Supporting information for:

CAPRAM reduction towards an operational multiphase halogen and DMS chemistry treatment in the chemistry transport model COSMO-MUSCAT(5.04e)

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Table S1 Implemented dry deposition, initial concentrations, and emission rates of chemical species for the open ocean simulation with COSMO-MUSCAT

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
NH_3	$1.0 \cdot 10^{-2}$	$1.28 \cdot 10^{9}$	$7.589 \cdot 10^{-10}$	
NO	$2.0 \cdot 10^{-4}$	$2.50 \cdot 10^{8}$	$4.151 \cdot 10^{-12}$	
NO_2	$2.0 \cdot 10^{-4}$	$5.00 \cdot 10^{8}$		
NO_3	$1.0 \cdot 10^{-2}$			
N_2O_5	$1.0 \cdot 10^{-2}$			
HONO		$2.50 \cdot 10^{8}$		
HNO_3	$7.0 \cdot 10^{-3}$	$2.00 \cdot 10^{9}$		
HO_2NO_2	$5.0 \cdot 10^{-3}$			
O_3	$1.5 \cdot 10^{-3}$	$7.50 \cdot 10^{11}$		
CO	$1.0 \cdot 10^{-3}$	$4.25 \cdot 10^{12}$	$1.416 \cdot 10^{-9}$	
CO_2		$1.02 \cdot 10^{16}$		
SO_2	$8.7 \cdot 10^{-3}$	$2.55 \cdot 10^{9}$		
SULF	$1.0 \cdot 10^{-2}$			
H_2		$1.28 \cdot 10^{13}$		
H_2O_2	$5.0 \cdot 10^{-3}$	$1.50 \cdot 10^{10}$		
CH_4		$4.50 \cdot 10^{13}$	$2.923 \cdot 10^{-11}$	
C_2H_6		$1.28 \cdot 10^{10}$	$1.661 \cdot 10^{-13}$	
C_3H_8		$2.31 \cdot 10^{10}$	$3.321 \cdot 10^{-13}$	
C_2H_2		$2.42 \cdot 10^{9}$	$1.661 \cdot 10^{-13}$	
C_2H_4		$2.55 \cdot 10^{9}$	$3.985 \cdot 10^{-12}$	
C_3H_6			$1.661 \cdot 10^{-12}$	
BIGENE		$9.50 \cdot 10^{8}$		
HCHO	$5.0 \cdot 10^{-3}$	$5.00 \cdot 10^{9}$	$2.956 \cdot 10^{-14}$	
CH_3CHO		$1.40 \cdot 10^{8}$	$1.513 \cdot 10^{-10}$	
C_2H_5CHO		$5.13 \cdot 10^{9}$	$9.083 \cdot 10^{-11}$	
HYAC		$3.83 \cdot 10^{8}$	$4.151 \cdot 10^{-12}$	
CH_3COCH_3		$1.10 \cdot 10^{10}$	$6.320 \cdot 10^{-12}$	
MEK		$6.89 \cdot 10^{8}$	$7.124 \cdot 10^{-16}$	
GLYOXAL		$2.55 \cdot 10^{8}$		

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
CH_3COCHO		$2.55 \cdot 10^{8}$		
CH_3OOH	$2.5 \cdot 10^{-3}$	$5.00 \cdot 10^{9}$		
CH_3CH_2OOH		$2.55 \cdot 10^{9}$		
CH_3COOOH		$2.55 \cdot 10^{7}$		
PAN	$1.0 \cdot 10^{-4}$	$2.50 \cdot 10^{8}$		
CH_3OH	$1.0 \cdot 10^{-2}$	$1.40 \cdot 10^{10}$	$9.797 \cdot 10^{-16}$	
CH_3CH_2OH	$5.0 \cdot 10^{-3}$	$2.00 \cdot 10^{9}$	$1.015 \cdot 10^{-11}$	
HCOOH	$1.0 \cdot 10^{-2}$	$6.25 \cdot 10^{9}$		
CH_3COOH		$5.00 \cdot 10^{9}$	$1.278 \cdot 10^{-12}$	
C_5H_8		$1.28 \cdot 10^{9}$	$2.341 \cdot 10^{-12}$	
APIN		$4.53 \cdot 10^{8}$	$2.541 \cdot 10^{-14}$	
BPIN		$3.02 \cdot 10^{8}$		
$CHBr_3$		$3.83 \cdot 10^{7}$	$2.225 \cdot 10^{-13}$	
C_3H_7I		$1.63 \cdot 10^{7}$	$8.170 \cdot 10^{-15}$	
CH_2I_2		$2.55 \cdot 10^{5}$	$1.876 \cdot 10^{-13}$	
CH_3I		$2.04 \cdot 10^{7}$	$2.458 \cdot 10^{-13}$	
CH_2ClI		$2.55 \cdot 10^{5}$	$1.524 \cdot 10^{-13}$	
CH_2BrI		$8.93 \cdot 10^{5}$	$8.751 \cdot 10^{-14}$	
HCl	$2.0 \cdot 10^{-2}$	$2.50 \cdot 10^{9}$		
HOCl	$2.0 \cdot 10^{-3}$			
$ClNO_2$	$1.0 \cdot 10^{-2}$			
$ClNO_3$	$1.0 \cdot 10^{-2}$			
HBr	$2.0 \cdot 10^{-2}$			
HOBr	$1.6 \cdot 10^{-3}$			
$BrNO_2$	$1.0 \cdot 10^{-2}$			
$BrNO_3$	$5.0 \cdot 10^{-3}$			
I_2			$1.744 \cdot 10^{-14}$	
HOI	$1.0 \cdot 10^{-2}$		$3.321 \cdot 10^{-13}$	
INO_3	$1.0 \cdot 10^{-2}$			
I_2O_2	$1.0 \cdot 10^{-2}$			
I_2O_3	$1.0 \cdot 10^{-2}$			

Specie	Dry deposition / s^{-1}	Initial concentration / molecules cm^{-3}	Emission rates / mol m^{-2} s^{-1}	Aerosol initial concentration / mol m^{-3}
I_2O_4	$1.0\cdot10^{-2}$			
DMS		$1.53\cdot10^{9}$	$1.026\cdot10^{-10}$	
DMSO	$5.0\cdot10^{-3}$			
DMSO2	$5.0\cdot10^{-3}$			
MSA	$5.0\cdot10^{-3}$			
SO_4^{2-}				$1.05\cdot10^{-8}$
NO_3^-				$2.05\cdot10^{-9}$
Cl^-				$9.76\cdot10^{-8}$
Br^-				$2.14\cdot10^{-10}$
NH_4^+				$5.72\cdot10^{-9}$
Mn^{3+}				$3.93\cdot10^{-15}$
Fe^{3+}				$4.80\cdot10^{-15}$
Cu^{2+}				$1.72\cdot10^{-13}$
$HC_2O_4^-$				$3.94\cdot10^{-11}$
MSA				$3.26\cdot10^{-10}$
H^+				$1.00\cdot10^{-11}$

Table S2 **Implemented gas-phase reactions in the CAPRAM-DM1.0red.**

Nr.	Reaction	Rate constant[(a)]	Comment
D1	$DMS + OH \rightarrow CH_3SCH_2O_2 - O_2$	$k = 1.12 \cdot 10^{-11} \exp(-250/T)$	
D2	$DMS + OH \rightarrow 0.9\ DMSO + 0.9\ HO_2 + 0.1\ CH_3SOH + 0.1\ CH_3O_2 - O_2$	**(1)**	
D3	$DMS + NO_3 \rightarrow CH_3SCH_2O_2 - O_2$	$k = 1.90 \cdot 10^{-13} \exp(520/T)$	
D4	$DMS + Cl \rightarrow 0.82\ CH_3SCH_2O_2 + 0.82\ HCl + 0.18\ DMSO + 0.18\ ClO - O_2$	$k = 1.88 \cdot 10^{-10}$	
D5	$DMS + ClO \rightarrow 0.73\ Cl + 0.73\ DMSO + 0.27\ HOCl + 0.27\ CH_3SCH_2O_2 - 0.27\ O_2$	$k = 1.70 \cdot 10^{-15} \exp(340/T)$	
D6	$DMS + BrO \rightarrow DMSO + Br$	$k = 1.50 \cdot 10^{-14} \exp(1000/T)$	
D7	$DMS + Cl_2 \rightarrow CH_3SCH_2Cl + HCl$	$k = 3.40 \cdot 10^{-14}$	
D8	$DMS + IO \rightarrow DMSO + I$	$k = 3.30 \cdot 10^{-13} \exp(-925/T)$	
D9	$CH_3SCH_2O_2 + HO_2 \rightarrow CH_3SCH_2OOH + O_2$	$k = 1.13 \cdot 10^{-13} \exp(1300/T)$	
D10	$CH_3SCH_2O_2 + NO \rightarrow CH_3S + HCHO + NO_2$	$k = 4.90 \cdot 10^{-12} \exp(260/T)$	
D11	$CH_3SCH_2O_2 + NO_3 \rightarrow CH_3S + HCHO + NO_2 + O_2$	$k = 2.30 \cdot 10^{-12}$	
D12	$CH_3SCH_2O_2 + CH_3O_2 \rightarrow 0.89\ CH_3S + 0.89\ HCHO + 0.11\ CH_3SCHO + O_2$	$k = 5.00 \cdot 10^{-13} \exp(400/T)$	
D13	$CH_3SCH_2Cl + OH \rightarrow CH_3SOH + ClCH_2O_2 - O_2$	$k = 2.50 \cdot 10^{-12}$	
D14	$CH_3SCH_2OOH + OH \rightarrow CH_3SCHO + OH + H_2O$	$k = 7.03 \cdot 10^{-11}$	
D15	$CH_3SCHO + OH \rightarrow CH_3S + CO + H_2O$	$k = 1.11 \cdot 10^{-11}$	
D16	$DMSO + OH \rightarrow MSIA + CH_3O_2 - O_2$	$k = 6.10 \cdot 10^{-12} \exp(800/T)$	
D17	$DMSO + NO_3 \rightarrow DMSO_2 + NO_2$	$k = 2.90 \cdot 10^{-13}$	
D18	$DMSO + Cl \rightarrow 0.43\ DMSO_2 + 0.43\ ClO + 0.57\ CH_3SO + 0.57\ HCHO + HCl - 0.43\ O_2$	$k = 1.45 \cdot 10^{-11}$	
D19	$DMSO + BrO \rightarrow CH_3SO_2CH_3 + Br$	$k = 1.00 \cdot 10^{-14}$	
D20	$CH_3SOH + OH \rightarrow CH_3SO + H_2O$	$k = 5.00 \cdot 10^{-11}$	
D21	$CH_3S + O_3 \rightarrow CH_3SO + O_2$	$k = 1.15 \cdot 10^{-12} \exp(430/T)$	
D22	$CH_3S + O_2 \rightarrow CH_3O_2 + SO_2 - O_2$	**(2)**	
D23	$CH_3S + O_2 \rightarrow CH_3SO_2$	**(3)**	
D24	$MSIA + OH \rightarrow CH_3O_2 + SO_2 + H_2O - O_2$	$k = 9.00 \cdot 10^{-11}$	
D25	$CH_3SO + O_3 \rightarrow CH_3O_2 + SO_2$	$k = 4.00 \cdot 10^{-13}$	
D26	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3 + O_2$	$k = 3.00 \cdot 10^{-13}$	
D27	$CH_3SO_2 \rightarrow CH_3O_2 + SO_2 - O_2$	$k = 5.00 \cdot 10^{+13} \exp(-9673/T)$	

