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

Supporting Information for:

Theoretical structural and spectroscopic characterization of Peroxyacetic Acid (CH_3-CO-OOH). Study of the Far Infrared region.

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Table S1

CCSD(T)-F12/CVTZ-F12 and MP2/AVTZ minimum energy structures

PAA-Cc

CCSD(T)-F12/CVTZ-F12 ENERGY=-304.21197782

C	0.0000000048	-0.1270278788	0.4802281595
C	0.0000000153	0.5297281555	1.8221135612
O	0.0000000078	0.7890532268	-0.5065815991
O	-0.0000000052	-1.3117179598	0.2537162843
O	-0.0000000023	0.1438362625	-1.7880553691
H	-0.0000000084	-0.7954638826	-1.5062798488
H	0.0000000232	1.6110710663	1.7333632272
H	-0.8810500518	0.1994724017	2.3668042306
H	0.8810497929	0.1994720810	2.3668044780

PAA-Ct

CCSD(T)-F12/CVTZ-F12 ENERGY=-304.20346221

C	-0.0000320237	-0.1440012020	0.4923338945
C	0.0000569015	0.6138273771	1.7894451234
O	-0.0000832954	0.7527834382	-0.5344128188
O	-0.0000284064	-1.3282686985	0.3560516743
O	0.0000976390	0.0263497878	-1.7847031707
H	-0.0003287029	0.7890775549	-2.3750506737
H	-0.8809333189	0.3207642671	2.3549347965
H	0.8807693265	0.3201833175	2.3550644878
H	0.0004194656	1.6879738380	1.6349339427

PAA-Ttg

CCSD(T)-F12/CVTZ-F12 ENERGY=-304.20198084

C	-0.0296771796	-0.0034034798	-0.5835185054
C	1.4574427171	-0.0050912063	-0.4256380566
O	-0.7935220679	0.0200923504	0.5576558833
O	-0.6357662461	-0.0080092211	-1.6136582386
O	0.0432624033	0.0323740940	1.7425350290
H	-0.4623932777	-0.5848504513	2.2833954784
H	1.8916218815	0.0182363180	-1.4185990857
H	1.7787252692	0.8570879272	0.1534394666
H	1.7791396911	-0.8949336069	0.1096771165

PAA-Cc (MP2/AVTZ)

C						
C	1	1.498200(1)				
O	1	1.359800(2)	2	110.417(9)		
O	1	1.220900(3)	2	127.105(10)	3	180.000(16)
O	3	1.456000(4)	1	110.144(11)	2	180.000(17)
H	5	0.984800(5)	3	99.284(12)	1	0.000(18)
H	2	1.085100(6)	1	111.330(13)	3	0.000(19)
H	2	1.087400(7)	1	108.539(14)	7	121.280(20)
H	2	1.087400(8)	1	108.539(15)	7	-121.280(21)

PAA-Ct (MP2/AVTZ)

C						
C	1	1.506900(1)				
O	1	1.377300(2)	2	107.553(9)		
O	1	1.207500(3)	2	127.370(10)	3	181.799(16)
O	3	1.468800(4)	1	108.081(11)	2	183.006(17)
H	5	0.971000(5)	3	96.091(12)	1	187.435(18)
H	2	1.088600(6)	1	108.761(13)	3	92.894(19)
H	2	1.085600(7)	1	108.322(14)	7	118.027(20)
H	2	1.086000(8)	1	111.650(15)	7	-120.172(21)

PAA-Ttg (MP2/AVTZ)

C						
C	1	1.499900(1)				
O	1	1.387500(2)	2	117.621(9)		
O	1	1.211000(3)	2	126.795(10)	3	179.396(16)
O	3	1.471800(4)	1	110.244(11)	2	-0.122(17)
H	5	0.970500(5)	3	97.183(12)	1	219.824(18)
H	2	1.084600(6)	1	107.409(13)	3	181.196 19)
H	2	1.087100(7)	1	110.455(14)	7	120.602(20)
H	2	1.086700(8)	1	110.435(15)	7	-120.614(21)

Table S2

Expansion coefficients of the 3D-Potential Energy Surface (in cm^{-1})
(positive values of the M, L and K index denote cosine functions; negative values denote sine functions)

