877439	-347.89623411	-347.2538314
20 [c]	-345.8782133	-347.918059	-347.2984433	-347.9193054	-347.93194221	
21 [c]	-345.8768851	-347.9171916		-347.9186493	-347.93162631	
22 [c]	-345.8778829	-347.917958		-347.9193155	-347.93034050	
23 [c]	-345.8770533	-347.9176716		-347.919115	-347.93030265	
24 [c]	-345.8478344	-347.8770982	-347.2533424	-347.8818084	-347.89949229	-347.2577899
25 [b]	-345.8521072	-347.8818308	-347.2578092	-347.8848978	-347.90289724	-347.2608584
26 [c]	-345.8529409	-347.8856773	-347.2628794	-347.8896913	-347.90745222	-347.2654261
27 [b]	-345.8457146	-347.8752977	-347.2500689	-347.8786856	-347.89628405	-347.2543011
28 [b]	-345.849509	-347.8848338	-347.2588171	-347.8882743	-347.90384105	-347.2616803
29 [b]	-345.852893	-347.8870186	-347.2608316	-347.8901554	-347.90614269	-347.2632956
30 [b]	-345.8559324	-347.8921163	-347.2661766	-347.8945218	-347.90957686	-347.2679479
31 [b]	-345.8483416	-347.8822655	-347.2562496	-347.8853953	-347.90098519	-347.2583138
32 [b]	-345.8293953	-347.8648648		-347.8709953	-347.88573097	
33 [b]	-345.8453976	-347.879985	-347.2549822	-347.8826925	-347.89953197	

34 [b]	-345.8327826	-347.8698098		-347.8757577	-347.89039045
35 [b]	-345.8380577	-347.870525	-347.2457144	-347.8723119	-347.88845360
36 [b]	-345.9227222	-347.9589025		-347.9601014	-347.96985541
37 [b]	-345.9469308	-347.986615		-347.9879703	-348.00133529
38 [b]	-345.9251549	-347.9610075		-347.9621246	-347.97137590
39 [b]	-345.9499146	-347.9887551		-347.9900362	-348.00328046
40 [e]				-347.8752027	-347.89652547
41 [e]				-347.8567028	-347.87984025
12 → 13 [b]	-345.8506354	-347.8778053			
14 → 15 [b]	-345.8509763	-347.8784322	-347.2538965	-347.8798536	
12 → 30 [c]	-345.8463178	-347.8774558			
14 → 29 [b]	-345.8443786	-347.8761468			
12 → 14 [b]	-345.8535782	-347.8833191			
29 → 30 [b]	-345.850087	-347.8821821		-347.8837211	
13 → 15 [b]	-345.8514736	-347.8819505	-347.2565625	-347.8832005	-347.89710834
28 → 31 [b]	-345.848055	-347.8808966		-347.8825713	

[a]CASSCF(4,4)/6-311++G(d,p) optimized geometries [b]CASSCF(10,8)/6-31++G(d,p) optimized geometries [C]CASSCF(8,7)/6-31++G(d,p) optimized geometries [d]UωB97xD/cc-pVTZ optimized geometries [e]RωB97xD/cc-pVTZ optimized geometries [f]cc-pVTZ basis set used [g]CASSCF(10,8)/6-31++G(d,p)//UCCSD(T)/cc-pVTZ triples correction 4.9 kcal/mol; UωB97xD/cc-pVTZ//UCCSD(T)/cc-pVTZ triples correction -0.1 kcal/mol [h]Energies calculated in solvent

Table S3. $\langle S^2 \rangle$ values of all diradical intermediates along cyclization pathway for substituted and unsubstituted allene oxide

	UωB97xD[a]	UCCSD(T)[a]	UωB97xD[b]	UωB97xD[c]	UCCSD(T)[b]
2	0.85	1.18	0.43		0.72
3	0.85	0.97	0.85		0.96
4	0.80	0.95	0.56		0.87
8	0.78	1.35	0.30	0.02	1.33
9	0.73	1.35	0.28	0.01	1.30
10	0.82	1.37	0.34	0.13	1.34
11	0.81	1.36	0.36	0.17	1.33
12	0.85	1.16	0.84	0.68	1.17
13	0.94	1.19	0.90	0.78	1.14
14	0.92	1.18	0.90	0.79	1.16
15	1.00	1.28	0.98	0.88	1.23
16	0.12	0.95	0.25	0.06	0.96
17	0.46	1.09	0.33	0.16	0.98
18	0.41	1.04	0.29	0.12	0.99
19	0.73	1.13	0.40	0.20	1.02
24	0.55	1.09	0.33	0.25	1.01
25	0.74	1.17	0.34	0.18	1.03
26	0.18	0.99	0.24	0.22	0.98
27	0.51	1.10	0.39	0.19	1.05
28	0.94	1.27	0.89	0.77	1.20
29	0.89	1.24	0.88	0.73	1.22
30	0.94	1.27	0.80	0.65	1.15
31	1.02	1.33	0.97	0.86	1.29
32	0.68		0.52	0.36	
33	0.82	1.23	0.60	0.44	
34	0.74		0.43	0.21	
35	0.93	1.25	0.75	0.66	
12 → 13	1.05				
14 → 15	1.05	1.32	1.05		
12 → 30	0.75				
14 → 29	0.81				
12 → 14	1.05				
29 → 30	1.05		1.05		
13 → 15	1.06	1.35	1.05	1.05	
28 → 31	1.05		1.05		

[a]CASSCF(10,8)/6-31++G(d,p) optimized geometry [b]UωB97xD/cc-pVTZ optimized geometry
[c]UωB97xD/cc-pVTZ optimized geometry [d]stable wavefunction confirmed

Cartesian coordinates (in Å)

Epoxide minima (**1**)

CASSCF(4,4)/6-311++G(d,p)

C	-0.00000000	0.26236802	0.00000000
C	0.84917006	-0.88662906	0.00000000
O	-0.64599405	-0.90906407	0.00000000
H	1.29189309	-1.23139509	0.91669107
H	1.29189309	-1.23139509	-0.91669107
C	-0.28540802	1.55269111	0.00000000
H	-1.30520510	1.88898913	0.00000000
H	0.50679904	2.27573116	0.00000000

ωB97xD/cc-pVTZ

C	0.26450302	-0.06370500	-0.00000800
C	-1.06796308	-0.58435005	0.00000100
O	-0.73027606	0.84014306	0.00000200
H	-1.51468112	-0.93772007	0.92160007
H	-1.51469711	-0.93771107	-0.92159407
C	1.57593212	-0.11337901	0.00000200
H	2.16316216	0.79266306	0.00000900
H	2.07359416	-1.06977308	-0.00000400

CASSCF(20,19,RASSCF(2,7,2,6))/cc-pVDZ -190.95842631 Hartree/particle

C	-0.00000000	0.26994856	0.00000000
C	0.81407284	-0.92790101	0.00000000
O	-0.68006476	-0.90835625	0.00000000
H	1.26901604	-1.30147631	0.93452632
H	1.26901604	-1.30147631	-0.93452632
C	-0.22609635	1.59051630	0.00000000
H	-1.24860708	1.98948907	0.00000000
H	0.62323413	2.28493046	0.00000000

Epoxide ring opening TS (**2**)

CASSCF(4,4)/6-311++G(d,p)

C	-0.07213301	0.00589400	-0.03702300
C	1.12684308	-0.78578706	-0.03230900
O	0.28891602	1.29654309	0.05547400
H	2.03268615	-0.35403903	-0.41374303
H	1.19322409	-1.67691112	0.56319304
C	-1.35458010	-0.41323903	-0.02882100
H	-2.17217316	0.28237702	-0.00358600
H	-1.56584211	-1.46498011	-0.00074000

ωB97xD/cc-pVTZ

C	0.11079501	0.03560300	0.01597300
C	-1.05093208	-0.81043506	0.03383500
O	-0.46815704	1.16595709	-0.06304701
H	-1.78420713	-0.61196605	0.80100406
H	-1.33355310	-1.44337811	-0.79954006
C	1.43181611	-0.29468502	0.03413600
H	2.19021817	0.47289104	0.08034601
H	1.72272613	-1.32810110	-0.08109501

CASSCF(20,19,RASSCF(2,7,2,6))/cc-pVDZ -190.90846012 Hartree/particle

C	-0.10120485	0.04224240	-0.01611361
C	1.05962109	-0.83928667	-0.04632558
O	0.45832384	1.20376570	0.07043202
H	1.86964662	-0.56100457	-0.73613708
H	1.31420804	-1.52641741	0.77994422
C	-1.44180384	-0.30977317	-0.04275256
H	-2.22722135	0.45744618	-0.09738392
H	-1.72289838	-1.35924514	0.12127116

Oxyallyl singlet (**3**)

CASSCF(4,4)/6-311++G(d,p)

C	0.00000000	0.00000000	0.14320901
C	0.00000000	1.22716409	-0.65697505
C	-0.00000000	-1.22716409	-0.65697505
H	0.00000000	1.19238209	-1.72904613
H	-0.00000000	-1.19238209	-1.72904613
H	0.00000000	2.18005116	-0.16252701
H	-0.00000000	-2.18005116	-0.16252701
O	0.00000000	0.00000000	1.35095010

ωB97xD/cc-pVTZ

C	0.00000000	0.00000000	0.12703500
C	0.00000000	1.21940600	-0.65390200
C	0.00000000	-1.21940600	-0.65390200
H	-0.00007500	1.20207800	-1.73487300
H	0.00007500	-1.20207800	-1.73487300
H	-0.00013800	2.17052400	-0.14017100
H	0.00013800	-2.17052400	-0.14017100
O	0.00000000	0.00000000	1.35433800

CASSCF(20,19,RASSCF(2,7,2,6))/cc-pVDZ -190.93476737 Hartree/particle

C	-0.00000123	0.16383536	-0.00000119
C	1.22034559	-0.67702613	0.00000020
C	-1.22033092	-0.67704983	0.00000018
H	1.16210430	-1.77483235	0.00000026
H	-1.16207006	-1.77485470	0.00000028
H	2.21274390	-0.20083342	0.00000068
H	-2.21273763	-0.20087471	0.00000075
O	-0.00001514	1.38660485	0.00000036

Oxyallyl triplet (**3**)

CASSCF(4,4)/6-311++G(d,p)

C	0.00000000	0.00000000	0.07994301
C	0.00000000	1.25721009	-0.62790304
C	-0.00000000	-1.25721009	-0.62790304
H	0.00000000	1.30006309	-1.70051412
H	-0.00000000	-1.30006309	-1.70051412
H	0.00000000	2.16905216	-0.06303100
H	-0.00000000	-2.16905216	-0.06303100
O	0.00000000	0.00000000	1.32278409

ωB97xD/cc-pVTZ

C	0.00000000	0.00000000	0.07023301
C	0.00000000	1.24996510	-0.62760605
C	-0.00000000	-1.24996510	-0.62760605
H	-0.00006300	1.30494710	-1.70706813
H	0.00006300	-1.30494710	-1.70706813
H	-0.00007900	2.16031016	-0.04758000
H	0.00007900	-2.16031016	-0.04758000
O	0.00000000	0.00000000	1.32739610

CASSCF(20,19,RASSCF(2,7,2,6))/cc-pVDZ -190.93367821 Hartree/particle

C	0.00000000	-0.00000000	0.09550877
C	0.00000000	1.26896549	-0.64211771
C	-0.00000000	-1.26896549	-0.64211771
H	0.00000000	1.30692915	-1.74122650
H	-0.00000000	-1.30692915	-1.74122650
H	0.00000000	2.20753385	-0.07156230
H	-0.00000000	-2.20753385	-0.07156230
O	0.00000000	-0.00000000	1.34474219

Cyclopropanone TS (**4**)

CASSCF(4,4)/6-311++G(d,p)

C	-0.02685100	0.15607901	-0.00000000
C	-0.02685100	-0.66334305	1.21059409
C	-0.02685100	-0.66334305	-1.21059409
H	-0.39596503	-1.67049612	1.19712009
H	-0.39596503	-1.67049612	-1.19712009
H	0.34744803	-0.25379402	2.13008815
H	0.34744803	-0.25379402	-2.13008815
O	0.07254401	1.35902910	-0.00000000

ωB97xD/cc-pVTZ

C	-0.18179608	-0.00000182	-0.09058107
C	0.68636642	-1.14342222	0.03956694
C	0.68634255	1.14343595	0.03956694
H	1.67215964	-1.15706336	-0.40204910
H	1.67213548	1.15709682	-0.40204910
H	0.35693099	-2.00248158	0.60948698
H	0.35688993	2.00248872	0.60948698
O	-1.40044917	-0.00001401	-0.04327407

Cyclopropanone (**5**)

CASSCF(4,4)/6-311++G(d,p)

C	-0.00000000	0.00000000	0.37382803
C	-0.00000000	0.80227406	-0.84669206
C	0.00000000	-0.80227406	-0.84669206
H	-0.91011006	1.29530709	-1.14411908
H	0.91011006	-1.29530709	-1.14411908
H	0.91011006	1.29530709	-1.14411908
H	-0.91011006	-1.29530709	-1.14411908
O	-0.00000000	0.00000000	1.56172611

ωB97xD/cc-pVTZ

C	-0.00000000	0.00000000	0.38205003
C	-0.00000000	0.78375306	-0.85500606
C	0.00000000	-0.78375306	-0.85500606
H	-0.91339507	1.28181810	-1.15289809
H	0.91339507	-1.28181810	-1.15289809
H	0.91339507	1.28181810	-1.15289809
H	-0.91339507	-1.28181810	-1.15289809
O	-0.00000000	0.00000000	1.57242112

CASSCF(20,19,RASSCF(2,7,2,6))/cc-pVDZ -190.98238024 Hartree/particle

C	0.00000000	-0.39348684	0.00000000
C	0.79964582	0.86787452	0.00000000
C	-0.80224794	0.86705080	0.00000000
H	1.30239598	1.17962164	0.92960534
H	-1.30598682	1.17743001	-0.92964740
H	1.30239598	1.17962164	-0.92960534
H	-1.30598682	1.17743001	0.92964740
O	0.00284930	-1.59534177	0.00000000

Z epoxide (**6**)

CASSCF(8,7)/6-31++G(d,p)

C	1.43416549	0.70267494	0.17370972
C	0.38464324	-0.23901917	-0.22810579
C	-0.90273811	0.10090291	-0.27280144
C	2.75765618	0.45597799	0.24824963
O	-1.66034521	1.17203768	-0.03223536
C	-2.29379804	-0.13375052	-0.48557171
H	1.09284677	1.69114513	0.43253096
H	0.62842778	-1.24702423	-0.50466673
H	3.39102501	1.26952174	0.56401976
C	3.47076399	-0.83289494	-0.05980543
H	4.01476604	-1.18543031	0.81274667
H	2.79882738	-1.62269683	-0.37150088
H	4.19928934	-0.68517116	-0.85289549
C	-3.17813843	-0.81492554	0.51928787
H	-4.15548953	-0.34478396	0.54776044
H	-3.31154626	-1.85701435	0.24320793
H	-2.73846881	-0.77238672	1.50792593
H	-2.67224202	-0.05625481	-1.49102285

CASSCF(10,8)/6-31++G(d,p)

C	1.43407377	0.70276912	0.17360310
C	0.38408575	-0.23846094	-0.22795328
C	-0.90314877	0.10202200	-0.27254089
C	2.75747590	0.45560443	0.24802952
O	-1.65924959	1.17366458	-0.03158351
C	-2.29358246	-0.13454438	-0.48590663
H	1.09328268	1.69147177	0.43227031
H	0.62735387	-1.24658595	-0.50451532
H	3.39122279	1.26896522	0.56350081
C	3.47001147	-0.83362838	-0.05984510
H	4.01403457	-1.18621926	0.81267414
H	2.79767971	-1.62321226	-0.37123841
H	4.19845510	-0.68641243	-0.85310714
C	-3.17764957	-0.81594464	0.51899389
H	-4.15546272	-0.34677327	0.54707815
H	-3.31005786	-1.85833227	0.24336920
H	-2.73824316	-0.77272064	1.50771640
H	-2.67186481	-0.05640073	-1.49136372

ωB97xD/cc-pVTZ

C	1.42916500	0.70136900	0.16444800
C	0.39619900	-0.23265700	-0.25638000
C	-0.88445200	0.09201000	-0.28841900
C	2.73649800	0.45656600	0.25381300
O	-1.66737300	1.15242700	-0.01209000
C	-2.28854900	-0.10183500	-0.47407200
H	1.07770600	1.69249300	0.42807000
H	0.64949500	-1.23885700	-0.55753600

H	3.37333000	1.26870600	0.58674000
C	3.43965400	-0.82732400	-0.05111700
H	3.95251700	-1.20546600	0.83616100
H	2.76485600	-1.60564900	-0.40181400
H	4.20389200	-0.67686000	-0.81673400
C	-3.14584300	-0.82303400	0.51953100
H	-4.11793900	-0.33867600	0.61078400
H	-3.30759300	-1.84935300	0.18794300
H	-2.66555300	-0.84514400	1.49575700
H	-2.68776700	-0.01118100	-1.47946700

