Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The Reactions of Formaldehyde Carbonyl Oxide with Methyl Peroxy Radical and Their Relevance in the Chemistry of the Atmosphere.

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(Electronic Supplementary Information)

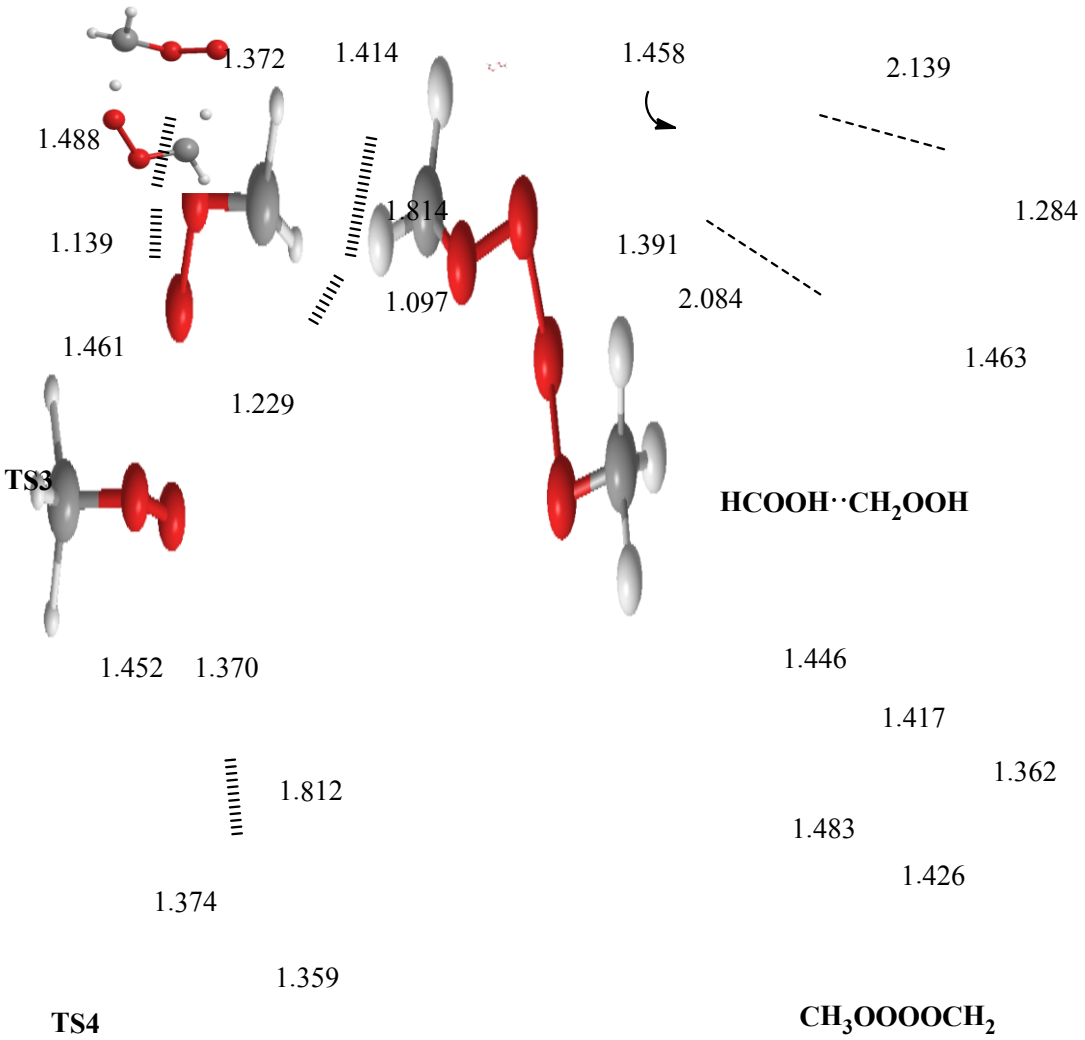
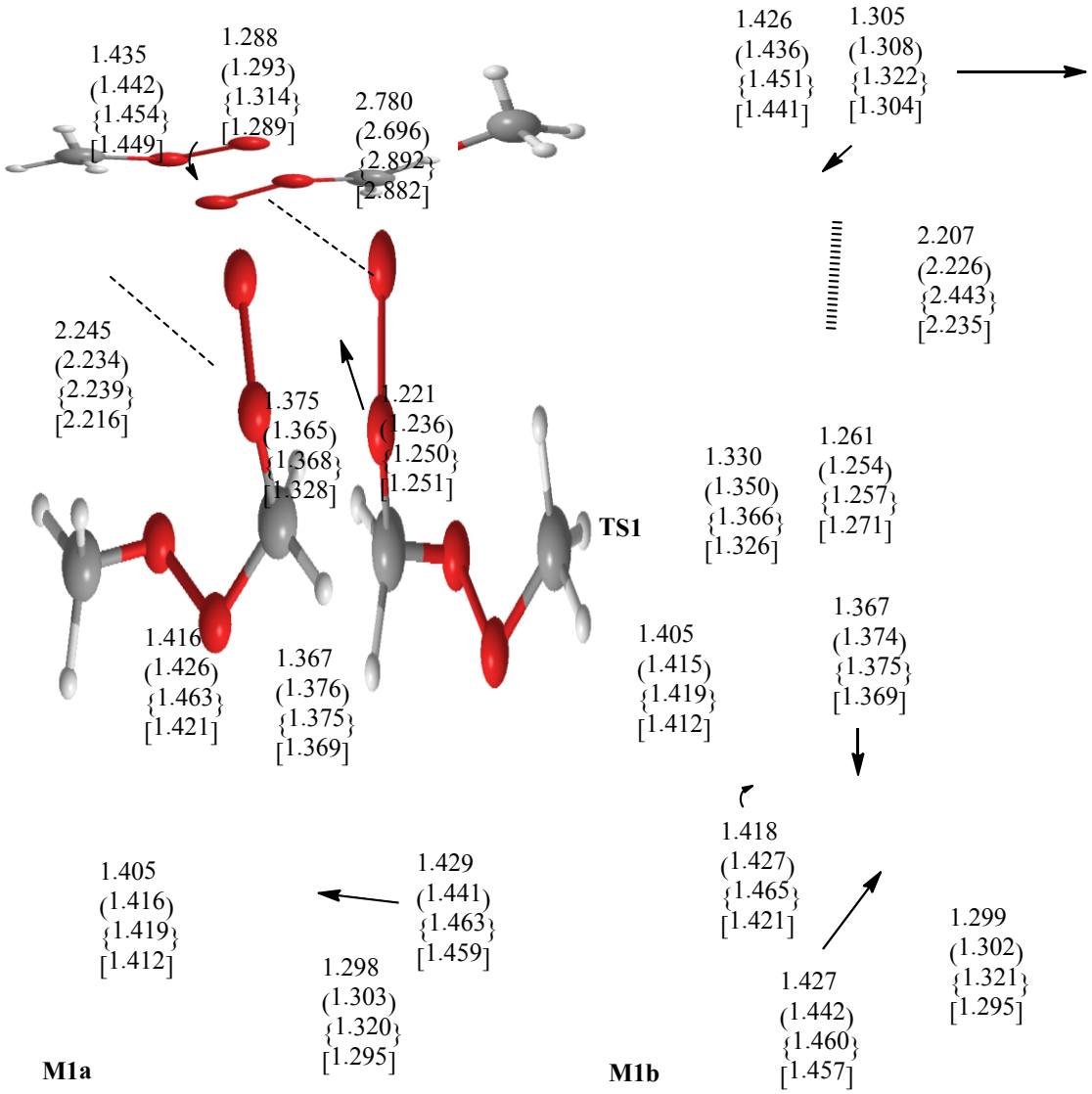


