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

The Atmospheric Oxidation of CH_3OOH by OH radical.

The effect of water vapor

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(Supplementary information)

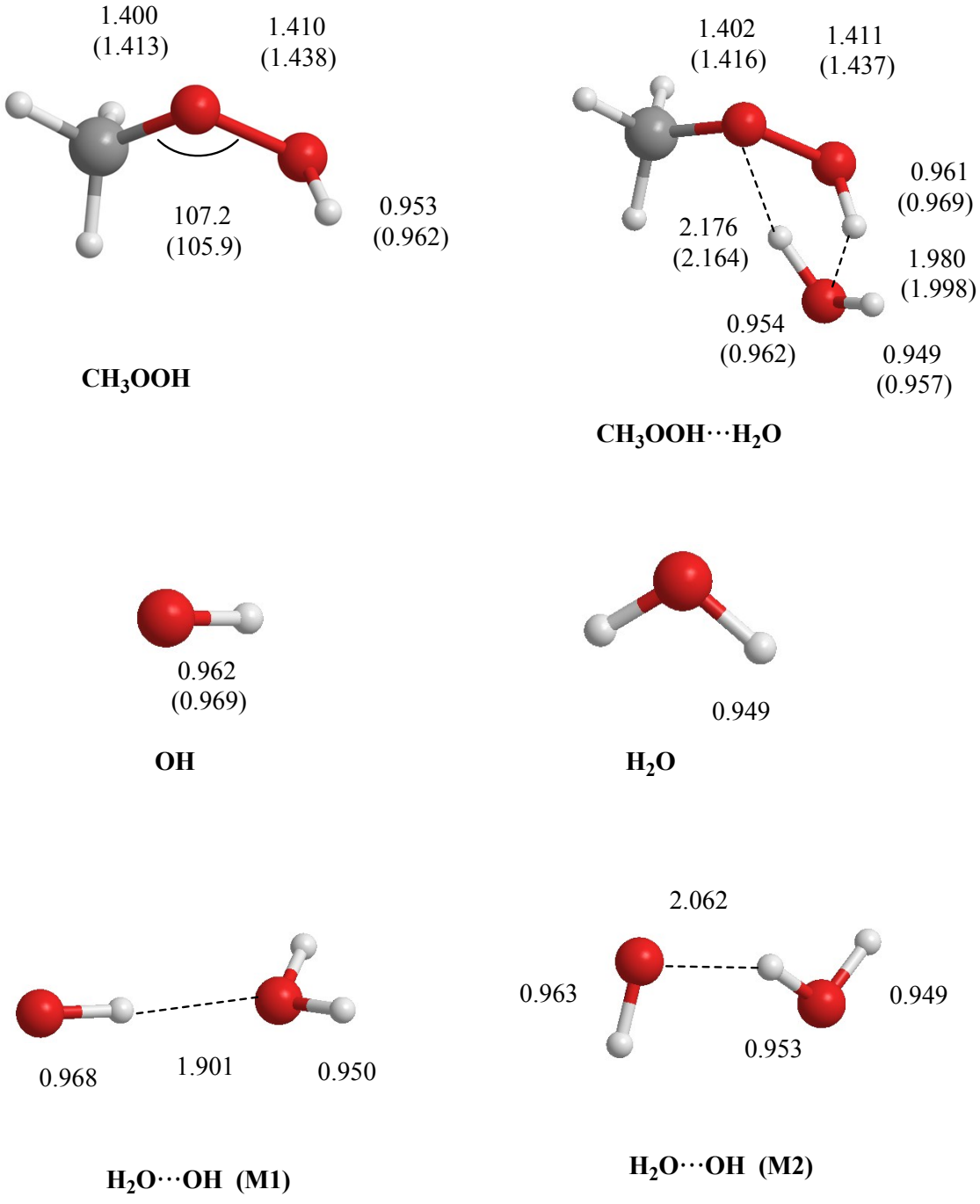

Figure S1 : Selected geometrical parameters (distances in Å, and angles in °) for the optimized structures of the reactants. Plain values obtained at BH&HLYP/6-311+G(2df,2p). Values in parenthesis optimized at QCISD/6-311+G(2df,2p)

Table S1: Calculated equilibrium constant (K_{eq} in cm^3 $molec^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the $CH_3OOH\cdots H_2O$, $H_2O\cdots OH$ (**M1**), and $H_2O\cdots OH$ (**M2**). The rate constants for the decomposition of the complexes into the reactants (in s^{-1}) are also give in each case.[a]

	$CH_3OOH\cdots H_2O$		$H_2O\cdots OH$ (**M1**)		$H_2O\cdots OH$ (**M2**)	
T	K_{eqa}	k_{-a}	K_{eqb}	k_{-b}	K_{eqc}	k_{-c}

275	.53175E-20	.24449E+15	.85660E-20	.50447E+14	.12968E-20	.33304E+15
280	.45089E-20	.29908E+15	.75569E-20	.59319E+14	.12195E-20	.36727E+15
290	.33034E-20	.43775E+15	.59659E-20	.80728E+14	.10869E-20	.44255E+15
298	.26187E-20	.58301E+15	.50009E-20	.10151E+15	.99849E-21	.50794E+15
300	.24763E-20	.62538E+15	.47930E-20	.10730E+15	.97846E-21	.52506E+15
310	.18951E-20	.87137E+15	.39118E-20	.14046E+15	.88875E-21	.61741E+15
325	.13134E-20	.13826E+16	.29613E-20	.20392E+15	.78088E-21	.77224E+15

a) Calculated according to the conventional transition state theory.

CH3OOH + OH

Table S2: Calculated, at different temperatures (T, in Kelvin) of the equilibrium constant (K_{eq} in cm^3 $molec^{-1}$) for the pre-reactive complexes, tunneling factor (Γ), rate constant (k_{uni} in s-1) of the unimolecular decomposition of the reactive complexes into the products, and the bimolecular rate constant (k_t =Keq· Γ ·k_{uni}, in cm^3 $molec^{-1}\cdot s^{-1}$)for the four elementary reactions in the oxidation of CH_3OOH by OH.

T	K_{eq}	Γ	k_{uni}	k_t
CH_3OOH + OH → ACR1 →ATS1a →ACP1				
275.00	6.22e-22	2.81	2.23e+09	3.90e-12
280.00	5.35e-22	2.70	2.54e+09	3.67e-12
290.00	4.01e-22	2.50	3.27e+09	3.28e-12
298.00	3.23e-22	2.37	3.94e+09	3.02e-12
300.00	3.06e-22	2.34	4.12e+09	2.96e-12
310.00	2.38e-22	2.21	5.12e+09	2.69e-12
325.00	1.69e-22	2.02	6.92e+09	2.36e-12
CH_3OOH + OH → ACR2 →ATS1b →ACP1				
275.00	8.51e-23	2.66	3.68e+09	8.33e-13
280.00	7.47e-23	2.55	4.00e+09	7.62e-13
290.00	5.84e-23	2.36	4.67e+09	6.43e-13
298.00	4.86e-23	2.23	5.25e+09	5.68e-13
300.00	4.64e-23	2.19	5.40e+09	5.48e-13
310.00	3.75e-23	2.05	6.19e+09	4.76e-13
325.00	2.79e-23	1.88	7.46e+09	3.91e-13
CH_3OOH + OH → ACR1 →ATS2a →ACP2				
275.00	6.22e-22	2.39	1.37e+09	2.04e-12
280.00	5.35e-22	2.31	1.54e+09	1.90e-12
290.00	4.01e-22	2.15	1.92e+09	1.65e-12
298.00	3.23e-22	2.04	2.27e+09	1.50e-12
300.00	3.06e-22	2.02	2.36e+09	1.46e-12
310.00	2.38e-22	1.91	2.86e+09	1.30e-12
325.00	1.69e-22	1.78	3.73e+09	1.12e-12
CH_3OOH + OH → ACR2 →ATS2b →ACP2				

275.00	8.51e-23	2.06	1.40e+09	2.46e-13
280.00	7.47e-23	2.00	1.53e+09	2.29e-13
290.00	5.84e-23	1.89	1.81e+09	2.00e-13
298.00	4.86e-23	1.81	2.06e+09	1.81e-13
300.00	4.64e-23	1.78	2.13e+09	1.76e-13
310.00	3.75e-23	1.70	2.47e+09	1.57e-13
325.00	2.79e-23	1.59	3.04e+09	1.35e-13

Table S3: Calculated and fitted overall rate constants ($k_{tot} = k_{5a}+k_{5b}$, in cm^3 $molec^{-1}\cdot s^{-1}$) and branching ratios, at different temperatures (T in K) for reactions 5a and 5b (Γ_{5a} and Γ_{5b}, in %) obtained from the calculated and fitted rate constants.

