

# Kinetic data for MANIC

January 9, 2011

*supplemental material to:*

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Modelling multi-phase halogen chemistry in the coastal marine boundary layer: investigation of the relative importance of local chemistry vs long-range transport.

*Atmos. Chem. Phys.*, 2010

# 1 Chemistry Scheme

This collection comprises a complete listing of all gas and aqueous phase species (Table 1), gas phase (Table 2) and aqueous phase (Table 3) reaction rates, as well as rates for the heterogeneous (particle surface) reactions (Table 4), aqueous phase equilibrium constants (Table 5), Henry constants and accommodation coefficients (Table 6). Unless otherwise indicated, the chemical rate constants are taken from Pechtl et al. (2006).

Table 1: Species

Gas phase
O <sup>1</sup> D, O <sub>2</sub> , O <sub>3</sub> , OH, HO <sub>2</sub> , H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O
NO, NO <sub>2</sub> , NO <sub>3</sub> , N <sub>2</sub> O <sub>5</sub> , HONO, HNO <sub>3</sub> , HNO <sub>4</sub> , PAN, NH <sub>3</sub>
CO, CO <sub>2</sub> , CH <sub>4</sub> , C <sub>2</sub> H <sub>6</sub> , C <sub>2</sub> H <sub>4</sub> , HCHO, HCOOH, ALD, HOCH <sub>2</sub> O <sub>2</sub> , CH <sub>3</sub> CO <sub>3</sub> , CH <sub>3</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> , EO <sub>2</sub> , ROOH
SO <sub>2</sub> , SO <sub>3</sub> , HOSO <sub>2</sub> , H <sub>2</sub> SO <sub>4</sub> , DMS, CH <sub>3</sub> SCH <sub>2</sub> OO, DMSO, DMSO <sub>2</sub> , CH <sub>3</sub> S, CH <sub>3</sub> SO, CH <sub>3</sub> SO <sub>2</sub> , CH <sub>3</sub> SO <sub>3</sub> , CH <sub>3</sub> SO <sub>2</sub> H, CH <sub>3</sub> SO <sub>3</sub> H
Cl, ClO, OCLO, HCl, HOCl, Cl <sub>2</sub> , Cl <sub>2</sub> O <sub>2</sub> , ClNO <sub>2</sub> , ClONO <sub>2</sub>
Br, BrO, HBr, HOBr, Br <sub>2</sub> , BrNO <sub>2</sub> , BrONO <sub>2</sub> , BrCl
I, IO, OIO, HI, HOI, INO <sub>2</sub> , IONO <sub>2</sub> , I <sub>2</sub> , ICl, IBr, HIO <sub>3</sub> , CH <sub>3</sub> I, C <sub>2</sub> H <sub>5</sub> I, C <sub>3</sub> H <sub>7</sub> I, CH <sub>3</sub> ClI, CH <sub>2</sub> BrI, CH <sub>2</sub> I <sub>2</sub> , I <sub>2</sub> O <sub>2</sub> , I <sub>2</sub> O <sub>3</sub> , I <sub>2</sub> O <sub>4</sub> , I <sub>2</sub> O <sub>5</sub>
Liquid phase (neutral)
O <sub>2</sub> , O <sub>3</sub> , OH, HO <sub>2</sub> , H <sub>2</sub> O <sub>2</sub> , H <sub>2</sub> O
NO, NO <sub>2</sub> , NO <sub>3</sub> , HONO, HNO <sub>3</sub> , HNO <sub>4</sub> , NH <sub>3</sub>
CO <sub>2</sub> , HCHO, HCOOH, CH <sub>3</sub> OH, CH <sub>3</sub> OO, CH <sub>3</sub> OOH, DOM, ROOH
SO <sub>2</sub> , H <sub>2</sub> SO <sub>4</sub> , DMS, DMSO, DMSO <sub>2</sub> , CH <sub>3</sub> SO <sub>2</sub> H, CH <sub>3</sub> SO <sub>3</sub> H
Cl, HCl, HOCl, Cl <sub>2</sub>
Br, HBr, HOBr, Br <sub>2</sub> , BrCl
IO, HI, HOI, I <sub>2</sub> , ICl, IBr
Liquid phase (ions)
H <sup>+</sup> , OH <sup>-</sup> , O <sub>2</sub> <sup>-</sup> , HO <sub>2</sub> <sup>-</sup>
NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> , NO <sub>4</sub> <sup>-</sup> , NH <sub>4</sub> <sup>+</sup>
HCO <sub>3</sub> <sup>-</sup> , CO <sub>3</sub> <sup>-</sup> , HCOO <sup>-</sup>
HSO <sub>3</sub> <sup>-</sup> , SO <sub>3</sub> <sup>2-</sup> , HSO <sub>4</sub> <sup>-</sup> , SO <sub>4</sub> <sup>2-</sup> , HSO <sub>5</sub> <sup>-</sup> , SO <sub>3</sub> <sup>-</sup> , SO <sub>4</sub> <sup>-</sup> , SO <sub>5</sub> <sup>-</sup> , CH <sub>3</sub> SO <sub>3</sub> <sup>-</sup> , CH <sub>2</sub> OHSO <sub>2</sub> <sup>-</sup> , CH <sub>2</sub> OHSO <sub>3</sub> <sup>-</sup>
Cl <sup>-</sup> , Cl <sub>2</sub> <sup>-</sup> , ClO <sup>-</sup> , ClOH <sup>-</sup>
Br <sup>-</sup> , Br <sub>2</sub> <sup>-</sup> , BrO <sup>-</sup> , BrCl <sub>2</sub> <sup>-</sup> , Br <sub>2</sub> Cl <sup>-</sup> , BrOH <sup>-</sup>
I <sup>-</sup> , IO <sub>2</sub> <sup>-</sup> , IO <sub>3</sub> <sup>-</sup> , ICl <sub>2</sub> <sup>-</sup> , IBr <sub>2</sub> <sup>-</sup> , IClBr <sup>-</sup>

