

Supporting Information

A unifying mechanism for the rearrangement of vinyl allene oxide geometric isomers to cyclopentenones

Adán B. González-Pérez,^[a] Alexander Grechkin,^[b] and Ángel R. de Lera*^[a]

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- [a] Dr. Adán B. González-Pérez, Prof. Dr. A. R. de Lera
Organic Chemistry Department
Universidade de Vigo
Lagoas-Marocosende s/n
36310 Vigo (Spain)
Fax: (+34)
E-mail: qolera@uvigo.es
- [b] Dr. Alexander Grechkin
Kazan Institute of Biochemistry and Biophysics
Russian Academy of Sciences
P.O. Box 30
420111 Kazan (Russia)

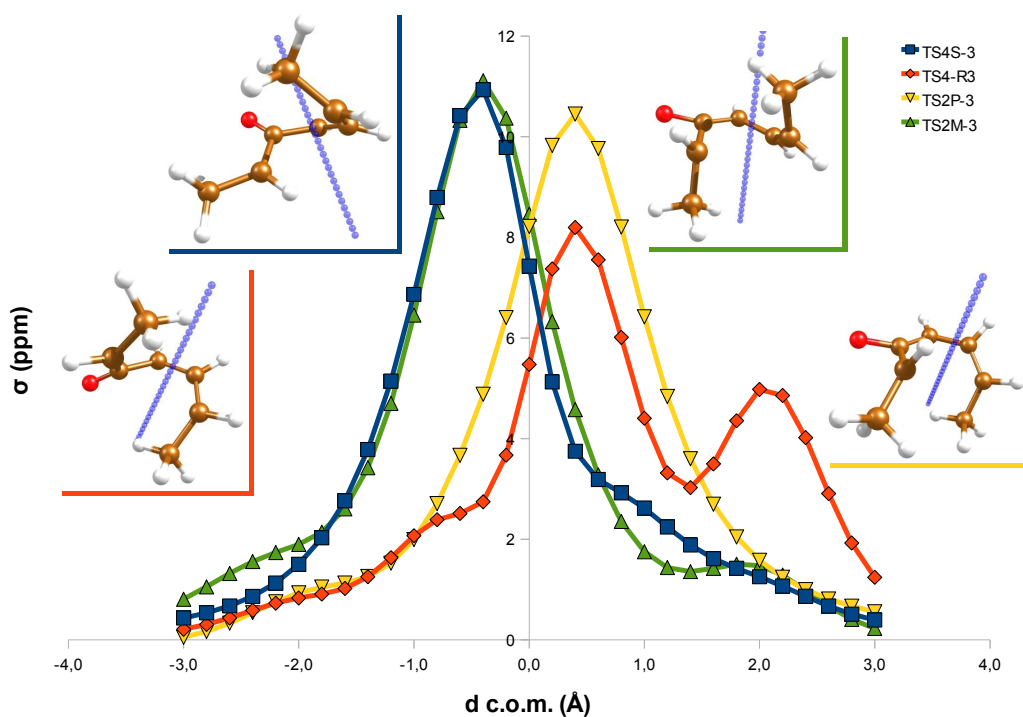


Figure S1. Graphical representation of the shielding constant (σ) calculated along a straight line made of points separated 0.2 \AA each that passes through the center of masses of a ring conformed by four atoms of the reacting system. The maximum shielding corresponds to the center of masses of the reacting ring.

Nucleus independent chemical shifts (NICS)^[1] have been calculated by gauge independent atomic orbital (GIAO) method.^[2]

[1] P. v. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao and N. J. R. v. E. Hommes, *J. Am. Chem. Soc.* **1996**, *118*, 6317-6318.

[2] K. Wolinski, J. F. Hinton and P. Pulay, *J. Am. Chem. Soc.* **1990**, *112*, 8251-8260.

Cartesian coordinates

S,E,Z-1

SCF Energy: -347.814092758

Num. Imaginary Frequencies: 0

C	1.259085	0.642530	-0.283813
C	0.431760	-0.524466	0.007586
C	-0.886852	-0.493527	-0.148176
C	2.591645	0.735326	-0.160349
O	-1.956407	-1.303975	0.007931
C	-2.165915	0.088096	-0.449032
H	0.720139	1.521068	-0.635460
H	0.879358	-1.448083	0.360326
H	3.051259	1.687586	-0.418344
H	-2.474073	0.132809	-1.492975
C	3.537402	-0.333617	0.301613
H	4.061674	-0.019253	1.211538
H	3.037356	-1.280908	0.515061
H	4.304033	-0.524621	-0.457990
C	-2.887794	0.996885	0.504449
H	-2.529549	0.843922	1.524744
H	-2.709801	2.040124	0.225445
H	-3.965132	0.811801	0.470537

TS1-2M

SCF Energy: -347.806390872

Num. Imaginary Frequencies: 1

C	-2.914749	-0.498063	0.812559
C	-2.462508	0.697518	0.029017
C	-1.362340	0.771280	-0.727116
C	-0.404925	-0.345514	-0.947311
C	0.739346	-0.444714	-0.291848
C	1.766800	-0.063483	0.635743
C	2.770446	1.014359	0.341168
O	1.818722	-1.262361	-0.228410
H	-1.160040	1.704924	-1.251153
H	-0.639161	-1.110262	-1.685106
H	-3.099536	1.579457	0.085684
H	1.625171	-0.319495	1.685143
H	-2.190832	-1.314249	0.753702
H	-3.879453	-0.862402	0.440437
H	-3.058066	-0.239285	1.867621
H	2.869966	1.163451	-0.736205
H	2.442120	1.954078	0.796037
H	3.747640	0.754365	0.757854

S,E,Z,M-2

SCF Energy: -347.811521036

Num. Imaginary Frequencies: 0

C	1.771399	1.337665	-0.662521
C	2.283721	0.299715	0.292840
C	1.716754	-0.885045	0.568773
C	0.453106	-1.425807	0.056736
C	-0.620142	-0.700976	-0.239200
O	-1.891055	-0.904209	-0.658997
C	-1.452628	0.465576	-0.315629
H	2.253108	-1.550324	1.242851
H	0.362375	-2.504015	-0.047390
H	3.221622	0.528119	0.794958
H	-1.365340	1.100734	-1.196528
C	-2.079708	1.086777	0.899153
H	1.187635	0.880420	-1.467895
H	1.125464	2.069733	-0.160733
H	2.600423	1.893658	-1.109634
H	-1.459499	1.920834	1.242370
H	-2.155788	0.355388	1.706538
H	-3.076571	1.471688	0.666519

TS2M-3

SCF Energy: -347.764405354

Num. Imaginary Frequencies: 1

C	0.777465	0.728991	0.324580
C	0.867246	-0.718215	0.205956
C	-0.025588	-1.460812	-0.529285
C	-1.105027	-0.676518	-1.049294
C	-1.715313	0.330294	-0.346205
C	-1.959820	0.390803	1.143722
O	1.960819	-0.871743	0.832369
H	0.681254	1.120521	1.335762
C	1.312697	1.631253	-0.720906
H	0.179147	-2.480480	-0.831470
H	-1.392224	-0.814715	-2.093177
H	-2.347748	1.005142	-0.924128
H	-3.030704	0.238247	1.326187
H	-1.708223	1.362484	1.583038
H	-1.411555	-0.385793	1.681414
H	0.908167	2.640702	-0.616957
H	1.126127	1.237567	-1.721670
H	2.399247	1.695495	-0.569367