T	calc k_{tot}	fitted k_{tot}	Calc. Γ_{5a}	Calc Γ_{5b}	Fitted Γ_{5a}	Fitted Γ_{5b}
275.00	7.03e-12	7.00e-12	67.43	32.57	67.43	32.57
280.00	6.56e-12	6.56e-12	67.53	32.47	67.63	32.37
290.00	5.77e-12	5.79e-12	67.94	32.06	67.88	32.12
298.00	5.27e-12	5.28e-12	68.12	31.88	68.12	31.88
300.00	5.14e-12	5.16e-12	68.09	31.91	68.22	31.78
310.00	4.63e-12	4.63e-12	68.47	31.53	68.47	31.53
325.00	4.00e-12	3.99e-12	68.75	31.25	68.67	31.33

Table S4: Kinetic equations S1 – S11 according to Scheme 2 of the main text. [M1] stands for the concentration of the M1 complex of the $H_2O\cdots OH$

$d[CH_3OOH]/dt =$ $- ka[CH_3OOH][H_2O] + k\_a[CH_3OOH\cdot\cdot H_2O]$ (S1)

$d[H_2O] /dt =$ $- ka[CH_3OOH][H_2O]+ k\_a[CH_3OOH\cdot\cdot H_2O]- kb[OH][H_2O] + k\_b[M1]$ (S2)

$d[OH]/dt =$ $- k1[CH_3OOH\cdot\cdot H_2O][OH] + k\_1[BCR1] - kb[OH][H_2O] + k\_b[M1]$ (S3)

$d[CH_3OOH\cdot\cdot H_2O]/dt =$ $- k1[CH_3OOH\cdot\cdot H_2O][OH] + k\_1[BCR1 + ka[CH_3OOH][H_2O] - k\_a[CH_3OOH\cdot\cdot H_2O]$ (S4)

$d[H_2O\cdots OH\ (M1)]/dt =$ $- k\_b[M1] + kb[OH][H_2O]+ k\_4[BCR1] - k4[CH_3OOH][M1] + k\_5[BCR2] - k5[CH_3OOH][M1]+ k\_6[BCR3] - k6[CH_3OOH][M1]$ (S5)

$d[BCR1]/dt =$ $k1[CH_3OOH\cdot\cdot H_2O][OH] - k\_1[BCR1] - k2[BCR1] + k\_2[BCR2] - k\_4[BCR1] + k4[CH_3OOH] [M1]$ (S6)

$d[BCR2]/dt =$ $k2[BCR1]- k\_2[BCR2]- k3[BCR2] + k\_3[BCR3] - k\_5[BCR2] + k5*[CH_3OOH] [M1] - k7[BCR2] - k8*[BCR2]$ (S7)

$$d[BCR3]/dt = k3[BCR2] - k\_3[BCR3] - k\_6[BCR3] + k6[CH_3OOH]\,[M1] - k9[BCR3] \quad (S8)$$

$$d[P1]/dt = + k7[BCR2] \quad (S9)$$

$$d[P2]/dt = + k8[BCR2] \quad (S10)$$

$$d[P3]/dt = + k9[BCR3] \quad (S11)$$

Table S5: Kinetic equations S12 – S25 according to Scheme 3 of the main text. [M2] stands for the concentration of the M2 complex of the $H_2O\cdots OH$

$$d[CH_3OOH]/dt = -ka[CH_3OOH][H_2O] + k\_a[CH_3OOH\cdot\cdot H_2O] \quad (S12)$$

$$d[H_2O]/dt = -ka[CH_3OOH][H_2O]] + k\_a[CH_3OOH\cdot\cdot H_2O] - kc[H_2O]][OH] + k\_c[M2] \quad (S13)$$

$$d[OH]/dt = -k1[CH3OOH\cdot\cdot H2O]*OH + k\_1*[BCR4] - kc[H2O]]*OH + k\_c[M2] \quad (S14)$$

$$d[CH_3OOH\cdot\cdot H_2O]/dt = -k1[CH_3OOH\cdot\cdot H_2O][OH] + k\_1*[BCR4] + ka[CH_3OOH][H_2O]] - k\_a[CH_3OOH\cdot\cdot H_2O] \quad (S15)$$

$$d[M2]/dt = kc[H2O][OH] - k\_c[M2] - k6[CH_3OOH][M2] + k\_6[BCR5] - k7[CH3OOH][M2] + k\_7[BCR7] - k8[CH_3OOH][M2] + k\_8[BCR8] - k9[CH3OOH][M2] + k\_9[BCR6] \quad (S16)$$

$$d[BCR4]/dt = k1[CH3OOH\cdot\cdot H2O][OH] - k\_1[BCR4] - k2[BCR4] + k\_2[BCR5] \quad (S17)$$

$$d[BCR5]/dt = k2[BCR4] - k\_2[BCR5] - k3[BCR5] + k\_3[BCR6] - k4[BCR5] + k\_4[BCR7] - k\_6[BCR5] + k6[CH_3OOH][M2] \quad (S18)$$

$$d[BCR6]/dt = k3[BCR5] - k\_3[BCR6] - k\_9[BCR6] + k9[CH3OOH][M2] - k10[BCR6] - k11[BCR6] \quad (S19)$$

$$d[BCR7]/dt = k4[BCR5] - k\_4[BCR7] - k5[BCR7] + k\_5[BCR8] - k\_7[BCR7] + k7[CH_3OOH][M2] - k12[BCR7] \quad (S20)$$

$$d[BCR8]/dt = k5[BCR7] - k\_5[BCR8] - k\_8[BCR8] + k8[CH3OOH][M2] - k13[BCR7] \quad (S21)$$

$$d[P1]/dt = k10[BCR6] \quad (S22)$$

$$d[P2]/dt = k11[BCR6] \quad (S23)$$

$$d[P3]/dt = k12[BCR7] \quad (S24)$$

d[P4]/dt = k13[BCR8] (S25)