Figure S1: Main geometrical parameters (distances in Angstrom) for some stationary points obtained at CASSCF(13,13)/6-311+G(2df,2p) level of theory.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M1b

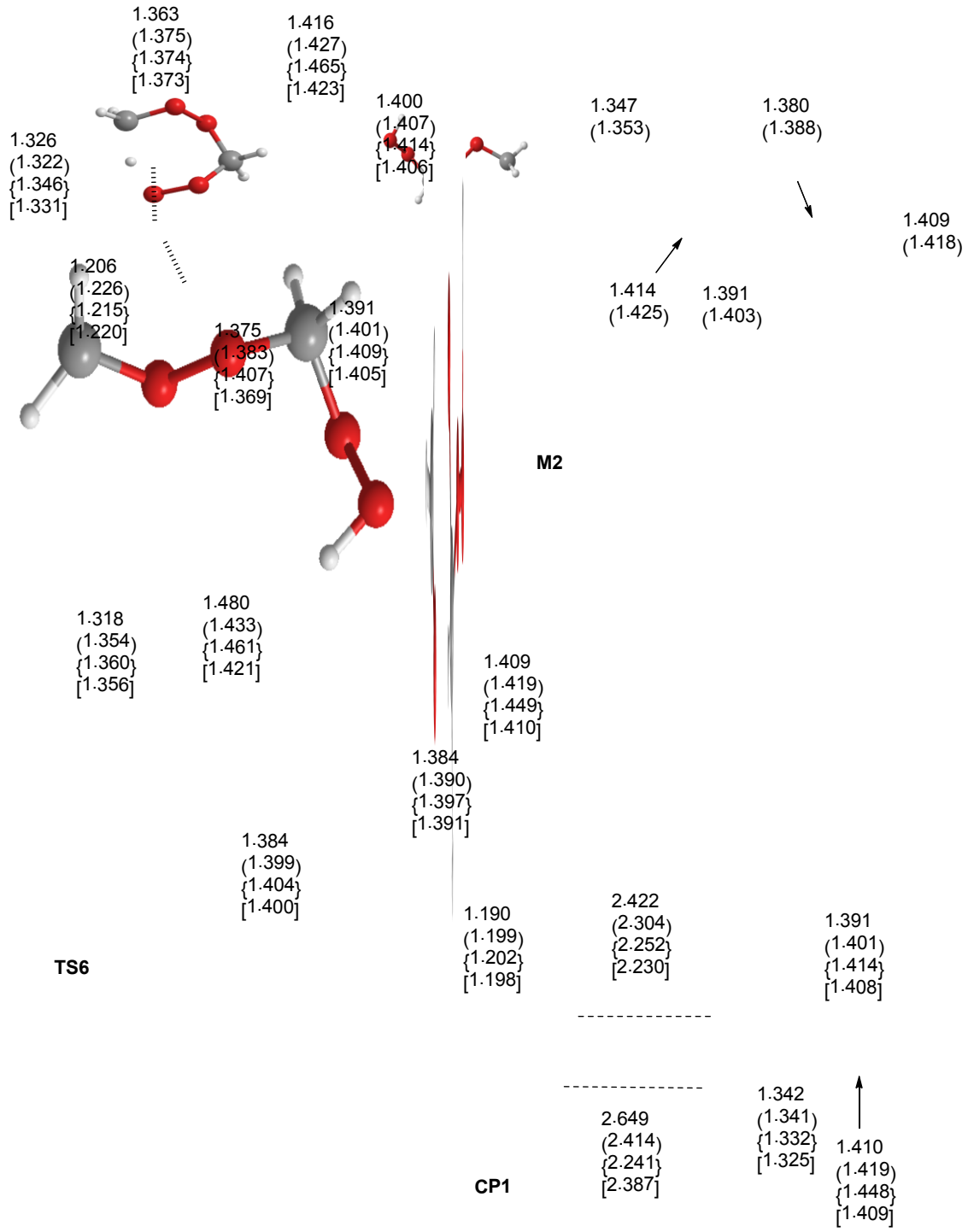

Figure S2: Main geometrical parameters (distances in Angstrom) for some stationary points obtained at BH&HLYP (plain text), M06-2X (in parenthesis), B3LYP (in braces), and M05 in brackets.

Table S1: Single point energies (in hartree) for the optimized energie at multireference levels of theory.