4R,5S-3

SCF Energy: -347.895145254

Num. Imaginary Frequencies: 0

C	-0.118244	0.710165	-0.241808
C	-1.211943	-0.362308	-0.188192
C	-0.561739	-1.646071	0.159571
C	0.729880	-1.431783	0.436369
C	1.141155	0.017064	0.320233
O	-2.393636	-0.175070	-0.396159
H	1.439441	-2.200276	0.731491
H	-1.095225	-2.587934	0.196209
C	2.402695	0.219805	-0.521374
H	1.340594	0.396486	1.333130
H	0.040382	0.915224	-1.310064
C	-0.524530	2.004047	0.456258
H	-1.446537	2.398027	0.022018
H	-0.700767	1.830491	1.522992
H	2.637058	1.285000	-0.611520
H	3.266559	-0.278686	-0.070177
H	2.264450	-0.184763	-1.529803
H	0.259484	2.761475	0.358653

TS1-2P

SCF Energy: -347.806612387

Num. Imaginary Frequencies: 1

C	-2.544777	0.980683	-0.714335
C	-2.412705	0.121399	0.507139
C	-1.467810	-0.799902	0.721290
C	-0.391902	-1.153644	-0.242946
C	0.846307	-0.707735	-0.113266
C	1.916262	0.057715	0.462143
C	2.053144	1.538512	0.251564
O	2.043204	-0.791504	-0.742560
H	-1.493975	-1.356449	1.657553
H	-0.616350	-1.814542	-1.077613
H	-3.161489	0.271684	1.284029
H	2.445321	-0.363449	1.316115
H	-1.759995	0.767913	-1.444215
H	-2.487249	2.042482	-0.448178
H	-3.517670	0.825704	-1.194485
H	1.506339	1.851094	-0.640835
H	1.642939	2.069273	1.116156

H 3.105377 1.816158 0.142421

S,E,Z,P-2

SCF Energy: -347.811258100

Num. Imaginary Frequencies: 0

C	-1.540423	1.562354	-0.162727
C	-2.320986	0.323377	0.156797
C	-1.874719	-0.940193	0.092574
C	-0.534267	-1.423339	-0.252785
C	0.620245	-0.818804	0.008451
O	1.935125	-1.107602	-0.143139
C	1.551388	0.143726	0.536032
H	-2.591202	-1.731577	0.305129
H	-0.460385	-2.404319	-0.716416
H	-3.357664	0.468228	0.453614
H	1.752834	0.108869	1.606520
C	1.941392	1.410934	-0.169585
H	-0.756835	1.355617	-0.898160
H	-2.195214	2.341452	-0.563584
H	-1.055744	1.976332	0.730814
H	1.392193	2.259454	0.248402
H	1.724263	1.342114	-1.237865
H	3.010980	1.596314	-0.035887

TS2P-3

SCF Energy: -347.762906680

Num. Imaginary Frequencies: 1

C	-1.670372	1.227089	-0.711429
C	-1.907568	0.185970	0.349285
C	-1.447984	-1.096847	0.384599
C	-0.258576	-1.587700	-0.256847
C	0.857723	-0.798493	-0.136832
O	2.102830	-0.909467	-0.392870
C	0.901415	0.415330	0.650828
H	-2.001935	-1.801121	1.008006
H	-0.178641	-2.605048	-0.623286
H	-2.722073	0.423961	1.033555
H	0.750591	0.305506	1.726839
C	1.443294	1.704207	0.175724
H	-0.948116	0.895650	-1.460295
H	-2.621667	1.431163	-1.217707
H	-1.330597	2.184678	-0.301014
H	0.747965	2.495063	0.487564
H	1.575350	1.722035	-0.905732
H	2.398894	1.926515	0.663064

4S,5S-3

SCF Energy: -347.893074988

Num. Imaginary Frequencies: 0

C	0.127283	0.645770	0.573415
C	1.239749	-0.228308	-0.017555
C	0.709464	-1.605345	-0.132639
C	-0.594186	-1.607673	0.167449
C	-1.146110	-0.238053	0.489281
O	2.353166	0.152280	-0.317868
H	-1.235926	-2.484524	0.147267
H	1.316175	-2.448058	-0.440336
H	-1.658483	-0.266728	1.459080
C	-2.173164	0.187332	-0.569379
H	0.393650	0.748403	1.634615
C	0.077734	2.041372	-0.038488
H	1.055110	2.518623	0.065353
H	-0.162092	2.006286	-1.104833
H	-2.584834	1.175340	-0.345793
H	-1.721360	0.220898	-1.565616
H	-3.003894	-0.524595	-0.601429
H	-0.668302	2.665544	0.462128

TS1-4E_in

SCF Energy: -347.763999622

Num. Imaginary Frequencies: 1

C	2.043687	-0.268598	-0.408361
C	1.100063	0.762431	-0.076896
C	-0.279594	0.633114	-0.051878
C	-1.002204	-0.605323	-0.173973
C	-2.340843	-0.761606	-0.089806
C	-3.368760	0.302452	0.140967
O	1.815619	1.787339	0.179754
H	-0.420743	-1.502484	-0.376210
H	-0.826097	1.559926	0.100518
H	-2.732112	-1.770292	-0.209095
H	2.815078	0.056422	-1.103164
C	2.266497	-1.531862	0.321564
H	-2.938835	1.302026	0.226398
H	-3.928399	0.098543	1.061537
H	-4.098412	0.315596	-0.676653
H	2.606203	-2.321759	-0.357606
H	1.394872	-1.853018	0.893355
H	3.090417	-1.367321	1.033187

2S,3S-4

SCF Energy: -347.822120354

Num. Imaginary Frequencies: 0

C	1.408372	0.492569	0.520681
C	1.298677	-0.803904	-0.151462
C	0.048765	-0.005906	-0.122275
C	-1.085966	-0.385953	0.750753
C	-2.385937	-0.188925	0.507009
C	-3.006306	0.454338	-0.697638
O	1.831635	-1.823294	-0.495060
H	-0.810300	-0.881292	1.680896
H	-0.194431	0.488423	-1.061915
H	-3.088443	-0.536301	1.262581
H	1.420753	0.448948	1.610567
C	2.149138	1.659625	-0.095829
H	-2.268175	0.824508	-1.412671
H	-3.638369	1.297853	-0.398707
H	-3.652106	-0.257658	-1.223582
H	1.720875	2.607395	0.243326
H	2.089713	1.628156	-1.188049
H	3.206939	1.635260	0.180610

TS4S-3

SCF Energy: -347.780314505

Num. Imaginary Frequencies: 1

C	1.861254	-0.559364	-0.286341
C	1.607101	0.739380	-0.681213
C	0.484161	1.459018	-0.258832
C	-0.686151	0.731597	0.186398
O	-1.454038	1.088007	1.101991
C	-0.952914	-0.372162	-0.697070
C	-2.190811	-1.155894	-0.513293
H	2.295222	1.196691	-1.391389
H	0.465343	2.545474	-0.249294
C	1.505039	-1.244552	1.001296
H	2.622424	-1.087009	-0.863833
H	-0.326349	-0.547910	-1.559824
H	-2.532276	-1.643408	-1.428463
H	-2.969162	-0.511560	-0.087454
H	0.825003	-0.665864	1.626524
H	1.064156	-2.230781	0.825448
H	2.435376	-1.414763	1.559084
H	-2.013509	-1.933073	0.247609

