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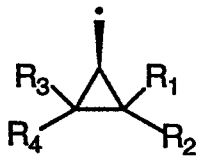


Table 1: Total energies, ZPE[a] and S^2 for the reactants for ring opening of methyl substituted cyclopropylcarbinyl radical.[b]

Rxn #	R1	R2	R3	R4	HF	ZPE[a]	MP2	PMP2	$<S^2>$
0	H	H	H	H	-155.466295	0.1007	-155.960429	-155.962971	0.767
1	Me	H	H	H	-194.501819	0.1314	-195.128235	-195.130757	0.767
2	H	Me	H	H	-194.503495	0.1311	-195.129773	-195.132275	0.766
3	H	H	Me	H	-194.501819	0.1314	-195.128235	-195.130757	0.767
4	H	H	H	Me	-194.503495	0.1311	-195.129771	-195.132272	0.767
5	Me	Me	H	H	-233.538505	0.1611	-234.299690	-234.302239	0.767
6	H	H	Me	Me	-233.538505	0.1611	-234.299690	-234.302239	0.767
7	H	Me	Me	H	-233.538897	0.1613	-234.297816	-234.300360	0.766
8	Me	H	H	Me	-233.538897	0.1613	-234.297816	-234.300360	0.767
9	Me	H	Me	H	-233.534976	0.1612	-234.294520	-234.297137	0.767
10	H	Me	H	Me	-233.538188	0.1608	-234.297286	-234.299848	0.767

a) In Hartree, using the HF/6-31G* optimized geometry; zero-point energy calculated at the HF/6-31G* level.

b) Reaction 0 at QCISD/6-31G* = -156.0082737; reaction 2 at QCISD/6-31G* = -195.1890556, both at the QCISD/6-31G* optimized geometry.

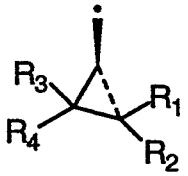


Table 2: Total energies, ZPE[a] and S^2 for the transition states for the ring opening of methyl substituted cyclopropylcarbinyl radical[b]

Rxn #	R1	R2	R3	R4	HF	ZPE[a]	MP2	PMP2	$<S^2>$
0	H	H	H	H	-155.447903	0.0991	-155.934282	-155.948184	0.943
1	Me	H	H	H	-194.485021	0.1297	-195.104481	-195.118053	0.936
2	H	Me	H	H	-194.485315	0.1295	-195.104137	-195.117957	0.941
3	H	H	Me	H	-194.484009	0.1294	-195.103115	-195.116919	0.940
4	H	H	H	Me	-194.485802	0.1292	-195.104483	-195.118318	0.942
5	Me	Me	H	H	-233.522502	0.1597	-234.276824	-234.290233	0.933
6	H	H	Me	Me	-233.521003	0.1591	-234.275097	-234.289110	0.940
7	H	Me	Me	H	-233.521295	0.1597	-234.273244	-234.286966	0.939
8	Me	H	H	Me	-233.522822	0.1595	-234.274978	-234.288471	0.934
9	Me	H	Me	H	-233.518924	0.1599	-234.271913	-234.285360	0.933
10	H	Me	H	Me	-233.520789	0.1596	-234.272648	-234.286381	0.939

a) In Hartree, using the HF/6-31G* optimized geometry; zero-point energy calculated at the HF/6-31G* level.

b) Reaction 0 at QCISD/6-31G* = -155.9901822, reaction 2 at QCISD/6-31G* = -195.1716459; reaction 4 at QCISD/6-31G* = -195.1717426 all at the QCISD/6-31G* optimized geometty.

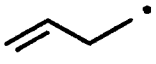
Unsubstituted Product 

Table 3: Total energies[a] for the product of the ring opening of cyclopropylcarbinyl radical.