Compound	Optimization Method [a]	CASSCF)/ 6-311+G(2df,2p) [b]	CASSCF)/ Aug-cc-pVTZ [c]	CASPT2/ Aug-cc-pVTZ [d]	CCSD(T)/ Aug-cc-pVTZ [e]
H_2COO	A	-188.768498	-188.7765984	-189.296789	-189.3317084
CH_3OO	A	-189.353421	-189.3615145	-189.920446	-189.9608154
CR1	A	-378.130100	-378.141944	-379.224026	--
CR1	B	--	-378.1395944	-379.227669	--
CR1	C	--	-378.1401056	-379.227201	-379.3033541
TS1	A	-378.111087	-378.1278026	-379.22211	-379.2903932
M1a	A	-378.200826	-378.1976294	-379.295884	-379.3717808
CR2	A	-378.130052	--	--	--
CR2	C	--	-378.1398968	-379.226854	--
TS2	A	-378.110122	-378.1255316	-379.218107	--
M1b	A	-378.201936	-378.1991821	-379.29658	-379.37248
TS4	A	-378.091338	-378.0990598	-379.194322	--
$CH_3OOOOCH_2$	A	-378.095529	-378.1013376	-379.196981	--
TS5	A	-378.105309	-378.1193405	-379.257354	-379.3303606
M2	A	-378.170893	-378.1673363	-379.281428	-379.3550257
TS6	A	-378.168637	-378.1656472	-379.281574	-379.3543071
CP1	A	-378.258625	-378.2494452	-379.340407	-379.4172187

TS3	A	-378.028662	-378.031865	-379.169377	--
HC(OOH)··CH2OOH	A	-378.103162	-378.096316	-379.191542	--
H_2CO	A	-113.987619	-114.0445231	-114.316512	-114.3426329
M3	A	-264.300071	-264.3040702	-265.021503	-265.0698667

a) A stands for optimized geometry at CASSCF(13,13)/6-311+G(2df,2p); B stands for optimized geometry at CASPT2 (13,13)/6-311+G(2df,2p); C stands for optimized geometry at QCISD/6-311+G(2df,2p).
b) Single point CASSCF(n,m)/6-311+G(2df,2p) energies at optimized geometries. (n,m) stands for (13,13) for all stationary points except H_2COO(12,9); CH_3OO (7,6); H_2CO(8,6) and M3(11,11).
c) Single point CASSCF(n,m)/aug-cc-pVTZ energies at optimized geometries. (n,m) stands for (19,15) for all stationary points except H_2COO(12,9); CH_3OO (7,6); H_2CO(8,6) and M3(11,11).
d) Single point CASPT2 energies over a CASSCF(n,m)/aug-cc-pVTZ wave function at optimized geometries. (n,m) stands for (19,15) for all stationary points except H_2COO(12,9); CH_3OO (7,6); H_2CO(8,6) and M3(11,11).
e) Single point UCCSD(T))/aug-cc-pVTZ energies at optimized geometries.

Table S2: Optimized energies (in hartree), obtained using different DFT functional and the aug-cc-pVTZ basis set.

Compound	B3LYP	BH&HLYP	M05	M06-2X
H_2COO	-189.662593	-189.544386	-189.55434	-189.57546
CH_3OO	-190.297724	-190.18894	-190.18409	-190.20980
CR1	-379.967665	-379.742398	-379.74746	-379.797318
TS1	-379.966319	-379.737782	-379.74562	-379.795947
M1a	380.031236	-379.817766	-379.81170	-379.872819
M1b	-380.031642	-379.818543	-379.81217	-379.873252
TS5	-379.991812	-379.767371	-379.76652	-379.83152
M2	(a)	-379.797775	(b)	-379.857679
TS6	(a)	-379.796765	-379.79088	-379.854713
CP1	-380.080102	-379.871041	-379.86603	-379.918754
H_2CO	-114.552147	-114.484475	-114.48187	-114.498984
$CH_2(O)OOH$	-265.523587	-265.382199	-265.37828	-265.413911

a) These species are not found at B3LYP level of theory.
b) Any attempt to optimize M2 leads to a stationary point having an imaginary frequency which involves a rotation of the CH_2 terminal group.

Table S3: Cartesian coordinates (in Angstrom) for the stationary points optimized in this work using the 6-311+G(2df,2p) basis set.

H_2COO CASSCF(12,9)

O	0.0017462527	-0.0009008537	0.0000000000
O	1.3586946040	0.0032534366	0.0000000000
C	1.9517820216	1.1341608270	0.0000000000
H	1.3731490947	2.0337964372	0.0000000000
H	3.0191280269	1.0802701528	0.0000000000

CH_3OO CASSCF(7,6)

O	-1.215903	0.043287	0.000000
O	0.007789	0.582625	0.000000
C	1.001751	-0.481318	0.000000
H	1.953862	0.024593	0.000000
H	0.880196	-1.077971	0.889022
H	0.880196	-1.077971	-0.889022

H_2CO CASSCF(8,6)

C	0.5403033440	-0.0000073769	0.0000007508
O	-0.6752665941	0.0000908180	0.0000702016
H	1.1056482513	0.9287083947	0.0006941032
H	1.1055509987	-0.9287918359	-0.0007650556

M3 ($CH_2(O)OOH$) CASSCF(11,11)

C	6.0	0.7037627367	0.4765988195	0.2505290269
O	8.0	1.3740559720	-0.6745767700	-0.1532632234
H	1.0	0.6104336458	0.4261448316	1.3266967550
H	1.0	1.2720874029	1.3419364553	-0.0603146915
O	8.0	-0.5644191811	0.6415780736	-0.3578957294
O	8.0	-1.4287299975	-0.3828863582	0.2154890358
H	1.0	-1.3840125788	-1.0550250519	-0.4797001733

CR1 CASPT2(13,13)

C	-1.710647	-1.179668	-0.119330
O	-1.879116	0.005543	0.309569
H	-2.081258	-1.949634	0.534366
H	-1.219493	-1.330407	-1.066619
O	1.092093	-1.024576	0.243755
O	1.779357	-0.107367	-0.406370
C	1.709375	1.157906	0.290682
O	-1.430709	1.018748	-0.445273
H	2.347489	1.826099	-0.275020
H	0.678604	1.493818	0.285016
H	2.083994	1.017630	1.298625