Table 2: Gas phase reactions.

no	reaction	$n$	$A [(cm^{-3})^{1-n} s^{-1}]$	$-E_a/R [K]$	reference
O 1	$O^1D + O_2 \rightarrow O_3$	2	$3.2 \times 10^{-11}$	70	
O 2	$O^1D + N_2 \rightarrow O_3$	2	$1.8 \times 10^{-11}$	110	
O 3	$O^1D + H_2O \rightarrow 2OH$	2	$2.2 \times 10^{-10}$		
O 4	$OH + O_3 \rightarrow HO_2 + O_2$	2	$1.7 \times 10^{-12}$	-940	
O 5	$OH + HO_2 \rightarrow H_2O + O_2$	2	$4.8 \times 10^{-11}$	250	
O 6	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2	$2.9 \times 10^{-12}$	-160	
O 7	$HO_2 + O_3 \rightarrow OH + 2O_2$	2	$1.0 \times 10^{-14}$	-490	
O 8	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	2	$2.3 \times 10^{-13}$	600	
O 9	$O_3 + hv \rightarrow O_2 + O^1D$	1	1		
O 10	$H_2O_2 + hv \rightarrow 2OH$	1	1		
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N 1	$NO + OH \xrightarrow{M} HONO$	3	2		Sander et al. (2006)
N 2	$NO + HO_2 \rightarrow NO_2 + OH$	2	$3.5 \times 10^{-12}$	250	
N 3	$NO + O_3 \rightarrow NO_2 + O_2$	2	$3.0 \times 10^{-12}$	-1500	
N 4	$NO + NO_3 \rightarrow 2NO_2$	2	$1.5 \times 10^{-11}$	170	
N 5	$NO_2 + OH \xrightarrow{M} HNO_3$	3	2		Sander et al. (2006)
N 6	$NO_2 + HO_2 \xrightarrow{M} HNO_4$	3	2		Sander et al. (2006)
N 7	$NO_2 + O_3 \rightarrow NO_3 + O_2$	2	$1.2 \times 10^{-13}$	-2450	
N 8	$NO_2 + hv \rightarrow NO + O_3$	1	1		
N 9	$NO_2 + NO_3 \xrightarrow{M} N_2O_5$	3	2		
N 10	$NO_3 + hv \rightarrow NO + O_3$	1	1		
N 11	$NO_3 + HO_2 \rightarrow 0.3HNO_3 + 0.7OH + 0.7NO_2 + O_2$	2	$4.0 \times 10^{-12}$		
N 12	$NO_3 + NO_3 \rightarrow NO_2 + NO_2 + O_2$	2	$8.5 \times 10^{-13}$		
N 13	$NO_3 + hv \rightarrow NO_2 + O_3$	1	1		
N 14	$N_2O_5 \xrightarrow{M} NO_2 + NO_3$	2	2		
N 15	$N_2O_5 + H_2O \rightarrow 2HNO_3$	2	$2.6 \times 10^{-22}$		
N 16	$N_2O_5 + hv \rightarrow NO_2 + NO_3$	1	1		
N 17	$HONO + OH \rightarrow NO_2$	2	$1.8 \times 10^{-11}$		
N 18	$HONO + hv \rightarrow NO + OH$	1	1	-390	
N 19	$HONO_3 + hv \rightarrow NO_2 + OH$	1	1		