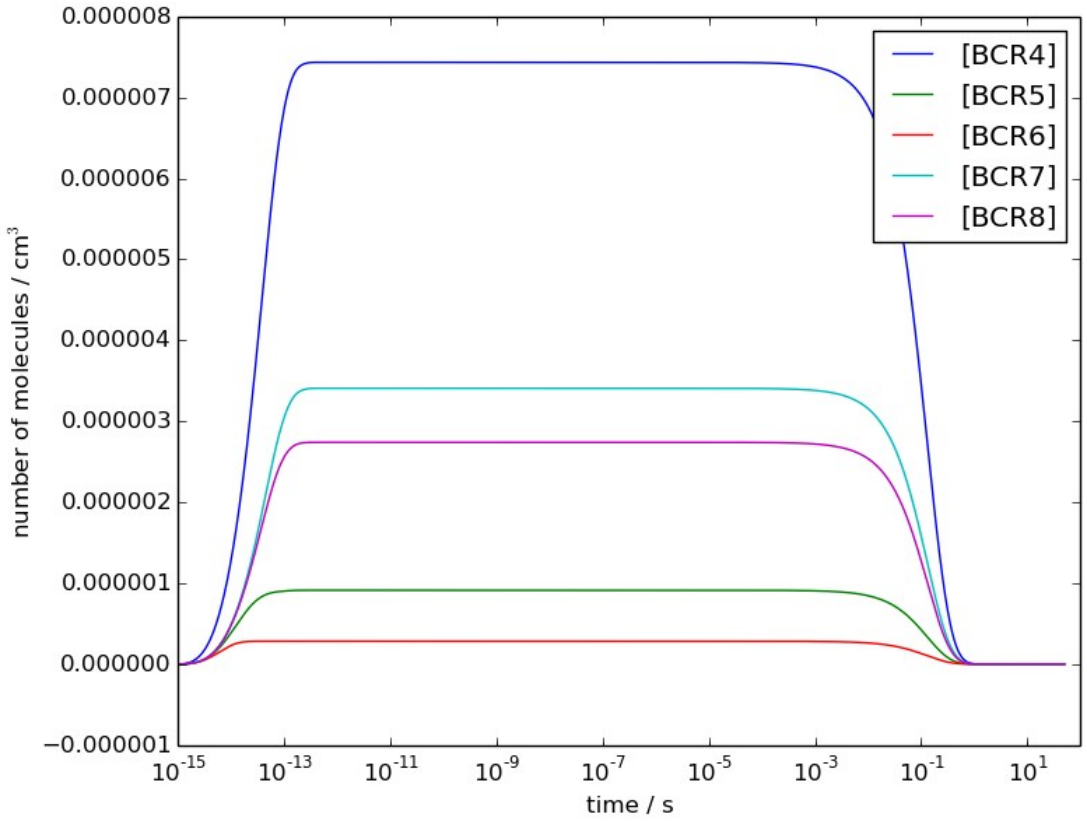

Figure S2 : Concentration of the **BCR4 – BCR8** pre-reactive complexes as a function of time in the steady state regime. For the numerical integration we have used [OH]=2 x 10^6 molecule·cm^{-3}, [CH_3OOH] = 6.45 x 10^{10} molecule·cm^{-3}, Temperatures ranging from 275 to 325 K and the water concentrations corresponding to RH of 20%, 40%, 60%, 80%, and 100% for each ttemperature.

Table S6: Calculated equilibrium constant (K_{eq} in cm^3 $molec^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the complexes from scheme 2 of the main text.. The rate constants for the decomposition of the complexes into the reactants (in s^{-1}) are also give in each case.[a, b]

T	K_{eq1}	K_{-1}	k_{eq4}	k_{-4}	k_{eq5}	k_{-5}	k_{eq6}	k-6
275	3.45e-21	3.77e+14	7.13e-22	1.83e+15	3.89e-20	3.35e+13	1.24e-20	1.05e+14
280	2.99e-21	4.50e+14	5.95e-22	2.27e+15	2.94e-20	4.60e+13	9.81e-21	1.38e+14
290	2.29e-21	6.32e+14	4.22e-22	3.43e+15	1.72e-20	8.41e+13	6.33e-21	2.29e+14
298	1.87e-21	8.15e+14	3.27e-22	4.68e+15	1.15e-20	1.33e+14	4.56e-21	3.36e+14
300	1.78e-21	8.67e+14	3.07e-22	5.05e+15	1.05e-20	1.48e+14	4.21e-21	3.68e+14
310	1.42e-21	1.17e+15	2.29e-22	7.23e+15	6.58e-21	2.51e+14	2.88e-21	5.74e+14
325	1.03e-21	1.76e+15	1.53e-22	1.19e+16	3.47e-21	5.24e+14	1.71e-21	1.06e+15

a) Calculated according to the conventional transition state theory.

b) The corresponding values for the $CH_3OOH + H_2O \leftrightarrow CH_3OOH\cdots H_2O$ and $H_2O\cdot\cdot OH \leftrightarrow H_2O\cdots OH$ (M1) are listed in Table S1

Table S7: Calculated rate constants (in s^{-1}) computed at different Temperatures (T in Kelvin) for the unimolecular reactions described in Scheme 2.

T	k_2	k_{-2}	k_3	k_{-3}	k_7	k_8	k_9
275	1.85e+12	3.35e+10	5.92e+11	1.72e+11	7.71e+08	7.39e+09	3.61e+09
280	1.87e+12	3.74e+10	6.21e+11	1.79e+11	8.32e+08	7.82e+09	3.83e+09
290	1.90e+12	4.61e+10	6.79e+11	1.93e+11	9.63e+08	8.75e+09	4.30e+09
298	1.93e+12	5.40e+10	7.28e+11	2.05e+11	1.08e+09	9.54e+09	4.71e+09
300	1.93e+12	5.61e+10	7.40e+11	2.08e+11	1.11e+09	9.75e+09	4.82e+09
310	1.97e+12	6.75e+10	8.02e+11	2.22e+11	1.28e+09	1.08e+10	5.37e+09
325	2.01e+12	8.73e+10	8.98e+11	2.43e+11	1.56e+09	1.26e+10	6.29e+09

Table S8: Calculated equilibrium constant (K_{eq} in cm^3 $molec^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the complexes from scheme 3 of the main text.. The rate constants for the decomposition of the complexes into the reactants (in s^{-1}) are also give in each case.[a, b]

T	K_{eq1}	k_{-1}	K_{eq6}	k_{-6}	K_{eq7}	k_{-7}	K_{eq8}	k_{-8}	K_{eq9}	k_{-9}
275	1.03e-19	1.26e+13	6.38e-20	2.04e+13	2.94e-19	4.43e+12	2.69e-19	4.85e+12	1.72e-20	7.59e+13
280	9.00e-20	1.49e+13	4.76e-20	2.84e+13	2.11e-19	6.40e+12	1.90e-19	7.10e+12	1.33e-20	1.02e+14
290	7.01e-20	2.06e+13	2.73e-20	5.30e+13	1.13e-19	1.29e+13	9.93e-20	1.46e+13	8.22e-21	1.76e+14
298	5.82e-20	2.61e+13	1.80e-20	8.50e+13	7.03e-20	2.18e+13	6.09e-20	2.51e+13	5.73e-21	2.67e+14
300	5.57e-20	2.77e+13	1.63e-20	9.54e+13	6.27e-20	2.48e+13	5.41e-20	2.87e+13	5.25e-21	2.95e+14
310	4.49e-20	3.67e+13	1.01e-20	1.65e+14	3.63e-20	4.57e+13	3.07e-20	5.39e+13	3.46e-21	4.78e+14
325	3.35e-20	5.41e+13	5.17e-21	3.52e+14	1.71e-20	1.07e+14	1.40e-20	1.30e+14	1.95e-21	9.35e+14

Table S9: Calculated rate constants (in s^{-1}) computed at different Temperatures (T in Kelvin) for the unimolecular reactions described in Scheme 3.

# T	k_2	k_{-2}	k_3	k_{-3}	k_4	k_{-4}	k_5	k_{-5}	k_{10}	k_{11}	k_{12}	k_{13}
275	4.50e+11	1.00e+12	1.19e+11	4.61e+11	3.46e+12	7.83e+11	3.09e+12	3.23e+12	2.72e+09	4.12e+09	9.42e+07	8.34e+07
280	4.51e+11	1.06e+12	1.24e+11	4.62e+11	3.43e+12	8.06e+11	3.08e+12	3.27e+12	2.94e+09	4.33e+09	1.09e+08	9.80e+07
290	4.53e+11	1.19e+12	1.34e+11	4.63e+11	3.38e+12	8.54e+11	3.08e+12	3.34e+12	3.39e+09	4.78e+09	1.21e+08	1.33e+08
298	4.55e+11	1.30e+12	1.42e+11	4.65e+11	3.34e+12	8.91e+11	3.07e+12	3.39e+12	3.78e+09	4.25e+09	1.49e+08	1.67e+08
300	4.56e+11	1.33e+12	1.44e+11	4.65e+11	3.34e+12	9.01e+11	3.07e+12	3.41e+12	3.88e+09	4.33e+09	1.57e+08	1.77e+08
310	4.59e+11	1.47e+12	1.54e+11	4.66e+11	3.29e+12	9.47e+11	3.06e+12	3.48e+12	4.40e+09	4.70e+09	2.01e+08	2.31e+08
325	4.61e+11	1.69e+12	1.70e+11	4.68e+11	3.24e+12	1.02e+12	3.05e+12	3.57e+12	5.23e+09	5.27e+09	2.82e+08	3.35e+08