E epoxide (**7**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.25515923	0.64851301	-0.27399029
C	-0.42070850	-0.52287148	0.00893820
C	0.90236156	-0.49891137	-0.14239672
C	-2.59500961	0.73963971	-0.15484326
O	1.93564952	-1.32471412	0.01179351
C	2.15683280	0.10794420	-0.45496216
H	-0.72596340	1.52462196	-0.61340480
H	-0.86456088	-1.44054158	0.34831593
H	-3.04667426	1.68544808	-0.40824899
C	-3.55158026	-0.33209715	0.29349814
H	-4.28288568	-0.53930733	-0.48349677
H	-3.05651375	-1.26326433	0.53811913
H	-4.10189160	-0.00790790	1.17300736
C	2.90246104	0.99720422	0.49856825
H	3.96889141	0.80558792	0.44345464
H	2.73187088	2.03831627	0.23968354
H	2.56819331	0.83456886	1.51555930
H	2.45994609	0.14015688	-1.48801628

ωB97xD/cc-pVTZ

C	-1.25326200	0.63798500	-0.28363800
C	-0.42900800	-0.52459300	0.00711700
C	0.88295200	-0.49564800	-0.14560200
C	-2.57724800	0.73299400	-0.16119700
O	1.94790300	-1.30030000	0.00757700
C	2.15430500	0.08800000	-0.44629000
H	-0.71538600	1.51219900	-0.63538800
H	-0.87696000	-1.44450000	0.35783900
H	-3.03389000	1.68198900	-0.41932000
C	-3.52180700	-0.32984500	0.30165400
H	-4.28786600	-0.51919500	-0.45340800
H	-3.02540500	-1.27438600	0.51492800
H	-4.04361900	-0.01432400	1.20799400
C	2.87400300	0.99606000	0.50198200
H	3.94850400	0.81802000	0.46321100
H	2.69149700	2.03538600	0.22643500
H	2.52265900	0.84142600	1.52029300
H	2.45762900	0.13606300	-1.48735500

Z-syn epoxide ring opening TS (**8**)

CASSCF(10,8)/6-31++G(d,p)

C	1.43249064	0.72902756	0.13389721
C	0.35575867	-0.21832337	-0.07312252
C	-0.96184007	0.15847356	-0.18770395
C	2.75883057	0.45539254	0.18249308
O	-1.48043108	1.33191710	-0.25745323
C	-2.11942526	-0.68593752	-0.35054180
H	1.13024567	1.75242010	0.28123089
H	0.56018109	-1.26581590	-0.19517185
H	3.42347667	1.28130464	0.37807392
H	-2.20108195	-1.28834053	-1.24444067
C	3.42629946	-0.87906313	-0.00776313
H	4.15603914	-0.82738877	-0.81157539
H	3.96228157	-1.16992704	0.89232345
H	2.72711852	-1.67028806	-0.24733729
C	-3.36675952	-0.54222339	0.46799087
H	-4.17182575	-0.08424259	-0.09863606
H	-3.70234367	-1.53577121	0.75664826
H	-3.19276956	0.04863511	1.35701201

RωB97xD/cc-pVTZ

C	1.41934900	0.72787400	0.15034400
C	0.35368400	-0.19563300	-0.12764100
C	-0.95154200	0.19515700	-0.21757700
C	2.72724800	0.44752200	0.21684100
O	-1.52529700	1.33658400	-0.26572700
C	-2.08617000	-0.65963100	-0.35769800
H	1.10688000	1.75031700	0.33047500
H	0.55134500	-1.24880500	-0.27871300
H	3.40088600	1.25919300	0.46808400
H	-2.15695700	-1.32156000	-1.22114700
C	3.37602200	-0.87740500	-0.01773800
H	4.14983300	-0.79661400	-0.78432700
H	3.87010500	-1.23270800	0.89004000
H	2.67077500	-1.64264900	-0.33576200
C	-3.27449300	-0.58523000	0.50683700
H	-4.14896500	-0.25177600	-0.05783900
H	-3.50566800	-1.60211400	0.84326000
H	-3.12044700	0.07812700	1.35154200

UωB97xD/cc-pVTZ

C	1.41959400	0.72181900	0.12437200
C	0.36423700	-0.20894300	-0.14194800
C	-0.94762900	0.17720300	-0.21809600
C	2.73220900	0.44921100	0.20271100
O	-1.51603200	1.32332400	-0.20661200
C	-2.13191000	-0.59878300	-0.41642700
H	1.10358500	1.74655600	0.28398400
H	0.56832100	-1.25982900	-0.29608100

H	3.40025000	1.27050200	0.43662800
H	-2.27830600	-1.11083800	-1.36598100
C	3.38736400	-0.87794200	0.00391400
H	4.15543000	-0.81655500	-0.77024200
H	3.89044900	-1.20047600	0.91895600
H	2.68487800	-1.65749100	-0.28368600
C	-3.27015900	-0.60579300	0.52385100
H	-4.16639800	-0.17981400	0.06765600
H	-3.50953200	-1.65038500	0.75189400
H	-3.04265900	-0.06889300	1.43950700

Z-anti epoxide ring opening TS (**9**)

CASSCF(10,8)/6-31++G(d,p)

C	1.41279131	-0.77419440	0.07402528
C	0.24166784	0.02981788	-0.20524623
C	-1.04014534	-0.47465590	-0.16201678
C	2.69860565	-0.34814594	0.12757279
O	-1.45683145	-1.63008207	0.20311491
C	-2.27729465	0.19929310	-0.46861074
H	1.22872873	-1.82332286	0.23448242
H	0.33302069	1.07982799	-0.41163127
H	3.45480259	-1.09315748	0.31508809
H	-2.95689005	-0.36258399	-1.08512403
C	3.20586808	1.05741765	-0.04363278
H	3.78163205	1.36177873	0.82649960
H	3.86782984	1.12233402	-0.90360377
H	2.41092832	1.77931708	-0.18244257
C	-2.83004560	1.33252894	0.33442345
H	-2.04471600	2.01507989	0.64123130
H	-3.57923115	1.87390115	-0.23355694
H	-3.31013708	0.95511414	1.23504794

RωB97xD/cc-pVTZ

C	1.39526800	-0.78014200	0.05269200
C	0.22492700	0.02700600	-0.14697300
C	-1.03873000	-0.50196900	-0.12200500
C	2.66632900	-0.35823600	0.08738900
O	-1.49501400	-1.64582100	0.20432400
C	-2.23844600	0.20091300	-0.43772300
H	1.20454400	-1.84023600	0.17653900
H	0.30621100	1.09039700	-0.33031700
H	3.43753300	-1.11017200	0.21232500
H	-2.90709900	-0.33260200	-1.10160500
C	3.15273900	1.04849700	-0.03326000
H	3.83299200	1.29225900	0.78530600
H	3.71682400	1.18286200	-0.95992600
H	2.34580700	1.77867200	-0.02609500
C	-2.72671900	1.38267400	0.28315900
H	-1.90114600	2.02593500	0.59059000
H	-3.47568100	1.93344200	-0.28440400
H	-3.21207200	1.03355100	1.20332300

UωB97xD/cc-pVTZ

C	1.39888100	-0.75783700	0.10541400
C	0.25899600	0.05457900	-0.19549100
C	-1.01687600	-0.44622300	-0.18168500
C	2.68167200	-0.36340700	0.15228200
O	-1.50534400	-1.57583400	0.16433500
C	-2.25972300	0.19658000	-0.46101500
H	1.18148400	-1.80031800	0.30907800
H	0.36782400	1.10310300	-0.43818800

H	3.42627400	-1.11720400	0.38209700
H	-2.89385300	-0.31945100	-1.16893700
C	3.21009800	1.01530900	-0.06945300
H	3.71150300	1.38470300	0.82846800
H	3.95650400	1.01709500	-0.86697200
H	2.43427700	1.73021400	-0.33610400
C	-2.81513300	1.29223300	0.35119900
H	-2.03470100	1.99457400	0.64766800
H	-3.63317700	1.80369200	-0.15398000
H	-3.22087600	0.86285400	1.27467200

E-syn epoxide ring opening TS (**10**)

CASSCF(10,8)/6-31++G(d,p)

C	1.20401317	-0.67716809	-0.16535512
C	0.39893032	0.50905518	0.03201928
C	-0.96860402	0.52024241	-0.12818107
C	2.55495338	-0.76709671	-0.08533161
O	-1.74939634	1.54264339	-0.15749191
C	-1.89309953	-0.56307567	-0.36589796
H	0.66873362	-1.58353430	-0.39700143
H	0.86856295	1.45498867	0.23113746
H	2.99301579	-1.73506602	-0.26770305
H	-1.84060107	-1.09669318	-1.30368771
C	3.52878346	0.33039999	0.24530872
H	3.04730899	1.28372336	0.42106113
H	4.09887376	0.07756583	1.13556860
H	4.24182235	0.46226640	-0.56445025
C	-3.12128367	-0.78823472	0.46534432
H	-4.02590320	-0.50522599	-0.06444623
H	-3.19857205	-1.85002732	0.68855239
H	-3.08022922	-0.23387886	1.39346500

RωB97xD/cc-pVTZ

C	1.17569700	-0.63639300	-0.19150200
C	0.39716000	0.55369700	-0.00060900
C	-0.96889300	0.56789600	-0.11067500
C	2.50740400	-0.75795600	-0.10055200
O	-1.81186500	1.52189800	-0.15449000
C	-1.81103200	-0.57073500	-0.31990800
H	0.62063500	-1.54103200	-0.42669400
H	0.88269500	1.50387200	0.17947300
H	2.93496500	-1.73439000	-0.29830100
H	-1.64464000	-1.20528100	-1.19034800
C	3.48375600	0.31032400	0.26781700
H	3.01282900	1.27830300	0.42403300
H	4.01682600	0.04606400	1.18434000
H	4.23979200	0.42545400	-0.51225400
C	-3.03457200	-0.83025000	0.45227300
H	-3.92366900	-0.69911400	-0.17059400
H	-3.03011800	-1.88587800	0.74552400
H	-3.11152000	-0.18267300	1.31968600

UωB97xD/cc-pVTZ

C	1.17143200	-0.63917700	-0.15012900
C	0.40698000	0.55513900	0.03234600
C	-0.95764400	0.56544500	-0.10526100
C	2.50780100	-0.76982500	-0.08533100
O	-1.81237100	1.51267000	-0.11022800
C	-1.86901400	-0.49953200	-0.40662500
H	0.60167900	-1.54121800	-0.35712100
H	0.88966300	1.50193400	0.23344700

H	2.92275600	-1.75570600	-0.26148800
H	-1.81373900	-0.97687700	-1.38307400
C	3.49993700	0.30305000	0.22072100
H	3.04002900	1.28078900	0.34641900
H	4.04845200	0.07088700	1.13693900
H	4.24177700	0.37953600	-0.57737700
C	-3.01148800	-0.86514100	0.45355700
H	-3.96515600	-0.68819900	-0.04822100
H	-2.95863000	-1.94379500	0.63945100
H	-2.99589100	-0.32846400	1.39717700

E-anti epoxide ring opening TS (**11**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.04376134	-0.59986440	-0.24174825
C	-0.31333188	0.63500118	-0.06340688
C	1.06468987	0.72132462	-0.11180036
C	-2.38465126	-0.77392954	-0.12517338
O	1.78747718	1.73824506	0.17438087
C	2.06200115	-0.26881845	-0.46758195
H	-0.46289921	-1.46616671	-0.51090900
H	-0.83720980	1.53719643	0.19433242
H	-2.76662310	-1.76561580	-0.30616042
H	2.79442953	0.07628786	-1.17699734
C	-3.41921021	0.26407014	0.21279685
H	-2.99145955	1.23679140	0.41831303
H	-4.12590743	0.37772822	-0.60531794
H	-3.98852955	-0.03956771	1.08738884
C	2.43902299	-1.42823674	0.40120888
H	1.58142963	-1.83624031	0.92255058
H	2.90366514	-2.20904789	-0.19303320
H	3.16473098	-1.11460685	1.14901669

RωB97xD/cc-pVTZ

C	-0.99366900	-0.60858800	-0.15199700
C	-0.27586200	0.62648500	-0.05177900
C	1.10025000	0.76680300	-0.06625100
C	-2.32542400	-0.76264800	-0.07850500
O	1.79472100	1.79421800	0.18223100
C	2.03328000	-0.26501500	-0.40402300
H	-0.41377100	-1.50697100	-0.32797000
H	-0.82535600	1.55122500	0.07751800
H	-2.71484300	-1.76973800	-0.17840100
H	2.80458800	0.06861900	-1.08889100
C	-3.35142900	0.30248900	0.12206400
H	-4.08931800	0.28163300	-0.68264200
H	-3.89808600	0.13334100	1.05304600
H	-2.92509700	1.30195800	0.16364900
C	2.25392300	-1.53523200	0.30246300
H	1.39012600	-1.85941600	0.87629500
H	2.58402000	-2.31456600	-0.38775200
H	3.08356000	-1.38559800	1.00546900

UωB97xD/cc-pVTZ

C	-1.03956100	-0.56303100	-0.27128900
C	-0.31689300	0.64638300	-0.03053500
C	1.05268900	0.72386200	-0.11893000
C	-2.36671800	-0.74784200	-0.15694100
O	1.86474600	1.66890200	0.14579600
C	2.03357700	-0.27148900	-0.44051600
H	-0.45152300	-1.41743600	-0.59271200
H	-0.83372600	1.54790400	0.27034900

H	-2.75380700	-1.73718300	-0.37290800
H	2.73097000	0.01331800	-1.21676400
C	-3.38422100	0.27226600	0.23389100
H	-2.95319600	1.25644900	0.40298600
H	-4.14938800	0.36830400	-0.53969600
H	-3.89981100	-0.02999300	1.14868800
C	2.35512900	-1.42938400	0.41453100
H	1.47554200	-1.80735100	0.93301600
H	2.83834100	-2.22249800	-0.15693600
H	3.07462000	-1.10732700	1.17634600

Oxyallyl (**12**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.40489710	0.64759805	-0.60057304
C	-0.34809803	-0.23071802	-0.28941702
C	1.05716908	0.20141201	-0.36113203
C	-2.75141920	0.35653503	-0.57084004
O	1.39874110	1.31707210	-0.71092805
C	2.01878215	-0.82210406	0.02971500
H	-1.11490208	1.64328512	-0.88735606
H	-0.54141004	-1.24361209	0.00776900
H	-3.42871525	1.15152108	-0.83490506
H	1.65746912	-1.80468713	0.27136002
C	-3.39418825	-0.95099407	-0.20614501
H	-4.04119829	-0.82726806	0.65862705
H	-4.01730629	-1.30697909	-1.02238407
H	-2.67586619	-1.72691912	0.02525900
C	3.48573925	-0.54943404	0.02250300
H	4.02258929	-1.26555409	0.63391705
H	3.87844128	-0.61060004	-0.99122007
H	3.68881127	0.45389503	0.37851403

UωB97xD/cc-pVTZ

C	1.40714200	0.72963000	-0.00315700
C	0.35841000	-0.18844500	-0.01031800
C	-1.03240200	0.25711100	-0.00496100
C	2.74143300	0.43654000	0.00183400
O	-1.35935000	1.44495500	0.00041800
C	-2.00212400	-0.81030500	-0.00385000
H	1.10909700	1.77192100	0.00281300
H	0.54937000	-1.25327700	-0.01613900
H	3.43363200	1.27071200	0.01616800
H	-1.64906700	-1.83450400	-0.01217200
C	3.36230500	-0.91622500	0.00339600
H	4.09654800	-0.99934500	-0.80059600
H	3.90544000	-1.08077700	0.93788300
H	2.63807900	-1.71930400	-0.11078200
C	-3.45293000	-0.54774400	0.00800900
H	-3.93536600	-0.99812800	-0.86458000
H	-3.92184200	-1.00357100	0.88521200
H	-3.64210200	0.52327500	0.01314100

Oxyallyl (**13**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.30140588	-0.81625597	-0.00161524
C	-0.13525088	-0.04239558	-0.00057239
C	1.20535902	-0.67618288	-0.00006120
C	-2.60663004	-0.34816730	-0.00127125
O	1.34833491	-1.88534323	0.00351941
C	2.37589611	0.20406293	-0.00392402
H	-1.15907490	-1.88277228	-0.00330802
H	-0.18781472	1.02836371	0.00152360
H	-3.38995541	-1.08727468	-0.00322879
C	-3.05846066	1.08397312	0.00132474
H	-3.67017885	1.29122526	-0.87312623
H	-3.67232343	1.28735239	0.87517399
H	-2.23585100	1.78760466	0.00389884
C	2.36824278	1.70601458	0.00094608
H	1.87853495	2.10821954	0.88410458
H	3.38401048	2.08191662	-0.00797388
H	1.86084382	2.11414841	-0.86925211
H	3.31862706	-0.31233122	-0.00492768

UωB97xD/cc-pVTZ

C	1.30613900	-0.79338900	-0.01147700
C	0.14891700	-0.02147500	-0.01150500
C	-1.16879700	-0.66147400	-0.00033300
C	2.59361300	-0.32817200	-0.00480400
O	-1.29857600	-1.88736400	0.00353000
C	-2.34036000	0.18198100	0.01422400
H	1.14854900	-1.86573400	-0.01384800
H	0.21477500	1.05620700	-0.00902700
H	3.38646100	-1.06718300	0.00045100
C	3.03505100	1.09317500	0.01056000
H	3.56804200	1.31285700	0.93964100
H	3.73978900	1.28302000	-0.80196200
H	2.21377200	1.80034800	-0.07999300
C	-2.43293200	1.65986800	-0.00981200
H	-1.47691100	2.16038900	-0.13603600
H	-3.09619200	1.98216900	-0.81724700
H	-2.88825700	2.02610300	0.91614900
H	-3.27121000	-0.37234300	0.05251700