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
N 20	$HNO_3 + OH \longrightarrow NO_3 + H_2O$	2	2		Sander et al. (2006)
N 21	$HNO_4 \xrightarrow{M} NO_2 + HO_2$	2	2		Sander et al. (2006), see note
N 22	$HNO_4 + OH \longrightarrow NO_2 + H_2O + O_2$	2	$1.3 \times 10^{-12}$		
N 23	$HNO_4 + h\nu \longrightarrow NO_2 + HO_2$	1	1	380	
N 24	$HNO_4 + h\nu \longrightarrow OH + NO_3$	1	1		
C 1	$CO + OH \xrightarrow{O_2} HO_2 + CO_2$	2	2		Sander et al. (2006)
C 2	$CH_4 + OH \xrightarrow{O_2} CH_3OO + H_2O$	2	$2.4 \times 10^{-12}$	-1175	
C 3	$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	2	$1.7 \times 10^{-11}$	-1232	
C 4	$C_2H_4 + OH \longrightarrow EO_2$	2	$1.66 \times 10^{-12}$	474	
C 5	$C_2H_4 + O_3 \longrightarrow HCHO + 0.4 HCOOH + 0.12 HO_2 + 0.42 CO + 0.06 CH_4$	2	$1.2 \times 10^{-14}$	-2633	
C 6	$HO_2 + CH_3OO \longrightarrow ROOH + O_2$	2	$4.1 \times 10^{-13}$	750	
C 7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	$7.5 \times 10^{-13}$	700	
C 8	$HO_2 + CH_3CO_3 \longrightarrow ROOH + O_2$	2	$4.5 \times 10^{-13}$	1000	
C 9	$CH_3OO + CH_3OO \longrightarrow 1.4 HCHO + 0.8 HO_2 + O_2$	2	$1.5 \times 10^{-13}$	220	
C 10	$C_2H_5O_2 + NO \longrightarrow ALD + HO_2 + NO_2$	2	$4.2 \times 10^{-12}$	180	
C 11	$2C_2H_5O_2 \longrightarrow 1.6 ALD + 1.2 HO_2$	2	$5.00 \times 10^{-14}$		
C 12	$EO_2 + NO \longrightarrow NO_2 + 2 HCHO + O_2$	2	$4.2 \times 10^{-12}$	180	
C 13	$EO_2 + EO_2 \longrightarrow 2.4 HCHO + 1.2 HO_2 + 0.4 ALD$	2	$5.00 \times 10^{-14}$		
C 14	$HO_2 + EO_2 \longrightarrow ROOH + O_2$	2	$3.00 \times 10^{-12}$		
C 15	$HCHO + h\nu \longrightarrow 2 HO_2 + CO$	1	1		
C 16	$HCHO + h\nu \longrightarrow CO + H_2$	1	1		
C 17	$HCHO + OH \xrightarrow{O_2} HO_2 + CO + H_2O$	2	$1.00 \times 10^{-11}$	600	
C 18	$HCHO + HO_2 \longrightarrow HOCH_2O_2$	2	$6.7 \times 10^{-15}$		
C 19	$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	2	$5.8 \times 10^{-16}$		
C 20	$ALD + OH \longrightarrow CH_3CO_3 + H_2O$	2	$6.9 \times 10^{-12}$	250	
C 21	$ALD + NO_3 \longrightarrow HNO_3 + CH_3CO_3$	2	$1.40 \times 10^{-15}$		
C 22	$ALD + h\nu \longrightarrow CH_3OO + HO_2 + CO$	1	1		
C 23	$ALD + h\nu \longrightarrow CH_4 + CO$	1	1		