Level of Theory[a]	Energy
HF/6-31G*	-155.4740188
ZPE (HF/6-31G*)	0.099928
MP2/6-31G*[b]	-155.973630
PMP2/6-31G*[b]	-155.968610
QCISD/6-31G*	-155.912511

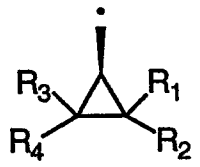
a) in Hartree.

b) The MP2 and PMP2 at HF/6-31G* optimized geometry.

Table 4: Total energies for the ring opening of the unsubstituted cyclopropylcarbinyl radical at the G2 level of theory.[a]

Level of Theory	Reactant	Transition State	Product
MP2/6-311G**	-156.069914	-156.043532	-156.068664
MP4/6-311G**	-156.137743	-156.115857	-156.140055
QCISD(T)/6-311G**	-156.139848	-156.124427	-156.143766
MP2/6-311+G**	-156.073366	-156.047981	-156.073220
MP4/6-311+G**	-156.141399	-156.120399	-156.144531
MP2/6-311 G(2df)	-156.144137	-156.118031	-156.143668
MP4/6-311 G(2df)	-156.198786	-156.175099	-156.202365
MP2/6-311+ G(3df, p)	-156.164980	-156.139457	-156.164325

Cartessian Coordinates of Reactants:



Reactant for Reaction 0; R1 = R2 = R3 = R4 = H
HF/6-31G* optimized geometry.

6	-.255477	-.000101	.483802
6	.902850	-.745974	-.134503
6	.902941	.745949	-.133979
6	-1.580920	.000260	-.160153
1	1.581532	-1.259631	.523860
1	.725427	-1.253325	-1.066845
1	.725602	1.253968	-1.065975
1	1.581714	1.259057	.524716
1	-1.669615	.001237	-1.231807
1	-2.480948	-.001594	.424742
1	-.280075	-.000516	1.560308

Reactant for Reaction 1and 3; R1 = Me; R2 = R3 = R4 = H
(HF/6-31G* optimized geometry)

6	1.564080	-.885477	.147141
6	.829496	.269265	-.402253
6	.085652	1.223631	.495722
6	-.688149	.345372	-.430406
1	.149849	2.277680	.287806
1	.059295	.986777	1.546520
1	-1.087750	.833821	-1.304715
1	1.306491	.719297	-1.257123
1	1.338002	-1.282415	1.119506
1	2.245213	-1.438438	-.472934
6	-1.562720	-.772562	.091073
1	-1.670332	-1.561765	-.647173
1	-2.554984	-.399444	.328132
1	-1.155939	-1.216889	.992318

Reactant for Reaction 2 and 4; R2 = Me; R1 = R3 = R4 = H
(HF/6-31G* optimized geometry)

6	-1.983153	-.514959	-.090969
6	-.669022	-.108685	.438180
6	-.064762	1.222589	.064130
6	.549949	-.033272	-.456555
1	.460996	1.768452	.829249
1	-.617263	1.846293	-.617528
1	.363390	-.246601	-1.496774
1	-.471393	-.438036	1.445149
1	-2.315412	-.165349	-1.052351
1	-2.548411	-1.295541	.383150
6	1.898143	-.500517	.043443
1	2.011402	-1.573729	-.078958
1	2.025035	-.271664	1.097344
1	2.704732	-.014761	-.498660

Reactant for Reaction 5 and 6 R1 = R2 = Me; R3 = R4 = H
(HF/6-31G* optimized geometry)

6	-2.080152	.119610	-.486303
6	-.830637	-.623673	-.240948
6	-.213327	-.696929	1.133853
6	.504790	.046046	.054336
1	.180122	-1.642910	1.465671
1	-.685153	-.124171	1.914932
1	-.743710	-1.522228	-.830074
1	-2.429694	.873265	.194644
1	-2.602335	.006779	-1.418468
6	.586143	1.557923	.135899
6	1.741007	-.596133	-.545943
1	.683758	1.995179	-.854059
1	1.453469	1.857567	.718370
1	-.289141	1.991543	.603978
1	2.622280	-.366793	.047952
1	1.916741	-.233125	-1.555184
1	1.646721	-1.676167	-.593127