Nr.	Reaction	Rate constant[(a)]	Comment
D28	$CH_3SO_3 + HO_2 \rightarrow MSA + O_2$	$k = 5.00\cdot10^{-11}$	
D29	$CH_3SO_3 \rightarrow CH_3O_2 + SULF - H_2O - O_2$	$k = 5.00\cdot10^{+13}\exp(-9946/T)$	
Photolysis reactions			
D30	$CH_3SCH_2OOH \rightarrow CH_3S + HCHO + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
D31	$CH_3SCHO \rightarrow CH_3S + CO + HO_2 - O_2$	$J = 2.792\cdot10^{-05}\cos(\chi)^{0.805}\exp(-0.338/\cos(\chi))$	
D32	$CH_3SCH_2Cl \rightarrow CH_3S + ClCH_2O_2 - O_2$	$J = 1.458\cdot10^{-04}\cos(\chi)^{0.314}\exp(-0.641/\cos(\chi))$	

(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}; J in s^{-1};

(1) $k = \frac{k1\times k3}{k2+k3}$ with $k1 = \frac{9.5\times10^{-39}\times[O_2]\times e^{5270/T}}{1+7.5\times10^{-29}\times[O_2]\times e^{5610/T}}$; $k2 = \frac{2.05\times10^{-14}\times[O_2]\times e^{2674/T}}{\left(1+5.5\times10^{-31}\times[O_2]\times e^{7460/T}\right)\times T}$

(2) $k = \frac{k1}{1+k2}$ with $k1 = 1.92\times10^{-10}\times e^{-5730/T}$; $k2 = 1.60\times10^{6}\times e^{-7310/T}$

(3) $k = \frac{k1}{1+k2}$ with $k1 = 3.43\times10^{-27}\times e^{-5140/T}$; $k2 = 2.86\times10^{-11}\times e^{-3560/T}$

Table S3 Implemented phase transfers in the CAPRAM-DM1.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2'

Species	$K_{H\,(298\,K)}$[(a)]	$-\Delta H/R$[(b)]	α	$D_{g\,(298\,K)}$[(c)]	Comment
D33③ DMS	0.56	4480	0.001	$1.08\cdot10^{-5}$	
D34③ DMSO	$1.00\cdot10^{7}$	2580	0.1	$1.01\cdot10^{-5}$	
D35② $DMSO_2$	$1.00\cdot10^{7}$	5390	0.1	$9.55\cdot10^{-6}$	
D36② MSIA	$1.00\cdot10^{8}$	1760	0.1	$1.11\cdot10^{-5}$	
D37② MSA	$5.09\cdot10^{13}$	1760	0.1	$1.04\cdot10^{-5}$	

(a) in M atm^{-1}; (b) in K; (c) in m^2 s^{-1}

Table S4 Implemented aqueous-phase reactions in the CAPRAM-DM1.0red

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2'

Nr.	Reaction	Rate constant[(a)]	Comment
D38	$DMS + O_3 \rightarrow DMSO + O_2$	$k = 8.61\cdot10^{+08}exp(-2600/T)$	
D39	$DMSO + OH \rightarrow MSIA + CH_3$	$k = 6.65\cdot10^{+09}exp(-1270/T)$	
D40③	$DMSO + SO_4^- \rightarrow MSIA + CH_3 + H^+ + SO_4^{2-}$	$k = 2.97\cdot10^{+09}exp(-1440/T)$	
D41③	$DMSO + Cl_2^- \rightarrow MSIA + HCl + CH_3 + Cl^- - H_2O$	$k = 1.60\cdot10^{+07}$	
D42②	$MSIA + O_3 \rightarrow MSA + O_2$	$k = 3.50\cdot10^{+07}$	
D43	$MSI^- + OH \rightarrow CH_3 + 0.135\ SO_2 + 0.765\ MS^- + 0.765\ SO_3 - 0.765\ MSI^- + 0.9\ OH^- + 0.1\ HSO_3^-$	$k = 1.20\cdot10^{+10}$	
D44③	$MSI^- + Cl_2^- \rightarrow CH_3 + 0.15\ SO_2 + 0.85\ MS^- + 0.85\ SO_3 - 0.85\ MSI^- + 2\ Cl^-$	$k = 8.00\cdot10^{+08}$	
D45②	$MSI^- + O_3 \rightarrow CH_3SO_3^- + O_2$	$k = 2.00\cdot10^{+06}$	
D46	$MS^- + OH \rightarrow HCHO + SO_3^- + H_2O – 0.5\ O_2$	$k = 1.29\cdot10^{+07}exp(-2630/T)$	
D47②	$MS^- + Cl_2^- \rightarrow CH_3 + SO_3 + 2\ Cl^-$	$k = 3.89\cdot10^{+03}$	

(a) k^{2nd} in $l^3\ mol^{-1}\ s^{-1}$

Table S5 Implemented aqueous-phase equilibria in the CAPRAM-DM1.0red

	Equilibrium	K[(a)]	$k_{f,\ 298}$[(b)]	E_A/R[(c)]	$k_{b,\ 298}$[(b)]	E_A/R[(c)]	Comment
D48②	$MSIA \rightleftharpoons MSI^- + H^+$	$5.0\cdot10^{-03}$	$2.50\cdot10^{08}$		$5.00\cdot10^{10}$		
D49②	$MSA \rightleftharpoons MS^- + H^+$	73	$3.65\cdot10^{12}$		$5.00\cdot10^{10}$		

(a) in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) k_{298}^{2nd} in $l^1\ mol^{-1}\ s^{-1}$, k_{298}^{1st} in s^{-1}; (c) in K