4R,5R-3

SCF Energy: -347.893074988

Num. Imaginary Frequencies: 0

C	-0.127283	0.645770	0.573416
C	-1.239749	-0.228308	-0.017555
C	-0.709465	-1.605344	-0.132638
C	0.594185	-1.607673	0.167450
C	1.146109	-0.238054	0.489281
O	-2.353165	0.152281	-0.317869
H	1.235925	-2.484525	0.147268
H	-1.316176	-2.448058	-0.440335
H	1.658483	-0.266728	1.459080
C	2.173164	0.187331	-0.569380
H	-0.393650	0.748403	1.634615
C	-0.077733	2.041372	-0.038488
H	0.162091	2.006286	-1.104833
H	-1.055108	2.518625	0.065356
H	3.003893	-0.524596	-0.601430
H	1.721359	0.220896	-1.565616
H	2.584833	1.175340	-0.345795
H	0.668305	2.665542	0.462128

TS1-4E_out

SCF Energy: -347.760857271

Num. Imaginary Frequencies: 1

C	1.828117	-0.566477	-0.332092
C	0.971944	0.566658	-0.112385
C	-0.398624	0.552957	-0.000466
C	-1.181022	-0.642042	-0.192772
C	-2.521113	-0.760617	-0.100813
C	-3.498671	0.312621	0.269310
O	1.817951	1.530308	-0.152671
H	-0.625578	-1.550605	-0.430142
H	-0.884286	1.505627	0.187402
H	-2.951671	-1.740226	-0.298996
H	1.679981	-1.185063	-1.222181
C	3.043842	-0.836678	0.460271
H	-3.024937	1.283537	0.427113
H	-4.033315	0.047230	1.189089
H	-4.255810	0.430247	-0.514648
H	3.040716	-1.902190	0.729242
H	3.096904	-0.209694	1.349550
H	3.947549	-0.679869	-0.141375

2S,3R-4

SCF Energy: -347.822098204

Num. Imaginary Frequencies: 0

C	1.907262	-0.912177	-0.179094
C	0.718456	-1.194619	0.362113
C	-0.243091	-0.214469	0.949840
C	-0.722459	0.978846	0.225180
O	-0.449390	2.046691	-0.254220
C	-1.716482	-0.089882	0.375006
C	-2.152749	-0.898704	-0.828678
H	0.401526	-2.235892	0.408192
H	-0.208077	-0.120542	2.036524
C	2.543678	0.437946	-0.319662
H	2.493451	-1.752515	-0.549890
H	-2.475464	0.053596	1.143048
H	-1.342548	-0.991357	-1.557480
H	-2.458184	-1.906178	-0.530259
H	1.922279	1.241005	0.080137
H	3.511557	0.451755	0.194240
H	2.740967	0.658611	-1.374538
H	-2.998073	-0.413660	-1.324441

TS4R-3

SCF Energy: -347.762342293

Num. Imaginary Frequencies: 1

C	-1.667822	0.488030	0.014482
C	-1.010781	0.296673	1.219208
C	0.119359	-0.508702	1.316665
C	0.881859	-0.735928	0.100917
C	1.224034	0.465692	-0.606130
C	1.174434	1.919249	-0.260864
O	1.290254	-1.861372	-0.259907
H	0.443732	-0.965859	2.246678
H	-1.377235	0.834923	2.093608
H	-2.357460	1.333811	-0.020680
C	-1.842407	-0.477538	-1.117574
H	0.572073	2.148927	0.617415
H	2.199696	2.272287	-0.080898
H	1.900801	0.240323	-1.433871
H	-1.149067	-1.318044	-1.091903
H	-2.866871	-0.871324	-1.057674
H	-1.759786	0.026579	-2.084752
H	0.800035	2.504504	-1.108891

4S,5R-3

SCF Energy: -347.895145254

Num. Imaginary Frequencies: 0

C	-1.141155	0.017064	0.320233
C	-0.729880	-1.431783	0.436369
C	0.561739	-1.646071	0.159571
C	1.211943	-0.362308	-0.188192
C	0.118244	0.710165	-0.241808
C	0.524530	2.004047	0.456258
O	2.393636	-0.175070	-0.396159
H	1.095225	-2.587934	0.196209
H	-1.439441	-2.200276	0.731490
H	-1.340593	0.396486	1.333130
C	-2.402695	0.219805	-0.521374
H	0.700767	1.830491	1.522992
H	1.446537	2.398027	0.022018
H	-0.040382	0.915224	-1.310064
H	-2.264450	-0.184763	-1.529803
H	-3.266558	-0.278687	-0.070177
H	-2.637058	1.285000	-0.611520
H	-0.259484	2.761475	0.358653

S,Z,Z-1

SCF Energy: -347.814427162

Num. Imaginary Frequencies: 0

C	-1.429959	0.700223	0.169406
C	-0.399141	-0.244602	-0.250073
C	0.888280	0.081253	-0.291118
C	-2.747198	0.460847	0.255794
O	1.670727	1.153960	-0.024500
C	2.299044	-0.106173	-0.477765
H	-1.072011	1.692720	0.434863
H	-0.656479	-1.256434	-0.543025
H	-3.381729	1.279984	0.589229
H	2.698384	-0.020915	-1.487859
C	-3.460282	-0.822127	-0.053759
H	-4.223285	-0.664059	-0.824581
H	-2.787943	-1.607728	-0.405803
H	-3.978990	-1.199534	0.835127
C	3.163854	-0.813428	0.526545
H	2.685000	-0.819827	1.508023
H	3.325262	-1.848422	0.209424
H	4.138380	-0.323425	0.606421

TS1-4Z_in

SCF Energy: -347.762602106

Num. Imaginary Frequencies: 1

C	2.103126	-0.654778	-0.368439
C	0.954676	0.189347	-0.216281
C	-0.356091	-0.202847	-0.132574
C	-1.422298	0.729509	0.142288
C	-2.738642	0.449967	0.213211
C	-3.393642	-0.879336	-0.010151
O	1.526198	1.341804	-0.254424
H	-1.106517	1.755921	0.316406
H	-0.558413	-1.259042	-0.285808
H	-3.411926	1.268806	0.459706
H	2.188016	-1.293989	-1.252457
C	3.288523	-0.588436	0.510970
H	-2.688292	-1.653749	-0.319728
H	-4.167546	-0.802977	-0.782517
H	-3.891600	-1.223938	0.904179
H	3.538900	-1.615213	0.812103
H	3.112017	0.039641	1.383203
H	4.161880	-0.210441	-0.033839

TS1-4Z_out

SCF Energy: -347.767894707

Num. Imaginary Frequencies: 1

C	-2.255750	0.199230	-0.441572
C	-1.040025	-0.492552	-0.139124
C	0.229095	0.034622	-0.163893
C	1.397086	-0.779060	0.061806
C	2.677775	-0.360555	0.100550
C	3.177724	1.044569	-0.040839
O	-1.499369	-1.642541	0.200511
H	1.199429	-1.839133	0.206216
H	0.317851	1.099355	-0.359441
H	3.445038	-1.116429	0.257717
H	-2.929134	-0.333697	-1.107553
C	-2.748149	1.374589	0.298896
H	2.376632	1.769244	-0.203050
H	3.877393	1.121715	-0.881332
H	3.728490	1.348564	0.857219
H	-3.527685	1.912056	-0.246650
H	-1.923766	2.038144	0.579638
H	-3.195839	1.015460	1.238205

S,E,Z-1

SCF Energy: -347.814092751

Num. Imaginary Frequencies: 0

C	-3.537388	-0.333607	0.301672
C	-2.591644	0.735313	-0.160368
C	-1.259089	0.642512	-0.283873
C	-0.431754	-0.524472	0.007543
C	0.886858	-0.493528	-0.148207
C	2.165928	0.088104	-0.449023
C	2.887760	0.996896	0.504492
O	1.956410	-1.303971	0.007935
H	-0.720156	1.521038	-0.635572
H	-0.879345	-1.448089	0.360293
H	-3.051266	1.687561	-0.418394
H	2.474128	0.132814	-1.492954
H	-4.061732	-0.019139	1.211520
H	-4.303962	-0.524750	-0.457952
H	-3.037315	-1.280846	0.515288
H	2.709845	2.040131	0.225427
H	2.529399	0.843990	1.524754
H	3.965093	0.811756	0.470695