CR1 CASSCF(13,13)

C	6.0	-1.8442203502	-1.1666690374	-0.1171531515
O	8.0	-2.1354761002	-0.0465999168	0.3431265624
H	1.0	-2.1831217277	-2.0025666444	0.4578428714
H	1.0	-1.2818205431	-1.2368058176	-1.0247337908
O	8.0	1.3417606486	-1.0796331963	0.2382248145
O	8.0	2.1080881458	-0.1390831024	-0.3319640598
C	6.0	1.8089359697	1.1627057901	0.2665340286
O	8.0	-1.7179656087	1.0595125730	-0.3505089072
H	1.0	2.4452179902	1.8543556421	-0.2618442921
H	1.0	0.7675216153	1.3913470889	0.1152671850
H	1.0	2.0607699602	1.1315286207	1.3146107396

CR1 QCISD

C	6.	-1.749654	-0.927750	-0.146433
O	8.	-1.850841	0.206730	0.389502
H	1.	-2.146262	-1.749140	0.431335
H	1.	-1.283146	-1.013346	-1.117765
O	8.	1.027870	-1.201268	0.219745
O	8.	1.802403	-0.359371	-0.437817
C	6.	1.861066	0.910609	0.246921
O	8.	-1.341407	1.261508	-0.307589
H	1.	2.537094	1.519709	-0.346108
H	1.	0.862207	1.337178	0.273203
H	1.	2.257435	0.747654	1.245680

TS1 CASSCF(13,13)

C	1.4250392959	0.8880814085	0.0215722187
O	1.5535871453	-0.3222869923	0.5132320513

H	1.6307912289	1.6592620027	0.7295740848
H	1.4289739096	1.0106031726	-1.0382961154
O	-0.7913350642	1.3213215074	0.0674587668
O	-1.3302071550	0.2300538937	-0.6008196078
C	-1.8919387191	-0.6731239136	0.3811333430
O	1.5028366233	-1.3317742170	-0.3730415592
H	-2.2812068015	-1.4947439216	-0.1991503192
H	-1.1240106055	-1.0190576797	1.0538304688
H	-2.6869858576	-0.1802352606	0.9206096683

M1a CASSCF(13,13)

C	-0.8345830094	0.9846927174	0.1063398171
O	-1.4836591317	-0.1397509383	-0.5314359885
H	-1.2544980011	1.8656215896	-0.3497046717
H	-1.0046052613	0.9251723902	1.1654103804
O	0.5300754879	1.0304435901	-0.2065206202
O	1.1678586663	-0.0025812731	0.6211807857
C	1.9902758757	-0.7566172024	-0.2848615145
O	-1.7315293307	-1.1123957696	0.3695971874
H	2.4832462893	-1.4840097116	0.3426549937
H	1.3817143575	-1.2488389451	-1.0288019496
H	2.7187430576	-0.1114004471	-0.7536064198

CR2 CASSCF(13,13)

C	1.844136	-1.088432	0.261868
O	2.041324	-0.064299	-0.419229
H	2.086949	-2.013371	-0.217516
H	1.444121	-0.997613	1.249964
O	-1.380718	-1.095933	0.356875
O	-2.084303	-0.210310	-0.362282
C	-1.853619	1.137554	0.160058
O	1.738182	1.148179	0.143857
H	-2.217161	1.186129	1.174050
H	-0.802663	1.365791	0.104631
H	-2.430447	1.778826	-0.486643

CR2 QCISD

C	1.614080	-0.988409	0.299781
O	1.801437	-0.004022	-0.461157
H	1.743577	-1.958183	-0.156709
H	1.337995	-0.813613	1.329878
O	-1.210495	-1.187580	0.122297
O	-1.955096	-0.234872	-0.404182
C	-1.664536	1.038295	0.214330
O	1.621140	1.235262	0.079948
H	-1.962072	0.990354	1.259052
H	-0.603069	1.252373	0.115085
H	-2.269574	1.759444	-0.327222

TS2 CASSCF(13,13)

C	1.151493	-0.997849	-0.332771
O	1.538697	0.238008	-0.573019
H	0.737481	-1.484586	-1.186648
H	1.546175	-1.495959	0.524871
O	-0.876787	-0.879549	0.644492
O	-1.768247	-0.395825	-0.309423
C	-1.928103	1.027316	-0.096717
O	2.248502	0.838844	0.393508
H	-2.317166	1.210515	0.893060
H	-0.987156	1.535052	-0.237773
H	-2.642132	1.334364	-0.845192

M1b CASSCF(13,13)

C	0.7815734179	-0.9732492840	-0.0577756901
O	1.3834438034	0.1981905419	-0.6503817884
H	0.5836124082	-1.6271188231	-0.8890485397
H	1.4581469267	-1.3921600431	0.6658050987
O	-0.3910953350	-0.6723190172	0.6458875774
O	-1.4058149708	-0.3884289813	-0.3797771130
C	-2.0115108997	0.8516581980	0.0221710958
O	1.9939903738	0.9207304885	0.3127012225
H	-2.4462843746	0.7529727243	1.0057911914
H	-1.2859567440	1.6508526915	0.0035546408
H	-2.7838226059	1.0236875044	-0.7126126955

TS4 CASSCF(13,13)

C	-2.2982550747	0.1652908748	-0.1575183873
O	-1.1947325923	-0.7719378192	-0.0533474064
O	-0.5609889432	-0.5653461781	1.1434550404
O	0.6148512551	0.7888702685	0.8882007516
O	1.2523209885	0.5334038415	-0.3016422266
C	2.2564190637	-0.3675011973	-0.1377226212
H	-1.9151216418	1.1735799702	-0.1787969632
H	-2.7779296369	-0.0825581496	-1.0911535806
H	-2.9746894009	0.0260389177	0.6715659897
H	2.6818374598	-0.4336750518	0.8415070421
H	2.8475475226	-0.4545354767	-1.0253496385

$CH_3OOOOCH_2$ CASSCF(13,13)