Reactant for Reaction 7 and 8; R2 = R3 = Me; R3 = R4 = H
(HF/6-31G* optimized geometry)

6	1.199316	1.675100	-.189921
6	.167050	.821762	.426511
6	.257011	-.698536	.456041
6	-.760800	-.027050	-.404256
1	-.127706	-1.141783	1.361700
1	-.538925	-.029556	-1.460896
1	-.275365	1.249444	1.311947
1	1.570201	1.480621	-1.179293
1	1.697880	2.428677	.391275
6	1.430265	-1.450052	-.132052
1	1.769756	-1.006887	-1.061301
1	1.156418	-2.480502	-.340764
1	2.271691	-1.461551	.554558
6	-2.237283	-.100791	-.085091
1	-2.677313	-1.013347	-.477891
1	-2.773547	.740723	-.514136
1	-2.406445	-.088441	.987407

Reactant for Reaction 9; R1 = R3 = Me; R2= R4 =H;
(HF/6-31G* optimized geometry)

6	.000634	1.818959	-.595914
6	.000335	.950044	.594703
6	.748123	-.370315	.658588
6	-.748389	-.369761	.658596
1	1.196982	-.571688	1.618427
1	-1.197385	-.570815	1.618438
1	.000561	1.504757	1.518055
1	.000214	1.429816	-1.595619
1	.001631	2.886190	-.478363
6	-1.585834	-.889390	-.490407
1	-1.712019	-1.965622	-.412787
1	-1.150685	-.680971	-1.459316
1	-2.573118	-.437566	-.473742
6	1.585177	-.890540	-.490428
1	1.150188	-.681753	-1.459329
1	1.710552	-1.966869	-.412844
1	2.572802	-.439460	-.473745

Reactant for Reaction 10; R2 = R4 = Me ; R1 = R3 = H
(HF/6-31G* optimized geometry)

6	-2.295281	-.000153	-.089971
6	-.855340	-.000052	-.400925
6	.141585	-.748259	.457988
6	.141528	.748244	.458029
1	-.281424	-1.194785	1.344139
1	-.281519	1.194689	1.344200
1	-.627688	.000002	-1.455221
1	-2.636783	-.000428	.929650
1	-3.031705	.000783	-.871222
6	1.242664	-1.582492	-.160965
1	.883222	-2.584675	-.374905
1	2.091500	-1.670955	.511661
1	1.602023	-1.160519	-1.092407
6	1.242527	1.582599	-.160900
1	2.091371	1.671088	.511711
1	.883004	2.584768	-.374772
1	1.601897	1.160710	-1.092376

Reactant for Reaction 0; R1 = R2 = R3 = R4 = H;
(QCISD/6-31G* optimized geometry)

6	-1.577314	.000061	-.161935
6	-.263888	-.000027	.490054
6	.905951	.749141	-.135734
6	.905935	-.749145	-.135868
1	1.590048	1.270461	.530747
1	.716728	1.264825	-1.075006
1	1.590007	-1.270600	.530533
1	.716697	-1.264659	-1.075229
1	-.285599	-.000135	1.579284
1	-1.656820	.000314	-1.246721
1	-2.495162	-.000390	.417285

Reactant for Reaction 2; R2 = Me; R1 = R3 =R4 = H;
(QCISD/6-31G* optimized geometry)

6	1.975720	-0.522704	0.100545
6	0.674313	-0.118658	-0.438441
6	0.062982	1.227775	-0.063823
6	-0.554991	-0.031772	0.461483
1	-0.467378	1.774896	-0.842160
1	0.629980	1.857983	0.618881
1	-0.360659	-0.250971	1.512393
1	0.467856	-0.452369	-1.455991
1	2.285924	-0.208140	1.094406
1	2.637713	-1.178185	-0.456659
6	-1.899373	-0.501404	-0.047020
1	-2.011376	-1.587237	0.069694
1	-2.014196	-0.262727	-1.112651
1	-2.719771	-0.012672	0.495623