TS1-2M

SCF Energy: -347.806390872

Num. Imaginary Frequencies: 1

C	-2.914749	-0.498063	0.812559
C	-2.462508	0.697518	0.029017
C	-1.362340	0.771280	-0.727116
C	-0.404925	-0.345514	-0.947311
C	0.739346	-0.444714	-0.291848
C	1.766800	-0.063483	0.635743
C	2.770446	1.014359	0.341168
O	1.818722	-1.262361	-0.228410
H	-1.160040	1.704924	-1.251153
H	-0.639161	-1.110262	-1.685106
H	-3.099536	1.579457	0.085684
H	1.625171	-0.319495	1.685143
H	-2.190832	-1.314249	0.753702
H	-3.879453	-0.862402	0.440437
H	-3.058066	-0.239285	1.867621
H	2.869966	1.163451	-0.736205
H	2.442120	1.954078	0.796037
H	3.747640	0.754365	0.757854

S,E,Z,M-2

SCF Energy: -347.811521036

Num. Imaginary Frequencies: 0

C	1.771399	1.337665	-0.662521
C	2.283721	0.299715	0.292840
C	1.716754	-0.885045	0.568773
C	0.453106	-1.425807	0.056736
C	-0.620142	-0.700976	-0.239200
O	-1.891055	-0.904209	-0.658997
C	-1.452628	0.465576	-0.315629
H	2.253108	-1.550324	1.242851
H	0.362375	-2.504015	-0.047390
H	3.221622	0.528119	0.794958
H	-1.365340	1.100734	-1.196528
C	-2.079708	1.086777	0.899153
H	1.187635	0.880420	-1.467895
H	1.125464	2.069733	-0.160733
H	2.600423	1.893658	-1.109634
H	-1.459499	1.920834	1.242370
H	-2.155788	0.355388	1.706538
H	-3.076571	1.471688	0.666519

TS2M-3

SCF Energy: -347.764405354

Num. Imaginary Frequencies: 1

C	0.777465	0.728991	0.324580
C	0.867246	-0.718215	0.205956
C	-0.025588	-1.460812	-0.529285
C	-1.105027	-0.676518	-1.049294
C	-1.715313	0.330294	-0.346205
C	-1.959820	0.390803	1.143722
O	1.960819	-0.871743	0.832369
H	0.681254	1.120521	1.335762
C	1.312697	1.631253	-0.720906
H	0.179147	-2.480480	-0.831470
H	-1.392224	-0.814715	-2.093177
H	-2.347748	1.005142	-0.924128
H	-3.030704	0.238247	1.326187
H	-1.708223	1.362484	1.583038
H	-1.411555	-0.385793	1.681414
H	0.908167	2.640702	-0.616957
H	1.126127	1.237567	-1.721670
H	2.399247	1.695495	-0.569367

4R,5S-3

SCF Energy: -347.895145254

Num. Imaginary Frequencies: 0

C	-0.118244	0.710165	-0.241808
C	-1.211943	-0.362308	-0.188192
C	-0.561739	-1.646071	0.159571
C	0.729880	-1.431783	0.436369
C	1.141155	0.017064	0.320233
O	-2.393636	-0.175070	-0.396159
H	1.439441	-2.200276	0.731491
H	-1.095225	-2.587934	0.196209
C	2.402695	0.219805	-0.521374
H	1.340594	0.396486	1.333130
H	0.040382	0.915224	-1.310064
C	-0.524530	2.004047	0.456258
H	-1.446537	2.398027	0.022018
H	-0.700767	1.830491	1.522992
H	2.637058	1.285000	-0.611520
H	3.266559	-0.278686	-0.070177
H	2.264450	-0.184763	-1.529803
H	0.259484	2.761475	0.358653

TS1-2P

SCF Energy: -347.806612387

Num. Imaginary Frequencies: 1

C	-2.544777	0.980683	-0.714335
C	-2.412705	0.121399	0.507139
C	-1.467810	-0.799902	0.721290
C	-0.391902	-1.153644	-0.242946
C	0.846307	-0.707735	-0.113266
C	1.916262	0.057715	0.462143
C	2.053144	1.538512	0.251564
O	2.043204	-0.791504	-0.742560
H	-1.493975	-1.356449	1.657553
H	-0.616350	-1.814542	-1.077613
H	-3.161489	0.271684	1.284029
H	2.445321	-0.363449	1.316115
H	-1.759995	0.767913	-1.444215
H	-2.487249	2.042482	-0.448178
H	-3.517670	0.825704	-1.194485
H	1.506339	1.851094	-0.640835
H	1.642939	2.069273	1.116156
H	3.105377	1.816158	0.142421

S,E,Z,P-2

SCF Energy: -347.811258100

Num. Imaginary Frequencies: 0

C	-1.540423	1.562354	-0.162727
C	-2.320986	0.323377	0.156797
C	-1.874719	-0.940193	0.092574
C	-0.534267	-1.423339	-0.252785
C	0.620245	-0.818804	0.008451
O	1.935125	-1.107602	-0.143139
C	1.551388	0.143726	0.536032
H	-2.591202	-1.731577	0.305129
H	-0.460385	-2.404319	-0.716416
H	-3.357664	0.468228	0.453614
H	1.752834	0.108869	1.606520
C	1.941392	1.410934	-0.169585
H	-0.756835	1.355617	-0.898160
H	-2.195214	2.341452	-0.563584
H	-1.055744	1.976332	0.730814
H	1.392193	2.259454	0.248402
H	1.724263	1.342114	-1.237865
H	3.010980	1.596314	-0.035887

TS2P-3

SCF Energy: -347.762906680

Num. Imaginary Frequencies: 1

C	-1.670372	1.227089	-0.711429
C	-1.907568	0.185970	0.349285
C	-1.447984	-1.096847	0.384599
C	-0.258576	-1.587700	-0.256847
C	0.857723	-0.798493	-0.136832
O	2.102830	-0.909467	-0.392870
C	0.901415	0.415330	0.650828
H	-2.001935	-1.801121	1.008006
H	-0.178641	-2.605048	-0.623286
H	-2.722073	0.423961	1.033555
H	0.750591	0.305506	1.726839
C	1.443294	1.704207	0.175724
H	-0.948116	0.895650	-1.460295
H	-2.621667	1.431163	-1.217707
H	-1.330597	2.184678	-0.301014
H	0.747965	2.495063	0.487564
H	1.575350	1.722035	-0.905732
H	2.398894	1.926515	0.663064

4S,5S-3

SCF Energy: -347.893074988

Num. Imaginary Frequencies: 0

C	0.127283	0.645770	0.573415
C	1.239749	-0.228308	-0.017555
C	0.709464	-1.605345	-0.132639
C	-0.594186	-1.607673	0.167449
C	-1.146110	-0.238053	0.489281
O	2.353166	0.152280	-0.317868
H	-1.235926	-2.484524	0.147267
H	1.316175	-2.448058	-0.440336
H	-1.658483	-0.266728	1.459080
C	-2.173164	0.187332	-0.569379
H	0.393650	0.748403	1.634615
C	0.077734	2.041372	-0.038488
H	1.055110	2.518623	0.065353
H	-0.162092	2.006286	-1.104833
H	-2.584834	1.175340	-0.345793
H	-1.721360	0.220898	-1.565616
H	-3.003894	-0.524595	-0.601429
H	-0.668302	2.665544	0.462128