C	-2.4729695502	0.2190707065	-0.0449772133
O	-1.3650117463	-0.6374724075	-0.4060757569
O	-0.4443976888	-0.6196197534	0.6706717942
O	0.4316891284	0.5594404057	0.4676082653
O	1.3863895945	0.1922083065	-0.5254838959
C	2.4139381174	-0.4751409837	0.0691818092
H	-2.1406503073	1.2418736004	0.0527557267
H	-3.1602314193	0.1248628447	-0.8711857383
H	-2.9292972995	-0.1272815830	0.8705289164
H	2.6924490384	-0.1452816227	1.0504300913
H	3.1573761329	-0.7379175135	-0.6556779987

TS3 CASSCF(13,13)

C	-0.1534984605	-0.1123435848	0.0208288548
O	0.1348823184	-0.1077673988	1.3620173775
H	0.7256440093	-0.1335489583	-0.6024867311
H	-0.9120420672	-0.8514196967	-0.1781947728
O	1.3134660246	0.6190184583	1.6469055488
H	0.3135501110	2.1254744056	1.7986456327
C	-0.6736001622	2.5891036961	1.9216804860
O	-1.4461068829	2.7549653970	0.9806221440
H	-1.0829640073	2.8887787292	2.8709382600
O	-0.8957462179	2.3785952969	-0.3190821794
H	-0.6536754249	1.2712654684	-0.2021862494

HC(OOH)···CH_2OOH CASSCF(13,13)

C	0.5587445792	-0.3837149071	-0.3287030739
O	-0.2592258371	-0.0724355990	0.7518571701
H	1.5179700320	-0.7902873695	-0.0810598996
H	-0.0254362235	-0.7943651600	-1.1286300826
O	0.6041391392	0.2818732876	1.8721554845
H	0.3728206895	1.2055810175	1.9657401132
C	-0.5736874302	3.1157394323	1.7935328495
O	-1.6325268581	3.3938420799	1.1229885314
H	-0.3159844061	4.0767154756	2.2412084583
O	-2.1904362161	2.2415676460	0.4147888556
H	-1.5402824688	1.5634460966	0.5876375935

TS5 CASCF(13,13)

C	0.8896001088	-1.0224034338	0.2269142309
O	-0.4529411119	-0.9469179914	0.7389334641
O	1.2647836250	0.1085054209	-0.4595579075
O	1.0493700514	1.2501811093	0.3632130515
H	1.4785707949	-1.1940663903	1.1163618605
H	0.9796812300	-1.8253345280	-0.4878359453
O	-1.2571904959	-0.3286562869	-0.3116020420
C	-1.3687769604	1.0075507359	0.0815146614
H	-1.7714322637	1.1360231761	1.0740503915
H	-1.8636330779	1.5519264976	-0.7040196291
H	-0.1326408923	1.4031726646	0.2058564460

M2 CASSCF(13,13)

C	0.8332920057	-0.9132408702	0.1959645727
O	-0.3983560251	-0.5851838440	0.8182181042
O	1.4196483509	0.1674750476	-0.4887426924
O	1.8653534797	1.1147252458	0.5371373626
H	1.4597633325	-1.2438824100	1.0077414208
H	0.6870945950	-1.6729801152	-0.5538249343
O	-1.3613874123	-0.4000381487	-0.2645476518
C	-1.9455619126	0.8437174774	-0.0783788338
H	-2.0833845083	1.1503474295	0.9399942278

H	-2.7186875497	0.9953129272	-0.8049093900
H	1.2000946588	1.7799226903	0.4572293091

TS6 CASSCF(13,13)

C	-0.6065124747	0.9351565989	0.0427607142
O	0.4710087634	0.2390878065	0.6428421256
O	-1.4921159570	0.0902725769	-0.6549723627
O	-2.1816829278	-0.7120482910	0.3580571037
H	-1.1058266169	1.4175758160	0.8672176826
H	-0.2466898502	1.6328209875	-0.6950716706
O	1.3442562277	-0.2011474863	-0.5021221152
C	2.6266195663	-0.2771816867	-0.0280111461
H	2.8954584645	0.3836748466	0.7676330807
H	3.1233634622	-1.2123887176	-0.1920962825
H	-1.6831130824	-1.5127378084	0.3150084014

CP1 CASSCF(13,13)

C	-0.7469097026	0.4313990078	-0.0016838687
O	-0.1613561140	-0.3648073736	0.9768635806
O	-1.9833515931	-0.0730465638	-0.4688166506
O	-2.9289301560	0.0922961826	0.6398526112
H	-0.8727140123	1.4203689826	0.4160496466
H	-0.0978426477	0.4462562032	-0.8650527804
O	2.6070711648	0.3587917510	-1.1318688215
C	3.2535596106	-0.0711220204	-0.2007317463
H	2.7823091847	-0.3833630474	0.7326994467
H	4.3406436945	-0.1661340748	-0.2522968904
H	-2.9798320927	-0.7957203295	0.9560637948

Table S4: Cartesian coordinates (in Amstrongs) for the optimizes stationary points using density functional methods.

Optimized at B3LYP/aug-cc-pVTZ

H_2COO

O	-1.177922	-0.202791	0.000000
O	0.000000	0.458950	0.000000
C	1.069980	-0.194863	0.000000
H	1.029606	-1.277362	0.000000
H	1.973891	0.397261	0.000000

CH_3OO

O	-1.217582	0.061370	0.000000
O	0.000000	0.564641	0.000000
C	1.002457	-0.479057	0.000000
H	1.959417	0.036976	0.000000
H	0.883249	-1.085362	0.895426
H	0.883249	-1.085362	-0.895426

CR1

C	-1.634106	-1.054025	-0.045351

O	-1.926802	0.078605	0.394125
H	-1.887469	-1.882959	0.601049
H	-1.163184	-1.150035	-1.014449
O	1.255186	-1.184762	-0.009026
O	2.098581	-0.208865	-0.259431
C	1.628547	1.069063	0.250494
O	-1.610744	1.172332	-0.364006
H	2.326697	1.801895	-0.145507
H	0.610736	1.245892	-0.096450
H	1.672249	1.040951	1.337955