A_{MLK}	M	L	K	A_{MLK}	M	L	K
4432.348	0	0	0	164.527	3	0	0
-0.789	6	0	0	652.049	0	1	0
-2126.888	0	2	0	339.762	0	3	0
100.403	0	4	0	564.904	0	0	1
369.374	0	0	2	6.913	0	0	3
-6.499	0	0	4	61.554	3	1	0
-45.135	3	2	0	121.356	3	3	0
46.589	3	4	0	-5.103	6	1	0
-4.951	6	2	0	-8.429	6	3	0
-6.595	6	4	0	-91.847	-3	-1	0
68.057	-3	-2	0	-138.752	-3	-3	0
-8.927	3	0	1	-0.825	3	0	2
-1.190	3	0	3	0.195	3	0	4
1.333	6	0	1	-0.317	6	0	2
-1.395	6	0	3	-0.693	6	0	4
-0.545	-3	0	-1	-2.605	-3	0	-2
-1.772	-3	0	-3	976.139	0	1	1
366.125	0	1	2	74.582	0	1	3
17.931	0	1	4	-319.321	0	2	1
-339.850	0	2	2	-84.583	0	2	3
-35.088	0	2	4	48.564	0	3	1
71.742	0	3	2	39.968	0	3	3
14.410	0	3	4	34.889	0	4	1
35.680	0	4	2	10.788	0	4	3
1.056	0	4	4	-571.714	0	-1	-1
-292.337	0	-1	-2	-36.732	0	-1	-3
300.196	0	-2	-1	152.892	0	-2	-2
60.747	0	-2	-3	-109.283	0	-3	-1
-56.080	0	-3	-2	-39.827	0	-3	-3
-0.037	3	1	1	-0.305	3	1	2
-1.248	3	1	3	0.421	3	1	4
18.343	3	2	1	3.387	3	2	2
1.417	3	2	3	0.211	3	2	4
31.789	3	3	1	29.086	3	3	2
12.999	3	3	3	1.099	3	3	4
12.015	3	4	1	13.625	3	4	2
8.060	3	4	3	0.142	3	4	4
-0.796	6	1	1	-0.520	6	1	2
-0.485	6	1	3	-0.080	6	1	4
-4.438	6	2	1	-0.533	6	2	2
1.674	6	2	3	1.428	6	2	4
-2.874	6	3	1	-0.966	6	3	2
-0.188	6	3	3	-0.003	6	3	4
-0.255	6	4	1	-0.687	6	4	2
-1.163	6	4	3	-0.638	6	4	4
0.346	3	-1	-1	-4.696	3	-1	-2
2.246	3	-1	-3	-19.471	3	-2	-1
-9.874	3	-2	-2	4.560	3	-2	-3
-39.600	3	-3	-1	-11.248	3	-3	-2
1.649	3	-3	-3	-3.659	6	-1	-1
-3.169	6	-1	-2	-2.329	6	-1	-3

-0.513	6	-2	-1	0.317	6	-2	-2
-0.723	6	-2	-3	3.151	6	-3	-1
3.974	6	-3	-2	1.594	6	-3	-3
-7.209	-3	-1	1	-3.312	-3	-1	2
-3.418	-3	-1	3	-1.893	-3	-1	4
-15.936	-3	-2	1	6.738	-3	-2	2
6.851	-3	-2	3	2.860	-3	-2	4
-31.874	-3	-3	1	-14.170	-3	-3	2
5.911	-3	-3	3	3.835	-3	-3	4
-11.353	-3	1	-1	-7.732	-3	1	-2
-1.681	-3	1	-3	-8.705	-3	2	-1
-7.381	-3	2	-2	-1.197	-3	2	-3
-52.402	-3	3	-1	-32.313	-3	3	-2
-17.463	-3	3	-3	-29.385	-3	4	-1
-17.439	-3	4	-2	-13.453	-3	4	-3

Table S3

Expansion coefficients of the kinetic energy parameters (cm^{-1})
(positive values of the M, L and K index denote cosine functions; negative values denote sine functions)