Oxyallyl (**14**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.20678311	-0.68720884	-0.29630112
C	-0.40555062	0.44834449	-0.10886891
C	-0.86080654	1.83658697	0.10877432
C	-0.75416728	-1.98660092	-0.46538033
O	-0.06252756	2.68888039	0.45977062
C	-2.25950374	2.17838260	-0.13920426
H	-2.27496470	-0.56086591	-0.31430097
H	0.66127909	0.34254351	-0.04079424
H	-1.50485623	-2.74782322	-0.59656769
C	0.66803827	-2.46762735	-0.46792914
H	1.38999087	-1.66330389	-0.42452090
H	0.84790408	-3.12396832	0.38021257
H	0.86769876	-3.04539345	-1.36629428
H	-2.95193699	1.42329607	-0.45264475
C	-2.72208673	3.58893816	0.02514926
H	-2.14402289	4.25736235	-0.60694902
H	-3.77145043	3.69076808	-0.22323845
H	-2.56951771	3.92536289	1.04722702

UωB97xD/cc-pVTZ

C	1.19720000	-0.73808200	-0.00441500
C	0.41947400	0.41585300	-0.01192400
C	-1.04131700	0.51681100	-0.00407600
C	2.56820800	-0.77740200	0.00167600
O	-1.57891000	1.62494700	0.00472200
C	-1.82491500	-0.69743300	-0.00662900
H	0.69579300	-1.69812000	0.00321800
H	0.90275800	1.38468400	-0.01655000
H	3.03528300	-1.75516700	0.02014600
C	3.49775900	0.38467000	0.00378100
H	2.99375100	1.33886500	-0.12680500
H	4.05282500	0.42301100	0.94508700
H	4.24050700	0.27991300	-0.78978000
H	-1.33405600	-1.66043900	-0.02486500
C	-3.29986500	-0.65849800	0.00817100
H	-3.65204700	0.36953600	0.04368500
H	-3.70940900	-1.14952200	-0.87999600
H	-3.69338900	-1.20785100	0.86858000

Oxyallyl (**15**)

CASSCF(10,8)/6-31++G(d,p)

C	0.94048109	-0.45854354	-0.48595835
C	0.22034729	0.51014820	0.20380603
C	-1.22882125	0.79380550	-0.00854464
C	2.32462157	-0.63651625	-0.42036391
O	-1.57386397	1.95123229	-0.20166020
C	-2.23906283	-0.25364206	0.04126505
H	0.39886530	-1.12673744	-1.13536114
H	0.73186550	1.24407666	0.80023830
H	2.75220998	-1.43202469	-1.00420253
C	3.25574761	0.20360433	0.41081708
H	3.19334453	1.25458815	0.14105243
H	3.02632568	0.12537217	1.47076256
H	4.28314193	-0.11175421	0.27278994
H	-3.24265794	0.10145218	-0.11329101
C	-2.03380310	-1.71762858	0.28392196
H	-1.09232766	-1.93115316	0.77216329
H	-2.83333429	-2.10284628	0.90889573
H	-2.06358357	-2.27819724	-0.64942533

UωB97xD/cc-pVTZ

C	0.92127400	-0.56573500	-0.34473700
C	0.22879500	0.54656600	0.09957300
C	-1.21691800	0.80193300	-0.03032400
C	2.29080500	-0.71185200	-0.28250400
O	-1.60989800	1.96614900	-0.11946300
C	-2.18837100	-0.26707800	-0.01870800
H	0.36708200	-1.37609400	-0.80132200
H	0.77773400	1.40168600	0.47465400
H	2.71772800	-1.62428100	-0.67848300
C	3.22642400	0.29980000	0.28908700
H	3.09521500	1.27538500	-0.18536900
H	3.05005900	0.44516300	1.35826500
H	4.26340700	-0.00070200	0.15897100
H	-3.19957900	0.08205600	-0.18992400
C	-1.98707400	-1.70928700	0.26214200
H	-1.09831200	-1.90130300	0.85986400
H	-2.85482400	-2.11700800	0.78117500
H	-1.88894500	-2.28017700	-0.66930000

Cyclopropanone ring closing TS (**16**)

CASSCF(10,8)/6-31++G(d,p)

C	1.17999303	0.59149223	0.49289536
C	0.22818661	0.14706792	-0.49866489
C	-1.15674349	0.57960822	-0.46954087
C	2.47967385	0.21251112	0.59199162
O	-1.62485726	1.65356087	-0.16699761
C	-1.74624455	-0.73811605	-0.42703218
H	0.80391318	1.29844896	1.21250534
H	0.53532617	-0.49595650	-1.29978674
H	3.05746681	0.65537359	1.38687638
H	-1.54407933	-1.41268178	-1.23833677
C	3.22630056	-0.74901812	-0.28967846
H	4.04758811	-0.24487150	-0.79220211
H	3.65831531	-1.54818152	0.30656895
H	2.60089071	-1.20331491	-1.04756315
C	-2.73689255	-1.13857153	0.62465724
H	-2.61875349	-2.17969666	0.90408447
H	-2.63832672	-0.52066861	1.50911523
H	-3.74912339	-1.00678073	0.24695252

UωB97xD/cc-pVTZ

C	1.23027800	0.68384100	0.34540500
C	0.25505400	0.03825900	-0.46890300
C	-1.11255100	0.48937800	-0.47313400
C	2.51628000	0.31204700	0.48607200
O	-1.54681800	1.60143900	-0.20288800
C	-1.76294000	-0.77566100	-0.33572600
H	0.87825900	1.56139200	0.87433900
H	0.52731600	-0.80830400	-1.08129900
H	3.13967800	0.92417800	1.12883800
H	-1.44427900	-1.60641700	-0.94925400
C	3.20306500	-0.84690400	-0.14994600
H	4.03535300	-0.50209200	-0.76760600
H	3.63257400	-1.49556100	0.61684100
H	2.54634300	-1.45041000	-0.77195100
C	-2.88748000	-0.96725000	0.60856300
H	-2.81596900	-1.91458600	1.14292000
H	-2.94693800	-0.13717500	1.30993000
H	-3.82803300	-0.98479300	0.04636400

Cyclopropanone ring closing TS (**17**)

CASSCF(8,7)/6-31++G(d,p)

C	1.24737283	-0.80824094	0.23307908
C	0.09403117	-0.11501308	-0.27324479
C	-1.23910327	-0.69413923	-0.17801737
C	2.52385310	-0.33768044	0.27304753
O	-1.56286631	-1.84886468	-0.33638346
C	-1.94432946	0.35766119	0.53740307
H	1.06643647	-1.80203960	0.60564794
H	0.19121130	0.85994942	-0.70667921
H	3.27586475	-1.00081869	0.66837526
C	3.02254168	1.00290849	-0.18853104
H	2.23104724	1.65144133	-0.54196116
H	3.53292138	1.51477644	0.62290066
H	3.74193995	0.88429532	-0.99459403
H	-2.33780872	0.08803698	1.50329052
C	-2.34006975	1.68243689	-0.04771454
H	-1.81629572	1.89756979	-0.97210775
H	-3.40386356	1.67334150	-0.27732634
H	-2.16430027	2.49676770	0.64739017

UωB97xD/cc-pVTZ

C	1.20737600	-0.84395300	0.15416600
C	0.06244100	-0.11134100	-0.27006200
C	-1.25044800	-0.70237500	-0.19218800
C	2.46817600	-0.37308700	0.21922500
O	-1.54573500	-1.88540100	-0.22726500
C	-1.95357400	0.37383500	0.45409100
H	1.02085300	-1.87538800	0.42823600
H	0.16821100	0.90384600	-0.61775700
H	3.23725900	-1.06537300	0.54398200
C	2.94319300	0.99973700	-0.11272900
H	2.14719300	1.66422200	-0.44101000
H	3.42227900	1.45238900	0.75850400
H	3.70050000	0.96076400	-0.89865100
H	-2.46405700	0.09662700	1.37146600
C	-2.16309300	1.75560300	-0.05006000
H	-1.64353800	1.94830400	-0.98672200
H	-3.23182200	1.89711700	-0.23923600
H	-1.87542500	2.51019000	0.68465300

Cyclopropanone ring closing TS (**18**)

CASSCF(10,8)/6-31++G(d,p)

C	1.21962817	-0.08098040	-0.77369252
C	0.24670829	0.40785747	0.17023817
C	-1.15072993	0.68708994	-0.15104993
C	2.53512117	-0.31996604	-0.52736973
O	-1.77146476	1.70783154	0.03697633
C	-1.64464668	-0.66269368	-0.32205196
H	0.87270867	-0.24531230	-1.78096289
H	0.54993722	0.67823864	1.16584787
H	3.13520884	-0.64658330	-1.36084733
H	-1.18610095	-1.28346438	-1.06820988
C	3.26804333	-0.15940877	0.77523868
H	3.79655085	-1.07558033	1.02355356
H	4.01198994	0.62950308	0.70007965
H	2.61293487	0.07846629	1.60330154
C	-2.83572324	-1.18219211	0.42756584
H	-2.69490596	-2.21512034	0.72721702
H	-3.03741610	-0.58269005	1.30708934
H	-3.71959590	-1.13834807	-0.20615081

UωB97xD/cc-pVTZ

C	1.19536700	-0.34372600	-0.70377300
C	0.26182900	0.43791100	0.03677400
C	-1.13697900	0.65150700	-0.26919200
C	2.50432100	-0.48266400	-0.41816700
O	-1.77850600	1.68249600	-0.14370300
C	-1.60014600	-0.69848700	-0.19520900
H	0.82926600	-0.82537900	-1.60337300
H	0.61225100	1.00710000	0.89055900
H	3.09979200	-1.07061200	-1.10762300
H	-1.04957600	-1.48419500	-0.68987300
C	3.24909800	0.09511000	0.73667500
H	3.77126300	-0.69530700	1.27971900
H	4.01406000	0.79165500	0.38587300
H	2.61087200	0.62365100	1.44055400
C	-2.83472500	-1.05214700	0.54639400
H	-2.66076000	-1.85322400	1.26670000
H	-3.24637000	-0.17839100	1.04690600
H	-3.58534600	-1.42029100	-0.16083300

Cyclopropanone ring closing TS (**19**)

CASSCF(10,8)/6-31++G(d,p)

C	-0.95669255	0.30257623	-0.59764622
C	-0.16124564	-0.63226739	0.12591407
C	1.29265711	-0.79388870	-0.02644001
C	-2.30168946	0.51106199	-0.45149732
O	1.84464102	-1.81088530	-0.37894623
C	1.95101831	0.36483821	0.58313220
H	-0.45981772	0.88175081	-1.35734786
H	-0.61513831	-1.29210459	0.84331627
H	-2.76075930	1.22223371	-1.11808541
H	2.47666030	0.17091498	1.50226470
C	-3.22801922	-0.16775845	0.51786529
H	-3.83199818	0.56903156	1.03970884
H	-3.91252433	-0.83055240	-0.00593101
H	-2.70391167	-0.75237898	1.26303813
C	1.93826117	1.76706423	0.04065477
H	2.89378733	2.24092916	0.24089228
H	1.78155779	1.78689425	-1.03196008
H	1.16927764	2.38060710	0.50377728

UωB97xD/cc-pVTZ

C	-0.91689400	0.32932700	-0.61397200
C	-0.06868900	-0.63510700	-0.00943900
C	1.37313300	-0.76224800	-0.11466500
C	-2.24605100	0.44843700	-0.40367100
O	2.00729100	-1.79051700	-0.25098200
C	1.80910800	0.45978000	0.51569400
H	-0.47709000	1.00012400	-1.33958700
H	-0.51295600	-1.41809700	0.59503800
H	-2.77316000	1.19376700	-0.98869800
H	2.42178500	0.29189600	1.39588400
C	-3.08938900	-0.35326100	0.52745200
H	-3.70022300	0.30534700	1.14753300
H	-3.78164900	-0.98418700	-0.03554700
H	-2.50777000	-0.99357400	1.18636400
C	1.58323300	1.87328900	0.10328300
H	2.44592100	2.47131300	0.39761500
H	1.45160600	1.98236500	-0.97134200
H	0.70850300	2.31388100	0.59249300

Cyclopropanone (**20**)

CASSCF(8,7)/6-31++G(d,p)

C	1.09397108	-0.41973103	0.72506406
C	-0.04590000	-0.01997500	-0.14344501
C	-1.29448610	-0.79305006	-0.15638101
C	2.40120718	-0.19954602	0.50145604
O	-1.83216514	-1.80442914	-0.50165704
C	-1.42493411	0.48812404	0.52737404
H	0.82302006	-0.94628407	1.62674813
H	0.19253301	0.47884904	-1.06869408
H	3.09043624	-0.56604104	1.24565810
C	3.03681723	0.49368704	-0.67324105
H	3.63980928	1.33256710	-0.33643203
H	3.69990128	-0.18632101	-1.20116709
H	2.31364518	0.87025607	-1.38544210
H	-1.42723211	0.43990903	1.60688512
C	-2.18724117	1.64794412	-0.07765801
H	-2.13390816	1.63063912	-1.16158309
H	-3.23486825	1.60284912	0.20190202
H	-1.78261214	2.59429120	0.26636002

ωB97xD/cc-pVTZ

C	1.08247200	-0.40914700	0.73385500
C	-0.04740800	-0.01597400	-0.12914900
C	-1.30283000	-0.79799800	-0.15366000
C	2.37423800	-0.20528300	0.49954200
O	-1.84324300	-1.80125500	-0.49825000
C	-1.39498800	0.49163900	0.52292200
H	0.80711600	-0.92155800	1.65013400
H	0.19226000	0.47910700	-1.06374200
H	3.07357700	-0.56534900	1.24629300
C	2.99325600	0.46536500	-0.68446900
H	3.61962300	1.30092500	-0.36578600
H	3.64232600	-0.22796200	-1.22323800
H	2.25792400	0.84739800	-1.38993100
H	-1.39833700	0.44182400	1.60774400
C	-2.12377700	1.66499300	-0.08216400
H	-2.07492700	1.63399700	-1.17097000
H	-3.17570800	1.65546700	0.20226600
H	-1.68368200	2.60462600	0.25197400

Cyclopropanone (**21**)

CASSCF(8,7)/6-31++G(d,p)

C	0.88823033	-0.13617517	0.74236580
C	-0.04046194	-0.35197065	-0.40149003
C	-1.42633175	-0.77590778	-0.18146912
C	2.22312475	0.01128563	0.66971430
O	-2.14001829	-1.64121957	0.23589571
C	-1.33636892	0.59960993	-0.65591663
H	0.43693741	-0.10550455	1.72027373
H	0.40317044	-0.68606851	-1.32450878
H	2.75107789	0.14448614	1.60072836
C	3.08675896	0.00380504	-0.56248940
H	3.68057045	0.91244210	-0.61068508
H	3.78134631	-0.83170983	-0.53740163
H	2.51428073	-0.06426734	-1.47891676
H	-1.52821399	0.74984853	-1.70780966
C	-1.66877368	1.77781424	0.23500497
H	-1.48205416	1.55853981	1.27992695
H	-1.07606822	2.64462733	-0.03827107
H	-2.71796709	2.03659549	0.13517897

ωB97xD/cc-pVTZ

C	0.87390500	0.07627300	0.69877700
C	-0.02173700	-0.26975300	-0.42126100
C	-1.35914700	-0.83742200	-0.15939300
C	2.20017900	0.15397800	0.65566600
O	-1.97316300	-1.72489000	0.34550400
C	-1.37834900	0.52248000	-0.68675600
H	0.38892000	0.26937700	1.64884800
H	0.44972000	-0.58025300	-1.34491500
H	2.70817700	0.41119300	1.57892900
C	3.09383500	-0.07858100	-0.51984000
H	3.69661000	0.80955200	-0.72054300
H	3.79142700	-0.89323000	-0.31552800
H	2.54960500	-0.32421300	-1.42960700
H	-1.57422200	0.62652000	-1.74780300
C	-1.81400600	1.68671800	0.16778700
H	-1.65640800	1.48953400	1.22720500
H	-1.26009700	2.58820500	-0.09467600
H	-2.87650100	1.88028600	0.02417400

Cyclopropanone (**22**)

CASSCF(8,7)/6-31++G(d,p)

C	0.94503065	-1.24596450	-0.08237445
C	-0.22195642	-0.48409042	0.46516500
C	-0.67409795	0.79907758	-0.08340911
C	2.20830272	-0.80170309	-0.19824992
O	-0.47876879	1.97679098	-0.15715146
C	-1.54743325	-0.31839188	-0.42769102
H	0.73126228	-2.26047605	-0.38040720
H	-0.42655322	-0.63140645	1.51749678
H	2.93427716	-1.49137608	-0.60040625
C	2.74077105	0.55084100	0.18946816
H	1.98032505	1.19285579	0.61260313
H	3.54111130	0.44093903	0.91675205
H	3.16211537	1.05636219	-0.67528282
H	-1.43459147	-0.69402860	-1.43480436
C	-2.92288474	-0.47861187	0.18432090
H	-2.95197380	-0.08108099	1.19390357
H	-3.66608591	0.05254782	-0.40140246
H	-3.20612884	-1.52560534	0.22538189