Table S6 **Implemented gas-phase reactions in the CAPRAM-HM3.0red**

Nr.	Reaction	Rate constant[(a)]	Comment
H1	$Cl + O_3 \rightarrow ClO$	$k = 2.80 \cdot 10^{-11} exp(-250/T)$	
H2	$ClO + HO_2 \rightarrow HOCl$	$k = 2.20 \cdot 10^{-12} exp(340/T)$	
H3	$HCl + OH \rightarrow Cl$	$k = 1.70 \cdot 10^{-12} exp(-230/T)$	
H4	$ClO + NO \rightarrow Cl + NO_2$	$k = 6.20 \cdot 10^{-12} exp(295/T)$	
H5	$Cl + NO_2 \rightarrow ClNO_2$	TROE	
H6	$ClO + NO_2 \rightarrow ClNO_3$	TROE	
H7	$ClNO_3 \rightarrow ClO + NO_2$	$k = [M]*2.75 \cdot 10^{-6} exp(11438/T)$	
H8	$Cl + CH_4 \rightarrow CH_3O_2 + HCl$	$k = 6.60 \cdot 10^{-12} exp(-1240/T)$	
H9	$Cl + C_2H_6 \rightarrow C_2H_5O_2 + HCl$	$k = 8.30 \cdot 10^{-11} exp(-100/T)$	
H10	$Cl + C_3H_8 \rightarrow C_3H_7O_2 + HCl$	$k = 1.40 \cdot 10^{-10}$	
H11	Cl + BIGALKANE → ALKO2 + HCl	$k = 1.21 \cdot 10^{-10} exp(55/T)$	
H12	$Cl + CH_3OH \rightarrow HCHO + HO_2 + HCl$	$k = 7.10 \cdot 10^{-11} exp(-75/T)$	
H13	$Cl + C_2H_5OH \rightarrow 0.92\ CH_3CHO + 0.92\ HO_2 + 0.08$ EO2 + HCl	$k = 6.05 \cdot 10^{-11} exp(155/T)$	
H14	Cl + ALKOH → 1.25 MEK + HO_2 + HCl	$k = 2.70 \cdot 10^{-11} exp(525/T)$	
H15	$Cl + CH_3OOH \rightarrow HCl + 0.6\ CH_3O_2 + 0.4\ HCHO + 0.4\ OH$	$k = 5.90 \cdot 10^{-11}$	
H16	$Cl + C_2H_5OOH \rightarrow HCl + CH_3CHO + OH$	$k = 1.07 \cdot 10^{-10}$	
H17	$ClO + CH_3O_2 \rightarrow Cl + O_2 + HCHO + HO_2$	$k = 1.80 \cdot 10^{-11} exp(-600/T)$	
H18	$Cl + HCHO \rightarrow HCl + CO + HO_2$	$k = 8.10 \cdot 10^{-11} exp(-34/T)$	
H19	$Cl + CH_3CHO \rightarrow HCl + CH_3CO_3$	$k = 8.00 \cdot 10^{-11}$	
H20	$Cl + C_2H_5CHO \rightarrow HCl + 1.5\ CH_3CO_3$	$k = 1.30 \cdot 10^{-10}$	
H21	Cl + HYAC → HCl + MGLY + HO_2	$k = 5.70 \cdot 10^{-11}$	
H22	$Cl + CH_3COCHO \rightarrow HCl + CH_3CO_3 + CO$	$k = 4.80 \cdot 10^{-11}$	
H23	Cl + GLYOXAL → HCl + 2.0 CO + HO_2	$k = 3.80 \cdot 10^{-11}$	
H24	Cl + MEK → HCl + MEKO2	$k = 3.05 \cdot 10^{-11} exp(80/T)$	
H25	Cl + MACR → 0.2 MACRO2 + 0.8 CC(O[O])(CCl)C=O + 0.2 HCl	$k = 2.55 \cdot 10^{-10}$	
H26	CC(O[O])(CCl)C=O + HO_2 → CH_3COCH_2Cl + CO +HO_2 + OH	$k = 1.00 \cdot 10^{-11}$	
H27	CC(O[O])(CCl)C=O + NO → CH_3COCH_2Cl + CO + HO_2 + NO_2	$k = 1.17 \cdot 10^{-11}$	
H28	CC(O[O])(CCl)C=O + CH_3O_2 → CH_3COCH_2Cl + CO + HO_2 + HCHO	$k = 1.00 \cdot 10^{-12}$	
H29	CC(O[O])(CCl)C=O + CH_3CO_3 → CH_3COCH_2Cl + CO + HO_2 + CH_3O_2	$k = 1.00 \cdot 10^{-11}$	

Nr.	Reaction	Rate constant[(a)]	Comment
H30	$OH + CC(OO)(CCl)C{=}O \rightarrow CH_3COCH_2Cl + CO + OH$	$k = 3.77\cdot10^{-11}$	
H31	$Cl + MVK \rightarrow CC(=O)C(O[O])CCl$	$k = 2.10\cdot10^{-10}$	
H32	$CC(=O)C(O[O])CCl + HO_2 \rightarrow CC(=O)C(OO)CCl$	$k = 1.82\cdot10^{-13}exp(1300/T)$	
H33	$CC(=O)C(O[O])CCl + NO \rightarrow ClCH_2CHO + NO_2 + CH_3CO_3$	$k = 2.70\cdot10^{-12}exp(360/T)$	
H34	$CC(=O)C(O[O])CCl+ NO_3 \rightarrow ClCH_2CHO + NO_2 + CH_3CO_3$	$k = 2.30\cdot10^{-12}$	
H35	$CC(=O)C(O[O])CCl + CH_3O_2 \rightarrow ClCH_2CHO + CH_3CO_3 + HCHO$	$k = 1.00\cdot10^{-12}$	
H36	$CC(=O)C(O[O])CCl + CH_3CO_3 \rightarrow ClCH_2CHO + CH_3CO_3 + CH_3O_2$	$k = 1.00\cdot10^{-11}$	
H37	$OH + CC(=O)C(OO)CCl \rightarrow ClCH_2CHO + CH_3CO_3 + OH$	$k = 3.95\cdot10^{-11}$	
H38	$Cl + BIGALD1 \rightarrow MALO2 + HO_2 + HCl$	$k = 1.35\cdot10^{-10}$	
H39	$Cl + TOL \rightarrow HCl + TOLO2$	$k = 6.20\cdot10^{-11}$	
H40	$Cl + XYL \rightarrow HCl + XYLNO2$	$k = 1.40\cdot10^{-10}$	
H41	$Cl + BZALD \rightarrow HCl + ACBZO2$	$k = 1.00\cdot10^{-10}$	
H42	$Cl + GLYALD \rightarrow HCl + HOCH_2CO_3$	$k = 7.00\cdot10^{-11}$	
H43	$Cl + CH_3COCH_3 \rightarrow HCl + CH_3COCH_2O_2$	$k = 3.20\cdot10^{-11}exp(-815/T)$	
H44	$Cl + C_2H_2 \rightarrow 0.26\ ClCHO + 0.21\ Cl + 0.53\ HCl + 0.21\ GLYOXAL + 1.32\ CO + 0.79\ HO_2$	TROE	
H45	$Cl + C_2H_4 \rightarrow ClCH_2CH_2O_2$	TROE	
H46	$ClCH_2CH_2O_2 + HO_2 \rightarrow ClCH_2CH_2OOH$	$k = 3.30\cdot10^{-13}exp(820/T)$	
H47	$ClCH_2CH_2O_2 + NO \rightarrow ClCH_2CHO + HO_2 + NO_2$	$k = 3.24\cdot10^{-12}exp(360/T)$	
H48	$ClCH_2CH_2O_2 + NO_3 \rightarrow ClCH_2CHO + HO_2 + NO_2$	$k = 2.30\cdot10^{-12}$	
H49	$ClCH_2CH_2O_2 + CH_3O_2 \rightarrow ClCH_2CHO + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 2.00\cdot10^{-12}$	HM2
H50	$ClCH_2CHO + NO_3 \rightarrow ClCH_2CO_3 + HNO_3$	$k = 1.40\cdot10^{-12}exp(-1860/T)$	
H51	$ClCH_2CHO + OH \rightarrow ClCH_2CO_3 + H_2O$	$k = 2.09\cdot10^{-11}$	
H52	$ClCH_2CO_3 + HO_2 \rightarrow 0.44\ ClCH_2O_2 + 0.44\ OH + 0.15\ ClCH_2COOH + 0.15\ O_3 + 0.41\ ClCH_2C(O)OOH$	$k = 5.20\cdot10^{-13}exp(980/T)$	
H53	$ClCH_2CO_3 + NO \rightarrow ClCH_2O_2 + NO_2$	$k = 7.50\cdot10^{-12}exp(290/T)$	
H54	$ClCH_2CO_3 + NO_2 \rightarrow ClPAN$	TROE	
H55	$ClCH_2CO_3 + NO_3 \rightarrow ClCH_2O_2 + NO_2$	$k = 4.00\cdot10^{-12}$	
H56	$ClCH_2CO_3 + CH_3O_2 \rightarrow 0.7\ ClCH_2O_2 + 0.3\ ClCH_2COOH + 0.7\ HO_2+ HCHO$	$k = 1.00\cdot10^{-11}$	
H57	$ClCH_2COOH + OH \rightarrow ClCH_2O_2$	$k = 1.90\cdot10^{-12}exp(190/T)$	
H58	$ClCH_2C(O)OOH + OH \rightarrow ClCH_2O_2$	$k = 4.29\cdot10^{-12}$	