$B_{\theta\theta}$	$B_{\alpha\alpha}$	$B_{\beta\beta}$	$B_{\theta\alpha}$	$B_{\theta\beta}$	$B_{\alpha\beta}$	**M**	**L**	**K**
5.6243	1.5428	20.0919	-0.1618	0.0009	-0.7741	0	0	0
0.0105	0.0030	-0.0073	0.0010	-0.0001	0.0005	3	0	0
-0.0001	0.0002	0.0008	-0.0005	-0.0003	-0.0004	6	0	0
0.0287	0.1075	0.2114	-0.5046	0.4924	-0.1070	0	1	0
0.1208	0.3369	0.2561	-0.0150	0.0068	-0.3473	0	2	0
0.0021	0.0286	0.0232	-0.0621	0.0590	-0.0303	0	3	0
0.0087	0.0123	0.0038	-0.0029	0.0025	-0.0039	0	4	0
0.0110	0.0745	1.0941	-0.0064	0.0033	-1.0528	0	0	1
0.0025	0.0504	0.4952	-0.0020	0.0020	-0.0783	0	0	2
0.0004	0.0087	0.0547	-0.0005	0.0011	-0.0260	0	0	3
0.0001	0.0014	0.0095	-0.0001	0.0003	-0.0034	0	0	4
0.0040	0.0132	0.0013	-0.0018	0.0012	-0.0081	3	1	0
-0.0001	0.0130	0.0092	-0.0027	0.0007	-0.0116	3	2	0
0.0058	0.0160	0.0103	-0.0047	0.0011	-0.0147	3	3	0
0.0020	0.0087	0.0031	-0.0025	0.0009	-0.0072	3	4	0
-0.0010	0.0001	0.0008	-0.0004	0.0000	-0.0004	6	1	0
-0.0005	-0.0005	0.0002	0.0006	-0.0003	0.0003	6	2	0
-0.0003	-0.0009	-0.0004	-0.0000	-0.0003	0.0008	6	3	0
-0.0005	-0.0007	-0.0007	-0.0003	0.0003	0.0007	6	4	0
-0.0084	-0.0095	-0.0094	0.0103	-0.0088	0.0069	-3	-1	0
-0.0039	-0.0224	-0.0162	0.0022	-0.0011	0.0210	-3	-2	0
-0.0060	-0.0114	-0.0106	0.0055	-0.0020	0.0127	-3	-3	0
-0.0001	-0.0007	-0.0042	-0.0000	-0.0002	0.0015	3	0	1
-0.0002	-0.0001	-0.0017	0.0002	-0.0001	0.0002	3	0	2
-0.0002	-0.0006	-0.0006	0.0001	-0.0001	0.0007	3	0	3
-0.0000	-0.0001	-0.0003	0.0000	-0.0000	0.0002	3	0	4
-0.0000	0.0001	0.0016	0.0000	-0.0000	-0.0002	6	0	1
0.0000	-0.0001	0.0006	0.0000	-0.0000	0.0000	6	0	2
-0.0000	0.0000	0.0004	0.0000	-0.0000	-0.0001	6	0	3
0.0000	0.0000	0.0003	-0.0000	0.0000	-0.0000	6	0	4
0.0006	-0.0002	-0.0002	-0.0001	0.0022	0.0012	-3	0	-1
0.0004	0.0000	-0.0002	-0.0001	0.0000	-0.0001	-3	0	-2
0.0001	-0.0004	-0.0010	0.0001	0.0001	0.0003	-3	0	-3
0.0122	0.0491	0.3644	-0.0200	0.0714	-0.0758	0	1	1