ωB97xD/cc-pVTZ

C	0.92512600	-1.26965200	-0.02206200
C	-0.23914400	-0.49447100	0.48448700
C	-0.64162100	0.81614400	-0.05134400
C	2.16335400	-0.81801400	-0.18266100
O	-0.43245700	1.98837700	-0.09862300
C	-1.50080100	-0.30466000	-0.43697900
H	0.71525100	-2.30633500	-0.26603100
H	-0.49117200	-0.65318500	1.53099500
H	2.89873400	-1.52263200	-0.55834700
C	2.67640000	0.55271800	0.11851100
H	1.90391300	1.22105600	0.49128100
H	3.47623400	0.49660800	0.86013500
H	3.11012600	1.00302100	-0.77645000
H	-1.34526900	-0.66638400	-1.44909500
C	-2.89265500	-0.47208300	0.11843400
H	-2.96989900	-0.03815100	1.11586100
H	-3.62479900	0.02674900	-0.51592400
H	-3.15741800	-1.52765100	0.18624400

Cyclopropanone (**23**)

CASSCF(8,7)/6-31++G(d,p)

C	0.74013805	-1.18146403	0.31257980
C	-0.21435693	-0.20044284	0.92013525
C	-0.74038403	0.96471010	0.20281507
C	1.95448480	-0.90813382	-0.19469517
O	-0.49384744	2.02974661	-0.28339949
C	-1.73776726	-0.08235346	0.39493624
H	0.41781948	-2.21047462	0.33281317
H	-0.13989958	-0.08902609	1.99296344
H	2.52786395	-1.74322580	-0.56672458
C	2.62673237	0.43456738	-0.28600296
H	2.02109417	1.23248884	0.12109899
H	3.57334905	0.41369137	0.24797549
H	2.84905298	0.67913644	-1.32118482
H	-2.44932683	0.08023899	1.19065803
C	-2.24646747	-0.90471589	-0.77088624
H	-1.48249260	-1.03562822	-1.52895647
H	-2.56698816	-1.88745789	-0.43982306
H	-3.09397007	-0.41072045	-1.23491618

ωB97xD/cc-pVTZ

C	0.72392500	-1.18712200	0.37143900
C	-0.24351800	-0.21589800	0.95000300
C	-0.72483000	0.97385400	0.23131000
C	1.90098900	-0.90323700	-0.17333800
O	-0.45691200	2.03395300	-0.24398200
C	-1.71117000	-0.09748500	0.37093700
H	0.42000100	-2.22749100	0.42915500
H	-0.22077200	-0.12595800	2.03255200
H	2.49029000	-1.74006500	-0.53515300
C	2.52655900	0.44465300	-0.33018600
H	1.90175600	1.24580300	0.05678300
H	3.49082700	0.47135900	0.18187400
H	2.72493000	0.65118500	-1.38375200
H	-2.46977500	0.03271900	1.13454300
C	-2.13175900	-0.89558600	-0.83887700
H	-1.32388000	-0.95942300	-1.56751900
H	-2.41436200	-1.91068400	-0.55871500
H	-2.98489400	-0.42414900	-1.32562900

Cyclopropanone ring closing TS (**24**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.26348109	1.31093487	-0.24653795
C	0.09914982	0.90828639	-0.46182383
C	0.67025270	-0.43706943	-0.42411475
C	-2.33494959	0.58443336	0.18648994
O	0.25682079	-1.44521053	-0.94913801
C	1.71337585	-0.32492830	0.59012541
H	-1.44487380	2.35655053	-0.43490355
H	0.79290371	1.69309300	-0.70216748
H	-3.26642354	1.12071505	0.25502040
H	1.60520851	-0.96111355	1.45293047
C	-2.36330202	-0.86092415	0.60518970
H	-1.60328472	-1.07578714	1.35054924
H	-3.32657426	-1.10521734	1.03806975
H	-2.18535889	-1.52331597	-0.23467486
C	3.02214689	0.38452717	0.39194452
H	3.80468361	-0.34239681	0.18195124
H	2.99354745	1.07572949	-0.44252590
H	3.31645029	0.93186756	1.28121649

UωB97xD/cc-pVTZ

C	-1.19585300	1.30638000	-0.30832200
C	0.15006400	0.86796400	-0.46700300
C	0.63680300	-0.49081100	-0.49970300
C	-2.25388300	0.61487900	0.16832600
O	0.08689600	-1.49905200	-0.92015700
C	1.70589800	-0.41833200	0.45782400
H	-1.36651400	2.34843200	-0.55594800
H	0.88829500	1.64634700	-0.59811800
H	-3.19972700	1.14412500	0.18978100
H	1.66930500	-1.18634200	1.22526200
C	-2.24480600	-0.76405600	0.72324600
H	-1.46934200	-0.86877500	1.48671100
H	-3.20426900	-1.01675100	1.16851700
H	-1.99113300	-1.49131100	-0.05215100
C	2.90837500	0.45573800	0.44893700
H	3.79343900	-0.17577800	0.32201700
H	2.90785100	1.18067600	-0.36176800
H	3.03734000	0.98122100	1.39711800

Cyclopropanone ring closing TS (**25**)

CASSCF(10,8)/6-31++G(d,p)

C	1.49493388	-0.72868052	-0.90244159
C	0.21277589	-1.19406770	-0.43243452
C	-0.74840349	-0.49409800	0.42259376
C	2.29320781	0.24651344	-0.38616929
O	-1.26339621	-0.91534750	1.43512984
C	-1.22276241	0.58031667	-0.42426952
H	1.87875373	-1.25752393	-1.75930717
H	-0.09842985	-2.17902768	-0.73616260
H	3.21740567	0.42810860	-0.91075607
C	2.08621310	1.08339408	0.84750864
H	1.27324326	0.73223822	1.46864279
H	2.99065572	1.07372028	1.44876911
H	1.88950539	2.12035239	0.58755837
H	-0.49513121	1.19138036	-0.92269333
C	-2.68028242	0.88694465	-0.58987684
H	-3.29473592	0.05909877	-0.25806674
H	-2.94695384	1.75303762	0.01342022
H	-2.92123735	1.11945965	-1.62190708

UωB97xD/cc-pVTZ

C	1.48082800	-0.62629900	-0.94994500
C	0.22512700	-1.15202400	-0.52298500
C	-0.75496900	-0.55567300	0.36513100
C	2.24334600	0.29217900	-0.31949300
O	-1.39688000	-1.10730200	1.24678800
C	-1.11796300	0.60713100	-0.38567300
H	1.88888400	-1.06055900	-1.85576900
H	-0.05051100	-2.13799100	-0.88220100
H	3.18017100	0.54903100	-0.80275300
C	2.00413300	0.95932900	0.99292900
H	1.17056300	0.52739400	1.54160800
H	2.90326100	0.89203100	1.60829300
H	1.80070600	2.02380300	0.85556700
H	-0.34633900	1.17544400	-0.88203000
C	-2.53027000	1.03814100	-0.50854800
H	-3.19808500	0.31072400	-0.05188100
H	-2.66329400	1.99110800	0.01495900
H	-2.81171400	1.21072800	-1.54860000

Cyclopropanone ring closing TS (**26**)

CASSCF(10,8)/6-31++G(d,p)

C	1.52928585	1.10925539	-0.34386709
C	0.15756835	1.31029484	0.07411351
C	-0.75302943	0.37431037	0.71462071
C	2.26230219	-0.03282251	-0.42291225
O	-0.56750199	-0.43841088	1.59102489
C	-1.82218216	0.46445809	-0.25587903
H	2.02043211	2.01369463	-0.66372731
H	-0.22669048	2.30691443	-0.04635898
H	3.27675155	0.08826402	-0.76447146
H	-2.26064847	1.42836122	-0.43688042
C	1.82161330	-1.44232519	-0.12970057
H	0.97143497	-1.72577211	-0.74333946
H	2.62557984	-2.13717181	-0.34325552
H	1.52541202	-1.56177788	0.90567742
C	-2.44953933	-0.74193022	-0.88836005
H	-2.63637935	-0.58256859	-1.94500001
H	-1.82653883	-1.61928239	-0.76732255
H	-3.40545009	-0.95081901	-0.41161218

UωB97xD/cc-pVTZ

C	1.64243600	1.06370000	-0.22991100
C	0.26282600	1.30365500	0.02983700
C	-0.69069800	0.40428800	0.63525300
C	2.27363200	-0.12600400	-0.32569200
O	-0.50871400	-0.48147900	1.46641600
C	-1.77488500	0.53292900	-0.28068700
H	2.23317700	1.95170000	-0.42647100
H	-0.10801400	2.28952000	-0.21997800
H	3.34018900	-0.08601600	-0.51644300
H	-2.03474900	1.51062800	-0.66135200
C	1.65089800	-1.47305800	-0.26318300
H	0.84209700	-1.55537100	-0.99470600
H	2.37813100	-2.25652800	-0.46198500
H	1.17926700	-1.63150400	0.71094400
C	-2.58416800	-0.63584900	-0.69720300
H	-2.70989300	-0.68169100	-1.77978900
H	-2.14357800	-1.55907500	-0.32632700
H	-3.58716200	-0.54779900	-0.26571000

Cyclopropanone ring closing TS (**27**)

CASSCF(10,8)/6-31++G(d,p)

C	1.23814327	-0.71277742	-1.01380157
C	-0.11109564	-1.11806303	-0.79971050
C	-1.09464867	-0.63280125	0.18750083
C	2.07547819	0.00342954	-0.19712104
O	-1.55266216	-1.31349488	1.07897217
C	-1.66922800	0.63629467	-0.25921101
H	1.66909813	-1.06189175	-1.93800801
H	-0.50332586	-1.88506754	-1.44543739
H	3.06521634	0.19012871	-0.58073061
C	1.82011672	0.51755003	1.19226033
H	0.90249539	0.14184519	1.62396277
H	2.63548169	0.22000520	1.84529994
H	1.78260633	1.60408089	1.20694994
H	-2.74034410	0.63194036	-0.37191039
C	-0.94314984	1.94107208	-0.39377838
H	0.05156623	1.81700539	-0.80417042
H	-1.49494556	2.61411274	-1.03991800
H	-0.84024744	2.42757206	0.57535291

UωB97xD/cc-pVTZ

C	1.08176800	-0.80086000	-1.01420000
C	-0.29593300	-1.03104900	-0.78989700
C	-1.20556500	-0.45965300	0.19193300
C	1.98499700	-0.27404500	-0.15140800
O	-1.98163400	-1.07721500	0.89812500
C	-1.35801200	0.90826800	-0.24411500
H	1.46576600	-1.14212400	-1.96919100
H	-0.78328300	-1.76386500	-1.42381800
H	3.00632100	-0.19363400	-0.50750000
C	1.76244800	0.14680000	1.25846900
H	0.77984600	-0.13158500	1.63421700
H	2.51950100	-0.30175300	1.90412000
H	1.86922400	1.23023200	1.36386400
H	-2.39614200	1.16370200	-0.43432600
C	-0.35885500	1.99369700	-0.35803100
H	0.58395600	1.65250300	-0.79255900
H	-0.74618500	2.81914400	-0.95186000
H	-0.11102700	2.38615500	0.63554300

Oxyallyl (**28**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.27979501	1.27074525	-0.34146768
C	0.05916793	0.92696376	-0.56551599
C	0.67962581	-0.42241900	-0.47815163
C	-2.31724184	0.54209332	0.23246504
O	0.14404002	-1.40834831	-0.96082463
C	1.96490797	-0.55190957	0.19225479
H	-1.53200593	2.28128208	-0.62051757
H	0.69539758	1.70718684	-0.94550184
H	-3.26662955	1.04660423	0.28396487
C	-2.25752415	-0.84204571	0.81401390
H	-2.12877502	-1.59290069	0.04191151
H	-1.42831841	-0.95128708	1.50696294
H	-3.17146814	-1.05710845	1.35618868
C	2.84473676	0.55677409	0.68221188
H	2.62896662	1.50603174	0.20790407
H	2.73087531	0.69686767	1.75546648
H	3.88735475	0.31492149	0.50089737
H	2.26901780	-1.56602411	0.38445867

UωB97xD/cc-pVTZ

C	-1.24872900	1.29295700	-0.26508700
C	0.09901300	0.92970300	-0.24738800
C	0.67168600	-0.41720500	-0.29741400
C	-2.37312400	0.57014400	0.04512400
O	0.03135200	-1.41270500	-0.64761700
C	2.06750600	-0.55752400	0.04027900
H	-1.43066600	2.33314700	-0.51696400
H	0.80309100	1.74773900	-0.32384800
H	-3.31342800	1.08992900	-0.10161600
C	-2.46827000	-0.79630600	0.62135600
H	-2.32955500	-1.55172600	-0.15430200
H	-1.68541600	-0.97894700	1.35597600
H	-3.43933300	-0.94376900	1.09195000
C	3.04276500	0.47593500	0.45808100
H	2.61276500	1.46769900	0.56720200
H	3.49472000	0.20038900	1.41526600
H	3.86787300	0.53050200	-0.25919100
H	2.42403900	-1.57955300	-0.02324100

Oxyallyl (**29**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.72632414	-0.83249158	-0.57892225
C	-0.43721136	-1.35433322	-0.32990972
C	0.75829215	-0.65951637	0.20169970
C	-2.29901894	0.36580441	-0.19834453
O	1.38297000	-1.11127275	1.14727821
C	1.22871694	0.47016079	-0.57803352
H	-2.37656225	-1.49778816	-1.12378104
H	-0.28766048	-2.40595829	-0.50150162
H	-3.30321859	0.53489897	-0.55047205
H	0.53258852	0.95567171	-1.23625817
C	-1.75059213	1.44068408	0.70031442
H	-0.88554315	1.11939849	1.26513761
H	-1.47485266	2.32813408	0.13630542
H	-2.51582573	1.74213583	1.40958396
C	2.61598010	1.00943450	-0.44440320
H	3.01328249	1.30233875	-1.41110384
H	2.62129677	1.89410983	0.19072982
H	3.27367934	0.27878521	0.00872875

UωB97xD/cc-pVTZ

C	-1.70969100	-0.83986400	-0.52362400
C	-0.45385000	-1.39433300	-0.25343100
C	0.78910600	-0.71659500	0.14002500
C	-2.22951600	0.37622200	-0.16742200
O	1.58087100	-1.24101400	0.92333400
C	1.09192000	0.50789700	-0.55396300
H	-2.39640600	-1.49959000	-1.04485400
H	-0.35361400	-2.47028900	-0.33067400
H	-3.23019000	0.58596500	-0.52877800
H	0.34983500	0.92145100	-1.22397300
C	-1.65437600	1.41131800	0.73869200
H	-0.78634800	1.05335400	1.28798500
H	-1.35538200	2.30567000	0.18556800
H	-2.41271900	1.73098200	1.45596200
C	2.39355200	1.18446500	-0.39901500
H	2.85978900	1.37027500	-1.36966700
H	2.25795600	2.16555400	0.06928800
H	3.05724100	0.59007500	0.22490500

Oxyallyl (**30**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.67778104	1.16833401	-0.02294443
C	-0.26340760	1.24932357	-0.04897578
C	0.72451884	0.18289129	-0.28029162
C	-2.52613610	0.08953008	0.10451346
O	0.48496834	-0.88908722	-0.80483924
C	2.05030115	0.53112633	0.21400241
H	-2.16736922	2.12813742	-0.07113890
H	0.14891838	2.24008798	0.02602664
H	-3.57567565	0.32953018	0.06520951
H	2.25916882	1.55734929	0.45400601
C	-2.19429651	-1.35710354	0.34554352
H	-1.89082909	-1.85134840	-0.57018936
H	-1.38331812	-1.47430412	1.05302226
H	-3.06548959	-1.86791504	0.74189545
C	3.14052560	-0.48351746	0.31491064
H	3.70521710	-0.52332256	-0.61551593
H	3.83413616	-0.23636549	1.11124624
H	2.73314852	-1.47265718	0.48360275

UωB97xD/cc-pVTZ

C	-1.64657700	1.17665100	-0.08261100
C	-0.24897700	1.22001600	0.01615300
C	0.71714900	0.14214300	-0.15879600
C	-2.51918200	0.12597600	-0.00886600
O	0.44884000	-0.98567900	-0.58048700
C	2.06469400	0.52153100	0.18978600
H	-2.11386900	2.14918500	-0.20257400
H	0.18245400	2.20496100	0.14916000
H	-3.56000200	0.37907600	-0.18032000
H	2.26569300	1.54810700	0.46973800
C	-2.25327900	-1.29538100	0.33661700
H	-1.94389500	-1.85217800	-0.54995400
H	-1.44236400	-1.39706800	1.05272600
H	-3.15390000	-1.75730600	0.74040600
C	3.17727000	-0.44568600	0.15974900
H	3.93666500	-0.13476500	-0.56452600
H	3.68091100	-0.49302900	1.12931200
H	2.81099700	-1.43305600	-0.11227000

Oxyallyl (**31**)

CASSCF(10,8)/6-31++G(d,p)

C	1.36191007	-0.61400203	-0.98734374
C	0.02527388	-1.01155374	-0.90951565
C	-0.98224182	-0.71541069	0.15600811
C	2.12944279	0.16212418	-0.12008925
O	-1.28863239	-1.60330996	0.94394335
C	-1.67740028	0.55484326	0.20145695
H	1.88736390	-0.98113877	-1.85425302
H	-0.32827842	-1.70440026	-1.65358678
H	3.14090999	0.35496781	-0.43478859
C	1.72596151	0.77419592	1.19310389
H	2.57488791	0.78642926	1.86906871
H	1.40454645	1.80605240	1.06706761
H	0.92698220	0.23227690	1.68167851
C	-1.38693765	1.76333063	-0.63170367
H	-0.50209549	1.64024643	-1.24206072
H	-2.22299308	1.98052529	-1.29304217
H	-1.24976313	2.63679561	0.00089595
H	-2.49855221	0.59355975	0.89597387