Nr.	Reaction	Rate constant[(a)]	Comment
H59	$ClPAN + OH \rightarrow ClCHO + CO + NO_2$	$k = 6.26\cdot10^{-13}$	
H60	$ClPAN \rightarrow ClCH_2CO_3 + NO_2$	TROE	
H61	$ClCH_2O_2 + HO_2 \rightarrow 0.3\ ClCH_2OOH + 0.7\ ClCHO$	$k = 3.20\cdot10^{-13}exp(820/T)$	
H62	$ClCH_2O_2 + NO \rightarrow ClCHO + HO_2 + NO_2$	$k = 4.05\cdot10^{-12}exp(360/T)$	
H63	$ClCH_2O_2 + NO_3 \rightarrow ClCHO + HO_2 + NO_2$	$k = 2.30\cdot10^{-12}$	
H64	$ClCH_2O_2 + CH_3O_2 \rightarrow 1.4\ HO_2 + ClCHO + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.50\cdot10^{-12}$	HM2
H65	$Cl + C_3H_6 \rightarrow 0.4\ CH_3CH(O_2)CH_2Cl + 0.5\ CH_3CH(Cl)CH_2O_2 + 0.1\ HYAC$	$k = 1.43\cdot10^{-14}exp(2886/T)$	
H66	$CH_3CH(O_2)CH_2Cl + NO \rightarrow CH_3COCH_2Cl + HO_2 + NO_2$	$k = 2.70\cdot10^{-12}exp(360/T)$	
H67	$CH_3CH(Cl)CH_2O_2 + NO \rightarrow CH_3CH(Cl)CHO + NO_2 + HO_2$	$k = 2.70\cdot10^{-12}exp(360/T)$	
H68	$CH_3CH(O_2)CH_2Cl + CH_3O_2 \rightarrow CH_3COCH_2Cl + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 4.00\cdot10^{-14}$	HM2
H69	$CH_3CH(Cl)CH_2O_2 + CH_3O_2 \rightarrow CH_3CH(Cl)CHO + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 6.48\cdot10^{-13}$	HM2
H70	$CH_3COCH_2Cl + OH \rightarrow CH_3COCHClO_2$	$k = 3.68\cdot10^{-13}$	
H71	$CH_3COCHClO_2 + HO_2 \rightarrow CH_3COCHClOOH$	$k = 3.30\cdot10^{-13}exp(820/T)$	
H72	$CH_3COCHClO_2 + NO \rightarrow ClCHO + CH_3CO_3 + NO_2$	$k = 2.70\cdot10^{-12}exp(360/T)$	
H73	$CH_3COCHClO_2 + NO_3 \rightarrow ClCHO + CH_3CO_3 + NO_2$	$k = 2.30\cdot10^{-12}$	
H74	$CH_3COCHClO_2 + CH_3O_2 \rightarrow ClCHO + CH_3CO_3 + 0.8\ HCHO + 0.2\ CH_3OH + HO_2$	$k = 2.00\cdot10^{-12}$	HM2
H75	$CH_3COCHClOOH + OH \rightarrow CH_3COCHClO_2$	$k = 8.34\cdot10^{-12}$	
H76	$ClCHO + NO_3 \rightarrow CO + Cl + HNO_3$	$k = 1.40\cdot10^{-12}exp(-1860/T)$	
H77	$ClCHO + OH \rightarrow CO + Cl + H_2O$	$k = 6.12\cdot10^{-12}$	
H78	$CH_3CH(Cl)CHO + OH \rightarrow CH_3CH(Cl)C(O)O_2$	$k = 4.90\cdot10^{-12}exp(405/T)$	
H79	$CH_3CH(Cl)CHO + NO_3 \rightarrow CH_3CH(Cl)C(O)O_2 + HNO_3$	$k = 3.24\cdot10^{-12}exp(-1860/T)$	
H80	$CH_3CH(Cl)C(O)O_2 + HO_2 \rightarrow 0.15\ CH_3CH(Cl)COOH + 0.15\ O_3 + 0.41\ CH_3CH(Cl)C(O)OOH + 0.44\ CH_3CH(Cl)O_2 + 0.44\ OH$	$k = 5.20\cdot10^{-13}exp(980/T)$	
H81	$CH_3CH(Cl)C(O)O_2 + NO \rightarrow CH_3CH(Cl)O_2 + NO_2$	$k = 7.50\cdot10^{-12}exp(290/T)$	
H82	$CH_3CH(Cl)CO_3 + NO_2 \rightarrow CH_3ClPAN$	TROE	
H83	$CH_3ClPAN \rightarrow CH_3CH(Cl)CO_3 + NO_2$	TROE	
H84	$CH_3CH(Cl)C(O)O_2 + NO_3 \rightarrow CH_3CH(Cl)O_2 + NO_2$	$k = 4.00\cdot10^{-12}$	

Nr.	Reaction	Rate constant[(a)]	Comment
H85	$CH_3CH(Cl)C(O)O_2 + CH_3O_2 \rightarrow 0.3\ CH_3CH(Cl)COOH + 0.7\ CH_3CH(Cl)O_2 + HCHO + HO_2$	$k = 1.00 \cdot 10^{-11}$	Estimated like $ClCH_2CO_3$
H86	CC(Cl)C(=O)OO + OH → CC(Cl)C(=O)O[O]	$k = 4.42 \cdot 10^{-12}$	
H87	$CH_3CH(Cl)COOH + OH \rightarrow CH_3CH(Cl)O_2$	$k = 1.20 \cdot 10^{-12}$	
H88	$CH_3CH(Cl)O_2 + HO_2 \rightarrow CH_3CH(Cl)OOH$	$k = 3.30 \cdot 10^{-13} exp(820/T)$	
H89	$CH_3CH(Cl)O_2 + NO \rightarrow CH_3CHO + Cl + NO_2$	$k = 4.05 \cdot 10^{-12} exp(360/T)$	
H90	$CH_3CH(Cl)O_2 + NO_3 \rightarrow CH_3CHO + Cl + NO_2$	$k = 2.30 \cdot 10^{-12}$	
H91	$CH_3CH(Cl)O_2 + CH_3O_2 \rightarrow 0.6\ CH_3CHO + 0.6\ Cl + 0.4\ CH_3C(O)Cl + 0.8\ HCHO + 0.2\ CH_3OH + 0.8\ HO_2$	$k = 2.65 \cdot 10^{-12}$	HM2
H92	$CH_3CH(Cl)OOH + OH \rightarrow CH_3CH(Cl)O_2 + H_2O$	$k = 1.90 \cdot 10^{-12} exp(190/T)$	
H93	$CH_3CH(Cl)OOH + OH \rightarrow CH_3C(O)Cl + OH + H_2O$	$k = 9.95 \cdot 10^{-12}$	
H94	$CH_3C(O)Cl + OH \rightarrow ClCOCH_2O_2 + H_2O$	$k = 3.88 \cdot 10^{-14}$	
H95	$ClCOCH_2O_2 + HO_2 \rightarrow ClCOCH_2OOH$	$k = 3.30 \cdot 10^{-13} exp(820/T)$	
H96	$ClCOCH_2O_2 + NO \rightarrow HCHO + Cl + CO + NO_2$	$k = 3.24 \cdot 10^{-12} exp(360/T)$	
H97	$ClCOCH_2O_2 + NO_3 \rightarrow HCHO + Cl + CO + NO_2$	$k = 2.30 \cdot 10^{-12}$	
H98	$ClCOCH_2O_2 + CH_3O_2 \rightarrow 2\ HCHO + Cl + CO + HO_2$	$k = 2.00 \cdot 10^{-12}$	HM2
H99	$Br + O_3 \rightarrow BrO$	$k = 1.70 \cdot 10^{-11} exp(-800/T)$	
H100	$BrO + HO_2 \rightarrow HOBr$	$k = 4.50 \cdot 10^{-12} exp(-500/T)$	
H101	$BrO + BrO \rightarrow 1.7\ Br + 0.15\ Br_2$	$k = 1.60 \cdot 10^{-12} exp(-210/T)$	
H102	$Br + NO_2 \rightarrow BrNO_2$	TROE	
H103	$BrO + NO \rightarrow Br + NO_2$	$k = 8.70 \cdot 10^{-12} exp(-260/T)$	
H104	$BrO + NO_2 \rightarrow BrNO_3$	TROE	
H105	$BrNO_3 \rightarrow BrO + NO_2$	$k = 2.79 \cdot 10^{13} exp(-12360/T)$	
H106	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	$k = 4.90 \cdot 10^{-11}$	
H107	$BrO + ClO \rightarrow 0.95\ Br + 0.5\ OClO + 0.45\ Cl + 0.05\ BrCl$	$k = 7.32 \cdot 10^{-12} exp(-200/T)$	Summation A-Factor Burkholder et al. (2015)
H108	$BrO + CH_3O_2 \rightarrow 0.25\ Br + 0.25\ HCHO + 0.25\ HO_2 + 0.75\ HOBr + 0.75\ HCOOH$	$k = 4.10 \cdot 10^{-13} exp(-800/T)$	
H109	$Br + C_2H_2 \rightarrow 0.17\ BrCHO + 0.09\ Br + 0.74\ HBr + 0.09\ GLYOXAL + 1.65\ CO + 0.91\ HO_2$	$k = 6.35 \cdot 10^{-15} exp(-440/T)$	
H110	$Br + HCHO \rightarrow HBr + CO + HO_2$	$k = 1.70 \cdot 10^{-11} exp(-800/T)$	
H111	$BrO + HCHO \rightarrow HOBr + CO + HO_2$	$k = 1.50 \cdot 10^{-14}$	