Table S10: Computed rate constants (in $cm^3 \cdot molecule^{-1} \cdot s^{-1}$) for the oxidation of CH_3OOH by OH without water vapor and including the effect of water vapor at different relative humidity (% RH), and different temperatures (T in Kelvin)

T	No water (0%RH)	20%RH	40%RH	60%RH	80%RH	100%RH
	Reaction 5a+w: $CH_3OOH + OH (+H_2O) \rightarrow CH_3O_2 + H_2O (+ H_2O)$					
275	4.74×10^{-12}	4.85×10^{-12}	4.96×10^{-12}	5.07×10^{-12}	5.19×10^{-12}	5.30×10^{-12}
280	4.43×10^{-12}	4.55×10^{-12}	4.66×10^{-12}	4.77×10^{-12}	4.88×10^{-12}	5.00×10^{-12}
290	3.92×10^{-12}	4.03×10^{-12}	4.14×10^{-12}	4.25×10^{-12}	4.36×10^{-12}	4.47×10^{-12}
298	3.59×10^{-12}	3.70×10^{-12}	3.80×10^{-12}	3.91×10^{-12}	4.02×10^{-12}	4.13×10^{-12}
300	3.50×10^{-12}	3.61×10^{-12}	3.72×10^{-12}	3.83×10^{-12}	3.94×10^{-12}	4.05×10^{-12}
310	3.17×10^{-12}	3.28×10^{-12}	3.39×10^{-12}	3.49×10^{-12}	3.60×10^{-12}	3.71×10^{-12}
325	2.75×10^{-12}	2.86×10^{-12}	2.97×10^{-12}	3.07×10^{-12}	3.18×10^{-12}	3.28×10^{-12}
	Reaction 5b+w: $CH_3OOH + OH (+H_2O) \rightarrow CH_2OOH + H_2O (+ H_2O)$					
275	2.29×10^{-12}	2.30×10^{-12}	2.30×10^{-12}	2.31×10^{-12}	2.32×10^{-12}	2.33×10^{-12}
280	2.13×10^{-12}	2.13×10^{-12}	2.14×10^{-12}	2.15×10^{-12}	2.16×10^{-12}	2.17×10^{-12}
290	1.85×10^{-12}	1.86×10^{-12}	1.87×10^{-12}	1.88×10^{-12}	1.89×10^{-12}	1.90×10^{-12}
298	1.68×10^{-12}	1.69×10^{-12}	1.70×10^{-12}	1.71×10^{-12}	1.72×10^{-12}	1.73×10^{-12}
300	1.64×10^{-12}	1.65×10^{-12}	1.66×10^{-12}	1.67×10^{-12}	1.68×10^{-12}	1.69×10^{-12}
310	1.46×10^{-12}	1.47×10^{-12}	1.49×10^{-12}	1.50×10^{-12}	1.51×10^{-12}	1.52×10^{-12}
325	1.25×10^{-12}	1.27×10^{-12}	1.28×10^{-12}	1.30×10^{-12}	1.31×10^{-12}	1.32×10^{-12}
	(Reaction 5a+w) + (Reaction 5b+w)					
275	7.02×10^{-12}	7.14×10^{-12}	7.26×10^{-12}	7.38×10^{-12}	7.51×10^{-12}	7.63×10^{-12}
280	6.56×10^{-12}	6.68×10^{-12}	6.80×10^{-12}	6.92×10^{-12}	7.04×10^{-12}	7.16×10^{-12}
290	5.77×10^{-12}	5.89×10^{-12}	6.02×10^{-12}	6.14×10^{-12}	6.26×10^{-12}	6.38×10^{-12}
298	5.26×10^{-12}	5.38×10^{-12}	5.50×10^{-12}	5.62×10^{-12}	5.74×10^{-12}	5.86×10^{-12}
300	5.14×10^{-12}	5.26×10^{-12}	5.38×10^{-12}	5.50×10^{-12}	5.62×10^{-12}	5.74×10^{-12}
310	4.63×10^{-12}	4.75×10^{-12}	4.87×10^{-12}	4.99×10^{-12}	5.11×10^{-12}	5.23×10^{-12}
325	4.01×10^{-12}	4.13×10^{-12}	4.25×10^{-12}	4.37×10^{-12}	4.49×10^{-12}	4.61×10^{-12}

Table S11. Increase (in percent) of the rate constant of Reaction 5a at different temnperatures (T in Kelvin), and relative humidity (%RH).

T	20%RH	40%RH	60%RH	80%RH	100%RH
275.00	2.39	4.78	7.17	9.55	11.93
280.00	2.54	5.07	7.60	10.12	12.65
290.00	2.83	5.66	8.48	11.30	14.11
298.00	3.06	6.12	9.17	12.21	15.25
300.00	3.13	6.25	9.37	12.47	15.57
310.00	3.41	6.82	10.21	13.59	16.96
325.00	3.89	7.76	11.60	15.43	19.24

Table S12. Increase (in percent) of the rate constant of Reaction 2 at different temnperatures (T in Kelvin), and relative humidity (%RH).

T	20%RH	40%RH	60%RH	80%RH	100%RH
275.00	0.33	0.66	0.99	1.32	1.65
280.00	0.39	0.78	1.17	1.56	1.95
290.00	0.52	1.03	1.55	2.07	2.58
298.00	0.60	1.20	1.79	2.39	2.99
300.00	0.63	1.26	1.89	2.52	3.15
310.00	0.81	1.62	2.42	3.23	4.03
325.00	1.13	2.25	3.37	4.49	5.60

Table S13. Increase (in percent) of the rate constant of Reaction 1 plus Reaction 2 at different temnperatures (T in Kelvin), and relative humidity (%RH).

T	20%RH	40%RH	60%RH	80%RH	100%RH
275.00	1.72	3.44	5.15	6.87	8.58
280.00	1.84	3.68	5.51	7.35	9.18
290.00	2.09	4.17	6.26	8.33	10.41
298.00	2.28	4.55	6.82	9.08	11.34
300.00	2.33	4.66	6.99	9.30	11.61
310.00	2.59	5.18	7.75	10.32	12.88
325.00	3.02	6.03	9.03	12.01	14.97

Table S14. Absolute energies, enthalpy and free energy corrections (in hartree) and ZPE (in Kcal/mol) and S (in Cal/Mol·Kelvin) [a,b]

Compound	E(QCISD)	ZPE	H	G	S	E(HF)/B1	E(CCSD(T))/B1	E(HF)/B2	E(CCSD(T))/B2
H_2O	-76.32100	13.63	0.02551	0.00410	45.0	-76.06063	-76.34228	-76.06602	-76.36358
CH_3OOH	-190.54940	34.92	0.06085	0.03030	64.3	-189.88092	-190.60555	-189.89298	-190.65514
OH	-75.62855	5.39	0.01190	-0.00832	42.6	-75.42167	-75.64557	-75.42667	-75.66449
ACR1	-266.18717	42.13	0.07493	0.03617	81.6	-265.30780	-266.26117	-265.32474	-266.32941
ACR2	-266.18643	41.88	0.07483	0.03378	86.4	-265.30784	-266.26004	-265.32477	-266.32820
ATS1a	-266.17519	39.14	0.06926	0.03284	76.7	-265.26911	-266.25071	-265.28595	-266.31894
ATS1b	-266.02416	39.66	0.07000	0.03362	76.6	-265.26693	-266.25252	-265.28376	-266.32073
ATS2a	-266.17277	39.91	0.07013	0.03473	74.5	-265.26914	-266.25036	-265.28604	-266.31895
ATS2b	-266.17241	39.82	0.07004	0.03453	74.7	-265.26886	-266.25010	-265.28576	-266.31866
$CH_3OOH\cdot\cdot H_2O$	-266.88183	50.87	0.08924	0.05043	81.7	-265.94841	-266.96002	-265.96578	-267.03062

a) Geometries optimized and characterized at QCISD/6-311+G(2df,2p). The ZPE and enthalpic and entropic corrections are obtained at this level of theory.

b) B1 stands for aug-cc-pVTZ; B2 stands for aug-cc-pVQZ basis sets.