UωB97xD/cc-pVTZ

C	1.31055300	-0.59543100	-0.99904400
C	0.03295600	-1.12254800	-0.86108900
C	-1.03507800	-0.81280400	0.11993200
C	2.00665400	0.27992600	-0.19586300
O	-1.52189400	-1.73237200	0.78055500
C	-1.59195000	0.50727900	0.21085500
H	1.86726900	-0.97870900	-1.84802500
H	-0.22129500	-1.96638000	-1.49111100
H	3.00428700	0.54063600	-0.52993000
C	1.58786900	0.88111300	1.09923100
H	2.41196300	0.84669600	1.81355800
H	1.33101400	1.93758100	0.97386200
H	0.72866400	0.38159000	1.54210700
C	-1.17365700	1.72656400	-0.51435100
H	-0.34894200	1.54736900	-1.19934600
H	-2.01694700	2.13500900	-1.07834200
H	-0.87841600	2.50869300	0.19251700
H	-2.45266500	0.57132300	0.86729700

5-membered ring closing TS (**32**)

CASSCF(8,7)/6-31++G(d,p)

C	-1.12298819	1.30634970	-0.14041811
C	0.16749485	1.06262253	0.18052847
C	0.67576570	-0.29682744	-0.05418945
C	-2.05405334	0.23594155	-0.51009625
O	-0.18135611	-1.21709353	-0.16649373
C	2.03567249	-0.60742770	-0.24034460
H	-1.46280611	2.32940702	-0.20790324
H	0.83959668	1.86631631	0.41415828
H	-2.56968314	0.37119575	-1.45049404
H	2.22967794	-1.60691182	-0.59001509
C	-2.78507007	-0.58103224	0.51559964
H	-3.07007002	-1.54363582	0.10460448
H	-2.17602085	-0.75145565	1.39307042
H	-3.69759563	-0.07094042	0.82645078
C	3.21109455	0.20257068	0.22052224
H	3.97322228	0.22473404	-0.55311442
H	2.95108711	1.22531861	0.46184454
H	3.66594464	-0.24046210	1.10373654

UωB97xD/cc-pVTZ

C	-1.14113700	1.31872700	-0.19734900
C	0.16385700	1.07862000	0.10170800
C	0.61069100	-0.26903600	-0.19434700
C	-2.06356500	0.26160500	-0.34958600
O	-0.26594200	-1.13417800	-0.49509300
C	1.97382800	-0.58085500	-0.24992600
H	-1.45053800	2.32046700	-0.47995900
H	0.86568900	1.87729800	0.28912200
H	-2.79102800	0.37220900	-1.15215700
H	2.20628400	-1.53257100	-0.71347300
C	-2.48169100	-0.67873800	0.72397600
H	-2.66635000	-1.67201800	0.31806000
H	-1.73910200	-0.74842500	1.51317100
H	-3.42149100	-0.31282500	1.15351500
C	3.09067500	0.16027600	0.39026000
H	3.90248200	0.31889700	-0.32404800
H	2.78919600	1.12515600	0.79237100
H	3.51645100	-0.41835700	1.21571300

5-membered ring closing TS (**33**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.67660949	-0.79250452	-0.55631676
C	-0.55072382	-1.49136454	-0.22790097
C	0.70624735	-0.79107893	0.13990017
C	-1.85825131	0.61821233	-0.34657801
O	1.43173010	-1.16664937	1.04551266
C	1.04932045	0.35071454	-0.70420943
H	-2.48577941	-1.32330229	-1.03385745
H	-0.52369923	-2.56522795	-0.27768902
H	-2.59447253	1.09258666	-0.97670331
H	0.55938159	0.44267398	-1.65353882
C	-1.53542142	1.37248478	0.91892569
H	-0.82626959	0.85453300	1.55018748
H	-1.14356812	2.36100820	0.70231597
H	-2.44860076	1.51074184	1.49631679
C	2.25010389	1.19216866	-0.41361821
H	3.15048529	0.72588211	-0.81078183
H	2.15501419	2.16960212	-0.87446024
H	2.39567392	1.31290337	0.65289428

UωB97xD/cc-pVTZ

C	-1.67636500	-0.73006100	-0.51024400
C	-0.60760300	-1.51286300	-0.18376000
C	0.67098200	-0.84817100	0.09086500
C	-1.71232800	0.65462000	-0.27072400
O	1.48396800	-1.23569800	0.92684300
C	0.90868000	0.31016000	-0.75194700
H	-2.53125000	-1.17369200	-1.01334700
H	-0.66186300	-2.59204500	-0.14130300
H	-2.39433700	1.23031000	-0.89034200
H	0.38122400	0.39382100	-1.68896800
C	-1.26388900	1.36605400	0.96682500
H	-0.62658800	0.75439300	1.60055800
H	-0.73881100	2.29507900	0.73564100
H	-2.14916600	1.64916300	1.54594800
C	2.01093300	1.23910400	-0.43851800
H	2.39513000	1.74926700	-1.31936800
H	1.66063100	2.00426500	0.26724900
H	2.81082500	0.70196500	0.07420500

5-membered ring closing TS (**34**)

CASSCF(8,7)/6-31++G(d,p)

C	1.47687606	1.21051226	0.18437187
C	0.21493216	1.37798306	-0.27268664
C	-0.70375928	0.24269479	-0.13452847
C	1.98383217	-0.10165285	0.58409405
O	-0.19660118	-0.89847478	0.04675262
C	-2.09508787	0.43790978	-0.12659578
H	2.10036317	2.07656077	0.34920576
H	-0.16887329	2.34720493	-0.53681706
H	2.43935973	-0.14681204	1.56358833
H	-2.46770588	1.37539731	-0.50277404
C	2.49390924	-1.10853888	-0.40542359
H	2.40011614	-2.11438859	-0.01045924
H	1.95311846	-1.05604483	-1.34041167
H	3.55020309	-0.93048504	-0.61022711
C	-3.07656330	-0.65316456	0.16933109
H	-3.44988456	-1.10913160	-0.74534206
H	-2.61603303	-1.43353334	0.76221717
H	-3.93268948	-0.25543092	0.70562378

UωB97xD/cc-pVTZ

C	1.50055000	1.19392400	0.20280600
C	0.23561600	1.35994400	-0.27299800
C	-0.64722400	0.23250100	-0.05318800
C	2.00957600	-0.09105700	0.47438500
O	-0.14395000	-0.85525900	0.36118000
C	-2.01553500	0.43205200	-0.23033600
H	2.06506100	2.05769700	0.53968000
H	-0.16168300	2.32001800	-0.57169100
H	2.62186100	-0.18305800	1.37033500
H	-2.33787300	1.34242300	-0.72027200
C	2.24253800	-1.15949400	-0.53157200
H	2.05468000	-2.14240300	-0.10279700
H	1.62654800	-1.02875200	-1.41588700
H	3.29821200	-1.12158300	-0.82588000
C	-3.02040000	-0.59789500	0.11836700
H	-3.31889500	-1.17314400	-0.76461200
H	-2.60024600	-1.30393600	0.83421300
H	-3.92679200	-0.14503400	0.52267800

5-membered ring closing TS (**35**)

CASSCF(10,8)/6-31++G(d,p)

C	-1.11467044	-0.20793564	1.24634748
C	0.08025330	-0.84760117	1.14312784
C	0.93841675	-0.71743706	-0.06768389
C	-1.77461190	0.51037620	0.17630152
O	1.46152865	-1.68880429	-0.58703950
C	1.16007955	0.62702945	-0.62168217
H	-1.60970551	-0.21190606	2.20558454
H	0.45507944	-1.45568328	1.94720583
H	-2.45263581	1.28980509	0.48660994
C	-2.00908969	-0.02114790	-1.21417414
H	-3.01426629	-0.43612631	-1.28000341
H	-1.94141734	0.76974187	-1.95412893
H	-1.31585465	-0.80477069	-1.48828778
C	1.41241469	1.85656517	0.20200394
H	0.89682681	1.83039208	1.15260593
H	2.47827044	1.96179056	0.40200700
H	1.09923918	2.74504916	-0.33629124
H	1.55548091	0.62304769	-1.62442931

UωB97xD/cc-pVTZ

C	-1.02176100	-0.16573500	1.26862700
C	0.17079500	-0.81283900	1.20381500
C	0.96406200	-0.65702000	-0.02825100
C	-1.66563200	0.38003400	0.13430500
O	1.61338900	-1.55843400	-0.54238900
C	0.92213500	0.67752200	-0.63015400
H	-1.50117900	-0.02198100	2.23376300
H	0.56364200	-1.40586800	2.01791900
H	-2.34848900	1.20381700	0.32235900
C	-1.86421800	-0.29718400	-1.18550500
H	-2.88061900	-0.70474500	-1.22211700
H	-1.77966100	0.40489500	-2.01543500
H	-1.17083100	-1.11812900	-1.34969400
C	1.08941400	1.96149000	0.10169600
H	0.73714600	1.90073400	1.12893200
H	2.15312000	2.22582800	0.12919500
H	0.57792300	2.77988100	-0.40654600
H	1.17306500	0.68542300	-1.68646300

5-membered ring (**36**)

CASSCF(8,7)/6-31++G(d,p)

C	-1.10243677	1.31079541	-0.12906910
C	0.22511712	1.24217292	0.04537973
C	0.65297191	-0.15270163	-0.11085856
C	-1.64484252	-0.06207670	-0.41603546
O	-0.45775276	-0.90595524	-0.36432965
C	1.87046079	-0.71461771	-0.04112776
H	-1.71593155	2.19040423	-0.08137224
H	0.88575909	2.05648846	0.26441829
H	-2.04014730	-0.12976476	-1.42582170
H	1.92882973	-1.77893430	-0.19426384
C	-2.67380529	-0.57250418	0.57725864
H	-2.94077650	-1.59791917	0.34739559
H	-2.28044415	-0.53560711	1.58742426
H	-3.57430293	0.03411422	0.53161644
C	3.15580329	0.01658497	0.23507404
H	3.63395311	-0.36516586	1.13334831
H	3.85900256	-0.11340645	-0.58332150
H	3.00646877	1.08151417	0.37148450

UωB97xD/cc-pVTZ

C	-1.08630000	1.30280500	-0.14078600
C	0.22652900	1.23040300	0.03497700
C	0.64753900	-0.15881200	-0.12453700
C	-1.62882200	-0.06703800	-0.41399800
O	-0.47030300	-0.90268300	-0.39642200
C	1.85495100	-0.71353500	-0.04452400
H	-1.70466100	2.18563700	-0.09006600
H	0.89583000	2.04421900	0.26000700
H	-2.06907000	-0.12636800	-1.41591400
H	1.92032000	-1.78273000	-0.20349100
C	-2.63941700	-0.56035700	0.60851100
H	-2.90334800	-1.59658400	0.40299300
H	-2.21834600	-0.49738600	1.61165900
H	-3.54664900	0.04365000	0.56854400
C	3.12280000	0.02055900	0.25313600
H	3.59855400	-0.36877800	1.15625700
H	3.84602900	-0.09131200	-0.55798200
H	2.96008200	1.08696300	0.40269900

5-membered ring (**37**)

CASSCF(10,8)/6-31++G(d,p)

C	0.61688237	-1.60802361	0.17608192
C	-0.69230850	-1.61418705	-0.12171977
C	-1.23731484	-0.24110483	-0.02130243
C	1.16417792	-0.22860547	0.48101872
O	-2.34776235	0.11183720	-0.33482992
C	-0.15428370	0.65421113	0.57370672
H	1.25304375	-2.47586182	0.16110630
H	-1.28796380	-2.45856781	-0.41312402
H	1.66265225	-0.23171092	1.44712743
H	-0.40066812	0.74228346	1.63041474
C	2.18465161	0.20821887	-0.57546349
H	1.74799884	0.22924899	-1.56901787
H	2.58345492	1.19329077	-0.35851766
H	3.01893443	-0.48721158	-0.59670036
C	-0.12083696	2.05542376	-0.02807162
H	0.62732921	2.67128735	0.46106462
H	0.09766851	2.03667664	-1.09018652
H	-1.08615865	2.53027050	0.10097235

UωB97xD/cc-pVTZ

C	-0.58707200	-1.60236900	0.15840600
C	0.70945000	-1.59810600	-0.13505800
C	1.24143800	-0.22491900	-0.01526800
C	-1.14054800	-0.24096000	0.48779900
O	2.34627500	0.15492200	-0.31003100
C	0.12569200	0.64425400	0.56980400
H	-1.22678500	-2.47569300	0.13215900
H	1.31312800	-2.43803900	-0.44323900
H	-1.64378600	-0.27784500	1.45711700
C	-2.17450700	0.18507000	-0.55694900
H	-2.99663000	-0.53053000	-0.59072900
H	-2.59061400	1.16439000	-0.32380600
H	-1.73048600	0.23087600	-1.55177800
C	0.07514500	2.03313000	-0.04571900
H	-0.16876000	1.99339800	-1.10690600
H	-0.66412400	2.66050800	0.45203200
H	1.05075800	2.50656800	0.05063800
H	0.38951700	0.75038900	1.62667400

5-membered ring (**38**)

CASSCF(8,7)/6-31++G(d,p)

C	-1.49041658	1.16232489	-0.11810095
C	-0.24299246	1.57469399	0.14722184
C	0.67266513	0.43931229	0.00825587
C	-1.47202215	-0.30462902	-0.45311964
O	-0.06046717	-0.65795539	-0.33097055
C	2.00479254	0.40868598	0.17266490
H	-2.38632421	1.75340226	-0.10563491
H	0.07365913	2.56242636	0.42001065
H	-1.75310997	-0.48071560	-1.48749961
H	2.48027861	1.33610159	0.44301008
C	-2.29585159	-1.18944562	0.46538896
H	-2.15457728	-2.23333000	0.20829232
H	-2.00196731	-1.04452276	1.49938723
H	-3.35191704	-0.95281709	0.36716581
C	2.87022038	-0.80949456	0.01015744
H	3.61952795	-0.65377111	-0.76200089
H	3.39948465	-1.03641284	0.93232206
H	2.28031120	-1.67540539	-0.26209880

UωB97xD/cc-pVTZ

C	-1.47183900	1.15755500	-0.12407300
C	-0.23963400	1.56757700	0.14567800
C	0.67312000	0.43821600	0.01208200
C	-1.44718100	-0.30607900	-0.44988000
O	-0.06671200	-0.66137800	-0.32594900
C	1.99464000	0.40683000	0.17140800
H	-2.37652000	1.74541900	-0.11583900
H	0.07842000	2.56053300	0.42066100
H	-1.74139600	-0.48192900	-1.49102100
H	2.47110200	1.34083800	0.43838700
C	-2.29286600	-1.17500100	0.46438800
H	-2.13317100	-2.22765100	0.23562600
H	-2.02858000	-0.99814200	1.50666900
H	-3.35079200	-0.94860300	0.32690800
C	2.84746400	-0.80902500	0.01018100
H	3.60834100	-0.65897200	-0.75925900
H	3.37458400	-1.04708500	0.93697300
H	2.24948500	-1.67381800	-0.27020800

5-membered ring (**39**)

CASSCF(10,8)/6-31++G(d,p)

C	-0.74624574	-1.42505352	0.45373080
C	0.54946588	-1.64233761	0.17581217
C	1.20690360	-0.36826675	-0.19395000
C	-1.15780101	0.02629589	0.32425308
O	2.38157484	-0.21006171	-0.42066696
C	0.14062487	0.72243098	-0.24810870
H	-1.44329749	-2.18525778	0.76119101
H	1.07500575	-2.57755474	0.22043870
H	-1.36383270	0.42128140	1.31790855
C	-2.40196560	0.22902620	-0.54064455
H	-3.26322012	-0.27190913	-0.10755621
H	-2.64391961	1.28404134	-0.62946091
H	-2.25181690	-0.16764382	-1.54081094
C	0.55556255	2.00113434	0.47452663
H	0.73748334	1.81290481	1.52888980
H	1.46532415	2.40333660	0.04453389
H	-0.22130493	2.75607524	0.39723918
H	-0.02228745	0.94584264	-1.30075395

UωB97xD/cc-pVTZ

C	-0.72576700	-1.42984400	0.42796300
C	0.55717100	-1.64283800	0.15044200
C	1.21202500	-0.36136400	-0.18669500
C	-1.13573500	0.01482500	0.32073400
O	2.38595400	-0.17323300	-0.38203400
C	0.11783000	0.70638200	-0.24153300
H	-1.43412900	-2.19544100	0.71906600
H	1.08529600	-2.58361000	0.18303300
H	-1.32822900	0.38863700	1.33213900
C	-2.39790900	0.22239600	-0.51027000
H	-3.25746200	-0.27311700	-0.05738200
H	-2.62941300	1.28424500	-0.59772300
H	-2.26642900	-0.17944100	-1.51634900
C	0.52255700	2.00070300	0.44534200
H	0.69322100	1.83541100	1.51025300
H	1.44484900	2.38623800	0.01398600
H	-0.25423200	2.75872300	0.34007800
H	-0.04214000	0.90266300	-1.30673200

Cyclopropanone to cyclopentenone rearrangement (**40**)