TS1-4E_in

SCF Energy: -347.763999622

Num. Imaginary Frequencies: 1

C	2.043687	-0.268598	-0.408361
C	1.100063	0.762431	-0.076896
C	-0.279594	0.633114	-0.051878
C	-1.002204	-0.605323	-0.173973
C	-2.340843	-0.761606	-0.089806
C	-3.368760	0.302452	0.140967
O	1.815619	1.787339	0.179754
H	-0.420743	-1.502484	-0.376210
H	-0.826097	1.559926	0.100518
H	-2.732112	-1.770292	-0.209095
H	2.815078	0.056422	-1.103164
C	2.266497	-1.531862	0.321564
H	-2.938835	1.302026	0.226398
H	-3.928399	0.098543	1.061537
H	-4.098412	0.315596	-0.676653
H	2.606203	-2.321759	-0.357606
H	1.394872	-1.853018	0.893355
H	3.090417	-1.367321	1.033187

2S,3S-4

SCF Energy: -347.822120354

Num. Imaginary Frequencies: 0

C	1.408372	0.492569	0.520681
C	1.298677	-0.803904	-0.151462
C	0.048765	-0.005906	-0.122275
C	-1.085966	-0.385953	0.750753
C	-2.385937	-0.188925	0.507009
C	-3.006306	0.454338	-0.697638
O	1.831635	-1.823294	-0.495060
H	-0.810300	-0.881292	1.680896
H	-0.194431	0.488423	-1.061915
H	-3.088443	-0.536301	1.262581
H	1.420753	0.448948	1.610567
C	2.149138	1.659625	-0.095829
H	-2.268175	0.824508	-1.412671
H	-3.638369	1.297853	-0.398707
H	-3.652106	-0.257658	-1.223582
H	1.720875	2.607395	0.243326
H	2.089713	1.628156	-1.188049
H	3.206939	1.635260	0.180610

TS4S-3

SCF Energy: -347.780314505

Num. Imaginary Frequencies: 1

C	1.861254	-0.559364	-0.286341
C	1.607101	0.739380	-0.681213
C	0.484161	1.459018	-0.258832
C	-0.686151	0.731597	0.186398
O	-1.454038	1.088007	1.101991
C	-0.952914	-0.372162	-0.697070
C	-2.190811	-1.155894	-0.513293
H	2.295222	1.196691	-1.391389
H	0.465343	2.545474	-0.249294
C	1.505039	-1.244552	1.001296
H	2.622424	-1.087009	-0.863833
H	-0.326349	-0.547910	-1.559824
H	-2.532276	-1.643408	-1.428463
H	-2.969162	-0.511560	-0.087454
H	0.825003	-0.665864	1.626524
H	1.064156	-2.230781	0.825448
H	2.435376	-1.414763	1.559084
H	-2.013509	-1.933073	0.247609

4R,5R-3

SCF Energy: -347.893074988

Num. Imaginary Frequencies: 0

C	-0.127283	0.645770	0.573416
C	-1.239749	-0.228308	-0.017555
C	-0.709465	-1.605344	-0.132638
C	0.594185	-1.607673	0.167450
C	1.146109	-0.238054	0.489281
O	-2.353165	0.152281	-0.317869
H	1.235925	-2.484525	0.147268
H	-1.316176	-2.448058	-0.440335
H	1.658483	-0.266728	1.459080
C	2.173164	0.187331	-0.569380
H	-0.393650	0.748403	1.634615
C	-0.077733	2.041372	-0.038488
H	0.162091	2.006286	-1.104833
H	-1.055108	2.518625	0.065356
H	3.003893	-0.524596	-0.601430
H	1.721359	0.220896	-1.565616
H	2.584833	1.175340	-0.345795
H	0.668305	2.665542	0.462128

TS1-4E_out

SCF Energy: -347.760857271

Num. Imaginary Frequencies: 1

C	1.828117	-0.566477	-0.332092
C	0.971944	0.566658	-0.112385
C	-0.398624	0.552957	-0.000466
C	-1.181022	-0.642042	-0.192772
C	-2.521113	-0.760617	-0.100813
C	-3.498671	0.312621	0.269310
O	1.817951	1.530308	-0.152671
H	-0.625578	-1.550605	-0.430142
H	-0.884286	1.505627	0.187402
H	-2.951671	-1.740226	-0.298996
H	1.679981	-1.185063	-1.222181
C	3.043842	-0.836678	0.460271
H	-3.024937	1.283537	0.427113
H	-4.033315	0.047230	1.189089
H	-4.255810	0.430247	-0.514648
H	3.040716	-1.902190	0.729242
H	3.096904	-0.209694	1.349550
H	3.947549	-0.679869	-0.141375

2S,3R-4

SCF Energy: -347.822098204

Num. Imaginary Frequencies: 0

C	1.907262	-0.912177	-0.179094
C	0.718456	-1.194619	0.362113
C	-0.243091	-0.214469	0.949840
C	-0.722459	0.978846	0.225180
O	-0.449390	2.046691	-0.254220
C	-1.716482	-0.089882	0.375006
C	-2.152749	-0.898704	-0.828678
H	0.401526	-2.235892	0.408192
H	-0.208077	-0.120542	2.036524
C	2.543678	0.437946	-0.319662
H	2.493451	-1.752515	-0.549890
H	-2.475464	0.053596	1.143048
H	-1.342548	-0.991357	-1.557480
H	-2.458184	-1.906178	-0.530259
H	1.922279	1.241005	0.080137
H	3.511557	0.451755	0.194240
H	2.740967	0.658611	-1.374538
H	-2.998073	-0.413660	-1.324441

TS4R-3

SCF Energy: -347.762342293

Num. Imaginary Frequencies: 1

C	-1.667822	0.488030	0.014482
C	-1.010781	0.296673	1.219208
C	0.119359	-0.508702	1.316665
C	0.881859	-0.735928	0.100917
C	1.224034	0.465692	-0.606130
C	1.174434	1.919249	-0.260864
O	1.290254	-1.861372	-0.259907
H	0.443732	-0.965859	2.246678
H	-1.377235	0.834923	2.093608
H	-2.357460	1.333811	-0.020680
C	-1.842407	-0.477538	-1.117574
H	0.572073	2.148927	0.617415
H	2.199696	2.272287	-0.080898
H	1.900801	0.240323	-1.433871
H	-1.149067	-1.318044	-1.091903
H	-2.866871	-0.871324	-1.057674
H	-1.759786	0.026579	-2.084752
H	0.800035	2.504504	-1.108891

4S,5R-3

SCF Energy: -347.895145254

Num. Imaginary Frequencies: 0

C	-1.141155	0.017064	0.320233
C	-0.729880	-1.431783	0.436369
C	0.561739	-1.646071	0.159571
C	1.211943	-0.362308	-0.188192
C	0.118244	0.710165	-0.241808
C	0.524530	2.004047	0.456258
O	2.393636	-0.175070	-0.396159
H	1.095225	-2.587934	0.196209
H	-1.439441	-2.200276	0.731490
H	-1.340593	0.396486	1.333130
C	-2.402695	0.219805	-0.521374
H	0.700767	1.830491	1.522992
H	1.446537	2.398027	0.022018
H	-0.040382	0.915224	-1.310064
H	-2.264450	-0.184763	-1.529803
H	-3.266558	-0.278687	-0.070177
H	-2.637058	1.285000	-0.611520
H	-0.259484	2.761475	0.358653