Table S15. Absolute energies, enthalpy and free energy corrections (in hartree) and ZPE (in Kcal/mol) and S (in Cal/Mol·Kelvin) [a,b]

Compound	E(BH&HLYP)	ZPE	H	G	S	E(HF)/B1	E(CCSD(T))/B1	E(HF)/B2	E(CCSD(T))/B2
CH_2OOH	-190.15560	26.65	0.04767	0.01674	65.1	-189.25280	-189.93743	-189.26502	-189.98652
CH_3OO	-190.18128	28.04	0.04943	0.01905	63.9	-189.28184	-189.95979	-189.29408	-190.00836
H_2O	-76.41851	13.94	0.02599	0.00461	45.0	-76.06105	-76.34201	-76.06648	-76.36338
H_2CO	-114.48040	17.37	0.03148	0.00671	52.1	-113.91520	-114.34187	-113.92273	-114.37162
CH_3OOH	-190.81746	35.81	0.06223	0.03177	64.1	-189.88295	-190.60402	-189.89516	-190.65395
OH	-75.73240	5.55	0.01216	-0.00805	42.5	-75.42187	-75.64546	-75.42688	-75.66442
ACR1	-266.55905	43.14	0.07649	0.03791	81.2	-265.30993	-266.25951	-265.32703	-266.32814
ATS1a	-266.54416	39.73	0.07024	0.03369	76.9	-265.27565	-266.24852	-265.29269	-266.31718
ACP1	-266.60671	43.69	0.07790	0.03738	85.3	-265.34557	-266.31023	-265.36315	-266.37989
ACR2	-266.55831	43.05	0.07649	0.03638	84.4	-265.31048	-266.25811	-265.32762	-266.32670
ATS1b	-266.54442	40.03	0.07074	0.03413	77.1	-265.27489	-266.24907	-265.29195	-266.31779
ATS2a	-266.54215	40.63	0.07135	0.03569	75.0	-265.26848	-266.24920	-265.28555	-266.31823
ACP2	-266.58536	42.56	0.07649	0.03470	88.0	-265.32119	-266.29133	-265.33873	-266.36146
ATS2b	-266.54193	40.55	0.07127	0.03546	75.4	-265.26824	-266.24892	-265.28531	-266.31794
$CH_3OOH\cdots H_2O$	-267.24708	52.05	0.09108	0.05238	81.4	-265.95082	-266.95816	-265.96836	-267.02920
$H_2O\cdots OH$ **M1**	-152.16086	21.54	0.04040	0.00841	67.3	-151.49003	-151.99686	-151.50043	-152.03708
$H_2O\cdots OH$ **M2**	-152.15677	20.91	0.03994	0.00633	70.7	-151.48643	-151.99332	-151.49684	-152.03350

BCR1	-342.98909	59.50	0.10545	0.05894	97.9	-341.37828	-342.61306	-341.40120	-342.70347
TSBCR1BCR2	-342.98884	59.12	0.10430	0.05937	94.6	-341.37900	-342.61347	-341.40143	-342.70313
BCR2	-342.99498	59.91	0.10563	0.06076	94.4	-341.38288	-342.61926	-341.40529	-342.70888
TSBCR2BCR3	-342.99227	59.37	0.10447	0.06015	93.3	-341.38106	-342.61676	-341.40343	-342.70639
BCR3	-342.99252	59.62	0.10549	0.05896	97.9	-341.38105	-342.61660	-341.40346	-342.70629
BTS1a	-342.97532	55.92	0.09878	0.05553	91.0	-341.34118	-342.60524	-341.36350	-342.69485
BCP1	-343.03557	59.48	0.10651	0.05638	105.5	-341.41465	-342.66267	-341.43755	-342.75331
BTS1b	-342.97643	56.15	0.09898	0.05617	90.1	-341.34162	-342.60656	-341.36392	-342.69615
BCP2	-343.03704	59.77	0.10663	0.05832	101.7	-341.41587	-342.66366	-341.43882	-342.75431
BTS1c	-342.97395	56.23	0.09943	0.05537	92.7	-341.34063	-342.60409	-341.36298	-342.69384
BCP3	-343.03724	59.77	0.10665	0.05762	103.2	-341.41367	-342.66473	-341.43662	-342.75547
BCR4	-342.98948	59.08	0.10533	0.05508	105.8	-341.37986	-342.61352	-341.40225	-342.70318
TSBCR4BCR5	-342.98948	59.06	0.10440	0.05752	98.7	-341.37982	-342.61348	-341.40222	-342.70312
BCR5	-342.99239	59.53	0.10542	0.05899	97.7	-341.38094	-342.61641	-341.40335	-342.70609
TSBCR5BCR6	-342.99037	59.28	0.10428	0.06034	92.5	-341.37979	-342.61403	-341.40228	-342.70382
BCR6	-342.99038	59.35	0.10527	0.05820	99.1	-341.37969	-342.61421	-341.40217	-342.70399
TSBCR5BCR7	-342.99210	59.18	0.10434	0.05981	93.7	-341.38080	-342.61674	-341.40318	-342.70636
BCR7	-342.99420	59.62	0.10547	0.05971	96.3	-341.38248	-342.61842	-341.40490	-342.70805
TSBC7BCR8	-342.99417	59.42	0.10445	0.06029	92.9	-341.38260	-342.61834	-341.40503	-342.70800
BCR8	-342.99477	59.79	0.10554	0.06038	95.0	-341.38285	-342.61914	-341.40525	-342.70874

BTS2a	-342.97917	57.68	0.10104	0.05915	88.2	-341.34552	-342.60871	-341.36790	-342.69858
BCP4	-343.01964	59.66	0.10563	0.06047	95.0	-341.39023	-342.65066	-341.41297	-342.74164
BTS2b	-342.97830	57.67	0.10111	0.05899	88.7	-341.34508	-342.60768	-341.36748	-342.69753
BCP5	-343.01881	59.38	0.10545	0.05936	97.0	-341.38975	-342.64975	-341.41251	-342.74076
BTS2c	-342.97851	57.72	0.10117	0.05908	88.6	-341.34557	-342.60769	-341.36797	-342.69756
BCP6	-343.01904	59.59	0.10556	0.06021	95.4	-341.38980	-342.64994	-341.41256	-342.74094
BTS2d	-342.97788	57.47	0.10092	0.05846	89.4	-341.34474	-342.60728	-341.36715	-342.69718
BCP7	-343.01827	59.34	0.10540	0.05923	97.2	-341.38928	-342.64917	-341.41206	-342.74019

a) Geometries optimized and characterized at BH&HLYP/6-311+G(2df,2p). The ZPE and enthalpic and entropic corrections are obtained at this level of theory.

b) B1 stands for aug-cc-pVTZ; B2 stands for aug-cc-pVQZ basis sets.

Table S16. Cartesian coordinates (in Å) optimized at QCISD(/6-311+G(2df,2p)

CH3OOH.