0.0021	0.0220	0.2258	-0.0085	0.0190	-0.0397	0	1	2
0.0005	0.0059	0.0923	-0.0023	0.0039	-0.0159	0	1	3
-0.0002	0.0012	0.0262	-0.0001	0.0001	-0.0044	0	1	4
0.0053	0.0241	0.1383	-0.0083	0.0067	-0.0612	0	2	1
0.0086	0.0028	-0.0906	-0.0052	0.0029	0.0007	0	2	2
0.0013	0.0028	-0.0862	-0.0015	0.0010	0.0030	0	2	3
0.0003	-0.0007	-0.0360	-0.0003	0.0004	0.0034	0	2	4
0.0011	0.0155	0.0440	0.0022	0.0012	-0.0218	0	3	1
0.0019	0.0114	0.0410	0.0010	-0.0011	-0.0130	0	3	2
0.0010	0.0063	0.0433	0.0003	0.0001	-0.0078	0	3	3
0.0003	0.0020	0.0200	0.0004	-0.0004	-0.0037	0	3	4
-0.0016	-0.0043	-0.0150	-0.0018	0.0025	0.0064	0	4	1
-0.0005	-0.0005	0.0196	-0.0019	0.0019	-0.0003	0	4	2
-0.0002	0.0003	0.0044	-0.0010	0.0006	-0.0012	0	4	3
-0.0001	-0.0004	-0.0020	-0.0004	0.0003	0.0004	0	4	4
-0.0102	-0.0210	-0.0828	0.0100	0.2809	-0.0244	0	-1	-1
-0.0030	-0.0143	-0.1223	-0.0140	0.0081	0.0251	0	-1	-2
-0.0011	-0.0053	-0.0533	-0.0001	0.0054	0.0088	0	-1	-3
-0.0090	-0.0168	0.1550	0.0060	0.0038	-0.1208	0	-2	-1
-0.0029	0.0166	0.1077	0.0051	-0.0018	-0.0085	0	-2	-2
-0.0014	-0.0025	0.0513	0.0019	-0.0004	-0.0077	0	-2	-3
-0.0008	-0.0089	0.0227	0.0017	0.0287	-0.0001	0	-3	-1
-0.0015	-0.0070	-0.0372	-0.0035	0.0015	0.0042	0	-3	-2
-0.0008	-0.0048	-0.0272	0.0002	0.0008	0.0060	0	-3	-3
0.0032	-0.0001	-0.0007	-0.0010	-0.0009	0.0000	3	1	1
0.0005	-0.0005	-0.0071	0.0000	-0.0003	0.0008	3	1	2
-0.0002	-0.0005	-0.0033	0.0003	-0.0003	0.0009	3	1	3
-0.0001	0.0000	-0.0001	0.0001	-0.0001	0.0002	3	1	4
0.0057	0.0017	0.0085	-0.0008	-0.0017	-0.0025	3	2	1
0.0035	0.0002	-0.0065	-0.0005	-0.0003	0.0008	3	2	2
0.0008	0.0003	-0.0044	-0.0002	0.0001	0.0004	3	2	3
0.0003	0.0000	-0.0013	-0.0000	0.0000	0.0002	3	2	4
0.0049	0.0027	0.0146	-0.0001	-0.0017	-0.0036	3	3	1
0.0067	0.0018	0.0043	-0.0006	-0.0007	-0.0011	3	3	2
0.0027	0.0021	0.0055	-0.0006	0.0004	-0.0016	3	3	3
0.0009	0.0002	0.0008	-0.0001	0.0001	-0.0004	3	3	4
0.0020	0.0017	0.0060	0.0003	-0.0012	-0.0022	3	4	1
0.0037	0.0020	0.0052	-0.0001	-0.0005	-0.0016	3	4	2
0.0019	0.0015	0.0045	-0.0004	0.0002	-0.0015	3	4	3
0.0006	0.0001	0.0003	-0.0000	0.0000	-0.0003	3	4	4
-0.0004	0.0002	0.0021	0.0001	-0.0000	-0.0004	6	1	1
-0.0001	0.0000	0.0012	0.0001	-0.0001	-0.0001	6	1	2
-0.0000	-0.0001	0.0011	0.0000	0.0000	-0.0001	6	1	3
0.0001	0.0002	0.0013	-0.0000	-0.0000	-0.0002	6	1	4
-0.0005	-0.0001	0.0000	-0.0000	-0.0000	-0.0001	6	2	1
-0.0001	0.0001	0.0013	0.0001	-0.0002	-0.0001	6	2	2
0.0001	0.0001	0.0013	0.0000	-0.0001	-0.0003	6	2	3
0.0001	0.0000	0.0007	-0.0000	-0.0000	-0.0000	6	2	4
-0.0002	0.0000	-0.0010	-0.0002	0.0000	-0.0000	6	3	1
0.0001	0.0001	0.0011	-0.0002	-0.0001	0.0000	6	3	2
0.0000	0.0001	0.0002	-0.0001	-0.0001	-0.0003	6	3	3
0.0000	0.0002	0.0005	-0.0000	-0.0001	-0.0002	6	3	4
-0.0000	-0.0002	-0.0006	-0.0002	0.0002	0.0003	6	4	1
0.0001	-0.0001	0.0004	-0.0002	-0.0000	0.0002	6	4	2
-0.0000	-0.0001	-0.0006	-0.0001	-0.0000	0.0000	6	4	3
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0001	6	4	4
-0.0021	-0.0010	-0.0004	0.0013	0.0017	-0.0010	3	-1	-1
-0.0010	0.0002	0.0039	0.0004	-0.0003	0.0000	3	-1	-2