Nr.	Reaction	Rate constant[(a)]	Comment
H112	$Br + CH_3CHO \rightarrow HBr + CH_3CO_3$	$k = 1.80\cdot10^{-11}exp(-460/T)$	
H113	$Br + C_2H_5CHO \rightarrow HBr + 1.5\ CH_3CO_3$	$k = 5.75\cdot10^{-11}exp(-610/T)$	
H114	$Br + C_2H_4 \rightarrow BrCH_2CH_2O_2$	$k = 2.25\cdot10^{-13}exp(-277/T)$	
H115	$BrCH_2CH_2O_2 + NO \rightarrow BrCH_2CHO + HO_2 + NO_2$	$k = 9.70\cdot10^{-12}$	
H116	$BrCH_2CH_2O_2 + CH_3O_2 \rightarrow BrCH_2CHO + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 2.00\cdot10^{-12}$	HM2
H117	$BrCH_2CHO + OH \rightarrow BrCH_2CO_3 + H_2O$	$k = 2.05\cdot10^{-12}$	
H118	$BrCH_2CO_3 + HO_2 \rightarrow$ $0.15\ BrCH_2COOH + 0.15\ O_3 + 0.41\ BrCH_2C(O)OOH + 0.44\ BrCH_2O_2 + 0.44\ OH$	$k = 5.20\cdot10^{-13}exp(980/T)$	
H119	$BrCH_2CO_3 + NO \rightarrow BrCH_2O_2 + NO_2$	$k = 7.50\cdot10^{-12}exp(290/T)$	
H120	$BrCH_2CO_3 + CH_3O_2 \rightarrow 0.7\ BrCH_2O_2 + 0.3\ BrCH_2COOH + 0.7\ HO_2 + HCHO$	$k = 1.00\cdot10^{-11}$	HM2
H121	$BrCH_2COOH + OH \rightarrow BrCH_2O_2 + H_2O$	$k = 1.90\cdot10^{-12}exp(190/T)$	
H122	$BrCH_2C(O)OOH + OH \rightarrow BrCH_2CO_3 + H_2O$	$k = 3.79\cdot10^{-12}$	
H123	$BrCH_2O_2 + HO_2 \rightarrow BrCH_2OOH$	$k = 4.28\cdot10^{-13}exp(820/T)$	
H124	$BrCH_2O_2 + NO \rightarrow BrCHO + HO_2 + NO_2$	$k = 4.05\cdot10^{-12}exp(360/T)$	
H125	$BrCH_2O_2 + NO_3 \rightarrow BrCHO + HO_2 + NO_2$	$k = 2.30\cdot10^{-12}$	
H126	$BrCH_2O_2 + CH_3O_2 \rightarrow 1.4\ HO_2 + BrCHO + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.00\cdot10^{-12}$	HM2
H127	$BrCH_2OOH + OH \rightarrow BrCH_2O_2 + H_2O$	$k = 1.90\cdot10^{-12}exp(190/T)$	
H128	$BrCH_2OOH + OH \rightarrow BrCHO + OH + H_2O$	$k = 5.79\cdot10^{-12}$	
H129	$BrCHO + NO_3 \rightarrow CO + Br + HNO_3$	$k = 1.40\cdot10^{-12}exp(-1860/T)$	
H130	$BrCHO + OH \rightarrow CO + Br + H_2O$	$k = 1.16\cdot10^{-12}$	
H131	$Br + C_3H_6 \rightarrow CH_3CH(O_2)CH_2Br$	$k = 3.60\cdot10^{-12}$	
H132	$CH_3CH(O_2)CH_2Br + NO \rightarrow CH_3COCH_2Br + HO_2 + NO_2$	$k = 2.70\cdot10^{-12}exp(360/T)$	
H133	$CH_3CH(O_2)CH_2Br + CH_3O_2 \rightarrow CH_3COCH_2Br + 0.8\ HCHO + 0.2\ CH_3OH + 1.4\ HO_2$	$k = 4.00\cdot10^{-14}$	HM2
H134	$CH_3COCH_2Br + OH \rightarrow CH_3COCHBrO_2$	$k = 8.80\cdot10^{-12}exp(-1320/T)$	
H135	$CH_3COCHBrO_2 + NO \rightarrow CH_3CO_3 + BrCHO + NO_2$	$k = 8.00\cdot10^{-12}$	
H136	$CH_3COCHBrO_2 + CH_3O_2 \rightarrow 0.4\ CH_3COC(O)Br + 0.6\ CH_3CO_3 + 0.6\ BrCHO + 0.8\ HO_2 + 0.8\ HCHO + 0.2\ CH_3OH$	$k = 2.00\cdot10^{-12}$	
H137	$I + O_3 \rightarrow IO$	$k = 2.10\cdot10^{-11}exp(-830/T)$	
H138	$I_2 + OH \rightarrow I + HOI$	$k = 2.10\cdot10^{-10}$	

Nr.	Reaction	Rate constant[(a)]	Comment
H139	$IO + HO_2 \rightarrow HOI$	$k = 1.40 \cdot 10^{-11} exp(540/T)$	
H140	$IO + IO \rightarrow 0.38\ OIO + 0.46\ I_2O_2 + 0.6\ I + 0.05\ I_2$	$k = 5.40 \cdot 10^{-11} exp(180/T)$	
H141	$OIO + OH \rightarrow HIO_3$	$k = 2.20 \cdot 10^{-10} exp(243/T)$	
H142	$IO + O_3 \rightarrow 0.83\ I + 0.17\ OIO$	$k = 1.20 \cdot 10^{-15}$	
H143	$IO + OIO \rightarrow I_2O_3$	$k = 1.00 \cdot 10^{-10}$	
H144	$I_2O_3 \rightarrow IO + OIO$	$k = 2.78 \cdot 10^{-11}$	
H145	$OIO + OIO \rightarrow I_2O_4$	$k = 1.00 \cdot 10^{-10}$	
H146	$I_2O_4 \rightarrow OIO + OIO$	$k = 1.67 \cdot 10^{+00}$	
H147	$I_2 + O_3 \rightarrow IO + I$	$k = 4.02 \cdot 10^{-15} exp(-2050/T)$	
H148	$I_2O_2 \rightarrow 0.995\ OIO + 0.995\ I + 0.01\ IO$	$k = 1.00 \cdot 10^{+01}$	
H149	$I_2 + NO_3 \rightarrow I + INO_3$	$k = 1.50 \cdot 10^{-12}$	
H150	$IO + NO \rightarrow I + NO_2$	$k = 7.15 \cdot 10^{-12} exp(300/T)$	
H151	$IO + NO_2 \rightarrow INO_3$	TROE	
H152	$INO_3 \rightarrow IO + NO_2$	$k = [M]*4.40 \cdot 10^{-05} exp(12060/T)$	
H153	$IO + CH_3O_2 \rightarrow I + HO_2 + HCHO$	$k = 2.00 \cdot 10^{-12}$	
H154	$IO + ClO \rightarrow 0.8\ I + 0.55\ OClO + 0.25\ Cl + 0.2\ ICl$	$k = 4.70 \cdot 10^{-12} exp(280/T)$	
H155	$IO + BrO \rightarrow 0.8\ OIO + Br + 0.2\ I$	$k = 1.50 \cdot 10^{-11} exp(510/T)$	
Photolysis reactions			
H156	$Cl_2 \rightarrow Cl + Cl$	$J = 3.827 \cdot 10^{-03} cos(\chi)^{0.543} exp(-0.244/cos(\chi))$	
H157	$ClO \rightarrow Cl + O(^3P)$	$J = 4.755 \cdot 10^{-04} cos(\chi)^{1.258} exp(-0.588/cos(\chi))$	
H158	$OClO \rightarrow ClO + O(^3P)$	$J = 1.332 \cdot 10^{-01} cos(\chi)^{0.416} exp(-0.244/cos(\chi))$	
H159	$HOCl \rightarrow Cl + OH$	$J = 4.615 \cdot 10^{-04} cos(\chi)^{0.656} exp(-0.240/cos(\chi))$	
H160	$ClNO_2 \rightarrow Cl + NO_2$	$J = 6.219 \cdot 10^{-04} cos(\chi)^{0.774} exp(-0.255/cos(\chi))$	
H161	$ClNO_3 \rightarrow Cl + NO_3$	$J = 6.420 \cdot 10^{-05} cos(\chi)^{0.648} exp(-0.217/cos(\chi))$	
H162	$ClNO_3 \rightarrow ClO + NO_2$	$J = 1.393 \cdot 10^{-05} cos(\chi)^{1.052} exp(-0.243/cos(\chi))$	
H163	$CC(=O)C(OO)CCl \rightarrow ClCH_2CHO + CH_3CO_3 + OH$	$J = 7.649 \cdot 10^{-05} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	
H164	$ClCH_2CH_2OOH \rightarrow ClCH_2CHO + HO_2 + OH$	$J = 7.649 \cdot 10^{-06} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	
H165	$ClCH_2CHO \rightarrow ClCH_2O_2 + HO_2 + CO$	$J = 4.642 \cdot 10^{-05} cos(\chi)^{0.762} exp(-0.353/cos(\chi))$	
H166	$ClCH_2C(O)OOH \rightarrow ClCH_2O_2 + OH$	$J = 7.649 \cdot 10^{-06} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	
H167	$ClCH_2OOH \rightarrow ClCHO + HO_2 + OH$	$J = 7.649 \cdot 10^{-06} cos(\chi)^{0.682} exp(-0.279/cos(\chi))$	