C	0.005942	0.000570	-0.004581
H	-0.000155	-0.000416	1.083959
O	1.373594	0.004837	-0.360393
H	-0.497846	-0.890681	-0.381493
H	-0.493256	0.894677	-0.377363
O	1.405910	0.075320	-1.796534
H	1.837367	-0.758922	-2.004562

OH

O	0.000000	0.000000	0.107651
H	0.000000	0.000000	-0.861206

ACR1

H	1.012748	0.530249	-0.859809
O	0.106172	0.865468	-0.864812
O	2.324423	-0.469937	0.577557
H	1.446754	-0.347178	0.982779
O	-0.409286	0.252201	0.329633
C	-1.445114	-0.618570	-0.091263
H	-1.856780	-1.033319	0.827156
H	-2.213140	-0.061961	-0.625625
H	-1.053466	-1.415865	-0.723573

ACR2

H	-0.819473	-0.263910	0.595059

C	-0.113348	0.024633	1.372703
O	0.920010	-0.102705	-2.341055
H	1.222019	-0.483796	-1.499416
H	-0.326682	1.036706	1.710039
H	-0.165189	-0.671820	2.209211
O	1.202502	0.093415	0.851494
O	1.486345	-1.225526	0.339867
H	2.323417	-1.409468	0.777618

ATS1a

H	0.946323	0.167224	-0.386682
O	0.181335	0.911516	-0.334915
O	1.968787	-0.512402	-0.028813
H	2.158469	-0.139145	0.843276
O	-0.757920	0.356789	0.558663
C	-1.520800	-0.592965	-0.174161
H	-2.263310	-0.953478	0.531926
H	-2.003989	-0.117792	-1.024289
H	-0.889530	-1.416183	-0.505981

ATS1b

H	0.884281	0.221328	-0.340044
O	0.136065	0.995904	-0.306321
O	1.974709	-0.453247	-0.126934
H	2.130278	-0.376044	0.825329
O	-0.836704	0.468499	0.528628
C	-1.491757	-0.593969	-0.161268

H	-2.255985	-0.951972	0.523970
H	-1.941212	-0.217645	-1.078193
H	-0.780310	-1.389290	-0.386140

ATS2a

H	-0.875154	0.669892	0.244967
C	0.235094	1.096888	0.247279
O	-1.846409	-0.325290	0.029386
H	-2.061992	-0.048054	-0.873054
H	0.254707	2.055941	-0.263576
H	0.507275	1.149127	1.300949
O	1.019243	0.215853	-0.474383
O	0.985725	-1.032156	0.225085
H	0.057407	-1.287394	0.093038

ATS2b

H	0.055613	0.068103	0.100370
C	0.013353	0.019159	1.288041
O	0.639383	-0.163753	-1.158111
H	0.041338	-0.873461	-1.433114
H	-0.488091	0.916967	1.640312
H	-0.493682	-0.906679	1.555637
O	1.322710	0.066508	1.729305
O	1.957080	-1.131312	1.271811
H	2.013395	-0.947905	0.319852

CH3OOH···H2O

C	-0.030331	0.011752	-0.019633

H	-0.032600	-0.028011	1.068611
O	1.335088	0.098537	-0.384707
H	-0.488262	-0.889449	-0.429392
H	-0.572057	0.892792	-0.360774
O	1.358980	0.215746	-1.817043
H	1.723050	-0.650203	-2.052821
O	2.504586	-2.308896	-1.258216
H	2.464880	-1.744998	-0.480324
H	3.411007	-2.610323	-1.312010

Table S17 Cartesian coordinates (in Å) optimized at BH&HLYP(/6-311+G(2df,2p)

CH3OOH

C	0.002360	-0.000337	0.000011
H	-0.004755	-0.000652	1.081645
O	1.355970	0.008035	-0.357436
H	-0.498254	-0.887750	-0.371680
H	-0.499454	0.885732	-0.369381
O	1.414885	0.080065	-1.765188
H	1.836134	-0.745684	-1.987898

CH2OOH

C	-0.161544	0.182748	0.121785
O	0.227111	-0.383680	1.282025
O	1.425804	0.207055	1.716539
H	1.126348	0.765570	2.430721
H	0.605208	0.597538	-0.502391

H	-1.039221	-0.290814	-0.271231

CH3OO

O	-1.196699	0.069728	0.000000
O	0.000000	0.554363	0.000000
C	0.983042	-0.476633	0.000000
H	1.936745	0.028175	0.000000
H	0.869295	-1.080552	0.888216
H	0.869295	-1.080552	-0.888216

H2O

H	0.000000	0.757548	-0.457704
O	0.000000	0.000000	0.114426
H	0.000000	-0.757548	-0.457704

H2CO

C	0.000000	0.000000	-0.520956
O	0.000000	0.000000	0.665681
H	0.000000	0.930143	-1.099855
H	0.000000	-0.930143	-1.099855

ACR1

H	0.943211	0.571695	-0.823244
O	0.038148	0.881297	-0.763690
O	2.273117	-0.533000	0.491396
H	1.405442	-0.492468	0.917622
O	-0.446432	0.138051	0.334171

C	-1.533187	-0.623016	-0.124323
H	-1.911847	-1.136579	0.748901
H	-2.300432	0.022245	-0.531896
H	-1.218839	-1.341136	-0.872425

ATS1a

H	0.918231	0.200274	-0.318135
O	0.148843	0.905209	-0.269035
O	1.992620	-0.530807	-0.032702
H	2.332925	-0.141580	0.774448
O	-0.814375	0.368956	0.538798
C	-1.545847	-0.593159	-0.182742
H	-2.318949	-0.929817	0.492835
H	-1.985809	-0.149815	-1.066361
H	-0.908274	-1.425696	-0.458081

ACP1

H	1.364646	-0.034221	-0.078253
O	-0.218942	1.249343	0.226339
O	1.812296	-0.857506	-0.257053
H	2.741004	-0.664168	-0.261112
O	-1.402418	0.744885	0.171602
C	-1.383881	-0.660575	-0.093038
H	-2.420052	-0.958836	-0.116039
H	-0.904767	-0.839809	-1.043422
H	-0.849529	-1.166484	0.696569

ACR2

H	0.938516	-0.769263	-1.203215
O	0.162000	-0.311210	-0.890933
O	-0.158708	2.539574	-1.431831
H	-0.031049	1.603918	-1.223602
O	0.287254	-0.421048	0.510631
C	-0.825995	-1.140657	0.972432
H	-0.716041	-1.159643	2.047814
H	-1.746685	-0.637323	0.706137
H	-0.827584	-2.151529	0.582159

ATS1b

H	0.356297	0.016805	0.005209
O	-0.107265	-0.050654	0.944083
O	0.405381	-0.077977	-1.310393
H	-0.401888	0.322312	-1.635373
O	0.182218	-1.305274	1.399499
C	-0.963240	-2.110792	1.279742
H	-0.694849	-3.057800	1.725305
H	-1.796247	-1.668837	1.810861
H	-1.215290	-2.250562	0.234611

ATS2a

H	-0.882722	0.643753	0.226345
C	0.235034	1.083179	0.240500
O	-1.864417	-0.271999	0.023731
H	-2.126507	0.012252	-0.853017

H	0.249177	2.028817	-0.280451
H	0.475716	1.154311	1.294042
O	1.029434	0.205544	-0.443029
O	1.023452	-1.016910	0.247488
H	0.136728	-1.344136	0.074083

ACP2

H	-2.551008	0.093495	0.114701
C	0.965232	1.481269	0.387512
O	-2.208315	-0.755055	-0.143075
H	-2.418543	-0.858275	-1.064313
H	1.264466	2.368290	-0.135961
H	1.298469	1.258591	1.382056
O	0.793536	0.442203	-0.449286
O	0.554859	-0.729822	0.288316
H	-0.398589	-0.833379	0.181796

ATS2b

H	0.065762	0.049664	0.080914
C	0.021050	0.010946	1.281050
O	0.573648	-0.140030	-1.161787
H	-0.003435	-0.848998	-1.448336
H	-0.475069	0.911553	1.611601
H	-0.494656	-0.902196	1.548458
O	1.315186	0.052360	1.719102
O	1.954936	-1.127495	1.308259
H	2.103677	-0.958179	0.374841

CH3OOH···H2O

C	-0.055908	0.037944	-0.014630
H	-0.057035	-0.008538	1.066290
O	1.295421	0.024627	-0.388174
H	-0.582868	-0.816785	-0.423043
H	-0.531604	0.953722	-0.342148
O	1.343763	0.150826	-1.792817
H	1.722939	-0.695779	-2.043062
O	2.571118	-2.313230	-1.277915
H	2.480741	-1.797299	-0.480435
H	3.487773	-2.548540	-1.350375

H_2O···OH (**M1**)

O	-0.026398	-1.255022	0.000000
H	-0.042831	0.645975	0.000000
H	0.232599	-1.758560	0.762530
H	0.232599	-1.758560	-0.762530
O	-0.026398	1.613915	0.000000

H_2O···OH (**M2**)