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
C 24	$\text{HOCH}_2\text{O}_2 + \text{NO} \longrightarrow \text{HCOOH} + \text{HO}_2 + \text{NO}_2$	2	$4.2 \times 10^{-12}$		
C 25	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \longrightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{O}_2$	2	$2.00 \times 10^{-12}$		
C 26	$2\text{HOCH}_2\text{O}_2 \longrightarrow 2\text{HCOOH} + \text{HO}_2 + 2\text{O}_2$	2	$1.00 \times 10^{-13}$		
C 27	$\text{HCOOH} + \text{OH} \xrightarrow{\text{O}_2} \text{HO}_2 + \text{H}_2\text{O} + \text{CO}_2$	2	$4.0 \times 10^{-13}$		
C 28	$\text{CH}_3\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PAN}$	2	$4.70 \times 10^{-12}$		
C 29	$\text{PAN} \longrightarrow \text{CH}_3\text{CO}_3 + \text{NO}_2$	1	$1.9 \times 10^{16}$	-13543	
C 30	$\text{CH}_3\text{CO}_3 + \text{NO} \longrightarrow \text{CH}_3\text{OO} + \text{NO}_2 + \text{CO}_2$	2	$4.2 \times 10^{-12}$	180	
C 31	$\text{CH}_3\text{OO} + \text{NO} \xrightarrow{\text{O}_2} \text{HCHO} + \text{NO}_2 + \text{HO}_2$	2	$3.0 \times 10^{-12}$	280	
C 32	$\text{ROOH} + \text{OH} \longrightarrow 0.7\text{CH}_3\text{OO} + 0.3\text{HCHO} + 0.3\text{OH}$	2	$3.8 \times 10^{-12}$	200	
C 33	$\text{ROOH} + h\nu \longrightarrow \text{HCHO} + \text{OH} + \text{HO}_2$	1			
S 1	$\text{SO}_2 + \text{OH} \xrightarrow{M} \text{HOSO}_2$	3	2		
S 2	$\text{HOSO}_2 + \text{O}_2 \longrightarrow \text{HO}_2 + \text{SO}_3$	2	$1.3 \times 10^{-12}$	330	Atkinson et al. (2006)
S 3	$\text{SO}_3 \xrightarrow{\text{H}_2\text{O}} \text{H}_2\text{SO}_4$	1	$3.9 \times 10^{-41} \times [\text{H}_2\text{O}]^2$	6830.6	Jayne et al. (1997)
S 4	$\text{CH}_3\text{SCH}_3 + \text{OH} \longrightarrow \text{CH}_3\text{SCH}_2\text{OO} + \text{H}_2\text{O}$	2	$1.12 \times 10^{-11}$	-250	Atkinson et al. (2006), see note
S 5	$\text{CH}_3\text{SCH}_3 + \text{OH} \xrightarrow{\text{O}_2} \text{CH}_3\text{SOCH}_3 + \text{HO}_2$	3			
S 6	$\text{CH}_3\text{SCH}_3 + \text{NO}_3 \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HNO}_3$	2		520	
S 7	$\text{CH}_3\text{SCH}_3 + \text{Cl} \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HCl}$	2			
S 8	$\text{CH}_3\text{SCH}_3 + \text{Br} \xrightarrow{\text{O}_2} \text{CH}_3\text{SCH}_2\text{OO} + \text{HBr}$	2			
S 9	$\text{CH}_3\text{SCH}_3 + \text{BrO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{Br}$	2			
S 10	$\text{CH}_3\text{SCH}_3 + \text{ClO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{Cl}$	2			
S 11	$\text{CH}_3\text{SCH}_3 + \text{IO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{I}$	2			
S 12	$\text{CH}_3\text{SCH}_2\text{OO} + \text{NO} \longrightarrow \text{HCHO} + \text{CH}_3\text{S} + \text{NO}_2$	2			
S 13	$\text{CH}_3\text{SCH}_2\text{OO} + \text{CH}_3\text{SCH}_2\text{OO} \xrightarrow{\text{O}_2} 2\text{HCHO} + 2\text{CH}_3\text{S}$	2			
S 14	$\text{CH}_3\text{S} + \text{O}_3 \longrightarrow \text{CH}_3\text{SO} + \text{O}_2$	2			
S 15	$\text{CH}_3\text{S} + \text{NO}_2 \longrightarrow \text{CH}_3\text{SO} + \text{NO}$	2			
S 16	$\text{CH}_3\text{SO} + \text{NO}_2 \xrightarrow{\text{O}_2} 0.82\text{CH}_3\text{SO}_2 + 0.18\text{SO}_2 + 0.18\text{CH}_3\text{OO}$	2			
S 17	$\text{CH}_3\text{SO} + \text{O}_3 \xrightarrow{\text{O}_2} \text{CH}_3\text{SO}_2 + \text{NO}$	2	$6.0 \times 10^{-13}$		

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
S 18	$CH_3SO_2 \rightarrow SO_2 + CH_3OO$	1	$1.9 \times 10^{13}$		
S 19	$CH_3SO_2 + NO_2 \rightarrow CH_3SO_3 + NO$	2	$2.2 \times 10^{-12}$		-8661
S 20	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	2	$3 \times 10^{-13}$		
S 21	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	2	$5 \times 10^{-11}$		
S 22	$CH_3SO_3 \xrightarrow{H_2O} CH_3OO + H_2SO_4$	1	$1.36 \times 10^{14}$		
S 23	$CH_3SOCH_3 + OH \rightarrow 0.95 CH_3SO_2H + 0.95 CH_3OO$ +0.05 DMSO <sub>2</sub>	2	$8.7 \times 10^{-11}$		-11071
S 24	$CH_3SO_2H + OH \rightarrow 0.95 CH_3SO_2 + 0.05 CH_3SO_3H$ +0.05 HO <sub>2</sub> + H <sub>2</sub> O	2	$9 \times 10^{-11}$		
S 25	$CH_3SO_2H + NO_3 \rightarrow CH_3SO_2 + HNO_3$	2	$1.0 \times 10^{-13}$		
Cl 1	$Cl + O_3 \rightarrow ClO + O_2$	2	$2.8 \times 10^{-11}$		-250
Cl 2	$Cl + HO_2 \rightarrow HCl + O_2$	2	$1.8 \times 10^{-11}$		170
Cl 3	$Cl + HO_2 \rightarrow ClO + OH$	2	$4.1 \times 10^{-11}$		-450
Cl 4	$Cl + H_2O_2 \rightarrow HCl + HO_2$	2	$1.1 \times 10^{-11}$		-980
Cl 5	$Cl + CH_3OO \rightarrow 0.5 ClO + 0.5 HCHO + 0.5 HO_2$ +0.5 HCl + 0.5 CO + 0.5 H <sub>2</sub> O	2	$1.6 \times 10^{-10}$		
Cl 6	$Cl + CH_4 \xrightarrow{O_2} HCl + CH_3OO$	2	$9.6 \times 10^{-12}$		-1360
Cl 7	$Cl + C_2H_6 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	$7.7 \times 10^{-11}$		-90
Cl 8	$Cl + C_2H_4 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	$1 \times 10^{-10}$		
Cl 9	$Cl + HCHO \xrightarrow{O_2} HCl + HO_2 + CO$	2	$8.1 \times 10^{-11}$		
Cl 10	$Cl + ROOH \rightarrow CH_3OO + HCl$	2	$5.7 \times 10^{-11}$		-30
Cl 11	$Cl + OCIO \rightarrow ClO + ClO$	2	$3.2 \times 10^{-11}$		
Cl 12	$Cl + ClONO_2 \rightarrow Cl_2 + NO_3$	2	$6.5 \times 10^{-12}$		170
Cl 13	$ClO + OH \rightarrow Cl + HO_2$	2	$7.4 \times 10^{-12}$		135
Cl 14	$ClO + OH \rightarrow HCl + O_2$	2	$6.0 \times 10^{-13}$		-270
Cl 15	$ClO + HO_2 \rightarrow HOCl + O_2$	2	$2.2 \times 10^{-12}$		-230
Cl 16	$ClO + CH_3OO \rightarrow Cl + HCHO + HO_2$	2	$3.3 \times 10^{-12}$		340
Cl 17	$ClO + NO \rightarrow Cl + NO_2$	2	$6.2 \times 10^{-12}$		-115
Cl 18	$ClO + NO_2 \xrightarrow{M} ClONO_2$	3 <sub>2</sub>			295
					M. Kanakidou, pers. comm.