TS1

C	1.581577	0.915080	-0.013026
O	1.646267	-0.188872	0.584005
H	1.789803	1.784160	0.593675
H	1.395835	0.936442	-1.077689
O	-0.828543	1.274639	0.162280
O	-1.384244	0.295444	-0.531264
C	-1.941528	-0.723345	0.338257
O	1.393127	-1.319129	-0.139760
H	-2.424448	-1.430608	-0.330629
H	-1.131523	-1.199583	0.883184
H	-2.660779	-0.256127	1.007072

M1a

C	-0.810237	0.967785	0.115344
O	-1.458906	-0.169746	-0.537662
H	-1.254295	1.862806	-0.319753
H	-0.993312	0.864018	1.182946
O	0.523765	1.025325	-0.211561
O	1.213039	0.027406	0.605918
C	2.008208	-0.741151	-0.283923
O	-1.919127	-1.047427	0.334530
H	2.534099	-1.438000	0.368436
H	1.390307	-1.288832	-0.996418
H	2.729498	-0.111847	-0.807606

M1b

C	0.891416	-0.954800	0.236684
O	-0.271481	-0.510760	0.820155
O	1.661111	0.121278	-0.380401
O	2.274742	0.851215	0.533771
H	1.491727	-1.377510	1.039701
H	0.706486	-1.649123	-0.581938
O	-1.225312	-0.261713	-0.263599
C	-1.823026	0.994091	0.016735
H	-2.334266	0.978352	0.980597
H	-2.551904	1.124053	-0.783090
H	-1.087549	1.798961	-0.011282

TS5

C	0.879115	-1.032328	0.235644
O	-0.432354	-0.930016	0.753956
O	1.293996	0.126817	-0.447129
O	1.075744	1.261580	0.360232
H	1.479130	-1.242628	1.125252
H	0.964915	-1.817275	-0.518557
O	-1.249488	-0.317389	-0.295928
C	-1.393242	0.999513	0.071838
H	-1.784252	1.146958	1.078562
H	-1.902087	1.527411	-0.729833
H	-0.116086	1.417339	0.209790

CP1

C	-0.543178	0.664503	0.124918
O	0.032909	0.221910	1.241497
O	-1.465558	-0.208114	-0.497740
O	-2.611409	-0.334201	0.379328
H	-1.028021	1.635670	0.342534
H	0.230306	0.849522	-0.649707
O	2.385349	0.467768	-1.178896
C	2.742030	-0.216110	-0.256959
H	2.060339	-0.465987	0.578752
H	3.767343	-0.621782	-0.199733
H	-2.357463	-1.098259	0.917085

H_2CO

C	0.000000	0.000000	-0.527125
O	0.000000	0.000000	0.673102
H	0.000000	0.939180	-1.111032
H	0.000000	-0.939180	-1.111032

$CH_2(O)OOH$

C	0.705111	0.446503	0.225992
O	1.346308	-0.664769	-0.136348
H	0.640272	0.432722	1.332446
H	1.273775	1.347562	-0.060799
O	-0.576657	0.653391	-0.331737
O	-1.452072	-0.373685	0.190006
H	-1.353558	-1.067954	-0.478019

Optimized at BH&HLYP/aug-cc-pVTZ

H_2COO

O	-1.162741	-0.235300	0.000000
O	0.000000	0.460664	0.000000
C	1.053343	-0.163876	0.000000
H	1.026710	-1.240566	0.000000
H	1.955161	0.420914	0.000000

CH_3OO

O	-1.197529	0.067369	0.000000
O	0.000000	0.555844	0.000000
C	0.983868	-0.475870	0.000000
H	1.937939	0.028978	0.000000
H	0.869541	-1.079730	0.888509
H	0.869541	-1.079730	-0.888509

CR1

C	-1.644436	-0.828730	-0.046187
O	-1.776589	0.274812	0.460398
H	-1.889069	-1.673857	0.572294
H	-1.306308	-0.909982	-1.064069
O	1.094765	-1.297422	-0.123303
O	2.042324	-0.451737	-0.336338
C	1.760985	0.837655	0.226787
O	-1.441735	1.366229	-0.306233
H	2.544987	1.481982	-0.140148
H	0.784822	1.172839	-0.096632
H	1.807019	0.760724	1.304105

TS1

C	1.433885	0.878973	0.041785
O	1.442919	-0.302104	0.482957
H	1.599085	1.644169	0.772630
H	1.442796	1.036999	-1.017961
O	-0.740033	1.256146	-0.009329
O	-1.257744	0.200955	-0.576423
C	-1.838068	-0.675217	0.387288
O	1.289331	-1.278217	-0.406755
H	-2.212235	-1.514768	-0.177521
H	-1.081815	-0.998164	1.085576
H	-2.642578	-0.160672	0.893854

M1a

C	-0.800338	0.962618	0.108771
O	-1.413634	-0.158304	-0.531733
H	-1.236297	1.846785	-0.334072
H	-0.993804	0.876652	1.167956
O	0.534336	1.027269	-0.179598
O	1.190892	0.046832	0.604086
C	1.957407	-0.736385	-0.275816
O	-1.752202	-1.084762	0.311973
H	2.471169	-1.442361	0.362061
H	1.325816	-1.262649	-0.980270
H	2.679694	-0.125359	-0.803106

M1b

C	0.871772	-0.939814	0.224202
O	-0.301933	-0.562492	0.814606
O	1.568763	0.161024	-0.356816

O	2.143389	0.888454	0.553540
H	1.484100	-1.360538	1.007707
H	0.706699	-1.621737	-0.597811
O	-1.236037	-0.303471	-0.220150
C	-1.764380	0.977138	0.015921
H	-2.242466	1.021819	0.986634
H	-2.502281	1.117784	-0.762013
H	-0.995682	1.735876	-0.058486

TS5

C	0.866805	-1.016801	0.232249
O	-0.435198	-0.916258	0.735284
O	1.269708	0.132286	-0.437063
O	1.062242	1.238504	0.357634
H	1.466948	-1.221871	1.111468
H	0.951317	-1.799048	-0.512018
O	-1.232174	-0.326789	-0.274224
C	-1.373156	0.986607	0.075175
H	-1.771655	1.139978	1.068990
H	-1.866560	1.513699	-0.725276
H	-0.122886	1.409672	0.211607