O	-0.005529	-1.423906	0.000000
H	0.790443	-1.939797	0.000000
H	0.265764	-0.510289	0.000000
O	-0.005529	1.534118	0.000000
H	-0.967739	1.568395	0.000000

BCR1

C	0.056343	-0.739035	-1.695688
O	0.598399	-1.157413	-0.463894
H	0.906382	-0.429009	-2.288328
H	-0.448306	-1.564520	-2.178987
H	-0.622588	0.093816	-1.559258
O	-0.455561	-1.667320	0.319537
H	-0.591863	-0.969252	0.961106
O	-0.801558	2.610069	-0.085405
H	-0.271325	2.091616	0.538831
O	0.714300	0.774886	1.461025
H	1.134326	0.201093	0.818091
H	1.315095	0.889903	2.186886

TSBCR1BCR2

C	-0.104997	0.167100	0.020481
O	0.317127	-0.197364	1.314926
H	0.798248	0.449614	-0.503152
H	-0.567793	-0.678022	-0.470762
H	-0.789415	1.005523	0.060237
O	-0.807069	-0.650549	2.028519
H	-1.060292	0.118430	2.538783
O	-1.181650	3.253762	1.767689
H	-0.480349	2.921712	2.349869
O	0.719766	1.781329	3.192095
H	0.965212	1.079900	2.586899

H	1.379723	1.830825	3.871568

BCR2

C	0.246779	-0.931986	-1.799014
O	0.244648	-0.820690	-0.399188
H	1.284341	-0.855134	-2.094993
H	-0.153069	-1.891461	-2.099600
H	-0.327200	-0.133059	-2.253192
O	-1.079874	-0.981026	0.049165
H	-1.328273	-0.081058	0.291349
O	-1.338386	1.706967	1.006022
H	-0.389055	1.711020	1.233968
O	1.334253	1.148954	1.276274
H	1.199955	0.355417	0.753677
H	1.842600	0.905215	2.039629

TSBCR2BCR3

C	-0.003033	0.004942	0.023186
O	-0.051319	0.047145	1.423544
H	1.048734	0.032620	-0.227899
H	-0.447235	-0.909925	-0.348678
H	-0.506902	0.861654	-0.409008
O	-1.405547	-0.049713	1.809654
H	-1.585192	0.836919	2.141036
O	-1.378197	2.310085	3.431900
H	-0.863008	1.695593	3.987062
O	-0.043145	0.126410	4.489544

H	-0.165905	-0.362104	3.678174
H	0.876136	0.050973	4.714483

BCR3

H	0.314223	0.535159	-0.858659
O	0.954285	0.518886	-0.138800
O	-0.735518	-0.397870	-2.277981
H	-0.266901	-1.213974	-2.024558
O	0.133740	0.379042	0.999668
C	0.124130	1.610545	1.669503
H	-0.474790	1.446512	2.555065
H	1.127855	1.903118	1.951817
H	-0.327673	2.384298	1.059247
O	0.991884	-2.190345	-1.067784
H	1.250756	-1.468799	-0.493701
H	0.873069	-2.956155	-0.520083

BTS1a

C	-0.050285	-0.053598	-0.072896
O	-0.004265	0.150523	1.322556
H	0.973277	0.025199	-0.410406
H	-0.442078	-1.037550	-0.291034
H	-0.659185	0.708325	-0.543640
O	-1.257167	-0.002536	1.848962
H	-1.792382	0.919046	1.652356
O	-2.158177	2.120026	1.632387
H	-1.459441	2.560314	2.136145
O	0.315574	2.596769	2.879071

H	0.600032	1.777038	2.479701
H	1.033340	3.211648	2.795958

BCP1

C	0.376129	-1.179110	-1.517226
O	1.215598	-0.959793	-0.376984
H	0.751870	-0.518071	-2.282472
H	0.463894	-2.212427	-1.814803
H	-0.636861	-0.912745	-1.259255
O	1.061602	-1.870044	0.527773
H	-1.992247	1.998434	-0.456560
O	-1.447044	1.232856	-0.331113
H	-0.725937	1.503112	0.240091
O	0.962516	1.577694	1.140294
H	1.326187	0.784983	0.753135
H	1.014828	1.459493	2.081027

BTS1b

C	0.008457	0.014671	0.027233
O	-0.012352	-0.006642	1.438926
H	1.054028	0.021632	-0.245007
H	-0.476235	-0.869426	-0.363318
H	-0.479526	0.908292	-0.341045
O	-1.305308	-0.080235	1.878969
H	-1.715080	0.924082	1.803174
O	-1.925709	2.146240	1.961717
H	-1.178448	2.419784	2.513268
O	0.582232	2.191389	3.226657

H	0.721844	1.360515	2.775280
H	0.735009	2.029206	4.149561

BCP2

C	-0.017453	-1.030189	-1.441826
O	0.786652	-1.179937	-0.265555
H	-0.477871	-0.057992	-1.354877
H	0.623683	-1.088734	-2.308634
H	-0.756302	-1.817220	-1.458404
O	1.396171	-2.318297	-0.222365
H	-1.002111	2.857146	-0.470024
O	-1.007958	1.926673	-0.286917
H	-0.430181	1.793818	0.467111
O	0.829322	1.029092	1.665840
H	0.995183	0.206032	1.210625
H	0.645235	0.806359	2.569946

BTS1c

H	0.031987	-0.161649	-0.088047
O	0.294809	-0.337279	0.948062
O	0.283631	0.099273	-1.294880
H	1.098467	-0.390847	-1.458766
O	0.135685	0.860116	1.583152
C	1.381725	1.504789	1.681874
H	1.189420	2.414340	2.232207
H	2.090062	0.887138	2.219974
H	1.760545	1.739589	0.694048
O	2.567450	-1.427549	-0.564341

H	2.120960	-1.363479	0.276130
H	2.835629	-2.332481	-0.665797

BCP3

H	-0.682548	0.318347	-2.859428
O	0.106211	-0.807644	1.858128
O	-0.251064	0.500283	-2.035038
H	0.246388	-0.286280	-1.804439
O	-0.186846	0.410510	2.146117
C	0.198782	1.328968	1.116187
H	-0.081920	2.301703	1.488014
H	1.267858	1.267609	0.974687
H	-0.323220	1.095488	0.200594
O	1.183095	-1.566738	-0.748513
H	0.869701	-1.404500	0.141326
H	1.274277	-2.506526	-0.841252

BCR4

C	-0.450586	-0.426638	0.435382
H	-0.374439	-0.328913	1.509840
O	0.805540	-0.045894	-0.058015
H	-0.679062	-1.452480	0.171095
H	-1.225003	0.231660	0.061896
O	0.736451	-0.105981	-1.467419
H	1.417061	-0.763194	-1.659161
O	2.870255	-1.851850	-1.428581
H	3.124679	-1.617203	-0.542192
H	3.642681	-1.736818	-1.970075

H	1.306339	1.652314	-1.936937
O	1.659150	2.516622	-2.198543

TS-BCR4-BCR5

C	0.076791	-0.033285	-0.037221
H	0.107060	-0.079200	1.042970
O	1.418566	-0.037423	-0.442741
H	-0.452784	-0.893347	-0.430191
H	-0.416766	0.878025	-0.351442
O	1.429516	0.075331	-1.850651
H	1.873225	-0.744865	-2.102690
O	2.970547	-2.199231	-2.163043
H	3.282614	-2.281252	-1.268080
H	3.744291	-2.093502	-2.705433
H	2.743754	1.436309	-2.106773
O	3.502325	2.011981	-2.290537

BCR5

C	0.001949	-0.001003	-0.001098
H	0.001346	-0.002461	1.080490
O	1.354500	-0.002732	-0.366923
H	-0.504941	-0.884889	-0.371231
H	-0.495617	0.888411	-0.367811
O	1.409259	0.056230	-1.775539
H	1.790597	-0.800039	-2.009016
O	3.181518	-1.848651	-2.678852

H	3.590390	-2.621996	-2.311089
H	3.834960	-1.149149	-2.667646
H	3.131654	0.917437	-2.104666
O	4.068512	0.895924	-2.363084