RωB97xD/cc-pVTZ

C	-1.59560900	0.72842500	-0.69084000
C	-0.48338100	1.44874400	-0.26787500
C	0.67791200	0.72549400	0.19755200
C	-1.84540200	-0.56255300	-0.29183400
O	1.42856800	1.07263300	1.11693600
C	0.95207600	-0.36716200	-0.69181400
H	-2.27547200	1.17464700	-1.41026400
H	-0.46075900	2.53121500	-0.27355300
H	0.33042200	-0.53823000	-1.55254500
C	2.19524600	-1.13606300	-0.51723600
H	2.95053100	-0.50087300	-0.04897400
H	2.01485600	-1.94627600	0.20215200
H	2.56194900	-1.57994600	-1.44033800
C	-1.50479100	-1.23078700	1.00263100
H	-1.06595200	-2.21644700	0.84315800
H	-0.83266600	-0.64751000	1.62497000
H	-2.43798200	-1.39391400	1.55082200
H	-2.58977400	-1.10031800	-0.87442000

Cyclopropanone to cyclopentenone rearrangement (**41**)

RωB97xD/cc-pVTZ

C	-1.00484800	0.33211400	1.20911500
C	0.10170900	-0.49069500	1.31678500
C	0.85523100	-0.75561200	0.10680700
C	-1.64947400	0.52429500	0.00555400
O	1.22374500	-1.88623900	-0.24567600
C	1.23786400	0.42926600	-0.59963500
H	-1.36014000	0.88689300	2.07301000
H	0.41806800	-0.93843500	2.24947900
H	1.91598300	0.17784100	-1.41409100
C	1.22798400	1.88172900	-0.27290500
H	2.25845900	2.20447400	-0.08698000
H	0.88475800	2.46659100	-1.12983300
H	0.62755000	2.14286300	0.59204800
C	-1.84099200	-0.44767500	-1.11076700
H	-1.74654300	0.04124500	-2.08046700
H	-1.16827700	-1.29927700	-1.07176200
H	-2.87082300	-0.81716500	-1.05064600
H	-2.31384200	1.38434500	-0.04507400

Rotation **12** to **13**

CASSCF(10,8)/6-31++G(d,p)

C	-1.40282933	0.73086290	-0.11449224
C	-0.30392875	-0.10230212	0.16252726
C	1.07099703	0.41412043	0.21277321
C	-2.72897891	0.35005011	-0.18148974
O	1.32674534	1.58282753	-0.02390092
C	2.18020024	-0.52854721	0.56873127
H	-1.17725289	1.76821467	-0.29020891
H	-0.43599008	-1.15062729	0.35315819
H	-3.44739387	1.12077670	-0.40543319
C	-3.29227775	-1.02727998	0.02406286
H	-2.53271894	-1.76789313	0.23886035
H	-4.00066189	-1.02878214	0.84862236
H	-3.83269143	-1.35246444	-0.86126212
H	2.53515546	-0.46497596	1.58459114
C	3.15308777	-0.94424020	-0.49754066
H	2.63766056	-1.29808581	-1.38588748
H	3.78131486	-0.10683606	-0.79640833
H	3.80099360	-1.73793035	-0.14225653

Rotation **14** to **15**

CASSCF(10,8)/6-31++G(d,p)

C	1.07161309	-0.63361882	-0.21816405
C	0.36360209	0.56047411	-0.02262426
C	-1.09081545	0.68684522	-0.15363195
C	2.44189504	-0.81034357	-0.10399064
O	-1.62260610	1.76621828	0.05466342
C	-1.94238611	-0.48421812	-0.53790244
H	0.49607402	-1.50427322	-0.48456685
H	0.86664137	1.47126196	0.24397192
H	2.82315699	-1.80090932	-0.28675559
C	3.46447119	0.23180078	0.24756940
H	3.03163703	1.20911440	0.41582119
H	4.00296960	-0.05334816	1.14777750
H	4.19934480	0.32559460	-0.54786476
H	-2.28115714	-0.49508732	-1.56089463
C	-2.81364253	-1.12252513	0.50598402
H	-2.24868253	-1.35259434	1.40473824
H	-3.62638002	-0.45713791	0.79219597
H	-3.25117922	-2.04285375	0.13482914

Rotation **12** to **30**

CASSCF(8,7)/6-31++G(d,p)

C	-1.62050341	-1.02059545	-0.13810055
C	-0.30254446	-0.66635239	-0.70708999
C	0.84520884	-0.30875941	0.12143318
C	-2.61774552	-0.16282570	0.13220912
O	0.82989422	-0.29350230	1.33915390
C	2.01425834	0.06257117	-0.66484964
H	-1.76363006	-2.06751458	0.08383564
H	-0.15194967	-0.75896040	-1.76802277
H	-3.52239610	-0.56983282	0.55460317
H	1.98955165	-0.08089376	-1.72905854
C	-2.59774432	1.32645085	-0.07370036
H	-2.70856974	1.84037589	0.87688174
H	-3.42321124	1.63703038	-0.70861695
H	-1.67470871	1.66446604	-0.52993569
C	3.25909285	0.55126557	-0.00637077
H	3.81072011	-0.28451435	0.42120611
H	3.90754615	1.06021652	-0.70979867
H	3.01735998	1.21711758	0.81448879

Rotation **14** to **29**

CASSCF(10,8)/6-31++G(d,p)

C	1.48404803	-0.80953280	0.70623894
C	0.33462958	-1.23882712	-0.12401350
C	-1.01728716	-0.66727236	-0.11557405
C	2.37230083	0.15914870	0.41890739
O	-1.97484647	-1.30834553	-0.51282249
C	-1.14269724	0.70798734	0.35568558
H	1.63973493	-1.38233769	1.60924622
H	0.41174598	-2.18815509	-0.62837390
H	3.17089833	0.31876439	1.12607445
C	2.39330404	1.04023412	-0.80012892
H	1.61322110	0.78494185	-1.50613316
H	2.27074953	2.08408773	-0.52280159
H	3.35043273	0.95483534	-1.30700783
H	-0.35388375	1.12236047	0.95369747
C	-2.42629224	1.45252201	0.20246644
H	-2.92297378	1.17596459	-0.72018621
H	-3.10830250	1.20661931	1.01530492
H	-2.26088595	2.52412408	0.22126819

Rotation **12** to **14**

CASSCF(10,8)/6-31++G(d,p)

C	1.30190300	0.05427393	0.74720355
C	0.42690122	0.10143038	-0.32839136
C	-1.03934693	0.36278163	-0.16358271
C	2.68652835	-0.12629913	0.66526411
O	-1.45245887	1.51530522	-0.11098900
C	-1.94662995	-0.76562966	-0.08775614
H	0.88261535	0.16736516	1.73461166
H	0.78864858	0.01281595	-1.33833785
H	3.24154089	-0.15067564	1.58588021
H	-1.52517755	-1.75378677	-0.13934896
C	3.44919138	-0.28837535	-0.62145545
H	4.51249951	-0.37263589	-0.43013520
H	3.14056504	-1.18113263	-1.16068234
H	3.29952315	0.56031187	-1.28410469
C	-3.42719446	-0.61347340	0.05983475
H	-3.94589063	-1.08088188	-0.77383313
H	-3.77454408	-1.10211813	0.96701456
H	-3.70822490	0.43004570	0.10014729

Rotation **29** to **30**

CASSCF(10,8)/6-31++G(d,p)

C	-1.83220952	-0.87659864	-0.38836891
C	-0.53965805	-1.35948431	-0.21607837
C	0.66637578	-0.60184646	0.25240218
C	-2.33882625	0.41574198	-0.20771137
O	0.92023147	-0.53590987	1.44866405
C	1.55007109	-0.01769182	-0.73855080
H	-2.55280735	-1.61209449	-0.70778542
H	-0.37120274	-2.41036705	-0.38094072
H	-3.38507816	0.54710805	-0.42046380
H	1.26482908	-0.09313361	-1.77287644
C	-1.58167839	1.63147695	0.25709735
H	-1.07870527	1.45725964	1.20238471
H	-0.82877898	1.93981628	-0.46394569
H	-2.26100208	2.46534793	0.39161187
C	2.81408367	0.69782452	-0.38193153
H	3.66169630	0.26373565	-0.90612029
H	2.75912809	1.74417953	-0.67446783
H	3.00111930	0.64889376	0.68213984

UωB97xD/cc-pVTZ

C	-1.85603100	-0.79344200	-0.39977400
C	-0.60527700	-1.35400500	-0.26305600
C	0.63152800	-0.66432600	0.22204700
C	-2.25165600	0.51334700	-0.16272900
O	0.91725300	-0.66661100	1.41800100
C	1.47722700	-0.03092200	-0.75055500
H	-2.63651000	-1.46888800	-0.73298100
H	-0.48555200	-2.41040900	-0.47232100
H	-3.29489000	0.74159300	-0.33845700
H	1.18481300	-0.08256100	-1.79240100
C	-1.38066200	1.62705900	0.31532500
H	-0.88677200	1.37754000	1.25675200
H	-0.58693700	1.85254200	-0.40378800
H	-1.95654100	2.53799100	0.46445100
C	2.69841200	0.71003400	-0.37261600
H	3.55812400	0.37166400	-0.95595600
H	2.57957600	1.77675900	-0.58928000
H	2.90541700	0.59019200	0.68811800

Rotation **13** to **15**

CASSCF(10,8)/6-31++G(d,p)

C	-1.07666684	-0.18779723	0.75123291
C	-0.19233255	-0.29723974	-0.31307049
C	1.23853530	-0.70527423	-0.13448881
C	-2.43866311	0.11189095	0.65239198
O	1.52537104	-1.89908388	-0.12434371
C	2.28810453	0.28138728	0.00494674
H	-0.68370161	-0.34909929	1.74281995
H	-0.53129881	-0.16585469	-1.32626007
H	-3.00358480	0.17119892	1.56537679
H	3.28063536	-0.12087427	0.10821847
C	-3.16615478	0.35243109	-0.64253835
H	-4.22051110	0.52791250	-0.46418587
H	-2.77333550	1.21959331	-1.16860849
H	-3.08220983	-0.49999424	-1.31189773
C	2.11018548	1.76728422	-0.00617837
H	2.53852128	2.20979575	0.88966626
H	2.62664618	2.20893376	-0.85572434
H	1.06782229	2.05496529	-0.05842886

UωB97xD/cc-pVTZ

C	-1.05674300	-0.19841800	0.74995100
C	-0.18740500	-0.31357800	-0.30981200
C	1.24884600	-0.69722400	-0.13486600
C	-2.40609100	0.09260600	0.65113800
O	1.56759500	-1.88672200	-0.12327000
C	2.24499500	0.32024000	0.00876000
H	-0.65242600	-0.35029200	1.74565400
H	-0.53728100	-0.18817300	-1.32804900
H	-2.97783400	0.16045700	1.56705700
H	3.25777800	-0.04552600	0.13191400
C	-3.11530700	0.32427600	-0.64067900
H	-4.17984900	0.48583100	-0.48684900
H	-2.71670900	1.20003600	-1.16175700
H	-2.99817100	-0.52496100	-1.31940200
C	2.00322000	1.77961300	-0.01066100
H	2.39240200	2.24700700	0.89826300
H	2.53722300	2.24674200	-0.84417700
H	0.94503000	2.01756100	-0.09947800

Rotation **28** to **31**

CASSCF(10,8)/6-31++G(d,p)

C	1.37775796	0.13913404	1.16477256
C	0.08765240	0.65960055	1.12845705
C	-0.81744713	0.79515926	-0.05919269
C	2.14391453	-0.43188127	0.14337245
O	-0.78994061	1.82948627	-0.71849721
C	-1.77440288	-0.23950891	-0.39161242
H	1.85873336	0.18595301	2.12853253
H	-0.30410929	1.08726857	2.03594562
H	3.11972251	-0.78538330	0.42658457
C	1.75180193	-0.60792064	-1.29988758
H	2.60873517	-0.92637661	-1.88235497
H	0.98053196	-1.36504859	-1.41990529
H	1.37953440	0.31281703	-1.73491677
C	-1.92722360	-1.55465100	0.30608906
H	-1.12140263	-1.74349512	1.00410590
H	-2.86471900	-1.59165786	0.85757162
H	-1.95217177	-2.36750879	-0.41474457
H	-2.43764909	-0.00205062	-1.20483150

UωB97xD/cc-pVTZ

C	1.36181100	-0.04275400	1.16492300
C	0.09770500	0.50345800	1.20883200
C	-0.78876100	0.80141700	0.03834000
C	2.08041200	-0.47546600	0.06236500
O	-0.73645000	1.90263200	-0.50929900
C	-1.71482400	-0.19234500	-0.41528500
H	1.86021600	-0.14720500	2.12256100
H	-0.30179100	0.80205100	2.17087700
H	3.06191700	-0.88874200	0.25530900
C	1.63906800	-0.40943400	-1.36175800
H	2.40417300	-0.80353300	-2.02718400
H	0.72354600	-0.98401100	-1.53119600
H	1.41912200	0.61692000	-1.66393400
C	-1.87342300	-1.54690300	0.15837200
H	-1.28909700	-1.67751300	1.06715200
H	-2.92413300	-1.75683800	0.37339500
H	-1.55273300	-2.30735300	-0.56195900
H	-2.32154900	0.09733100	-1.26535900

Z epoxide (**6**) solvent optimized

ωB97xD/cc-pVTZ

C	-1.43104500	-0.70879100	0.15222700
C	-0.39445500	0.22344600	-0.26846500
C	0.88818700	-0.09825600	-0.28832300
C	-2.73810600	-0.45340400	0.24709100
O	1.66420800	-1.16231200	0.01181900
C	2.29065300	0.09975900	-0.47050900
H	-1.08869800	-1.70592600	0.40996800
H	-0.64634500	1.22729500	-0.58147100
H	-3.38132700	-1.26306200	0.57634700
C	-3.43124400	0.83792700	-0.04162200
H	-3.93569500	1.20872800	0.85448900
H	-2.75633800	1.61690500	-0.39230700
H	-4.20705500	0.69814000	-0.79862400
C	3.13901800	0.83739100	0.51249400
H	4.11141400	0.35500800	0.61525100
H	3.30269300	1.85295400	0.14856100
H	2.65659400	0.89106700	1.48746600
H	2.69305200	-0.01102800	-1.47159400

E epoxide (**7**) solvent optimized

ωB97xD/cc-pVTZ

C	-1.25184800	0.64226100	-0.28203200
C	-0.42791700	-0.52351700	0.00495600
C	0.88489500	-0.48929200	-0.14791100
C	-2.57795600	0.73270500	-0.15828400
O	1.94286100	-1.30979000	0.00963500
C	2.15536400	0.09308200	-0.44638000
H	-0.71344800	1.51880600	-0.62886600
H	-0.87587800	-1.44540700	0.35371700
H	-3.03706000	1.68284300	-0.41111600
C	-3.52061800	-0.33251100	0.29945600
H	-4.29168900	-0.51186200	-0.45407900
H	-3.02780500	-1.28122300	0.50588300
H	-4.04161200	-0.01913300	1.20797000
C	2.87447200	0.99442200	0.50253900
H	3.94887800	0.81409800	0.46033900
H	2.69379000	2.03215900	0.21792800
H	2.52272700	0.84962000	1.52320000
H	2.46086600	0.13551800	-1.48612200

Z-syn epoxide ring opening TS (**8**) solvent optimized

UωB97xD/cc-pVTZ

C	1.42122100	0.73087600	0.13396200
C	0.33798200	-0.17040600	-0.17583800
C	-0.95947900	0.23487100	-0.22688700
C	2.72400000	0.42719600	0.21771600
O	-1.51776700	1.39653200	-0.19402200
C	-2.10588300	-0.61395900	-0.40252200
H	1.13406900	1.76014600	0.32544200
H	0.52359800	-1.22035700	-0.36236400
H	3.40848000	1.22725600	0.48025300
H	-2.21462700	-1.17787000	-1.32784700
C	3.35303900	-0.90833300	-0.00507700
H	4.12546800	-0.84748200	-0.77612300
H	3.85177000	-1.25440400	0.90450900
H	2.63773500	-1.67193900	-0.30609400
C	-3.22564000	-0.66695700	0.52534700
H	-4.15062100	-0.35622300	0.02965700
H	-3.38082400	-1.73145400	0.74834200
H	-3.06435900	-0.09965600	1.43619900

Z-anti epoxide ring opening TS (**9**) solvent optimized

RωB97xD/cc-pVTZ

C	1.39827700	-0.77612700	0.06413100
C	0.22706000	0.03361500	-0.16716900
C	-1.03077200	-0.48239700	-0.14298200
C	2.67069400	-0.35904900	0.10808700
O	-1.50349700	-1.63598700	0.19210900
C	-2.24576700	0.21447400	-0.43972900
H	1.21162000	-1.83480700	0.21466700
H	0.31640100	1.09157100	-0.37686700
H	3.43518200	-1.11010200	0.27924500
H	-2.89534300	-0.27971600	-1.15278600
C	3.16905800	1.03959900	-0.04409100
H	3.68832400	1.36178800	0.86264400
H	3.90015300	1.09855200	-0.85459100
H	2.37676900	1.75759100	-0.25000400
C	-2.74433300	1.35631500	0.30717200
H	-1.93374100	2.00322500	0.64525500
H	-3.52185300	1.89524100	-0.23116300
H	-3.21483300	0.94596400	1.21421300

UωB97xD/cc-pVTZ

C	1.39849400	-0.77494500	0.06700100
C	0.22895000	0.03525900	-0.16899200
C	-1.02967900	-0.47951900	-0.14587900
C	2.67158000	-0.35927700	0.11119200
O	-1.50360300	-1.63243700	0.19008000
C	-2.24692900	0.21372200	-0.44098000
H	1.21043100	-1.83283800	0.22122900
H	0.31968000	1.09259500	-0.38112800
H	3.43481300	-1.11062200	0.28653900
H	-2.89444400	-0.28012000	-1.15602300
C	3.17195000	1.03807800	-0.04596800
H	3.69130500	1.36290100	0.85976700
H	3.90344500	1.09299000	-0.85639500
H	2.38074400	1.75638900	-0.25488600
C	-2.74950800	1.35157500	0.31036500
H	-1.94091200	2.00267700	0.64536800
H	-3.53135500	1.88751400	-0.22463900
H	-3.21403100	0.93865100	1.21909400