Cartessian Coordinates of Transition States:

Transition State for Reaction 0; R1 = R2 = R3 = R4 =H;

(HF/6-31G* optimized geometry)

6	-1.604998	-.105784	-.179905
6	-.400320	.155707	.485527
6	.813103	.726208	-.157787
6	1.145758	-.715261	-.099020
1	1.409825	1.385523	.454554
1	.660208	1.135123	-1.145661
1	1.737323	-1.107643	.706045
1	.984807	-1.339019	-.956400
1	-.382984	.080403	1.557659
1	-1.704477	.055451	-1.238941
1	-2.425964	-.575051	.329848

Transition State for Reaction 1; R1 = Me; R2 = R3 = R4 =H

(HF/6-31G* optimized geometry)

6	2.079313	-.624334	.089151
6	1.208026	.240433	-.393375
6	.081746	.873462	.391723
6	-1.280338	.543012	-.162756
1	.216643	1.952369	.392565
1	.150935	.547950	1.428591
1	-1.841643	1.305365	-.672561
1	1.275496	.531672	-1.430392
1	2.050125	-.947076	1.116311
1	2.859003	-1.042077	-.523010
6	-1.865333	-.827763	-.000728
1	-1.170971	-1.597577	-.330239
1	-2.782309	-.939362	-.568703
1	-2.097763	-1.040122	1.043351

Transition State for Reaction 2; R2 = Me; R1 = R3 = R4 =H
(HF/6-31G* optimized geometry)

6	2.042151	-.501924	.137073
6	.859164	-.086417	-.485894
6	.080839	1.122776	-.099845
6	-.705965	.034895	.527174
1	-.397543	1.657389	-.908192
1	.586483	1.799206	.573894
1	-.515200	-.173413	1.564181
1	.565369	-.574259	-1.397857
1	2.441775	.024208	.986177
1	2.524003	-1.418493	-.149437
6	-1.982726	-.482049	-.073984
1	-2.155980	-1.521414	.185941
1	-1.968192	-.408071	-1.157292
1	-2.841494	.091163	.275441

Transition State for Reaction 3; R3 = Me; R1 = R2 = R4 =H
(HF/6-31G* optimized geometry)

6	-1.658482	-.729369	.205242
6	-.851932	.190998	-.477583
6	.638437	.261292	-.447964
6	.255039	1.333855	.501249
1	1.053549	.631260	-1.375579
1	.193716	2.358299	.186758
1	.236537	1.128829	1.554793
1	-1.329899	.820419	-1.206609
1	-1.251896	-1.467854	.870783
1	-2.728811	-.655499	.149184
6	1.433609	-.917941	.081349
1	1.075076	-1.242610	1.051807
1	2.477793	-.643748	.193597
1	1.373909	-1.762105	-.598488

Transition State for Reaction 4; R4 = Me; R1 = R3 = R2 =H
(HF/6-31G* optimized geometry)

6	1.998065	-.469153	-.111434
6	.710985	-.265219	.403369
6	-.503855	-.002638	-.416149
6	-.149264	1.356740	.054694
1	-.333807	-.149338	-1.474533
1	-.619991	1.767886	.928576
1	.418286	2.018543	-.570005
1	.545866	-.451978	1.450084
1	2.195705	-.397700	-1.166520
1	2.840325	-.596962	.543121
6	-1.819332	-.605730	.039344
1	-2.653596	-.147252	-.482685
1	-1.969597	-.452996	1.104083
1	-1.842777	-1.674204	-.151067

Transition State for Reaction 5; R1 = R2 = Me; R3 = R4 = H
(HF/6-31G* optimized geometry)

6	-2.154945	.189261	-.472222
6	-1.074050	-.645748	-.159469
6	-.268462	-.565972	1.092378
6	.631483	.055495	.088587
1	.048614	-1.506612	1.520114
1	-.665529	.094895	1.849812
1	-.921131	-1.517171	-.770185
1	-2.455439	.991978	.177145
1	-2.656049	.106681	-1.419211
6	.785639	1.552051	.041374
1	-.110034	2.061598	.375907
1	1.006761	1.895885	-.964828
1	1.606347	1.872887	.683497
6	1.747843	-.763938	-.505161
1	2.656903	-.663576	.089284
1	1.984453	-.443630	-1.515683
1	1.500053	-1.819831	-.538774