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R [K]$	reference
Cl 19	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$	2	$2$	$1.0 \times 10^{-12}$	Atkinson et al. (2006)
Cl 20	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$	2	$1.0 \times 10^{-12}$	$-1590$	
Cl 21	$\text{ClO} + \text{ClO} \rightarrow 2\text{Cl} + \text{O}_2$	2	$3.0 \times 10^{-11}$	$-2450$	
Cl 22	$\text{ClO} + \text{ClO} \rightarrow \text{Cl} + \text{OCIO}$	2	$3.5 \times 10^{-13}$	$-1370$	
Cl 23	$\text{OCIO} + \text{OH} \rightarrow \text{HOCl} + \text{O}_2$	2	$4.5 \times 10^{-13}$	$800$	
Cl 24	$\text{OCIO} + \text{NO} \rightarrow \text{ClO} + \text{NO}_2$	2	$1.1 \times 10^{-13}$	$350$	M. Kanakidou, pers. comm.
Cl 25	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	1	$2$		
Cl 26	$\text{HOCl} + \text{OH} \rightarrow \text{ClO} + \text{H}_2\text{O}$	2	$3.0 \times 10^{-12}$	$-500$	
Cl 27	$\text{HCl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	2	$1.8 \times 10^{-12}$	$-240$	
Cl 28	$\text{ClNO}_2 + \text{OH} \rightarrow \text{HOCl} + \text{NO}_2$	2	$2.4 \times 10^{-12}$	$-1250$	
Cl 29	$\text{ClONO}_2 + \text{OH} \rightarrow 0.5\text{ClO} + 0.5\text{HNO}_3 + 0.5\text{HOCl} + 0.5\text{NO}_2$	2	$1.2 \times 10^{-12}$	$-330$	
Cl 30	$\text{ClONO}_2 \rightarrow \text{ClO} + \text{NO}_2$	1	$2$		
Cl 31	$\text{OCIO} + hv \xrightarrow{\text{O}_2, \text{O}_3} \text{O}_3 + \text{ClO}$	1	$1$		
Cl 32	$\text{Cl}_2\text{O}_2 + hv \rightarrow \text{Cl} + \text{Cl} + \text{O}_2$	1	$1$		
Cl 33	$\text{Cl}_2 + hv \rightarrow 2\text{Cl}$	1	$1$		
Cl 34	$\text{HOCl} + hv \rightarrow \text{Cl} + \text{OH}$	1	$1$		
Cl 35	$\text{ClNO}_2 + hv \rightarrow \text{Cl} + \text{NO}_2$	1	$1$		
Cl 36	$\text{ClONO}_2 + hv \rightarrow \text{Cl} + \text{NO}_3$	1	$1$		
Br 1	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	2	$1.7 \times 10^{-11}$	$-800$	
Br 2	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	2	$7.7 \times 10^{-12}$	$-450$	
Br 3	$\text{Br} + \text{C}_2\text{H}_4 \xrightarrow{\text{O}_2} \text{HBr} + \text{C}_2\text{H}_5\text{O}_2$	2	$5 \times 10^{-14}$		
Br 4	$\text{Br} + \text{HCHO} \xrightarrow{\text{O}_2} \text{HBr} + \text{CO} + \text{HO}_2$	2	$1.7 \times 10^{-11}$		
Br 5	$\text{Br} + \text{ROOH} \rightarrow \text{CH}_3\text{OO} + \text{HBr}$	2	$2.66 \times 10^{-12}$	$-800$	
Br 6	$\text{Br} + \text{NO}_2 \xrightarrow{M} \text{BrNO}_2$	3	$2$	$-1610$	Sander et al. (2006)
Br 7	$\text{Br} + \text{BrONO}_2 \rightarrow \text{Br}_2 + \text{NO}_3$	2	$4.9 \times 10^{-11}$		
Br 8	$\text{BrO} + \text{OH} \rightarrow \text{Br} + \text{HO}_2$	2	$1.8 \times 10^{-11}$	$250$	
Br 9	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	2	$4.5 \times 10^{-12}$	$500$	
Br 10	$\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{HOBr} + \text{HCHO}$	2	$4.1 \times 10^{-12}$		
Br 11	$\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{Br} + \text{HCHO} + \text{HO}_2$	2	$1.6 \times 10^{-12}$		

