Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Decomposition of the simplest ketohydroxyperoxide in the ozonolysis of ethylene

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All coordinates are given in Å and rotational constants and frequencies in cm-1. All calculations were performed at the FC-CCSD(T)/ANO1 level of theory, unless mentioned differently.

Cis-HPA geometry (AE-CCSDT(T)/PCVQZ):

H	-0.653307753	-1.393890498	-0.001262273
O	-1.34100672	-0.798261467	-0.331838814
O	-1.063996348	0.364103221	0.48197313
C	-0.04699031	1.06863575	-0.171591385
H	0.076022752	2.001251373	0.384339065
H	-0.325043289	1.318662502	-1.200942329
C	1.26966643	0.333226734	-0.191012174
O	1.411117208	-0.795455637	0.212365884
H	2.117823115	0.897104898	-0.617817185

Be-B_0 (FC-CCSDT(T)/ANO0), ordered A to C according to main text):

0.00129742
0.00335065
0.00178410

Vibrational frequencies:

Harmonic Frequency (FC-CCSD(T)/ANO1)	Anharmonic Contribution (FC-CCSD(T)/ANO0)	Fundamental Frequency
169.61	-13.62	155.99
201.02	-12.44	188.58
281.53	-8.64	272.90
424.68	-7.97	416.71
482.57	-64.20	418.37
705.44	-12.92	692.53
809.29	-24.87	784.42
844.35	-23.71	820.65
886.65	-11.10	875.55
1087.66	-27.64	1060.03
1131.83	-28.34	1103.49
1277.94	-32.86	1245.08
1389.99	-47.00	1342.99
1401.48	-38.82	1362.67
1409.73	-43.14	1366.59
1437.06	-28.75	1408.31
1781.81	-19.81	1762.00
2946.85	-156.32	2790.53
3022.13	-131.94	2890.18
3082.24	-154.29	2927.95
3726.50	-191.86	3534.64

Trans-HPA geometry (AE-CCSDT(T)/PCVQZ):

H	2.285550766	0.667103097	-0.765010022
O	1.592064706	0.821748645	-0.114000845
O	1.272647989	-0.545144633	0.252799323
C	-0.012850583	-0.780259582	-0.273844829
H	-0.241040581	-1.811574149	0.003103947
H	-0.036172572	-0.68695306	-1.360368363
C	-1.052089235	0.131078713	0.34260864
O	-2.145592041	0.286386991	-0.137197346
H	-0.741248344	0.62603373	1.27810432

Be-B_0 (FC-CCSDT(T)/ANO0), ordered A to C according to main text):

-0.00325843
0.00179559
0.00140359

Harmonic frequencies:

Harmonic Frequency (FC-CCSD(T)/ANO1)	Anharmonic Contribution (FC-CCSD(T)/ANO0)	Fundamental Frequency
75.65	-5.62	70.03
164.93	-6.03	158.90
217.43	-48.30	169.13
309.36	-5.66	303.71
428.89	-10.22	418.66
574.04	-11.53	562.51
738.76	-11.44	727.32
856.91	-31.04	825.87
1059.79	-26.82	1032.97
1070.30	-32.09	1038.21
1120.42	-29.22	1091.19
1267.73	-29.69	1238.05
1334.46	-41.11	1293.34
1367.06	-3.42	1363.65
1411.61	-35.94	1375.68
1447.58	-46.30	1401.29
1789.35	-35.60	1753.75
2966.25	-153.97	2812.28
3047.26	-132.51	2914.75
3106.18	-152.29	2953.89
3788.68	-196.63	3592.06

Cis-formylmethoxy geometry:

O	-1.406974549	0.570635736	0.014210298
C	-0.729905806	-0.614479997	-0.012546925
C	0.791993008	-0.513563324	0.016763261
H	-1.073785518	-1.31702047	0.763559918
H	-1.00490631	-1.09725981	-0.970177624
H	1.302539524	-1.496308971	0.069768475
O	1.409298992	0.522068414	-0.008750803

Rotational constants:

0.7014478404
0.2036150749
0.1625260286

Harmonic frequencies:

134
263
592
724
848
901
1080
1180
1298
1369
1412
1800
2913
2929
2986

Trans-formylmethoxy geometry:

O	-1.730451594	0.2344304	-0.146329008
C	-0.609473816	-0.49964484	0.12540543
C	0.656165141	0.353942605	0.168703982
H	-0.752914977	-0.87737853	1.157572893
H	-0.476352247	-1.375874093	-0.520658157
H	0.49504439	1.391597176	0.512934857
O	1.741684683	-0.070826856	-0.146774158

Rotational constants:

1.2771117744
0.1529822308
0.1438598490

Harmonic frequencies:

103
338
506
673
987
1002
1104
1136
1252
1368
1397
1787
2909
2963
30393