S,Z,Z-1

SCF Energy: -347.814427162

Num. Imaginary Frequencies: 0

C	-1.429959	0.700223	0.169406
C	-0.399141	-0.244602	-0.250073
C	0.888280	0.081253	-0.291118
C	-2.747198	0.460847	0.255794
O	1.670727	1.153960	-0.024500
C	2.299044	-0.106173	-0.477765
H	-1.072011	1.692720	0.434863
H	-0.656479	-1.256434	-0.543025
H	-3.381729	1.279984	0.589229
H	2.698384	-0.020915	-1.487859
C	-3.460282	-0.822127	-0.053759
H	-4.223285	-0.664059	-0.824581
H	-2.787943	-1.607728	-0.405803
H	-3.978990	-1.199534	0.835127
C	3.163854	-0.813428	0.526545
H	2.685000	-0.819827	1.508023
H	3.325262	-1.848422	0.209424
H	4.138380	-0.323425	0.606421

TS1-4Z_in

SCF Energy: -347.762602106

Num. Imaginary Frequencies: 1

C	2.103126	-0.654778	-0.368439
C	0.954676	0.189347	-0.216281
C	-0.356091	-0.202847	-0.132574
C	-1.422298	0.729509	0.142288
C	-2.738642	0.449967	0.213211
C	-3.393642	-0.879336	-0.010151
O	1.526198	1.341804	-0.254424
H	-1.106517	1.755921	0.316406
H	-0.558413	-1.259042	-0.285808
H	-3.411926	1.268806	0.459706
H	2.188016	-1.293989	-1.252457
C	3.288523	-0.588436	0.510970
H	-2.688292	-1.653749	-0.319728
H	-4.167546	-0.802977	-0.782517
H	-3.891600	-1.223938	0.904179
H	3.538900	-1.615213	0.812103
H	3.112017	0.039641	1.383203
H	4.161880	-0.210441	-0.033839

TS1-4Z_out

SCF Energy: -347.767894707

Num. Imaginary Frequencies: 1

C	-2.255750	0.199230	-0.441572
C	-1.040025	-0.492552	-0.139124
C	0.229095	0.034622	-0.163893
C	1.397086	-0.779060	0.061806
C	2.677775	-0.360555	0.100550
C	3.177724	1.044569	-0.040839
O	-1.499369	-1.642541	0.200511
H	1.199429	-1.839133	0.206216
H	0.317851	1.099355	-0.359441
H	3.445038	-1.116429	0.257717
H	-2.929134	-0.333697	-1.107553
C	-2.748149	1.374589	0.298896
H	2.376632	1.769244	-0.203050
H	3.877393	1.121715	-0.881332
H	3.728490	1.348564	0.857219
H	-3.527685	1.912056	-0.246650
H	-1.923766	2.038144	0.579638
H	-3.195839	1.015460	1.238205

S,E,E-1

SCF Energy: -347.815222595

Num. Imaginary Frequencies: 0

C	-1.327045	-0.003261	0.083967
C	-0.215487	-0.914023	-0.167972
C	1.043138	-0.580638	0.090452
C	-2.612096	-0.283992	-0.166248
O	2.285488	-1.106829	-0.003650
C	2.122126	0.272982	0.504354
H	-1.071327	0.969004	0.506967
H	-0.416556	-1.899183	-0.580617
H	2.338082	0.345239	1.569681
C	2.665467	1.369486	-0.366959
H	2.441748	1.170905	-1.417340
H	2.206411	2.322850	-0.087011
H	3.748050	1.460916	-0.241793
C	-3.756165	0.650111	0.089622
H	-4.301345	0.869104	-0.835890
H	-4.477489	0.211278	0.788897
H	-3.409191	1.598148	0.511814
H	-2.861908	-1.257620	-0.588807

TS1-2M

SCF Energy: -347.806147057

Num. Imaginary Frequencies: 1

C	-2.383658	-0.181784	0.294048
C	-1.365991	-0.163996	-0.569352
C	-0.168276	-1.038921	-0.462603
C	0.984724	-0.600719	0.014990
C	1.910070	0.355185	0.556362
C	2.588882	1.396471	-0.286822
O	2.240182	-1.053028	0.248744
H	-1.415548	0.512730	-1.424722
H	-0.227880	-2.071885	-0.798138
H	1.878665	0.543179	1.628906
H	2.583040	1.103609	-1.339086
H	2.062513	2.350685	-0.185962
H	3.623406	1.539662	0.038125
C	-3.612083	0.672199	0.191846
H	-3.576404	1.321793	-0.687806
H	-4.514551	0.054202	0.124512
H	-3.723642	1.303731	1.080393

H -2.333062 -0.864096 1.143009

S,E,E,M-2

SCF Energy: -347.811783616

Num. Imaginary Frequencies: 0

C	1.944039	0.188085	-0.310226
C	1.439482	-0.820739	0.411002
C	0.093454	-1.390812	0.266876
C	-0.957693	-0.676738	-0.114780
O	-2.281374	-0.838206	-0.342732
C	-1.684408	0.510519	-0.465829
H	2.066215	-1.277538	1.177204
H	-0.061172	-2.440326	0.500865
H	-1.649807	0.847341	-1.501366
C	-2.106043	1.525714	0.556996
H	-1.368279	2.333416	0.592600
H	-2.167411	1.067684	1.546440
H	-3.077608	1.956458	0.299341
C	3.302782	0.788676	-0.107744
H	3.229383	1.853777	0.141809
H	3.844105	0.288743	0.701045
H	3.905449	0.716475	-1.020418
H	1.340447	0.611392	-1.113427

TS2M-3

SCF Energy: -347.772173362

Num. Imaginary Frequencies: 1

C	-0.876937	0.826439	-0.427378
C	-1.288369	-0.531350	-0.129045
C	-0.453082	-1.523291	0.317755
C	0.927611	-1.149976	0.412714
C	1.523655	-0.260782	-0.432148
O	-2.532626	-0.343356	-0.329045
H	-1.066312	1.166729	-1.442765
C	-0.687707	1.849881	0.628022
H	-0.838422	-2.455523	0.712546
H	1.510603	-1.536255	1.251157
H	-0.050107	2.664140	0.272536
H	-0.279586	1.412543	1.540621
H	-1.671770	2.283154	0.852615
C	2.850900	0.388376	-0.174537
H	3.312511	-0.001460	0.737905
H	3.545760	0.235321	-1.007482
H	2.740584	1.473100	-0.046062
H	1.081317	-0.090680	-1.411005

TS1-2P

SCF Energy: -347.806342901

Num. Imaginary Frequencies: 1

C	-2.234680	0.097061	-0.396602
C	-1.394665	-0.624341	0.348785
C	-0.134325	-1.225223	-0.162534
C	1.048621	-0.672013	0.046600
C	1.978434	0.316950	0.515052
C	2.189493	1.628291	-0.186070
O	2.353956	-0.899156	-0.238104
H	-1.650147	-0.815281	1.392871
H	-0.173199	-2.164548	-0.709753
H	2.295717	0.266058	1.556085
H	1.870013	1.560965	-1.228290
H	1.602400	2.407368	0.309877
H	3.244045	1.916751	-0.152085
C	-3.525830	0.683284	0.091720
H	-4.375930	0.276936	-0.467954
H	-3.684850	0.473459	1.153493
H	-3.541268	1.769796	-0.049699
H	-1.980710	0.277683	-1.441419

S,E,E,P-2

SCF Energy: -347.811874550

Num. Imaginary Frequencies: 0

C	-1.860807	0.299869	-0.140890
C	-1.452135	-0.968603	-0.014426
C	-0.078802	-1.449395	-0.216988
C	0.992015	-0.717074	0.060902
O	2.340572	-0.802113	-0.011334
C	1.720911	0.429282	0.525785
H	-2.185190	-1.728330	0.257179
H	0.075853	-2.455606	-0.596389
H	1.876568	0.532029	1.599034
C	1.891006	1.674505	-0.296840
H	1.162371	2.425628	0.024506
H	1.730395	1.462646	-1.356296
H	2.893018	2.092205	-0.163294
C	-3.256678	0.780300	0.120048
H	-3.683994	1.253638	-0.771426
H	-3.913782	-0.042068	0.418120
H	-3.272480	1.531754	0.918154
H	-1.140398	1.051692	-0.464455