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
Br 12	$BrO + HCHO \xrightarrow{O_2} HOBr + CO + HO_2$	2	$1.5 \times 10^{-14}$		
Br 13	$BrO + NO \longrightarrow Br + NO_2$	2	$8.7 \times 10^{-12}$	260	Sander et al. (2006)
Br 14	$BrO + NO_2 \xrightarrow{M} BrONO_2$	3			
Br 15	$BrO + BrO \longrightarrow 2Br + O_2$	2	$2.4 \times 10^{-12}$		
Br 16	$BrO + BrO \longrightarrow Br_2 + O_2$	2	$2.9 \times 10^{-14}$	40	
Br 17	$HBr + OH \longrightarrow Br + H_2O$	2	$5.5 \times 10^{-12}$	860	
Br 18	$BrONO_2 \longrightarrow BrO + NO_2$	1		205	M. Kanakidou, pers. comm.
Br 19	$BrO + hv \xrightarrow{O_2} Br + O_3$	1	1		
Br 20	$Br_2 + hv \longrightarrow 2Br$	1	1		
Br 21	$HOBr + hv \longrightarrow Br + OH$	1	1		
Br 22	$BrNO_2 + hv \longrightarrow Br + NO_2$	1	1		
Br 23	$BrONO_2 + hv \longrightarrow Br + NO_3$	1	1		
I 1	$I + O_3 \longrightarrow IO + O_2$	2	$1.9 \times 10^{-11}$	-830	
I 2	$I + HO_2 \longrightarrow HI + O_2$	2	$1.5 \times 10^{-11}$	-1090	
I 3	$I + NO_2 \xrightarrow{M} INO_2$	3			
I 4	$I + NO_3 \longrightarrow IO + NO_2$	2	$4.5 \times 10^{-10}$		
I 5	$I + I \longrightarrow I_2$	2	$2.99 \times 10^{-11}$		
I 6	$IO + HO_2 \longrightarrow HOI + O_2$	2	$1.4 \times 10^{-11}$	540	
I 7	$IO + NO \longrightarrow I + NO_2$	2	$7.15 \times 10^{-12}$	300	
I 8	$IO + NO_2 \xrightarrow{M} IONO_2$	3			
I 9	$IO + IO \longrightarrow 0.3OIO + 0.3I + 0.7I_2O_2$	2	$5.4 \times 10^{-11}$		
I 10	$OIO + OH \longrightarrow 0.5HOIO_2 + 0.5HOI$	2	$2.0 \times 10^{-10}$	180	
I 11	$OIO + NO \longrightarrow NO_2 + IO$	2	$5.1 \times 10^{-13}$	712	
I 12	$HI + OH \longrightarrow I + H_2O$	2	$1.6 \times 10^{-11}$	440	
I 13	$HI + NO_3 \longrightarrow I + HNO_3$	2	$1.3 \times 10^{-12}$	-1830	
I 14	$INO_2 \xrightarrow{M} I + NO_2$	2	2.4		
I 15	$INO_2 \xrightarrow{M} IO + NO_2$	2	$1.1 \times 10^{15}$	-12060	
I 16	$I_2 + OH \longrightarrow I + HOI$	2	$2.1 \times 10^{-10}$		
I 17	$I_2 + NO_3 \longrightarrow I + IONO_2$	2	$1.5 \times 10^{-12}$		