E-syn epoxide ring opening TS (**10**) solution

UωB97xD/cc-pVTZ

C	1.16031000	-0.63596100	-0.20400900
C	0.38893600	0.56368300	-0.01158200
C	-0.97061100	0.58503900	-0.11985900
C	2.49212500	-0.76455300	-0.10167600
O	-1.81073500	1.56083700	-0.11384500
C	-1.84781300	-0.52573600	-0.37638900
H	0.59960400	-1.53312100	-0.45546900
H	0.88051500	1.50416700	0.20671900
H	2.91593000	-1.74409100	-0.29597300
H	-1.75808000	-1.06363500	-1.31865100
C	3.47318800	0.29725600	0.27182100
H	3.01226500	1.27191500	0.42317000
H	4.00034200	0.02831400	1.19141500
H	4.23807200	0.40286800	-0.50203600
C	-2.96798000	-0.89297000	0.48009700
H	-3.91480600	-0.82356300	-0.06344400
H	-2.84558400	-1.96444000	0.69019000
H	-3.01130000	-0.32565300	1.40442400

E-anti epoxide ring opening TS (**11**) solvent optimized

RωB97xD/cc-pVTZ

C	0.99633500	0.59872300	-0.16568300
C	0.27431800	-0.63895900	-0.02082500
C	-1.08674100	-0.75994200	-0.07269300
C	2.32680500	0.75459100	-0.09698100
O	-1.83247000	-1.78383500	0.15753500
C	-2.02348500	0.27942000	-0.39041200
H	0.41119800	1.49105800	-0.36128300
H	0.82345200	-1.55955100	0.14261500
H	2.71571500	1.75956000	-0.22347000
H	-2.75915300	-0.00233800	-1.13592500
C	3.35543000	-0.30253400	0.13157400
H	2.93418400	-1.30287500	0.21394100
H	4.08699200	-0.30670700	-0.68050000
H	3.91463100	-0.09789400	1.04890900
C	-2.24229700	1.52631200	0.32402900
H	-1.45936400	1.77820400	1.03217300
H	-2.40868200	2.32841700	-0.40340200
H	-3.20140600	1.43713800	0.85260400

UωB97xD/cc-pVTZ

C	1.01444900	0.58192500	-0.20635000
C	0.29528300	-0.64803800	-0.01502900
C	-1.06582200	-0.74338000	-0.09533300
C	2.34366100	0.75331500	-0.12170200
O	-1.85524700	-1.73163100	0.15020700
C	-2.02618700	0.27412500	-0.40913500
H	0.42194200	1.45830800	-0.45113300
H	0.83163400	-1.56085700	0.21617400
H	2.72761600	1.75466600	-0.28559500
H	-2.73042400	0.00594900	-1.18781200
C	3.37300400	-0.28758300	0.16939600
H	2.95307600	-1.28501700	0.28737600
H	4.11666400	-0.32416400	-0.63082000
H	3.91804700	-0.04189800	1.08516800
C	-2.29455000	1.48106500	0.36439500
H	-1.50712400	1.72951100	1.07000800
H	-2.48900600	2.30756200	-0.32690900
H	-3.23948300	1.34041600	0.90443800

Oxyallyl (**12**) solvent optimized

UωB97xD/cc-pVTZ

C	1.41421600	0.74931700	-0.00264000
C	0.34588500	-0.15554700	-0.01171400
C	-1.03035300	0.28030800	-0.00622200
C	2.73637600	0.41705000	0.00352100
O	-1.37381100	1.48446900	-0.00003800
C	-1.96999600	-0.79668500	-0.00475200
H	1.15797400	1.80248100	0.00445900
H	0.53178400	-1.22077600	-0.01948300
H	3.45137900	1.23255000	0.01789000
H	-1.58634300	-1.80881200	-0.01485400
C	3.32350800	-0.94501900	0.00309400
H	4.04057500	-1.04001300	-0.81610100
H	3.89273000	-1.09842900	0.92458700
H	2.58654700	-1.74003500	-0.08212600
C	-3.42674800	-0.59831100	0.00968800
H	-3.88330200	-1.07715600	-0.86259200
H	-3.86757300	-1.08926200	0.88330900
H	-3.69060900	0.45702000	0.01935600

Oxyallyl (**13**) solvent optimized

UωB97xD/cc-pVTZ

C	1.30525200	-0.81414500	-0.00789600
C	0.13868600	-0.04532600	-0.01613100
C	-1.17169200	-0.65809200	-0.00316400
C	2.58178400	-0.32730300	-0.00009700
O	-1.33039600	-1.90110600	0.00342000
C	-2.31329100	0.20726600	0.01159400
H	1.17727800	-1.89027900	-0.00369200
H	0.20854800	1.03135700	-0.02712000
H	3.38546200	-1.05547900	0.00784400
C	3.00600300	1.09405200	0.00816000
H	3.59036400	1.29894300	0.90990400
H	3.67288100	1.28987900	-0.83563500
H	2.18041900	1.80097200	-0.03176300
C	-2.37968600	1.68111600	-0.00482700
H	-1.41766100	2.17928100	-0.08410700
H	-3.01176700	2.00879800	-0.83617900
H	-2.88068100	2.03523700	0.90246900
H	-3.26401000	-0.31527000	0.04508000

Oxyallyl (**14**) solvent optimized

UωB97xD/cc-pVTZ

C	1.18433600	-0.74477400	0.02374500
C	0.40913200	0.41689800	-0.01144300
C	-1.03590700	0.52544900	0.00440500
C	2.55259900	-0.77442200	0.01894300
O	-1.57553200	1.65392500	0.02709900
C	-1.80957100	-0.68012800	-0.01812500
H	0.68753600	-1.70560000	0.07164800
H	0.91103200	1.37711400	-0.03919900
H	3.02019300	-1.75140100	0.06868000
C	3.48601000	0.37829900	-0.02706800
H	2.99595400	1.33764500	-0.17570500
H	4.05856000	0.42702600	0.90414400
H	4.21765100	0.23547000	-0.82598000
H	-1.30749200	-1.63553700	-0.06444500
C	-3.28127400	-0.68486100	-0.00908700
H	-3.69485500	0.31197200	0.12372600
H	-3.66220500	-1.10246200	-0.94801300
H	-3.65407400	-1.34439000	0.78013500

Oxyallyl (**15**) solvent optimized

UωB97xD/cc-pVTZ

C	-0.91776300	0.56155200	-0.29825300
C	-0.20440100	-0.57973300	0.05860300
C	1.23171600	-0.79408300	-0.02962800
C	-2.28357000	0.69030400	-0.23720600
O	1.66264500	-1.96747700	-0.08632000
C	2.17720500	0.28870800	-0.01264300
H	-0.37673100	1.41326200	-0.68729500
H	-0.74995800	-1.47210100	0.34184200
H	-2.70316300	1.63070600	-0.57629900
H	3.20126400	-0.04018900	-0.15053600
C	-3.26197400	-0.31188400	0.25309100
H	-3.77236000	0.07269100	1.14103000
H	-4.03867000	-0.47662200	-0.49797800
H	-2.81625400	-1.27108600	0.50646300
C	1.95945200	1.73126500	0.22910000
H	2.85342400	2.17036000	0.67193800
H	1.78778800	2.26202900	-0.71562500
H	1.10951200	1.93399100	0.87862900

Cyclopropanone ring closing TS (**16**) solvent optimized

UωB97xD/cc-pVTZ

C	1.26744300	0.71159300	0.31922400
C	0.26210500	-0.00410100	-0.39746000
C	-1.08891000	0.44078000	-0.44372600
C	2.55364300	0.33203000	0.43218000
O	-1.52170300	1.59557400	-0.23449000
C	-1.76942500	-0.78305100	-0.27208900
H	0.95609400	1.63497000	0.79270500
H	0.51821800	-0.92014800	-0.90830400
H	3.20914200	0.98591500	0.99840800
H	-1.40069200	-1.66454500	-0.77654600
C	3.20570500	-0.87615100	-0.13214900
H	4.00361600	-0.57628100	-0.81659600
H	3.68807600	-1.43887100	0.67093500
H	2.52645700	-1.53882200	-0.66309400
C	-2.98899500	-0.89888200	0.55281000
H	-3.04206000	-1.85791100	1.06667800
H	-3.07235500	-0.08115400	1.26808500
H	-3.86226300	-0.84105100	-0.10909600

Cyclopropanone ring closing TS (**17**) solvent optimized

UωB97xD/cc-pVTZ

C	1.08196600	-0.41826800	0.73353100
C	-0.04709900	-0.01468000	-0.12801400
C	-1.29655000	-0.78990200	-0.15727600
C	2.37396800	-0.20802500	0.49627400
O	-1.83187000	-1.80564800	-0.50335300
C	-1.40045100	0.48789400	0.52240000
H	0.80496200	-0.93585400	1.64674700
H	0.18772100	0.48293200	-1.06307900
H	3.07697100	-0.57159800	1.23911800
C	2.98754100	0.47703100	-0.68063000
H	3.62816400	1.29809400	-0.35019300
H	3.62853200	-0.21288100	-1.23530700
H	2.25181400	0.88076700	-1.37449300
H	-1.41501500	0.41894700	1.60658300
C	-2.12728900	1.66427700	-0.07816300
H	-2.05992700	1.65122300	-1.16651900
H	-3.18307600	1.64387600	0.19401800
H	-1.69770200	2.59971600	0.28123100

Cyclopropanone ring closing TS (**18**) solvent optimized

UωB97xD/cc-pVTZ

C	1.18856200	-0.43603800	-0.66542800
C	0.27150000	0.43965700	-0.00897300
C	-1.11925700	0.62446500	-0.28724400
C	2.49801400	-0.53180000	-0.36974000
O	-1.75720300	1.69030000	-0.18521100
C	-1.60272800	-0.69318900	-0.14691500
H	0.81460500	-1.02192400	-1.49651300
H	0.65659800	1.10915700	0.75442900
H	3.09175600	-1.19168600	-0.99353100
H	-1.03860300	-1.51470200	-0.56186100
C	3.25103900	0.16540500	0.70551100
H	3.75556600	-0.57110600	1.33579400
H	4.03867400	0.78360800	0.26725300
H	2.63254000	0.79478100	1.34129500
C	-2.86673000	-1.00394500	0.55471600
H	-2.73539900	-1.81623600	1.27130900
H	-3.27977500	-0.12852900	1.05267600
H	-3.60074200	-1.35309600	-0.18072900

Cyclopropanone ring closing TS (**19**) solvent optimized

UωB97xD/cc-pVTZ

C	-0.91525900	0.34953400	-0.63351400
C	-0.05146000	-0.63180600	-0.06769900
C	1.37406700	-0.73871700	-0.13585300
C	-2.23842900	0.43294100	-0.38665300
O	2.01769800	-1.79817800	-0.20157500
C	1.80707500	0.47142500	0.47132100
H	-0.50121200	1.04265400	-1.35182800
H	-0.50351900	-1.45491700	0.47771300
H	-2.79228400	1.18295300	-0.94142900
H	2.48598800	0.30337700	1.30405500
C	-3.04782200	-0.39155800	0.54778300
H	-3.64343000	0.25873800	1.19236900
H	-3.76037500	-1.00025000	-0.01584600
H	-2.45395600	-1.04976400	1.17806200
C	1.51681300	1.88904800	0.13434500
H	2.36918500	2.49841500	0.43574300
H	1.33958400	2.04761700	-0.92675200
H	0.64852900	2.27140400	0.68213500

Cyclopropanone (**20**) solvent optimized

ωB97xD/cc-pVTZ

C	1.08196600	-0.41826800	0.73353100
C	-0.04709900	-0.01468000	-0.12801400
C	-1.29655000	-0.78990200	-0.15727600
C	2.37396800	-0.20802500	0.49627400
O	-1.83187000	-1.80564800	-0.50335300
C	-1.40045100	0.48789400	0.52240000
H	0.80496200	-0.93585400	1.64674700
H	0.18772100	0.48293200	-1.06307900
H	3.07697100	-0.57159800	1.23911800
C	2.98754100	0.47703100	-0.68063000
H	3.62816400	1.29809400	-0.35019300
H	3.62853200	-0.21288100	-1.23530700
H	2.25181400	0.88076700	-1.37449300
H	-1.41501500	0.41894700	1.60658300
C	-2.12728900	1.66427700	-0.07816300
H	-2.05992700	1.65122300	-1.16651900
H	-3.18307600	1.64387600	0.19401800
H	-1.69770200	2.59971600	0.28123100

Cyclopropanone (**21**) solvent optimized

ωB97xD/cc-pVTZ

C	0.87359400	0.09844600	0.69620800
C	-0.01479600	-0.25550200	-0.42874300
C	-1.33549100	-0.83998800	-0.16881000
C	2.20168100	0.17628500	0.65433500
O	-1.93056500	-1.73796000	0.36107000
C	-1.39205800	0.51084400	-0.69210300
H	0.37989400	0.30750200	1.63898600
H	0.45452900	-0.54576900	-1.36024700
H	2.70827100	0.44980800	1.57470900
C	3.09677700	-0.07246100	-0.51494900
H	3.69565700	0.81602000	-0.72952300
H	3.80198500	-0.87591100	-0.28892600
H	2.55743200	-0.34242700	-1.42135900
H	-1.57805100	0.61090700	-1.75504800
C	-1.86411800	1.65449500	0.16983000
H	-1.70842700	1.45404600	1.22961800
H	-1.33080600	2.57073400	-0.08619200
H	-2.92950700	1.82605400	0.01480600

Cyclopropanone (**22**) solvent optimized

ωB97xD/cc-pVTZ

C	0.92690500	-1.25876100	-0.04230600
C	-0.23611900	-0.48729500	0.47533000
C	-0.65286600	0.81181700	-0.05967100
C	2.17056300	-0.81413000	-0.18717900
O	-0.44685300	1.99181500	-0.11913600
C	-1.50962700	-0.30595800	-0.43211300
H	0.70867300	-2.28869600	-0.30751100
H	-0.47824500	-0.63792800	1.52549800
H	2.90367700	-1.51566800	-0.57401600
C	2.69343900	0.54498700	0.14294100
H	1.93402500	1.20090100	0.56448100
H	3.51460600	0.46619600	0.85961900
H	3.10329200	1.02517800	-0.74882200
H	-1.36295700	-0.66131700	-1.44844100
C	-2.89308200	-0.48107200	0.14035800
H	-2.95705500	-0.06514900	1.14658100
H	-3.63461700	0.02379900	-0.47943600
H	-3.15185800	-1.53936700	0.19097900

Cyclopropanone (**23**) solvent optimized

ωB97xD/cc-pVTZ

C	0.70624500	-1.18352600	0.28474600
C	-0.22335600	-0.20998700	0.92280300
C	-0.71752200	0.97054100	0.21171000
C	1.90707900	-0.91185800	-0.21411200
O	-0.44218500	2.01154600	-0.31778300
C	-1.71490400	-0.07040100	0.41413200
H	0.34621100	-2.20682500	0.24519900
H	-0.14680700	-0.11143900	2.00168000
H	2.46612400	-1.73912600	-0.64072400
C	2.59300600	0.41416600	-0.24323900
H	2.03001300	1.19145900	0.27044900
H	3.57842100	0.33625100	0.22200100
H	2.75937400	0.73790000	-1.27357500
H	-2.42400000	0.08793400	1.21873400
C	-2.21950300	-0.87011200	-0.76127400
H	-1.45590900	-0.96601900	-1.53409200
H	-2.51502000	-1.87230600	-0.44889300
H	-3.08719100	-0.38313300	-1.20711600

Cyclopropanone ring closing TS (**24**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.22256600	1.28046500	-0.34500200
C	0.14399100	0.87654800	-0.45027400
C	0.64522900	-0.45954300	-0.52172500
C	-2.25805500	0.58220300	0.16377200
O	0.07845800	-1.46781800	-0.98019800
C	1.73341200	-0.45517100	0.39794900
H	-1.41692200	2.30420000	-0.64716500
H	0.87116700	1.67487800	-0.49943400
H	-3.22434800	1.07385800	0.15045600
H	1.74580400	-1.30233300	1.08018100
C	-2.20184200	-0.75744900	0.80341400
H	-1.30494200	-0.87317200	1.41539200
H	-3.07863400	-0.92725400	1.42599300
H	-2.15874400	-1.54410900	0.04454800
C	2.87999000	0.47630900	0.49675800
H	3.79622600	-0.10965300	0.36933000
H	2.87479700	1.25946400	-0.25692400
H	2.94697400	0.92650300	1.48986000

Cyclopropanone ring closing TS (**25**) solvent optimized

UωB97xD/cc-pVTZ

C	1.49030200	-0.64821300	-0.91750000
C	0.23625800	-1.17786300	-0.48264300
C	-0.77711400	-0.57368800	0.33191500
C	2.24400300	0.28103800	-0.29487900
O	-1.49080500	-1.15926000	1.16966400
C	-1.09193300	0.60400600	-0.38446100
H	1.90720700	-1.10734700	-1.80668600
H	0.00884800	-2.19603200	-0.78751900
H	3.18885600	0.52219200	-0.77096400
C	1.99469200	0.98323900	0.99200600
H	1.16271700	0.56693000	1.55629200
H	2.89684300	0.94811600	1.60629300
H	1.78484100	2.04085900	0.81363800
H	-0.30049600	1.14161500	-0.88304100
C	-2.47186100	1.11853900	-0.49929900
H	-3.20342500	0.40834500	-0.11782000
H	-2.55439700	2.03910300	0.09091800
H	-2.71064400	1.38794700	-1.52926800