Transition State for Reaction 6; R1 = R2 = H; R3 = R4 = Me
(HF/6-31G* optimized geometry)

6	2.093343	.081002	-.437324
6	.856069	-.571175	-.348103
6	-.457206	.025845	.046990
6	-.029993	-.653342	1.296782
1	-.376084	-1.642503	1.532207
1	.466676	-.097767	2.069126
1	.803992	-1.573340	-.736044
1	2.222942	1.113942	-.174393
1	2.977259	-.474634	-.691032
6	-1.667080	-.580276	-.651781
6	-.538885	1.544527	.110760
1	-1.599407	-1.662789	-.692033
1	-1.747680	-.212815	-1.670653
1	-2.581091	-.323568	-.124188
1	.278433	1.973598	.678130
1	-1.464331	1.846630	.591485
1	-.518196	1.973761	-.886546

Transition State for Reaction 7; R2 = R3 = Me; R1 = R4 = H
(HF/6-31G* optimized geometry)

6	-1.486607	-1.495431	-.219646
6	-.462870	-.841575	.477674
6	-.163938	.622241	.453595
6	.865272	.073478	-.464496
1	.241236	.978090	1.392264
1	.638418	.097926	-1.515855
1	.070775	-1.410761	1.217994
1	-2.145876	-.979143	-.892364
1	-1.578629	-2.564702	-.167797
6	-1.196892	1.587158	-.099664
1	-1.548439	1.283193	-1.079318
1	-.767661	2.579337	-.199477
1	-2.057251	1.653565	.559090
6	2.297955	-.129852	-.058128
1	2.758372	-.944654	-.607830
1	2.381101	-.355171	1.000766
1	2.890446	.766204	-.243483

Transition State for Reaction 8; R1 = R4 = Me; R2 = R3 = H
(HF/6-31G* optimized geometry)

6	-1.011531	1.842157	-.167593
6	-.025038	1.007402	.374698
6	.689619	-.072362	-.363497
6	-.290863	-.835012	.445916
1	.463075	-.073344	-1.422341
1	.048368	-1.211699	1.395893
1	.372781	1.260916	1.341897
1	-1.355511	1.725526	-1.179730
1	-1.518007	2.564592	.445738
6	-1.542621	-1.433472	-.129721
1	-1.919951	-.844351	-.958121
1	-2.330257	-1.498627	.614076
1	-1.358537	-2.440683	-.501997
6	2.171675	-.265074	-.100078
1	2.514577	-1.215749	-.497631
1	2.382459	-.255441	.965237
1	2.753553	.527023	-.561363

Transition State for Reaction 9; R1 = R3 = Me; R2 = R4 = H
(HF/6-31G* optimized geometry)

6	-1.567119	-1.026217	-.591616
6	-.974101	-.502071	.565141
6	-.144882	.738427	.656061
6	.877281	-.342418	.677466
1	-.253517	1.234399	1.611332
1	1.215520	-.662291	1.647292
1	-1.271975	-.930491	1.505206
1	-1.439366	-.580870	-1.560472
1	-2.111343	-1.951632	-.546986
6	1.732084	-.731724	-.497048
1	2.580197	-.057656	-.611158
1	1.180271	-.722638	-1.429126
1	2.127261	-1.733527	-.365260
6	-.171481	1.753583	-.473570
1	-.032488	1.302013	-1.447663
1	.616739	2.487599	-.336843
1	-1.121990	2.277613	-.484924

Transition State for Reaction 10; R2 = R3 = Me; R1 = R4 = H
(HF/6-31G* optimized geometry)