Nr.	Reaction	Rate constant[(a)]	Comment
H168	$CH_3CH(O)CH_2Cl \rightarrow CH_3O_2 + ClCH_2CO_3$	$J = 5.804\cdot10^{-06}\cos(\chi)^{1.092}\exp(-0.377/\cos(\chi))$	
H169	$CH_3CH(O)CHClOOH \rightarrow ClCHO + CH_3CO_3 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
H170	$ClCHO \rightarrow HO_2 + CO + Cl$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	
H171	$CH_3CH(Cl)CHO \rightarrow CH_3CH(Cl)O_2 + HO_2 + CO$	$J = 2.879\cdot10^{-05}\cos(\chi)^{1.067}\exp(-0.358/\cos(\chi))$	
H172	$CH_3CH(Cl)OOH \rightarrow CH_3CHO + Cl + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
H173	$CH_3C(O)Cl \rightarrow CH_3CO_3 + Cl$	$J = 5.804\cdot10^{-06}\cos(\chi)^{1.092}\exp(-0.377/\cos(\chi))$	
H174	$ClCOCH_2OOH \rightarrow ClCOCH_2O_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
H175	$Br_2 \rightarrow Br + Br$	$J = 4.773\cdot10^{-02}\cos(\chi)^{0.193}\exp(-0.213/\cos(\chi))$	
H176	$BrO \rightarrow Br + O(^3P)$	$J = 6.368\cdot10^{-02}\cos(\chi)^{0.605}\exp(-0.269/\cos(\chi))$	
H177	$HOBr \rightarrow Br + OH$	$J = 3.464\cdot10^{-03}\cos(\chi)^{0.441}\exp(-0.214/\cos(\chi))$	
H178	$BrNO_2 \rightarrow Br + NO_2$	$J = 7.443\cdot10^{-03}\cos(\chi)^{0.355}\exp(-0.236/\cos(\chi))$	
H179	$BrNO_3 \rightarrow 0.29\ Br + 0.29\ NO_3 + 0.71\ BrO + 0.71\ NO_2$	$J = 2.194\cdot10^{-04}\cos(\chi)^{0.492}\exp(-0.215/\cos(\chi))$	
H180	$BrCl \rightarrow Br + Cl$	$J = 1.650\cdot10^{-02}\cos(\chi)^{0.297}\exp(-0.224/\cos(\chi))$	
H181	$BrCH_2CHO \rightarrow BrCH_2O_2 + HO_2 + CO$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	
H182	$BrCH_2C(O)OOH \rightarrow BrCH_2O_2 + OH$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
H183	$BrCH_2OOH \rightarrow BrCHO + OH + HO_2$	$J = 7.649\cdot10^{-06}\cos(\chi)^{0.682}\exp(-0.279/\cos(\chi))$	
H184	$BrCHO \rightarrow HO_2 + CO + Br$	$J = 4.642\cdot10^{-05}\cos(\chi)^{0.762}\exp(-0.353/\cos(\chi))$	
H185	$CH_3COCH_2Br \rightarrow 0.7\ CO + 0.7\ Br + 0.7\ CH_3CO_3 + 0.3\ BrCH_2CO_3 + 0.3\ CH_3O_2$	$J = 3.523\cdot10^{-04}\cos(\chi)^{0.885}\exp(-0.283/\cos(\chi))$	
H186	$CH_3COC(O)Br \rightarrow CO + Br + CH_3CO_3$	$J = 1.853\cdot10^{-04}\cos(\chi)^{0.583}\exp(-0.225/\cos(\chi))$	
H187	$CHBr_3 \rightarrow 3\ Br + CO + HO_2$	$J = 2.228\cdot10^{-06}\cos(\chi)^{1.471}\exp(-0.230/\cos(\chi))$	
H188	$I_2 \rightarrow I + I$	$J = 2.165\cdot10^{-01}\cos(\chi)^{0.125}\exp(-0.185/\cos(\chi))$	
H189	$IO \rightarrow I + O(^3P)$	$J = 2.640\cdot10^{-03}\cos(\chi)^{0.240}\exp(-0.240/\cos(\chi))$	
H190	$OIO \rightarrow 0.96\ I + 0.04\ IO + 0.04\ O(^3P)$	$J = 4.054\cdot10^{-02}\cos(\chi)^{0.119}\exp(-0.185/\cos(\chi))$	
H191	$HOI \rightarrow I + OH$	$J = 1.469\cdot10^{-02}\cos(\chi)^{0.342}\exp(-0.236/\cos(\chi))$	
H192	$INO_3 \rightarrow 0.85\ I + 0.85\ NO_3 + 0.15\ IO + 0.15\ NO_2$	$J = 6.599\cdot10^{-02}\cos(\chi)^{0.530}\exp(-0.243/\cos(\chi))$	
H193	$ICl \rightarrow I + Cl$	$J = 3.403\cdot10^{-02}\cos(\chi)^{0.179}\exp(-0.207/\cos(\chi))$	
H194	$IBr \rightarrow I + Br$	$J = 1.000\cdot10^{-01}\cos(\chi)^{0.149}\exp(-0.197/\cos(\chi))$	
H195	$C_3H_7I \rightarrow I + C_3H_7O_2$	$J = 3.731\cdot10^{-05}\cos(\chi)^{1.292}\exp(-0.217/\cos(\chi))$	
H196	$CH_2I_2 \rightarrow 2\ I + 2\ HO_2$	$J = 1.496\cdot10^{-02}\cos(\chi)^{0.801}\exp(-0.265/\cos(\chi))$	
H197	$CH_3I \rightarrow I + CH_3O_2$	$J = 1.206\cdot10^{-05}\cos(\chi)^{1.254}\exp(-0.231/\cos(\chi))$	
H198	$ClCH_2I \rightarrow I + ClCH_2O_2$	$J = 6.910\cdot10^{-04}\cos(\chi)^{1.057}\exp(-0.238/\cos(\chi))$	

Nr.	Reaction	Rate constant[(a)]	Comment
H199	$BrCH_2I \rightarrow I + BrCH_2O_2$	$J = 4.261\cdot10^{-04}\cos(\chi)^{0.976}\exp(-0.250/\cos(\chi))$	
(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}; J in s^{-1}			

Table S7 **Parameters for pressure dependent reactions.**

	Reaction	TYPE	k_0[(a)]	k_∞[(a)]	F_C
H5	$Cl + NO_2 \rightarrow ClNO_2$	TROE	$1.80\cdot10^{-31}*(T/298)^{-2.0}$	$1.00\cdot10^{-10}*(T/298)^{-1.0}$	0.6
H6	$ClO + NO_2 \rightarrow ClNO_3$	TROE	$1.60\cdot10^{-31}*(T/298)^{-3.4}$	$7.00\cdot10^{-11}$	0.4
H44	$Cl + C_2H_2 \rightarrow 0.26\ ClCHO + 0.21\ Cl + 0.53\ HCl + 0.21$ GLYOXAL $+ 1.32\ CO + 0.79\ HO_2$	TROE	$6.10\cdot10^{-30}*(T/298)^{-3.0}$	$2.00\cdot10^{-10}$	0.6
H45	$Cl + C_2H_4 \rightarrow ClCH_2CH_2O_2$	TROE	$1.85\cdot10^{-29}*(T/298)^{-3.3}$	$6.00\cdot10^{-10}$	0.4
H54	$ClCH_2CO_3 + NO_2 \rightarrow ClPAN$	TROE	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
H60	$ClPAN \rightarrow ClCH_2CO_3 + NO_2$	TROE	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
H82	$CH_3CH(Cl)CO_3 + NO_2 \rightarrow CH_3ClPAN$	TROE	$2.70\cdot10^{-28}*(T/298)^{7.1}$	$1.20\cdot10^{-11}*(T/298)^{0.9}$	0.3
H83	$CH_3ClPAN \rightarrow CH_3CH(Cl)CO_3 + NO_2$	TROE	$4.90\cdot10^{-03}\exp(-12100/T)$	$5.40\cdot10^{+16}\exp(-13830/T)$	0.3
H102	$Br + NO_2 \rightarrow BrNO_2$	TROE	$4.20\cdot10^{-31}*(T/298)^{-2.4}$	$2.70\cdot10^{-11}$	0.55
H104	$BrO + NO_2 \rightarrow BrNO_3$	TROE	$4.70\cdot10^{-31}*(T/298)^{-3.1}$	$1.80\cdot10^{-11}$	0.4
H151	$IO + NO_2 \rightarrow INO_3$	TROE	$7.70\cdot10^{-31}(T/300)^{-5.0}$	$1.60\cdot10^{-11}$	0.6
(a) k^{2nd} in cm^3 $molecules^{-1}$ s^{-1}; k^{1st} in s^{-1}					

Rate constants calculated with TROE formula: $k(T)= \frac{k_0(T)[M]}{1+\frac{k_0(T)[M]}{k_\infty(T)}} \times F_C^{\left\{1+log_{10}\left(\frac{k_0(T)[M]}{k_\infty(T)}\right)^2\right\}^{-1}}$