TS2P-3

SCF Energy: -347.769163971

Num. Imaginary Frequencies: 1

C	-1.599176	0.115613	-0.283041
C	-1.178803	-1.153385	-0.024973
C	0.167363	-1.614118	-0.216030
C	1.149646	-0.688824	0.017434
O	2.424001	-0.660345	0.105536
C	0.929710	0.667738	0.464007
H	-1.892705	-1.849680	0.419694
H	0.404366	-2.662079	-0.355639
H	0.605640	0.796804	1.498530
C	1.417991	1.871574	-0.252694
H	0.618668	2.622461	-0.244695
H	1.705536	1.642858	-1.279259
H	2.271103	2.316511	0.270056
H	-1.011260	0.733886	-0.957161
C	-2.929018	0.669931	0.138224
H	-3.535271	0.949612	-0.731530
H	-3.493910	-0.053907	0.732926
H	-2.810452	1.575123	0.745226

TS1-4E_in

SCF Energy: -347.761899293

Num. Imaginary Frequencies: 1

C	-1.671109	0.684114	-0.371368
C	-1.145303	-0.616594	-0.063685
C	0.172353	-0.948186	0.135747
C	1.254846	-0.011093	-0.028919
C	2.556832	-0.303454	0.143998
O	-2.211066	-1.330321	-0.136397
H	0.994090	1.013634	-0.303790
H	0.399629	-1.983434	0.378237
H	-1.320985	1.204452	-1.267910
C	-2.820339	1.289624	0.330844
H	-2.564490	2.332871	0.562430
H	-3.078979	0.741201	1.235896
H	-3.699666	1.332409	-0.323656
C	3.682157	0.665893	-0.042859
H	3.317680	1.644243	-0.370678
H	4.241072	0.805770	0.890178
H	4.397896	0.301891	-0.789420
H	2.825660	-1.312296	0.457334

2S,3S-4

SCF Energy: -347.823421861

Num. Imaginary Frequencies: 0

C	-1.465516	-0.520438	0.501914
C	-1.348985	0.847190	-0.011879
C	-0.232862	-0.057322	-0.377729
C	1.114115	0.079095	0.221694
C	2.250958	-0.233992	-0.403871
O	-1.814992	1.951408	-0.085073
H	1.154333	0.470889	1.238985
H	-0.254985	-0.431019	-1.402428
H	-1.232766	-0.641476	1.560750
C	-2.463075	-1.508921	-0.063446
H	-2.086802	-2.531498	0.034543
H	-2.650709	-1.313478	-1.123683
H	-3.419182	-1.436279	0.462230
C	3.621361	-0.094061	0.187497
H	4.242511	0.575078	-0.418342
H	3.579235	0.307794	1.203946
H	4.133633	-1.062110	0.222525
H	2.198685	-0.618463	-1.423018

TS4S-3

SCF Energy: -347.788997205

Num. Imaginary Frequencies: 1

C	-1.695986	0.126527	0.362212
C	-1.324325	-0.916144	-0.451512
C	-0.013919	-1.416296	-0.439518
C	1.069189	-0.621064	0.102218
O	2.030137	-1.074915	0.752844
C	0.999359	0.721868	-0.402507
C	2.150979	1.631997	-0.209007
H	-2.063516	-1.354077	-1.121012
H	0.210245	-2.418730	-0.794523
H	0.184181	1.019030	-1.047395
H	2.216860	2.401858	-0.980630
H	3.074233	1.042792	-0.157426
H	2.070523	2.129246	0.768482
C	-2.998603	0.846444	0.265283
H	-3.556087	0.764770	1.205391
H	-2.827749	1.916416	0.097406
H	-3.619335	0.468100	-0.550615
H	-1.050618	0.389923	1.194551

TS1-4E_out

SCF Energy: -347.765307293

Num. Imaginary Frequencies: 1

C	1.900113	0.602992	0.446540
C	1.364155	-0.673156	0.065210
C	0.025565	-1.010689	-0.020593
C	-1.080274	-0.094887	0.082198
C	-2.369262	-0.455049	-0.068855
O	2.399082	-1.384608	-0.171575
H	-0.865633	0.948088	0.314758
H	-0.191943	-2.059463	-0.213893
H	2.703801	0.537834	1.176555
C	1.722102	1.881827	-0.269035
H	1.778669	2.730135	0.421724
H	0.803474	1.913756	-0.857005
H	2.566364	1.996990	-0.966285
H	-2.594827	-1.501458	-0.274357
C	-3.535726	0.476162	0.031838
H	-4.226286	0.160110	0.822576
H	-3.216551	1.500276	0.247176
H	-4.109757	0.487395	-0.902462

2S,3R-4

SCF Energy: -347.823478666

Num. Imaginary Frequencies: 0

C	1.748953	0.298334	-0.090416
C	0.933848	-0.308920	0.775400
C	-0.462582	0.117900	1.060874
C	-1.259549	0.844280	0.058246
O	-1.359370	1.832054	-0.620662
C	-1.705105	-0.533461	0.298081
C	-1.518716	-1.603954	-0.754684
H	1.284524	-1.186936	1.319399
H	-0.685205	0.325300	2.107493
H	-2.575135	-0.653273	0.942323
H	-0.597210	-1.440511	-1.320020
H	-1.461906	-2.593690	-0.291881
H	-2.354747	-1.596416	-1.459414
C	3.149589	-0.139787	-0.393803
H	3.866334	0.650553	-0.144812
H	3.421126	-1.038812	0.167276
H	3.269294	-0.352089	-1.461978
H	1.389255	1.183096	-0.615273

TS4R-3

SCF Energy: -347.773123978

Num. Imaginary Frequencies: 1

C	-1.390679	-0.472639	-0.411058
C	-0.802664	-0.951628	0.737731
C	0.587372	-1.044517	0.825624
C	1.407431	-0.321966	-0.130775
C	1.123788	1.078555	-0.235797
C	0.204657	2.018485	0.476029
O	2.368064	-0.857956	-0.724698
H	1.080399	-1.690224	1.546432
H	-1.432495	-1.246663	1.576219
H	-0.472978	1.533645	1.178108
H	0.805141	2.757096	1.023412
H	1.902044	1.582714	-0.813124
H	-0.395438	2.594239	-0.241466
C	-2.813092	-0.053767	-0.512565
H	-2.855794	1.034769	-0.664042
H	-3.304860	-0.506815	-1.379509
H	-3.379468	-0.288780	0.392129
H	-0.791948	-0.421471	-1.315709

S,Z,E-1

SCF Energy: -347.815711412

Num. Imaginary Frequencies: 0

C	-1.435655	0.092552	-0.035948
C	-0.203486	-0.625667	-0.344727
C	0.993520	-0.051336	-0.327007
C	-2.652437	-0.466339	-0.030028
O	1.528633	1.167123	-0.067435
C	2.422278	0.044710	-0.423638
H	-1.332435	1.150753	0.202104
H	-0.251655	-1.679669	-0.601640
H	2.860863	0.172046	-1.412938
C	3.347159	-0.435656	0.658294
H	2.818857	-0.513817	1.610920
H	3.741926	-1.421820	0.394798
H	4.190459	0.251639	0.771692
C	-3.924597	0.258350	0.289885
H	-4.633656	0.201318	-0.544220
H	-4.421423	-0.184952	1.160862
H	-3.738348	1.314498	0.505626
H	-2.744340	-1.526666	-0.268712