6	2.308911	-.329166	-.077117
6	.990675	-.017655	-.433584
6	.008284	.675955	.446625
6	-.425320	-.743179	.544390
1	.461554	1.034438	1.361723
1	-.065692	-1.291698	1.396194
1	.700737	-.140560	-1.462842
1	2.685728	-.120295	.908709
1	2.944628	-.883645	-.742698
6	-1.586339	-1.335848	-.208007
1	-2.528324	-1.155999	.309843
1	-1.471470	-2.410066	-.309287
1	-1.685954	-.923117	-1.205767
6	-.903201	1.729423	-.159128
1	-.349237	2.645319	-.339613
1	-1.726671	1.959479	.510485
1	-1.323356	1.408967	-1.105826

Transition State for Reaction 0 R1 = R2 = R3 = R4 = H
(QCISD/6-31G* optimized geometry)

6	-1.605115	-.119985	-.182034
6	-.421319	.156386	.487127
6	.799727	.729129	-.155176
6	1.185007	-.702670	-.103422
1	1.387010	1.412654	.462493
1	.635012	1.139825	-1.154562
1	1.764123	-1.097117	.725403
1	1.000396	-1.347492	-.955446
1	-.391669	.055361	1.570642
1	-1.703815	.054490	-1.251902
1	-2.440854	-.594877	.324400

Transition State for Reaction 2; R2 = Me; R1 = R3 = R4 = H
(QCISD/6-31G* optimized geometry)

6	2.049474	-0.494511	0.143684
6	0.877384	-0.101410	-0.485309
6	0.083751	1.111400	-0.116206
6	-0.730311	0.056398	0.539273
1	-0.394188	1.640178	-0.945915
1	0.602372	1.806684	0.549505
1	-0.520112	-0.159958	1.584000
1	0.552507	-0.634937	-1.377491
1	2.461559	0.070775	0.977642
1	2.547731	-1.422863	-0.122444
6	-1.990646	-0.480153	-0.073047
1	-2.171745	-1.523578	0.214347
1	-1.946333	-0.434202	-1.169589
1	-2.869700	0.107563	0.239574

Transition State Reaction 4 R4 = Me; R1= R2 = R3 = H
(QCISD/6-31G* optimized geometry)

6	1.998484	-0.456760	-0.110623
6	0.722622	-0.272014	0.402390
6	-0.498293	0.001254	-0.415502
6	-0.190063	1.375812	0.051392
1	-0.318124	-0.143223	-1.486591
1	-0.652886	1.768577	0.952775
1	0.407383	2.047265	-0.555842
1	0.551209	-0.439556	1.465827
1	2.193697	-0.387973	-1.179260
1	2.854867	-0.595430	0.543742
6	-1.803497	-0.629240	0.037170
1	-2.655327	-0.177346	-0.486902
1	-1.950724	-0.477476	1.114846
1	-1.805612	-1.709146	-0.157561

Unsubstituted Ring Opening Product; R1 = R2 = R3 = R4 = H;
(HF/6-31G* optimized geometry)

6	-1.790647	-.047825	-.265777
6	-.666781	-.190033	.410255
6	.613625	.554086	.130637
6	1.758109	-.363890	-.200225
1	.446494	1.259850	-.683844
1	.879438	1.152694	.999815
1	2.772859	-.036331	-.060440
1	1.592827	-1.225006	-.822990
1	-.630280	-.891842	1.229096
1	-1.873816	.636865	-1.092982
1	-2.673361	-.610260	-.017995

Unsubstituted Ring Opening Product; R1 = R2 = R3 = R4 = H;
(QCISD/6-31G* optimized geometry)

6	-1.794991	-.049801	-.268290
6	-.660638	-.187583	.423243
6	.618960	.557551	.129606
6	1.752680	-.362344	-.214434
1	.433550	1.271976	-.693358
1	.897364	1.169626	1.001538
1	2.784681	-.070317	-.037881
1	1.571266	-1.248305	-.817758
1	-.620024	-.891608	1.257395
1	-1.872396	.637652	-1.110304
1	-2.690505	-.615956	-.020380