M2

C	0.824072	-0.892104	0.195035
O	-0.391525	-0.563829	0.786032
O	1.421895	0.159856	-0.469220
O	1.858502	1.099186	0.486612
H	1.432955	-1.232770	1.022440
H	0.691409	-1.657558	-0.558354
O	-1.329190	-0.368564	-0.254135
C	-1.947503	0.813877	-0.068272
H	-2.039232	1.165738	0.941123
H	-2.708102	0.977978	-0.805516
H	1.144587	1.734365	0.490138

TS6

C	-0.607350	0.907716	0.039944
O	0.447296	0.231509	0.628822
O	-1.482500	0.083244	-0.645022
O	-2.185321	-0.694254	0.296844
H	-1.108697	1.398698	0.865349
H	-0.253613	1.613710	-0.700162
O	1.366017	-0.156309	-0.465268
C	2.577523	-0.308754	0.027605
H	2.935540	0.389401	0.758342
H	3.099608	-1.203473	-0.249777
H	-1.643736	-1.478403	0.364570

CP1

C	-0.646610	0.410958	0.016168

O	-0.082581	-0.315569	0.993005
O	-1.851524	-0.089130	-0.467554
O	-2.820766	0.060165	0.544920
H	-0.781683	1.424233	0.403383
H	0.027855	0.447708	-0.839677
O	2.434703	0.397952	-1.106029
C	3.047181	-0.067692	-0.197750
H	2.550433	-0.402982	0.717051
H	4.135500	-0.179397	-0.239663
H	-2.799860	-0.791327	0.977224

H_2CO

C	0.000000	0.000000	-0.521398
O	0.000000	0.000000	0.666069
H	0.000000	0.930412	-1.100085
H	0.000000	-0.930412	-1.100085

$CH_2(O)OOH$

C	0.694461	0.453254	0.232994
O	1.347891	-0.653727	-0.147826
H	0.615769	0.419175	1.322617
H	1.262300	1.338108	-0.055346
O	-0.561161	0.627981	-0.340743
O	-1.417938	-0.356317	0.189609
H	-1.358145	-1.054703	-0.459764

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H_2COO

O	-1.161095	-0.230328	0.000000
O	-0.008760	0.460499	0.000000
C	1.059049	-0.168076	0.000000
H	1.024426	-1.251768	0.000000
H	1.958853	0.431510	0.000000

CH_3OO

O	-1.201211	0.063156	0.000000
O	-0.002839	0.560933	0.000000
C	0.988872	-0.475947	0.000000
H	1.949410	0.031411	0.000000
H	0.864564	-1.081346	0.894908
H	0.864564	-1.081346	-0.894908

CR1

C	-1.452329	-0.730484	-0.009358
O	-1.615799	0.353969	0.560127
H	-1.560709	-1.615100	0.603962
H	-1.228776	-0.740067	-1.069725
O	1.144416	-1.438841	-0.157394
O	2.068191	-0.538603	-0.245327

C	1.594303	0.760566	0.163352
O	-1.455670	1.487702	-0.183213
H	2.425465	1.437713	-0.007828
H	0.720028	1.039072	-0.423987
H	1.337644	0.716585	1.220067

TS1

C	1.429722	0.859676	0.044476
O	1.353310	-0.313693	0.481459
H	1.653978	1.619006	0.779319
H	1.403403	1.020270	-1.024383
O	-0.751282	1.306011	0.025333
O	-1.212820	0.234821	-0.567589
C	-1.782560	-0.677144	0.383923
O	1.084113	-1.276785	-0.426116
H	-2.030538	-1.569566	-0.181538
H	-1.042325	-0.898959	1.147087
H	-2.669459	-0.215537	0.814131

M1a

C	-0.782419	0.985844	0.113081
O	-1.315238	-0.154638	-0.589179
H	-1.254785	1.861401	-0.327586
H	-1.004701	0.846028	1.169244
O	0.564906	1.121507	-0.128815
O	1.234890	0.134686	0.652009
C	1.870313	-0.745037	-0.257250
O	-1.468538	-1.179782	0.199567
H	2.412772	-1.445239	0.375214
H	1.138031	-1.276616	-0.864738
H	2.567809	-0.197818	-0.891296

M1b

C	0.854037	-0.959564	0.216190
O	-0.332832	-0.657938	0.838243
O	1.472648	0.211405	-0.353491
O	1.922602	0.998062	0.581013
H	1.512687	-1.355028	0.986181
H	0.714918	-1.630694	-0.629536
O	-1.278210	-0.364213	-0.189867
C	-1.693057	0.973442	0.015408
H	-2.141148	1.086635	1.002252
H	-2.441794	1.148468	-0.754857
H	-0.857907	1.663467	-0.104201

TS5

C	0.869832	-1.023824	0.234228
O	-0.435105	-0.914123	0.749110
O	1.267241	0.134385	-0.445793
O	1.072424	1.236576	0.365718

H	1.481515	-1.224496	1.115777
H	0.944628	-1.809943	-0.517964
O	-1.224760	-0.325645	-0.283132
C	-1.373678	0.993726	0.072482
H	-1.781083	1.135617	1.072923
H	-1.875555	1.518418	-0.734261
H	-0.130066	1.419289	0.214740

M2

C	0.829138	-0.940640	0.191544
O	-0.395795	-0.724615	0.840891
O	1.287493	0.171437	-0.500310
O	1.573553	1.190892	0.443366
H	1.501294	-1.221101	1.003734
H	0.737603	-1.717327	-0.568132
O	-1.356063	-0.441209	-0.172816
C	-1.730884	0.852684	-0.047325
H	-1.821377	1.238261	0.959301
H	-2.405955	1.145563	-0.836637
H	0.738860	1.682230	0.452267