Table S8 **Implemented phase transfers in the CAPRAM-HM3.0red**

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Species	$K_{H\ (298\ K)}$ (a)	$-\Delta H/R$ (b)	α	$D_{g\ (298\ K)}$ (c)	Comment
H200③●	Cl_2	$9.15\cdot10^{-2}$	2490	0.08	1.28	
H201	Cl	$2.00\cdot10^{-1}$		0.05	1.82	
H202②●	HCl	$1.10\cdot10^{0}$	2020	0.1026	1.89	
H203③	HOCl	$6.60\cdot10^{2}$	5862	0.5	1.51	
H204③●	$ClNO_2$	$2.40\cdot10^{-2}$		0.01	1.27	
H205③	$ClNO_3$	$2.10\cdot10^{5}$	8700	0.1	1.18	
H206	ClCHO	$3.00\cdot10^{3}$	7216	0.02	1.23	
H207③●	Br_2	$7.60\cdot10^{-1}$	4100	0.08	1.00	
H208	Br	$1.20\cdot10^{0}$		0.05	1.29	
H209③	HBr	$1.30\cdot10^{0}$	10239	0.0481	1.26	
H210③	HOBr	$9.30\cdot10^{1}$	5862	0.5	1.16	
H211③	$BrNO_3$	$2.10\cdot10^{5}$	8700	0.8	1.01	
H212③	BrCl	$9.40\cdot10^{-1}$	-5600	0.33	1.05	
H213	$BrCH_2CO_3$	$6.69\cdot10^{2}$	5893	0.019	0.84	
H214②	$BrCH_2COOH$	$1.52\cdot10^{5}$	9300	0.0322	0.84	
H215	BrCHO	$7.40\cdot10^{1}$		0.02	1.02	
H216	I_2	$3.00\cdot10^{0}$	4431	0.0126	0.86	
H217③	HOI	$4.50\cdot10^{2}$	5862	0.5	1.08	
H218	HIO_3	$2.10\cdot10^{5}$	8700	0.0126	0.98	
H219③	INO_3	$2.10\cdot10^{5}$	8700	0.123	0.96	
H220③	I_2O_2	$1.00\cdot10^{4}$		0.123	0.80	
H221③	ICl	$1.10\cdot10^{2}$	5600	0.0126	0.98	
H222③	IBr	$2.40\cdot10^{1}$	5600	0.0126	0.88	

(a) in $M\ atm^{-1}$; (b) in K; (c) in $m^2\ s^{-1}$

Table S9 **Implemented aqueous-phase reactions in the CAPRAM-HM3.0red**

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	k_{298} (a)	E_A/R (b)	Comment
H223●	$Cl_2^- + H_2O_2 \rightarrow 2\ Cl^- + H^+ + HO_2$	$6.20 \cdot 10^5$	3340	
H224②●	$Cl_2^- + H_2O \rightarrow H^+ + Cl^- + ClOH^-$	$2.34 \cdot 10^1$		
H225②	$HOCl + HO_2 \rightarrow Cl + H_2O + O_2$	$7.50 \cdot 10^6$		
H226	$HOCl + OH \rightarrow ClO + H_2O$	$2.00 \cdot 10^9$		
H227●	$Cl_2^- + HSO_3^- \rightarrow 2\ Cl^- + H^+ + SO_3^-$	$1.70 \cdot 10^8$	400	
H228③	$HOCl + HSO_3^- \rightarrow Cl^- + H^+ + HSO_4^{2-}$	$7.60 \cdot 10^8$		
H229	$Cl^- + HSO_5^- \rightarrow HOCl + SO_4^{2-}$	$1.80 \cdot 10^{-3}$	7352	
H230●	$Cl_2^- + Fe_2^+ \rightarrow 2\ Cl^- + Fe_3^+$	$1.00 \cdot 10^7$	3030	
H231②●	$Cl^- + FeO_2^+ \rightarrow Fe_3^+ + ClOH^- + OH- - H_2O$	$1.00 \cdot 10^2$		
H232●	$Cl_2^- + Mn_2^+ \rightarrow MnCl_2^+$	$2.00 \cdot 10^7$	4090	
H233●	$MnCl_2^+ \rightarrow 0.588\ Cl_2^- + 0.588\ Mn^{2+} + 0.824\ Cl^- + 0.412\ Mn^{3+}$	$5.10 \cdot 10^5$		
H234	$2\ ClO \rightarrow Cl^- + ClO_3^- + 2\ H^+$	$2.50 \cdot 10^9$		
H235	$OH + ClO_3^- \rightarrow ClO + O_2 + OH^-$	$1.00 \cdot 10^6$		
H236	$Cl_2 + H_2O_2 \rightarrow 2\ H^+ + 2\ Cl^- + O_2$	$1.83 \cdot 10^2$	5387	
H237③	$ClNO_3 \rightarrow HOCl + HNO_3$	$1.62 \cdot 10^6$	2800	
H238②	$Cl_2^- + HC_2O_4^- \rightarrow 2\ Cl^- + H^+ + C_2O_4^-$	$1.30 \cdot 10^6$		
H239②	$Cl_2^- + C_2O_4^{2-} \rightarrow 2\ Cl^- + C_2O_4^-$	$4.00 \cdot 10^6$		
H240②	$ClCHO \rightarrow CO + H^+ + Cl^-$	$1.00 \cdot 10^4$		
H241	$Br + H_2O_2 \rightarrow H^+ + Br^- + HO_2$	$4.00 \cdot 10^9$		
H242②	$Br_2^- + HO_2 \rightarrow Br^- + 0.5\ Br_2 + 0.5\ H_2O_2 + 0.5\ O_2$	$8.80 \cdot 10^9$		
H243	$BrO + BrO \rightarrow BrO_2^- + HOBr + H^+$	$2.80 \cdot 10^9$		
H244	$HOBr + OH \rightarrow BrO + H_2O$	$2.00 \cdot 10^9$		
H245②	$HOBr + HO_2 \rightarrow Br + H_2O + O_2$	$1.00 \cdot 10^9$		
H246②	$HOBr + H_2O_2 \rightarrow H^+ + Br^- + H_2O + O_2$	$3.50 \cdot 10^6$		
H247③	$HOBr + HSO_3^- \rightarrow H+ + Br^- + HSO_4^-$	$5.00 \cdot 10^9$		
H248	$Br^- + HSO_5^- \rightarrow HOBr + SO_4^{2-}$	$1.00 \cdot 10^0$	5338	

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	k_{298} (a)	E_A/R (b)	Comment
H249	$Br^- + NO_3 \rightarrow Br + NO_3^-$	$3.80 \cdot 10^{9}$		
H250	$Br_2^- + Fe^{2+} \rightarrow 2\ Br^- + Fe^{3+}$	$3.60 \cdot 10^{6}$	3330	
H251●	$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.30 \cdot 10^{6}$	4330	
H252●	$MnBr_2^+ \rightarrow 0.577\ Br_2^- + 0.577\ Mn^{2+} + 0.846\ Br^- + 0.423\ Mn^{3+}$	$5.20 \cdot 10^{5}$		
H253	$BrO_3^- + SO_4^- \rightarrow BrO + O_2 + SO_4^{2-}$	$1.40 \cdot 10^{6}$		
H254	$Br + O_3 \rightarrow BrO + O_2$	$1.50 \cdot 10^{8}$		
H255	$BrO_3^- + HSO_3^- \rightarrow BrO_2^- + SO_4^{2-} + H^+$	$2.70 \cdot 10^{-2}$		
H256	$BrO_3^- + OH \rightarrow BrO + O_2 + OH^-$	$5.00 \cdot 10^{6}$		
H257③	$BrNO_3 \rightarrow HOBr + HNO_3$	$1.00 \cdot 10^{9}$		
H258	$BrO_3^- + HC_2O_4^- \rightarrow BrO_2^- + 2\ CO_2 + H_2O$	$7.47 \cdot 10^{-4}$		
H259②	$BrCHO \rightarrow CO + H^+ + Br^-$	$1.00 \cdot 10^{4}$		
H260②	$CH_2BrCO_3 + H_2O \rightarrow CH_2BrCOOH + HO_2$	$3.55 \cdot 10^{5}$		
H261	$Br_2^- + HCOO^- \rightarrow 2\ Br^- + COOH$	$4.90 \cdot 10^{3}$		
H262③	$Br^- + HOCl \rightarrow BrCl + H_2O - H^+$	$1.30 \cdot 10^{6}$		
H263②	$BrO_2^- + HOCl \rightarrow 0.85\ ClO_3^- + 0.93\ HOBr + 0.08\ ClO_2^- + 0.07\ BrO_3^- + 0.92\ Cl^- + 0.92\ H^+ - 0.85\ HOCl$	$1.60 \cdot 10^{2}$		
H264	$I^- + O_3 \rightarrow HOI + O_2$	$2.17 \cdot 10^{9}$	8790	
H265②	$IO + IO \rightarrow HOI + HIO_3 + H^+ - H_2O - H_2O_2$	$1.50 \cdot 10^{9}$		
H266③	$HOI + HSO_3^- \rightarrow H^+ + I^- + HSO_4^-$	$5.00 \cdot 10^{9}$		
H267	$HOI + OH \rightarrow IO + H_2O$	$7.00 \cdot 10^{9}$		
H268③	$INO_3 \rightarrow HOI + HNO_3$	$1.62 \cdot 10^{6}$	2800	
H269	$I_2O_2 + H^+ \rightarrow HIO_3 + HOI + H^+$	$3.20 \cdot 10^{4}$		
H270	$IO_3^- + OH \rightarrow IO + O_2 + OH^-$	$1.08 \cdot 10^{5}$		

(a) k_{298}^{2nd} in $l^1\ mol^{-1}\ s^{-1}$; k_{298}^{1st} in s^{-1}; (b) in K

Table S10 **Implemented aqueous-phase equilibrium reactions in the CAPRAM-HM3.0red**