Cyclopropanone ring closing TS (**26**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.68611900	-1.05082800	-0.17498400
C	-0.28647300	-1.28894300	-0.04087400
C	0.68139400	-0.42298300	0.56132700
C	-2.30775300	0.14328300	-0.26296900
O	0.49585500	0.43244500	1.45173000
C	1.79472500	-0.51501700	-0.30930500
H	-2.29488400	-1.94029300	-0.29793400
H	0.07960700	-2.24028700	-0.40587900
H	-3.38724500	0.11875700	-0.36429200
H	2.00060400	-1.46086900	-0.79140500
C	-1.66661000	1.48169800	-0.31853400
H	-0.74762300	1.46454000	-0.90803100
H	-2.34627900	2.21897500	-0.74232200
H	-1.37861300	1.81144500	0.68420200
C	2.68499000	0.62647500	-0.59106200
H	2.87968500	0.72436600	-1.66022700
H	2.28672300	1.55843300	-0.19375800
H	3.65626500	0.44326200	-0.11578600

Cyclopropanone ring closing TS (**27**) solvent optimized

UωB97xD/cc-pVTZ

C	1.04151600	-0.86509600	-0.98045100
C	-0.34134600	-1.04573800	-0.71856400
C	-1.23427800	-0.39947800	0.20032900
C	1.97557900	-0.35637200	-0.14441500
O	-2.12329500	-0.97904100	0.84715200
C	-1.28829300	0.95890500	-0.22107200
H	1.39240700	-1.25735300	-1.92825200
H	-0.83772500	-1.82551300	-1.28992700
H	2.99557000	-0.34247600	-0.51405000
C	1.80004600	0.12917400	1.24510900
H	0.80958000	-0.06904400	1.65143600
H	2.54884000	-0.33223000	1.89234300
H	1.97621200	1.20790100	1.29501200
H	-2.31299800	1.29456200	-0.36404000
C	-0.23871500	1.97712300	-0.41334400
H	0.66797500	1.58180100	-0.87845300
H	-0.61594300	2.80822400	-1.00597000
H	0.07537900	2.37535100	0.55912400

Oxyallyl (**28**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.24325100	1.26881300	-0.30000800
C	0.11135800	0.90195400	-0.20826400
C	0.69002700	-0.42363700	-0.28746800
C	-2.37604400	0.56761600	-0.00456600
O	0.04823000	-1.43736200	-0.64369900
C	2.08419900	-0.54141100	0.02526300
H	-1.40575600	2.29904000	-0.60254200
H	0.81221800	1.72525800	-0.20713700
H	-3.31094000	1.07701200	-0.21472600
C	-2.51712000	-0.75327400	0.65537500
H	-2.84920400	-1.50480300	-0.06717200
H	-1.59689300	-1.10517500	1.10947400
H	-3.29700700	-0.69176400	1.41813500
C	3.04882700	0.48760800	0.45855900
H	2.63270100	1.48490400	0.56816900
H	3.48764700	0.19356900	1.41746200
H	3.88439200	0.52780500	-0.24788900
H	2.46902900	-1.55296700	-0.05753000

Oxyallyl (**29**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.67005800	-0.85745000	-0.54196800
C	-0.40814600	-1.39827600	-0.23445200
C	0.81717200	-0.71597600	0.13761300
C	-2.22388900	0.33389600	-0.17171300
O	1.66379700	-1.26574500	0.87449500
C	1.05480300	0.53158100	-0.51652800
H	-2.32643700	-1.52430100	-1.09236500
H	-0.31828100	-2.47906900	-0.27039700
H	-3.22250100	0.52321500	-0.55093000
H	0.27727400	0.93680300	-1.14883900
C	-1.70452600	1.37104100	0.75859300
H	-0.82679000	1.04973600	1.31665100
H	-1.44309800	2.28473400	0.21785600
H	-2.49139400	1.64734300	1.46400000
C	2.32098900	1.27123100	-0.40139400
H	2.69896000	1.55633300	-1.38625200
H	2.14605900	2.21091100	0.13683100
H	3.07777100	0.70396900	0.13658000

Oxyallyl (**30**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.63598100	1.16521100	-0.11637200
C	-0.23350900	1.19275400	0.04001200
C	0.72433000	0.13640500	-0.19033600
C	-2.51188600	0.12778300	-0.03187100
O	0.45887300	-0.97186800	-0.70567900
C	2.04490300	0.49602200	0.22582500
H	-2.08457000	2.14024600	-0.28159600
H	0.19555600	2.16375000	0.25474700
H	-3.54749000	0.36756900	-0.25047500
H	2.21619500	1.50199500	0.58648300
C	-2.27403600	-1.26530800	0.41880600
H	-2.33871700	-1.95613100	-0.42720900
H	-1.30849700	-1.40111400	0.89397500
H	-3.06451100	-1.55471700	1.11531600
C	3.18143500	-0.43595900	0.18917100
H	3.95196300	-0.05711200	-0.49138500
H	3.65704900	-0.50204200	1.17198000
H	2.88050800	-1.42894600	-0.13781600

Oxyallyl (**31**) solvent optimized

UωB97xD/cc-pVTZ

C	1.13819200	-1.07886800	-0.76468900
C	-0.24470400	-1.20833700	-0.62806000
C	-1.22048100	-0.43207400	0.14099500
C	2.03322500	-0.33195600	-0.04037700
O	-2.07575000	-1.04387700	0.81543200
C	-1.31626500	0.98601400	-0.00549000
H	1.57879300	-1.73413300	-1.50915800
H	-0.69360800	-2.07534800	-1.10073100
H	3.07231100	-0.42053400	-0.33775300
C	1.78376600	0.53683300	1.13521600
H	2.54243500	0.34969100	1.89806300
H	1.87904900	1.59286200	0.86358900
H	0.79884200	0.39492500	1.57795800
C	-0.45068900	1.90898400	-0.76074300
H	0.32566400	1.41125200	-1.33521900
H	-1.06441000	2.51454700	-1.43374900
H	0.02315600	2.62037400	-0.07498500
H	-2.19449700	1.41379800	0.46741000

5-membered ring closing TS (**32**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.13216600	1.30669900	-0.21311300
C	0.17254000	1.05488300	0.08555000
C	0.62357300	-0.29072300	-0.19254500
C	-2.07715900	0.27397900	-0.34441800
O	-0.26378200	-1.16491400	-0.51073400
C	1.97943200	-0.58835900	-0.21676400
H	-1.42592600	2.30754200	-0.51638400
H	0.87564500	1.85304000	0.27278100
H	-2.80945600	0.38881000	-1.14187400
H	2.23848900	-1.55099200	-0.64626000
C	-2.49845800	-0.64739000	0.73503800
H	-2.76794700	-1.62583000	0.33827600
H	-1.74907300	-0.75114700	1.51500300
H	-3.40862800	-0.22535900	1.17953900
C	3.08993400	0.18945900	0.38655900
H	3.89358700	0.32888800	-0.34170800
H	2.78600000	1.16448200	0.76131800
H	3.53138000	-0.36140200	1.22334600

5-membered ring closing TS (**33**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.63903900	-0.77611200	-0.51975600
C	-0.53876000	-1.52266000	-0.17442900
C	0.70785900	-0.82867400	0.08065500
C	-1.75065000	0.58792400	-0.25444800
O	1.57197600	-1.23511600	0.88763900
C	0.88115500	0.35093200	-0.72357300
H	-2.45473000	-1.24820600	-1.06036200
H	-0.57196900	-2.60291600	-0.10393800
H	-2.46242200	1.13482800	-0.86674400
H	0.31118800	0.44818600	-1.63365000
C	-1.32274500	1.32317500	0.97188500
H	-0.67977100	0.73731600	1.62442900
H	-0.82069900	2.26214100	0.72943000
H	-2.22555500	1.59612500	1.52877900
C	1.94385200	1.32800800	-0.43483400
H	2.23892400	1.89462300	-1.31588200
H	1.58398300	2.04386600	0.31791800
H	2.81521800	0.83940000	0.00590600

5-membered ring closing TS (**34**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.49961400	1.19057200	-0.18735800
C	-0.22014000	1.33728000	0.25739900
C	0.66233700	0.21452800	0.02209900
C	-2.05226100	-0.07192900	-0.44856500
O	0.14864400	-0.87532000	-0.42474500
C	2.01083000	0.42597900	0.23040300
H	-2.05451500	2.06607400	-0.51137000
H	0.18469300	2.29191300	0.56548100
H	-2.69828300	-0.14294700	-1.32242300
H	2.30732400	1.34858400	0.71352900
C	-2.26173000	-1.14465300	0.54623200
H	-2.16930800	-2.12999800	0.09049100
H	-1.60108300	-1.05961300	1.40421400
H	-3.29963100	-1.05236900	0.89198700
C	3.05250300	-0.57967400	-0.08258900
H	3.32445200	-1.15939600	0.80696000
H	2.69824000	-1.29068500	-0.83052000
H	3.96741000	-0.10161900	-0.43611000

5-membered ring closing TS (**35**) solvent optimized

UωB97xD/cc-pVTZ

C	-0.99320900	-0.29737500	1.25176400
C	0.23943000	-0.87926500	1.14473600
C	1.02364000	-0.57786900	-0.04363100
C	-1.68589600	0.23730800	0.15542300
O	1.80195800	-1.38678900	-0.57832100
C	0.85266100	0.75795600	-0.59181000
H	-1.45909900	-0.20413000	2.22957300
H	0.65317200	-1.51816100	1.91432100
H	-2.42509200	0.99980200	0.38422600
C	-1.83693800	-0.36823900	-1.20182800
H	-2.83749200	-0.81094100	-1.26638500
H	-1.78526200	0.38526200	-1.98877800
H	-1.10973700	-1.14967000	-1.41042600
C	0.86174100	2.03127900	0.17415800
H	0.58429300	1.90325300	1.21793900
H	1.87575100	2.44831200	0.14395500
H	0.21096100	2.77656400	-0.28621400
H	1.10826200	0.84125200	-1.64452300

5-membered ring (**36**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.08920900	1.29823600	-0.14220200
C	0.22484200	1.23116400	0.03318800
C	0.65050900	-0.15682000	-0.12378900
C	-1.63516700	-0.06713300	-0.41326500
O	-0.46750600	-0.90745900	-0.39677800
C	1.85948400	-0.71265300	-0.04472400
H	-1.71177300	2.17897400	-0.09414300
H	0.89396100	2.04690800	0.25580600
H	-2.07380400	-0.12835700	-1.41408000
H	1.92995900	-1.78306500	-0.20360700
C	-2.64145800	-0.55799600	0.60990100
H	-2.91343000	-1.59335400	0.40452100
H	-2.22526000	-0.49330700	1.61622800
H	-3.54649600	0.04914600	0.56569000
C	3.12612300	0.02349200	0.25397600
H	3.60695100	-0.37330900	1.15200300
H	3.84902700	-0.08219000	-0.55928800
H	2.96017600	1.08848700	0.41258100

5-membered ring (**37**) solvent optimized

UωB97xD/cc-pVTZ

C	-0.57260400	-1.60058700	0.14104000
C	0.72726700	-1.58358200	-0.15158200
C	1.23974200	-0.21702800	-0.01004300
C	-1.13284800	-0.25241000	0.49061700
O	2.36066300	0.16933700	-0.28326600
C	0.12409600	0.64646000	0.56132000
H	-1.20447400	-2.47953900	0.10747900
H	1.33690500	-2.41817100	-0.46610100
H	-1.61756800	-0.30811500	1.46765700
C	-2.19171400	0.16761100	-0.53004400
H	-3.00307100	-0.56111500	-0.54926000
H	-2.61803500	1.13773700	-0.27579400
H	-1.77154200	0.22945400	-1.53498200
C	0.05265100	2.02736300	-0.07082600
H	-0.16955500	1.97321900	-1.13680100
H	-0.71363600	2.63665700	0.40804700
H	1.00841700	2.53853900	0.04633100
H	0.38771300	0.76967600	1.61666500

5-membered ring (**38**) solvent optimized

UωB97xD/cc-pVTZ

C	-1.47251100	1.15421000	-0.12589100
C	-0.24079200	1.56761000	0.14511700
C	0.67412900	0.43861100	0.01363200
C	-1.45354600	-0.30700200	-0.44937000
O	-0.06490400	-0.66516400	-0.32283900
C	1.99803800	0.40622500	0.16985900
H	-2.37964300	1.73953500	-0.12068800
H	0.07656300	2.56205600	0.41937000
H	-1.74412500	-0.48349700	-1.48993800
H	2.47504400	1.34140800	0.43468400
C	-2.30094400	-1.17025300	0.46402700
H	-2.14906000	-2.22557300	0.23650100
H	-2.04586200	-0.99300600	1.50992800
H	-3.35624100	-0.93778100	0.31743000
C	2.85624400	-0.80672500	0.01024200
H	3.61911800	-0.65473300	-0.75799200
H	3.38767400	-1.04028200	0.93672200
H	2.27205600	-1.68287300	-0.26899800

5-membered ring (**39**) solvent optimized

UωB97xD/cc-pVTZ

C	-0.73184400	-1.41141100	0.45252200
C	0.55283700	-1.63308600	0.17405600
C	1.19657100	-0.36696400	-0.19170600
C	-1.13837800	0.02678900	0.31622800
O	2.37920700	-0.19172600	-0.41792700
C	0.12309900	0.70997400	-0.23970500
H	-1.44006000	-2.17098000	0.75964000
H	1.07757200	-2.57619400	0.22293900
H	-1.34688000	0.41366900	1.31888000
C	-2.38746400	0.21610000	-0.53724500
H	-3.25089100	-0.27505100	-0.08613000
H	-2.61991900	1.27646600	-0.64393400
H	-2.24225000	-0.20162200	-1.53548900
C	0.53582000	1.99066200	0.46901800
H	0.72696900	1.80428300	1.52746900
H	1.44191000	2.40649600	0.02802900
H	-0.25132100	2.74186700	0.39537100
H	-0.03263500	0.92249100	-1.30236100

Cyclopropanone to cyclopentenone rearrangement (**40**)

RωB97xD/cc-pVTZ

C	-1.60035500	0.77526100	-0.61420400
C	-0.47052900	1.48111900	-0.22290700
C	0.72425100	0.76504200	0.12258500
C	-1.84497700	-0.53019300	-0.25449700
O	1.56247000	1.16937000	0.97771400
C	0.90743400	-0.38585900	-0.68654400
H	-2.32148000	1.25832600	-1.26649000
H	-0.47536800	2.56383500	-0.16395300
H	0.26877000	-0.54591100	-1.53819300
C	2.05026900	-1.28706400	-0.47232300
H	2.92220100	-0.72944600	-0.12147000
H	1.80367200	-1.98894200	0.33707500
H	2.30207100	-1.86835900	-1.35684300
C	-1.46390300	-1.25495400	0.99059800
H	-1.03963800	-2.23554500	0.76821600
H	-0.77394500	-0.70497000	1.62453700
H	-2.38597500	-1.44446400	1.54994400
H	-2.61321000	-1.03959400	-0.83078300

Cyclopropanone to cyclopentenone rearrangement (**41**)

RωB97xD/cc-pVTZ

C	-1.00761300	0.01666100	1.24217800
C	0.20903200	-0.63360800	1.25206800
C	0.99970900	-0.60190700	0.04784800
C	-1.69999800	0.26436400	0.07361400
O	1.63806300	-1.61425700	-0.37107000
C	1.06770600	0.65844500	-0.59542900
H	-1.43263100	0.38880100	2.16974800
H	0.58221800	-1.15180400	2.12746600
H	1.67085300	0.61564800	-1.50172200
C	0.84204100	2.05195100	-0.12127100
H	1.81789400	2.54132800	-0.02450500
H	0.29100300	2.63257200	-0.86486300
H	0.32726700	2.12673300	0.83167400
C	-1.79428400	-0.57440600	-1.14945700
H	-1.76703700	0.03781300	-2.05142900
H	-1.04193400	-1.35463300	-1.21279800
H	-2.78462200	-1.04418400	-1.13395000
H	-2.46707100	1.03278400	0.13163600

Rotation **13** to **15**

UωB97xD/cc-pVTZ

C	-1.04452000	-0.17609900	0.74129500
C	-0.18109300	-0.32550700	-0.32150600
C	1.25192500	-0.69300000	-0.13166100
C	-2.39579100	0.11088300	0.64925100
O	1.57545100	-1.89106900	-0.09884900
C	2.24144700	0.32484900	0.00507800
H	-0.62932000	-0.28581800	1.73889000
H	-0.52157600	-0.21476000	-1.34500000
H	-2.94527500	0.23542700	1.57402300
H	3.25657700	-0.02637900	0.15430300
C	-3.13740700	0.29281400	-0.62932700
H	-4.21026500	0.17978200	-0.47921400
H	-2.97106300	1.29205300	-1.04715500
H	-2.82210000	-0.42397000	-1.39034200
C	1.99502100	1.77742700	-0.03272000
H	2.24873300	2.22665300	0.93382600
H	2.65250600	2.25432600	-0.76542100
H	0.96069100	2.02304200	-0.26556900