-0.0000	0.0003	0.0024	0.0000	0.0000	-0.0004	3	-1	-3
-0.0055	-0.0034	-0.0092	0.0020	0.0002	0.0040	3	-2	-1
-0.0039	-0.0002	0.0014	0.0009	-0.0003	0.0004	3	-2	-2
-0.0004	0.0003	0.0039	0.0002	-0.0002	-0.0005	3	-2	-3
-0.0056	-0.0038	-0.0039	0.0016	0.0002	0.0046	3	-3	-1
-0.0040	0.0005	-0.0027	0.0009	-0.0003	-0.0011	3	-3	-2
-0.0007	0.0001	0.0023	0.0002	-0.0003	0.0001	3	-3	-3
0.0001	-0.0004	-0.0009	0.0000	-0.0003	0.0004	6	-1	-1
-0.0000	-0.0001	-0.0010	0.0001	0.0001	0.0003	6	-1	-2
-0.0000	-0.0002	-0.0011	0.0000	-0.0000	0.0003	6	-1	-3
0.0002	-0.0002	-0.0010	0.0000	0.0004	0.0002	6	-2	-1
0.0003	-0.0000	-0.0003	-0.0001	0.0001	0.0002	6	-2	-2
0.0000	-0.0002	-0.0003	-0.0001	0.0001	0.0002	6	-2	-3
0.0003	0.0000	0.0003	0.0001	0.0004	-0.0002	6	-3	-1
0.0004	0.0000	0.0004	-0.0001	0.0001	-0.0000	6	-3	-2
0.0001	-0.0001	0.0004	-0.0001	0.0001	0.0001	6	-3	-3
-0.0034	-0.0011	-0.0109	0.0016	-0.0008	0.0024	-3	-1	1
-0.0007	-0.0001	0.0029	0.0004	-0.0004	0.0006	-3	-1	2
0.0001	0.0003	0.0001	-0.0000	-0.0000	-0.0004	-3	-1	3
0.0001	0.0002	0.0004	0.0000	-0.0000	-0.0001	-3	-1	4
-0.0061	-0.0022	-0.0188	0.0013	0.0007	0.0040	-3	-2	1
-0.0033	0.0004	0.0088	0.0009	-0.0004	-0.0010	-3	-2	2
0.0001	0.0010	0.0074	0.0001	-0.0002	-0.0015	-3	-2	3
0.0003	0.0004	0.0028	-0.0000	-0.0001	-0.0005	-3	-2	4
-0.0045	-0.0032	-0.0209	0.0003	0.0011	0.0044	-3	-3	1
-0.0039	-0.0001	0.0004	0.0007	0.0002	0.0003	-3	-3	2
-0.0002	0.0004	0.0026	0.0001	-0.0002	-0.0006	-3	-3	3
0.0003	0.0003	0.0016	0.0000	-0.0001	-0.0002	-3	-3	4
-0.0020	-0.0010	-0.0003	0.0014	0.0038	0.0023	-3	1	-1
-0.0006	-0.0006	0.0007	0.0002	-0.0001	0.0004	-3	1	-2
0.0000	-0.0006	-0.0005	0.0003	0.0000	0.0003	-3	1	-3
-0.0056	-0.0041	-0.0050	0.0017	-0.0001	0.0014	-3	2	-1
-0.0044	-0.0005	0.0036	0.0010	-0.0001	0.0006	-3	2	-2
-0.0009	-0.0018	0.0012	0.0005	-0.0002	0.0010	-3	2	-3
-0.0063	-0.0062	-0.0037	0.0013	0.0017	0.0050	-3	3	-1
-0.0071	-0.0032	-0.0117	0.0005	0.0007	0.0023	-3	3	-2
-0.0026	-0.0031	-0.0090	0.0008	-0.0004	0.0029	-3	3	-3
-0.0027	-0.0032	-0.0043	0.0006	0.0006	0.0014	-3	4	-1
-0.0036	-0.0015	-0.0097	0.0002	0.0005	0.0014	-3	4	-2
-0.0017	-0.0019	-0.0069	0.0005	-0.0002	0.0019	-3	4	-3

Tabla S3a

Expansion coefficients of the 1D-Potential Energy Surface and the kinetic parameter corresponding to the torsion of the methyl group (in cm^{-1})

$V_M(\theta)$	$B_M(\theta)$	M
29.496	5.6470	0
-37.127	0.0003	3
7.631	0.0008	6

Tabla S3b

Expansion coefficients of the 1D-Potential Energy Surface and the kinetic parameter corresponding to the torsion of C-O single bond (in cm^{-1})

$V_L(\alpha)$	$B_L(\alpha)$	L
3054.848	1.4136	0
792.763	0.0574	1
-2053.496	0.2558	2
257.506	0.0273	3
18.266	0.0043	4
-17.705	0.0126	5
12.927	0.0093	6

Tabla S3c

Expansion coefficients of the 1D-Potential Energy Surface and the kinetic parameter corresponding to the torsion of the OH group (in cm^{-1})

$V_K(\beta)$	$B_K(\beta)$	K
1318.880	19.2417	0
-789.858	-0.3256	1
-327.329	-0.1443	2
-120.180	-0.1249	3
-57.448	-0.0498	4
-17.813	-0.0145	5
-6.266	-0.0045	6