TS1-4Z_out

SCF Energy: -347.769277456

Num. Imaginary Frequencies: 1
 C 2.428534 0.020122 -0.413943
 C 1.084291 0.426769 -0.143433
 C -0.041757 -0.354685 -0.219238
 C -1.370557 0.166245 -0.020525
 C -2.490320 -0.578765 -0.053803
 O 1.282750 1.641701 0.228359
 H -1.445187 1.238334 0.158041
 H 0.094494 -1.412600 -0.432495
 H 2.990056 0.694464 -1.054857
 C 3.142670 -1.036087 0.326556
 H 4.028242 -1.389287 -0.207557
 H 2.470402 -1.861959 0.580393
 H 3.487251 -0.605849 1.279246
 H -2.398123 -1.653601 -0.215777
 C -3.877499 -0.044790 0.119840
 H -4.376223 -0.515390 0.975583
 H -3.871587 1.036976 0.280004
 H -4.493502 -0.257546 -0.762169

TS1-4Z_in

SCF Energy: -347.763912890
 Num. Imaginary Frequencies: 1
 C 2.344945 -0.518369 -0.315449
 C 1.040305 0.068752 -0.242464
 C -0.164738 -0.579025 -0.191416
 C -1.417500 0.111690 -0.005381
 C -2.621278 -0.487349 0.010760
 O 1.365112 1.314225 -0.309606
 H -1.354047 1.189835 0.138295
 H -0.157267 -1.660538 -0.308580
 H 2.604495 -1.153784 -1.167683
 C 3.447175 -0.175162 0.607390
 H 3.882067 -1.115507 0.974276
 H 3.104396 0.441769 1.436992
 H 4.254559 0.346712 0.079871
 C -3.923499 0.215995 0.234992
 H -4.601613 0.074516 -0.614999
 H -4.436872 -0.181062 1.119007
 H -3.776594 1.290009 0.380016
 H -2.672474 -1.564952 -0.150939

PARENT SYSTEMS

cyclopentene

SCF Energy: -194.0863712107
 Num. Imaginary Frequencies: 0
 C -0.008625 -1.217935 -0.144580
 H -0.010242 -1.535740 -1.180542
 C -1.229550 -0.310786 0.107194
 C -0.659197 1.077240 -0.052266
 H -1.269203 1.958926 -0.104121
 C 0.674941 1.067465 -0.049557
 C 1.225694 -0.329066 0.110300
 H 1.621101 -0.466782 1.113317
 H 2.035704 -0.544434 -0.576780
 H -0.016184 -2.110918 0.466497
 H 1.298298 1.939775 -0.100929
 H -1.632769 -0.445394 1.130750
 H -2.046274 -0.516940 -0.574737

ts_vinylcyclopropane_to_cyclopentene

SCF Energy: -193.9795846370
 Num. Imaginary Frequencies: 1
 C 1.355628 -0.882972 -0.378491
 H 1.189569 -0.877287 -1.439942

C 1.169744 0.413143 0.370945
 C -0.088634 1.119330 -0.072601
 H -0.038706 2.153250 -0.354859
 C -1.260186 0.435226 -0.170655
 C -1.392358 -0.924063 0.231055
 H -0.780519 -1.343257 1.000321
 H -2.233314 -1.505954 -0.092292
 H 2.093427 -1.580413 -0.020937
 H -2.110294 0.913235 -0.623919
 H 1.146857 0.214461 1.440152
 H 2.027814 1.061985 0.209962

vinylcyclopropane

SCF Energy: -194.0507299618
 Num. Imaginary Frequencies: 0
 C -1.454268 -0.446593 -0.492938
 H -1.176501 -0.605792 -1.518040
 C -1.134640 0.887415 0.108364
 C -0.348365 -0.349930 0.515874
 H -0.586834 -0.748980 1.486757
 C 1.067135 -0.569542 0.109350
 C 1.961874 0.381313 -0.166153
 H 1.719566 1.425699 -0.107563
 H 2.965371 0.130896 -0.454112
 H -2.366577 -0.932718 -0.202970
 H 1.372574 -1.600998 0.046783
 H -1.822642 1.301793 0.820675
 H -0.655369 1.614121 -0.518512

Vinyl allene oxide

SCF Energy: -267.8267441776
 Num. Imaginary Frequencies: 0
 C -2.813382 0.025683 0.004839
 C -1.542445 0.381056 -0.004789
 C -0.417872 -0.551357 -0.004974
 C 0.828712 -0.144767 -0.001891
 C 1.878879 0.814323 0.002483
 O 2.081854 -0.663776 0.002167
 H -1.292629 1.428058 -0.012091
 H -0.612188 -1.607411 -0.005681
 H -3.595785 0.759576 0.005148
 H 2.180659 1.294160 -0.909626
 H 2.173877 1.292897 0.917574
 H -3.112126 -1.006697 0.013330

ts_epoxide_opening

SCF Energy: -267.7411090937
 Num. Imaginary Frequencies: 1
 C -1.531728 1.217832 -0.015434
 C -1.000141 -0.108481 -0.038422
 C 0.302210 -0.540453 -0.038702
 C 1.452449 0.345875 -0.032511
 C 2.723574 -0.080855 0.022744
 O -2.040189 -0.956647 0.055006
 H 1.264830 1.402817 -0.084291
 H 0.475706 -1.600649 -0.019111
 H 3.543247 0.610710 0.019096
 H -2.524393 1.373848 -0.386187
 H 2.966017 -1.126550 0.068586
 H -1.082078 1.989495 0.575809

vinylcyclopropanone

SCF Energy: -267.8005941582
 Num. Imaginary Frequencies: 0
 C -1.045670 -1.113417 -0.498735
 H -0.709661 -1.239676 -1.512088
 C -1.045969 0.231226 0.061618

C	0.058398	-0.631235	0.572015
H	-0.086684	-1.052757	1.552386
C	1.469703	-0.439582	0.146278
C	1.994103	0.724746	-0.242362
H	1.417978	1.630925	-0.249703
H	3.019071	0.793162	-0.553363
H	-1.776378	-1.825260	-0.160579
H	2.084138	-1.323488	0.150552
O	-1.566482	1.298333	0.067488

ts_vinylcyclopropanone_to_cyclopentenone

SCF Energy: -267.7743932105

Num. Imaginary Frequencies: 1

C	0.826960	1.393512	-0.013705
H	-0.064224	1.803491	-0.435537
C	1.091989	-0.031153	-0.049172
C	-0.104441	-0.763445	0.353743
H	0.084186	-1.611939	0.988168
C	-1.469842	-0.627689	-0.186052
C	-2.338102	0.364779	0.029277
H	-2.105313	1.202773	0.657453
H	-3.317506	0.336720	-0.408112
H	1.553139	2.050281	0.422251
H	-1.792398	-1.469098	-0.778661
O	2.200342	-0.541031	-0.156263

cyclopentenone

SCF Energy: -267.8880217839

Num. Imaginary Frequencies: 0

C	0.047061	-1.194567	-0.003772
H	-0.158466	-1.805334	-0.872778
C	-0.875089	0.014965	-0.001032
C	-0.025663	1.225253	-0.000095
H	-0.427602	2.218017	0.000316
C	1.265108	0.877957	0.000700
C	1.474161	-0.618175	0.000369
H	2.039091	-0.929208	0.871297
H	2.044158	-0.928131	-0.867684
H	-0.163138	-1.813946	0.883772
H	2.087432	1.567112	0.001660
O	-2.091868	-0.017639	0.000799