TS-BCR5BCR6

C	-0.020482	0.002829	0.042628
H	-0.003169	0.088206	1.120664
O	1.318281	0.116669	-0.355257
H	-0.435618	-0.957511	-0.242491
H	-0.618654	0.803127	-0.377025
O	1.359831	0.057721	-1.756758
H	1.661353	-0.834344	-1.958520
O	1.781386	-2.116836	-3.381567
H	1.422133	-1.534217	-4.050209
H	2.540104	-2.542877	-3.760239
O	0.506336	0.304617	-4.404116
H	0.621691	0.558768	-3.475297

BCR6

C	-1.093774	1.576187	1.091858
H	-1.113837	2.538452	1.585135
O	-0.122071	1.698041	0.090096
H	-0.828674	0.804446	1.806243
H	-2.067427	1.366548	0.664181
O	-0.075845	0.488297	-0.621420

H	0.706395	0.038139	-0.284670
O	1.512228	-1.679152	-0.028423
H	0.802326	-2.182158	-0.426303
H	2.328488	-2.042779	-0.347786
O	-1.155285	-2.051797	-1.142434
H	-1.120413	-1.087036	-1.042660

TSBCR5BCT7

C	0.004332	0.001558	-0.000820
H	0.016032	0.013248	1.080620
O	1.351362	0.005090	-0.385456
H	-0.498155	-0.890571	-0.355842
H	-0.504615	0.882306	-0.372706
O	1.388068	0.051611	-1.798112
H	1.859251	-0.764999	-2.010244
O	3.363849	-1.823325	-2.215937
H	3.552616	-2.654451	-1.798652
H	3.958751	-1.175902	-1.836396
H	3.236559	0.903669	-1.189745
O	4.190738	0.747445	-1.155265

BCR7

C	0.012985	0.021340	-0.010729
O	0.013570	0.013990	1.392449
H	1.028065	0.029445	-0.385550
H	-0.492311	0.933696	-0.298073
H	-0.518641	-0.837378	-0.403288

O	0.724793	-1.123493	1.820420
H	0.029761	-1.665225	2.217286
O	-2.057669	0.498672	3.222759
H	-1.298470	0.515789	2.614110
O	-1.405052	-2.273520	3.165824
H	-1.876185	-1.472167	3.397927
H	-2.047626	-2.957592	3.028808

TSBCR7BCR8

C	-0.037632	-0.045822	0.029628
O	0.032603	0.028830	1.429547
H	0.957673	-0.056993	-0.394700
H	-0.561581	0.846983	-0.284594
H	-0.583921	-0.927099	-0.285080
O	0.770556	-1.078234	1.888757
H	0.088953	-1.628833	2.294366
O	-2.034523	0.543918	3.261951
H	-1.280386	0.540675	2.646424
O	-1.380980	-2.212884	3.212784
H	-1.867542	-1.426984	3.462860
H	-1.942773	-2.965561	3.341253

BCR8

C	-0.050235	-0.084457	0.056441
O	0.023914	0.040956	1.453342
H	0.944166	-0.129725	-0.367518
H	-0.558238	0.805733	-0.289721

H	-0.613901	-0.966195	-0.224055
O	0.739660	-1.061860	1.955568
H	0.036765	-1.612808	2.326244
O	-1.995268	0.559152	3.330905
H	-1.273509	0.567083	2.677464
O	-1.516267	-2.231805	3.074211
H	-1.905384	-1.418216	3.399273
H	-1.578484	-2.874301	3.769789

BTS2a

C	-0.001794	0.117934	-0.123388
H	-0.321461	0.315050	0.890393
O	1.315271	0.468387	-0.220387
H	-0.121088	-1.034344	-0.279759
H	-0.621037	0.605082	-0.865622
O	1.691605	0.441651	-1.573390
H	2.129623	-0.420760	-1.637352
O	2.485651	-2.185541	-1.523058
H	1.649470	-2.472799	-1.147653
H	3.172185	-2.500762	-0.948461
O	-0.179701	-2.453395	-0.576002
H	-0.769553	-2.390385	-1.329182

BCP4

C	-1.137428	1.301458	0.682360
H	-1.538591	1.471830	1.663704

O	0.198287	1.210374	0.700638
H	-1.398473	-0.930424	0.450958
H	-1.584293	1.727254	-0.195552
O	0.703013	1.253981	-0.609506
H	1.034854	0.346544	-0.720024
O	1.338978	-1.383070	-0.793350
H	0.518084	-1.735521	-0.434553
H	2.046632	-1.744655	-0.274367
O	-1.183151	-1.848061	0.273458
H	-1.910822	-2.205994	-0.220762

BTS2b

C	-0.010268	0.021112	-0.032583
H	-0.083324	0.066081	1.045140
O	1.316712	0.010849	-0.359175
H	-0.526371	-0.967017	-0.380837
H	-0.559487	0.813092	-0.525879
O	1.448293	0.246317	-1.737407
H	1.490566	-0.653853	-2.094491
O	1.172872	-2.377827	-2.493753
H	0.416979	-2.560926	-1.930976
H	1.814522	-3.057981	-2.332323
O	-1.049332	-2.285060	-0.716118
H	-1.014666	-2.647361	0.170348

BCP5

C	-0.474370	1.323020	1.184023

H	-0.503966	1.386955	2.255585
O	0.736800	0.963726	0.740292
H	-1.464501	-0.655364	0.711395
H	-1.045305	1.983890	0.560313
O	0.821105	1.162757	-0.647387
H	0.822196	0.248512	-0.978560
O	0.587505	-1.441999	-1.400925
H	-0.169002	-1.692838	-0.862861
H	1.284531	-2.055135	-1.203832
O	-1.610264	-1.510765	0.303311
H	-1.987449	-2.073536	0.967968

BTS2c

C	-0.018912	0.068258	-0.020975
O	-0.005999	0.063703	1.345637
H	0.973196	0.117570	-0.452055
H	-0.656479	0.880924	-0.339995
H	-0.478350	-0.921526	-0.432866
O	1.021722	-0.783787	1.789538
H	0.552103	-1.619143	1.930732
O	-1.197747	-2.126049	-0.843746
H	-2.068748	-1.726724	-0.873276
O	-0.484018	-3.098256	1.723670
H	-0.794842	-2.958904	0.825657
H	-0.124230	-3.975631	1.762279

BCP6

C	0.349680	1.627713	-0.758408
O	0.112818	1.323927	0.523995
H	1.352952	1.493250	-1.114576
H	-0.268378	2.438062	-1.097115
H	-0.734370	-0.179710	-1.589640
O	1.119314	0.477346	1.015051
H	0.652058	-0.372232	1.079600
O	-1.155156	-1.041024	-1.626770
H	-2.070591	-0.883046	-1.824988
O	-0.294195	-1.857092	0.884864
H	-0.677197	-1.749950	0.008035
H	0.127595	-2.706942	0.903277

BTS2d

C	0.198504	-0.161341	-0.697593
O	0.058982	-1.504379	-0.491374
O	1.333486	-2.072626	-0.334231
H	1.393962	-2.154343	0.628287
H	-0.769091	0.229439	-0.979910
H	0.482112	0.371814	0.302345
H	0.975599	0.074766	-1.413580
O	0.959018	0.970207	1.539708
H	1.764181	1.342370	1.176446
O	1.294718	-1.727862	2.392237
H	1.865055	-1.919127	3.125293
H	1.204246	-0.774129	2.333505

BCP7

C	-0.595868	0.612317	-1.638224
O	-0.853496	-0.536108	-1.000526
O	0.329865	-1.274683	-0.839295
H	0.455000	-1.233743	0.123037
H	-1.497566	1.103294	-1.952630
H	-0.110566	1.700663	0.279761
H	0.305883	0.655571	-2.218591
O	0.128793	1.864898	1.193856
H	0.684509	2.634496	1.194090
O	0.590646	-0.806937	1.833988
H	1.323810	-1.026311	2.394256
H	0.505699	0.150975	1.829983