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
I 18	$CH_3I + OH \rightarrow HCHO + I$	2	$4.3 \times 10^{-12}$	-1120	
I 19	$C_3H_7I + OH \rightarrow CH_3OO + I$	2	$1.2 \times 10^{-12}$		
I 20	$IO + hv \xrightarrow{O_2} I + O_3$	1	1		
I 21	$OIO + hv \rightarrow I + O_2$	1	$1 \times 10^{-12}$		
I 22	$HOI + hv \rightarrow I + OH$	1	1		
I 23	$INO_2 + hv \rightarrow I + NO_2$	1	1		
I 24	$IONO_2 + hv \rightarrow I + NO_3$	1	1		
I 25	$I_2 + hv \rightarrow 2I$	1	1		
I 26	$CH_3I + hv \rightarrow I + CH_3OO$	1	1		
I 27	$C_2H_5I + hv \rightarrow I + ROOH$	1	1		
I 28	$C_3H_7I + hv \rightarrow I + ROOH$	1	1		
I 29	$CH_2ClI + hv \rightarrow I + Cl + 2HO_2 + CO$	1	1		
I 30	$CH_2BrI + hv \rightarrow I + Br + 2HO_2 + CO$	1	1		
I 31	$CH_2I_2 + hv \rightarrow I + IO + HCHO$	1	1		
I 32	$I_2O_2 \rightarrow 2IO$	1	0.04	(at 290K)	Kaltsoyannis and Plane (2008)
I 33	$I_2O_2 \rightarrow OIO + I$	1	10.0	(at 290K)	Kaltsoyannis and Plane (2008)
I 32	$I + IONO_2 \rightarrow I_2 + NO_3$	2	$5.5 \times 10^{-11}$	(at 290K)	Kaltsoyannis and Plane (2008)
I 33	$IO + OIO \rightarrow I_2O_3$	2	$1.5 \times 10^{-10}$		Gómez Martín et al. (2005)
I 34	$OIO + OIO \rightarrow I_2O_4$	2	$1.0 \times 10^{-10}$		(rate after Saiz-Lopez et al., 2008)
I 35	$I_2O_2 + O_3 \rightarrow I_2O_3 + O_2$	2	$1.0 \times 10^{-12}$		Saunders and Plane (2005)
I 36	$I_2O_3 + O_3 \rightarrow I_2O_4 + O_2$	2	$1.0 \times 10^{-12}$		(rate after Saiz-Lopez et al., 2008)
I 37	$I_2O_4 + O_3 \rightarrow I_2O_5 + O_2$	2	$1.0 \times 10^{-12}$		Saunders and Plane (2005)
I 38	$I_2O_4 \rightarrow 2OIO$	1	0.4	(at 290K)	(rate after Saiz-Lopez et al., 2008)
I 39	$I_2O_2 + hv \rightarrow IO + IO$	1	0.06 (at midday)		Kaltsoyannis and Plane (2008)
I 40	$I_2O_3 + hv \rightarrow IO + OIO$	1	0.06 (at midday)		estimated by Mahajan et al. (2009)
					estimated by Mahajan et al. (2009)

Table 2: Continued

no	reaction	$n$	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R [K]$	reference
I 41	$I_2O_4 + h\nu \longrightarrow OIO + OIO$	1	0.06 (at midday)		estimated by Mahajan et al. (2009)
Hx 1	$Cl + CH_3I \longrightarrow HCl + HCHO + I$	2	$2.9 \times 10^{-11}$		-1000
Hx 2	$Cl + BrCl \longrightarrow Br + Cl_2$	2	$1.5 \times 10^{-11}$		
Hx 3	$Cl + Br_2 \longrightarrow BrCl + Br$	2	$1.2 \times 10^{-10}$		
Hx 4	$I_2 + Cl \longrightarrow I + ICl$	2	$2.09 \times 10^{-10}$		
Hx 5	$Br + OCIO \longrightarrow BrO + ClO$	2	$2.6 \times 10^{-11}$		-1300
Hx 6	$Br + Cl_2 \longrightarrow BrCl + Cl$	2	$1.1 \times 10^{-15}$		
Hx 7	$Br + BrCl \longrightarrow Br_2 + Cl$	2	$3.3 \times 10^{-15}$		
Hx 8	$I_2 + Br \longrightarrow I + IBr$	2	$1.2 \times 10^{-10}$		
Hx 9	$I + BrO \longrightarrow IO + Br$	2	$1.2 \times 10^{-11}$		
Hx 10	$BrO + ClO \longrightarrow Br + OCIO$	2	$1.6 \times 10^{-12}$		430
Hx 11	$BrO + ClO \longrightarrow Br + Cl + O_2$	2	$2.9 \times 10^{-12}$		220
Hx 12	$BrO + ClO \longrightarrow BrCl + O_2$	2	$5.8 \times 10^{-13}$		170
Hx 13	$IO + ClO \longrightarrow 0.8 I + 0.55 OCIO + 0.45 O_2 + 0.25 Cl + 0.2 ICl$	2	$4.7 \times 10^{-12}$		280
Hx 14	$IO + BrO \longrightarrow Br + 0.8 OIO + 0.2 I + 0.2 O_2$	2	$1.5 \times 10^{-11}$		510
Hx 15	$BrCl + h\nu \longrightarrow Br + Cl$	1	1		
Hx 16	$ICl + h\nu \longrightarrow I + Cl$	1	1		
Hx 17	$IBr + h\nu \longrightarrow I + Br$	1	1		

$n$  is the order of the reaction.<sup>1</sup> Photolysis rates are calculated from actinic fluxes measured at Roscoff during the RHaMBLe campaign. (Damian et al., 2002).<sup>2</sup> Special rate functions (pressure and/or humidity dependent). Notes: Self dissociation rates of  $N_2O_5$  and  $HNO_4$  are calculated by dividing their formation rates (reactions N9 and N6 respectively) by the equilibrium constants given in Sander et al. (2006).  $CH_3SCH_3$  reacts with OH and  $O_2$  to form  $CH_3SCH_2OO$ , however the second step of this process (that involving  $O_2$ ) is extremely rapid, so it is assumed that the process is controlled only by the first reaction rate. The temperature dependence is  $k = A \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$ , where  $T_0 = 298$  K.