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	K[(a)]	$k_{f,\,298}$[(b)]	E_A/R[(c)]	$k_{b,\,298}$[(b)]	E_A/R[(c)]	Comment
H271②●	$Cl + Cl^- \rightleftharpoons Cl_2^-$	$1.4\cdot10^{5}$	$8.50\cdot10^{9}$		$6.00\cdot10^{4}$		
H272③●	$Cl_2 + H_2O \rightleftharpoons H^+ + Cl^- + HOCl$	$1.90\cdot10^{-5}e^{-4500/T}$	$4.00\cdot10^{-1}$	8000	$2.10\cdot10^{4}$	3500	
H273③●	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72\cdot10^{6}\,e^{6890/T}$	$5.00\cdot10^{11}$	-6890	$2.90\cdot10^{5}$		
H274②●	$Cl^- + OH \rightleftharpoons ClOH^-$	$7.00\cdot10^{-1}$	$4.30\cdot10^{9}$		$6.10\cdot10^{9}$		
H275②	$Cl + OH^- \rightleftharpoons ClOH^-$	$7.83\cdot10^{8}$	$1.80\cdot10^{10}$		$2.30\cdot10^{1}$		
H276②●	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	$5.10\cdot10^{6}$	$2.1\cdot10^{10}$		$4.10\cdot10^{3}$		
H277②●	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	$2.20\cdot10^{-4}$	$1.00\cdot10^{4}$		$4.50\cdot10^{7}$		
H278②●	$Cl^- + SO_4^- \rightleftharpoons Cl + SO_4^{2-}$	$1.20\cdot10^{0}$	$2.52\cdot10^{8}$		$2.10\cdot10^{8}$		
H279②●	$Cl^- + NO_3 \rightleftharpoons Cl + NO_3^-$	$3.40\cdot10^{0}\,e^{-4300/T}$	$3.40\cdot10^{8}$	4300	$1.00\cdot10^{8}$		
H280	$HOCl + NO_2^- \rightleftharpoons ClNO_2 + OH^-$	$3.97\cdot10^{-4}$	$1.99\cdot10^{7}$		$5.00\cdot10^{10}$		
H281③	$Cl_2 + SO_4^{2-} \rightleftharpoons Cl^- + HOCl + HSO_4^-$	$1.14\cdot10^{-3}$	$3.20\cdot10^{1}$		$2.80\cdot10^{3}$		
H282③●	$Cl^- + NO_2^+ \rightleftharpoons ClNO_2$	$1.44\cdot10^{8}$	$3.90\cdot10^{10}$		$2.70\cdot10^{2}$		
H283②●	$Br + Br^- \rightleftharpoons Br_2^-$	$6.32\cdot10^{5}$	$1.20\cdot10^{10}$		$1.90\cdot10^{4}$		
H284③	$Br_2 + H_2O \rightleftharpoons H^+ + Br^- + HOBr$	$1.06\cdot10^{-10}e^{-7500/T}$	$1.70\cdot10^{0}$	7500	$1.60\cdot10^{10}$		
H285③	$HBr \rightleftharpoons H^+ + Br^-$	$1.00\cdot10^{9}$	$5.00\cdot10^{11}$		$5.00\cdot10^{2}$		
H286②●	$Br^- + OH \rightleftharpoons BrOH^-$	$3.33\cdot10^{2}$	$1.10\cdot10^{10}$		$3.30\cdot10^{7}$		
H287②	$Br + OH^- \rightleftharpoons BrOH^-$	$3.10\cdot10^{3}$	$1.30\cdot10^{10}$		$4.20\cdot10^{6}$		
H288②●	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.80\cdot10^{12}$	$4.40\cdot10^{10}$		$2.45\cdot10^{-2}$		
H289②●	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	$7.00\cdot10^{1}$	$1.90\cdot10^{8}$		$2.70\cdot10^{6}$		
H290	$HOBr + HOBr \rightleftharpoons H^+ + Br^- + BrO_2^-$	$6.70\cdot10^{-12}$	$2.00\cdot10^{-5}$		$3.00\cdot10^{6}$		
H291	$HOBr + BrO_2^- \rightleftharpoons H^+ + Br^- + BrO_3^-$	$1.70\cdot10^{0}$	$3.20\cdot10^{0}$		$2.00\cdot10^{0}$		
H292②	$CH_2BrCOOH \rightleftharpoons CH_2BrCOO^- + H^+$	$1.75\cdot10^{-5}\,e^{46/T}$	$8.75\cdot10^{5}$	-46	$5.00\cdot10^{10}$		
H293③	$Br_2 + SO_4^{2-} + H_2O \rightleftharpoons HOBr + Br^- + HSO_4^-$	$6.15\cdot10^{-6}$	$2.28\cdot10^{4}$		$3.70\cdot10^{9}$		
H294③	$BrCl \rightleftharpoons HOBr + H^+ + Cl^- - H_2O$	$1.80\cdot10^{-5}$	$1.00\cdot10^{5}$		$5.60\cdot10^{9}$		
H295③	$BrCl^- \rightleftharpoons Br^- + Cl$	$1.60\cdot10^{-7}$	$1.90\cdot10^{3}$		$1.20\cdot10^{10}$		
H296③	$BrCl^- \rightleftharpoons Br + Cl^-$	$6.10\cdot10^{-4}$	$6.10\cdot10^{4}$		$1.00\cdot10^{8}$		
H297③	$BrCl^- + Br^- \rightleftharpoons Br_2^- + Cl^-$	$1.86\cdot10^{3}$	$8.00\cdot10^{9}$		$4.30\cdot10^{6}$		

② reactions that run in the cloud mode 'sub#1', ③ reactions that run in the aerosol mode 'sub#2', ● already included in CAPRAM3.0red

	Reaction	K(a)	$k_{f,\,298}$(b)	E_A/R(c)	$k_{b,\,298}$(b)	E_A/R(c)	Comment
H298③	$BrCl^- + Cl^- \rightleftharpoons Br^- + Cl_2^-$	$2.75 \cdot 10^{-8}$	$1.10 \cdot 10^{2}$		$4.00 \cdot 10^{9}$		
H299③	$Br_2Cl^- \rightleftharpoons BrCl + Br^-$	$5.60 \cdot 10^{-5}$	$4.30 \cdot 10^{5}$		$7.70 \cdot 10^{9}$		
H300③	$Br_2Cl^- \rightleftharpoons Br_2 + Cl^-$	$7.60 \cdot 10^{-1}$	$3.80 \cdot 10^{4}$		$5.00 \cdot 10^{4}$		
H301③	$BrCl_2^- \rightleftharpoons BrCl + Cl^-$	$1.70 \cdot 10^{-1}$	$1.70 \cdot 10^{5}$		$1.00 \cdot 10^{6}$		
H302③	$BrCl_2^- \rightleftharpoons Br^- + Cl_2$	$1.50 \cdot 10^{-6}$	$9.00 \cdot 10^{3}$		$6.00 \cdot 10^{9}$		
H303	$I_2 + OH^- \rightleftharpoons I_2OH^-$	$5.00 \cdot 10^{0}$	$1.00 \cdot 10^{10}$		$2.00 \cdot 10^{9}$		
H304	$I_2OH^- \rightleftharpoons HOI + I^-$	$8.30 \cdot 10^{0}$	$2.49 \cdot 10^{9}$		$3.00 \cdot 10^{8}$		
H305	$HOI + H^+ + I^- \rightleftharpoons I_2 + H_2O$	$1.47 \cdot 10^{12}$	$4.40 \cdot 10^{12}$		$3.00 \cdot 10^{0}$		
H306②	$HIO_3 \rightleftharpoons H^+ + IO_3^-$	$1.70 \cdot 10^{-1}$	$8.50 \cdot 10^{9}$		$5.00 \cdot 10^{10}$		
H307③	$HOI + H^+ + Cl^- \rightleftharpoons ICl$	$1.20 \cdot 10^{4}$	$2.90 \cdot 10^{10}$		$2.40 \cdot 10^{6}$		
H308③	$HOI + H^+ + Br^- \rightleftharpoons IBr$	$5.10 \cdot 10^{6}$	$4.10 \cdot 10^{12}$		$8.00 \cdot 10^{5}$		
H309③	$ICl + Br^- \rightleftharpoons IBr + Cl^-$	$3.30 \cdot 10^{3}$	$1.65 \cdot 10^{14}$		$5.00 \cdot 10^{10}$		

(a) in M^{m-n}, n order of reaction of forward reaction, m order of reaction of backward reaction; (b) k_{298}^{2nd} in $l^1\ mol^{-1}\ s^{-1}$, k_{298}^{1st} in s^{-1}; (c) in K

Table S11 **Measured values of HCl and BrO in marine environments.**

HCl	BrO*	Location	Comment	Reference
daily average: 133 – 675 ppt		Bermuda		Keene and Savoie (1999)
range: 30-250 ppt		Hawaii		Pszenny et al. (2004)
median: 351 ppt		Appledore Island		Keene et al. (2007)
daily median: 82-682 ppt		North to South Atlantic		Keene et al. (2009)
median: 206 ppt		Cape Verde	range: 26 – 613 ppt	Sander et al. (2013)
	max. 1-3.6 ppt	Canary Island	in remote ocean below detection limit	Leser et al. (2003)
	average 2.3 ppt	Mace Head	Coastal region	Saiz-Lopez et al. (2004)
	average max. 2.5 ± 1.1 ppt	Cape Verde		Read et al. (2008)
	< 0.5 ppt	Eastern tropical Pacific	MBL: below detection limit	Volkamer et al. (2015)
	0.03 ± 0.26 ppt	Western tropical Pacific	clean MBL outflow	Chen et al. (2016)
	0.17-1.64 ppt	Western Pacific	between 0.5 – 7 km height	Le Breton et al. (2017)

DL – Detection Limit; * for a more detailed overview on measurements before 2003 see Sander et al. (2003)

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