TS6

C	-0.598455	0.920314	-0.007704
O	0.456647	0.245257	0.615538
O	-1.483780	0.064579	-0.652069
O	-2.162090	-0.681717	0.345733
H	-1.089208	1.450964	0.808635
H	-0.228733	1.586220	-0.787167
O	1.295328	-0.259627	-0.430369
C	2.574737	-0.250672	0.011787
H	2.756476	0.138149	0.999204
H	3.190353	-0.999215	-0.460590
H	-1.566510	-1.431168	0.478247

CP1

C	-0.613583	0.536608	0.018177
O	-0.008110	-0.046552	1.063440
O	-1.715019	-0.161079	-0.494392
O	-2.728296	-0.132586	0.499178
H	-0.915988	1.549297	0.335916
H	0.104533	0.628417	-0.812008
O	2.382480	0.442082	-1.099299
C	2.908712	-0.145568	-0.196094
H	2.339853	-0.465894	0.691420
H	3.984268	-0.385333	-0.219627
H	-2.526202	-0.924474	1.014367

H_2CO

C	-0.001136	0.000634	0.003418
O	0.001560	-0.000203	1.199260

H	0.936988	-0.000215	-0.576426
H	-0.940391	0.002247	-0.574635

$CH_2(O)OOH$

C	0.688035	0.454451	0.228626
O	1.309974	-0.671362	-0.155097
H	0.616877	0.417282	1.329287
H	1.276174	1.336957	-0.058968
O	-0.578948	0.658240	-0.333588
O	-1.430557	-0.351565	0.181861
H	-1.298377	-1.070235	-0.450580

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H_2COO

O	-1.163987	-0.202695	0.000000
O	-0.024404	0.448947	0.000000
C	1.062114	-0.179485	0.000000
H	1.050251	-1.262722	0.000000
H	1.948499	0.437792	0.000000

CH_3OO

O	-1.207907	0.076829	0.000000
O	-0.009667	0.559372	0.000000
C	0.989817	-0.480330	0.000000
H	1.945654	0.036118	0.000000
H	0.872732	-1.087564	0.894779
H	0.872731	-1.087564	-0.894779

CR1

C	-1.705039	-0.861399	-0.054310
O	-1.839844	0.286963	0.422754
H	-2.068777	-1.664420	0.570634
H	-1.249651	-0.991079	-1.027777
O	1.143238	-1.296404	-0.093972
O	2.044810	-0.424906	-0.391617
C	1.795791	0.865423	0.219955
O	-1.402969	1.334941	-0.265186
H	2.572895	1.515322	-0.171319
H	0.800012	1.209577	-0.057707
H	1.886297	0.758494	1.299219

TS1

C	1.463361	0.894577	0.020609
8	1.506017	-0.279909	0.503423
H	1.636113	1.685755	0.733634
H	1.440561	1.023395	-1.051472
O	-0.742939	1.253026	0.033560
O	-1.283012	0.226555	-0.561929
C	-1.877089	-0.688839	0.379780

O	1.349944	-1.295899	-0.333665
H	-2.283694	-1.492710	-0.226161
H	-1.110803	-1.065996	1.051239
H	-2.662915	-0.171856	0.927084

M1a

C	-0.789902	0.970286	0.120366
O	-1.400242	-0.159909	-0.571191
H	-1.239173	1.863147	-0.310903
H	-1.003320	0.841793	1.179757
O	0.547221	1.065638	-0.159941
O	1.238706	0.100478	0.620233
C	1.946499	-0.738378	-0.268773
8	-1.752416	-1.107216	0.238537
H	2.497004	-1.411917	0.385317
H	1.271068	-1.309655	-0.907041
H	2.647596	-0.163930	-0.876110

M1b

C	0.863645	-0.950082	0.218693
O	-0.314250	-0.605161	0.824882
O	1.574093	0.191665	-0.342661
O	2.101326	0.929161	0.582640
H	1.486987	-1.384412	0.996733
H	0.716887	-1.607536	-0.636497
O	-1.275465	-0.338416	-0.187912
C	-1.749780	0.976164	0.016138
H	-2.204606	1.081182	1.002428
H	-2.509762	1.107150	-0.752300
H	-0.957131	1.714326	-0.114810

TS5

C	0.871523	-1.025163	0.235856
O	-0.437234	-0.920725	0.740112
O	1.291799	0.138039	-0.430190
O	1.074877	1.243582	0.347989
H	1.465134	-1.248383	1.126022
H	0.963347	-1.801251	-0.526608
O	-1.230576	-0.320701	-0.276883
C	-1.382178	0.997649	0.075035
H	-1.777264	1.152967	1.079257
H	-1.899660	1.509347	-0.730376
H	-0.124376	1.414618	0.203615

TS6

C	-0.579931	0.884336	-0.013898
O	0.472991	0.218435	0.623820
O	-1.500429	0.047120	-0.635262
O	-2.246163	-0.627484	0.352468
H	-1.043984	1.451454	0.794012

H	-0.212867	1.525576	-0.815296
O	1.320479	-0.318917	-0.382214
C	2.610404	-0.202913	0.018991
H	2.799477	0.105339	1.033149
H	3.261201	-0.862317	-0.532600
H	-1.736414	-1.437545	0.478073

CP1

C	-0.565823	0.631049	0.116724
O	-0.008168	0.237289	1.251912
O	-1.504938	-0.241035	-0.465385
O	-2.641946	-0.297238	0.364791
H	-1.023895	1.624832	0.284609
H	0.213181	0.763484	-0.659749
O	2.362277	0.449592	-1.164376
C	2.795162	-0.202067	-0.257279
H	2.169225	-0.497883	0.607700
H	3.847609	-0.541877	-0.232208
H	-2.430036	-1.031229	0.954338

H_2CO

C	-0.000713	0.000593	0.010396
O	0.000881	-0.000140	1.205701
H	0.934974	-0.000228	-0.583663
H	-0.938120	0.002237	-0.580817

$CH_2(O)OOH$

C	0.697971	0.439359	0.223358
O	1.337744	-0.663445	-0.138369
H	0.641578	0.424397	1.329936
H	1.261503	1.342979	-0.060635
O	-0.582222	0.644571	-0.322549
O	-1.446558	-0.348872	0.172957
H	-1.326837	-1.065218	-0.463155