Table 3: Aqueous phase reactions

no	reaction	$n$	$k_0 [(M^{1-n}) s^{-1}]$	$-E_a/R [K]$	reference
O 1	$O_3 + OH \rightarrow HO_2$	2	$1.1 \times 10^8$		
O 2	$O_3 + O_2^- \rightarrow OH + OH^-$	2	$1.5 \times 10^9$		
O 3	$OH + OH \rightarrow H_2O_2$	2	$5.5 \times 10^9$		
O 4	$OH + HO_2 \rightarrow H_2O$	2	$7.1 \times 10^9$		
O 5	$OH + O_2^- \rightarrow OH^-$	2	$1.0 \times 10^{10}$		
O 6	$OH + H_2O_2 \rightarrow HO_2$	2	$2.7 \times 10^7$	-1684	
O 7	$HO_2 + HO_2 \rightarrow H_2O_2$	2	$9.7 \times 10^5$	-2500	
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	$1.0 \times 10^8$	-900	
N 1	$HONO + OH \rightarrow NO_2$	2	$1.0 \times 10^{10}$		
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3 + H^+$	3	$4.6 \times 10^3$		
N 3	$NO_3^- + OH^- \rightarrow NO_3^- + OH$	2	$8.2 \times 10^7$	-6800	
N 4	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	2	$1.0 \times 10^8$	-2700	
N 5	$NO_2 + HO_2 \rightarrow HNO_4$	2	$1.8 \times 10^9$		
N 6	$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	2	$5.0 \times 10^5$	-6950	
N 7	$NO_2^- + OH \rightarrow NO_2 + OH^-$	2	$1.0 \times 10^{10}$		
N 8	$NO_4^- \rightarrow NO_2^- + O_2$	1	$8.0 \times 10^{-1}$		
C 1	$HCHO + OH \rightarrow HCOOH + HO_2$	2	$7.7 \times 10^8$	-1020	
C 2	$HCOOH + OH \rightarrow HO_2 + CO_2$	2	$1.1 \times 10^8$	-991	
C 3	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	2	$3.1 \times 10^9$	-1240	
C 4	$CH_3OO + HO_2 \rightarrow CH_3OOH$	2	$4.3 \times 10^5$		
C 5	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	2	$5.0 \times 10^7$		
C 6	$CH_3OH + OH \rightarrow HCHO + HO_2$	2	$9.7 \times 10^8$		
C 7	$CH_3OOH + OH \rightarrow CH_3OO$	2	$2.7 \times 10^7$	-1715	
C 8	$CH_3OOH + OH \rightarrow HCHO + OH$	2	$1.1 \times 10^7$	-1715	
C 9	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	2	$6.5 \times 10^8$		
C 10	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	2	$4.3 \times 10^5$		
C 11	$CO_3^- + HCOO^- \rightarrow 2HCO_3^- + HO_2$	2	$1.5 \times 10^5$		
C 12	$HCO_3^- + OH \rightarrow CO_3^-$	2	$8.5 \times 10^6$		
C 13	$DOM + OH \rightarrow HO_2$	2	$5.0 \times 10^9$		

Table 3: Continued

no	reaction	$n$	$k_0 [(M^{1-n}) s^{-1}]$	$-E_a/R [K]$	reference
S 1	$\text{SO}_3^- + \text{O}_2 \longrightarrow \text{SO}_5^-$	2	$1.5 \times 10^9$		
S 2	$\text{HSO}_3^- + \text{O}_3 \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{O}_2$	2	$3.7 \times 10^5$	-5500	
S 3	$\text{SO}_3^{2-} + \text{O}_3 \longrightarrow \text{SO}_4^{2-} + \text{O}_2$	2	$1.5 \times 10^9$	-5300	
S 4	$\text{HSO}_3^- + \text{OH} \longrightarrow \text{SO}_3^-$	2	$4.5 \times 10^9$		
S 5	$\text{SO}_3^- + \text{OH} \longrightarrow \text{SO}_3^- + \text{OH}^-$	2	$5.5 \times 10^9$		
S 6	$\text{HSO}_3^- + \text{HO}_2 \longrightarrow \text{SO}_4^{2-} + \text{OH} + \text{H}^+$	2	$3.0 \times 10^3$		
S 7	$\text{HSO}_3^- + \text{O}_2^- \longrightarrow \text{SO}_4^{2-} + \text{OH}$	2	$3.0 \times 10^3$		
S 8	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \longrightarrow \text{SO}_4^{2-} + \text{H}^+$	2	$5.2 \times 10^6 \times \frac{[\text{H}^+]}{[\text{H}^+] + 0.1M}$	-3650	
S 9	$\text{HSO}_3^- + \text{NO}_2 \xrightarrow{\text{NO}_2} \text{HSO}_4^- + \text{HONO} + \text{HONO}$	2	$2.0 \times 10^7$		
S 10	$\text{SO}_3^{2-} + \text{NO}_2 \xrightarrow{\text{NO}_2} \text{SO}_4^{2-} + \text{HONO} + \text{HONO}$	2	$2.0 \times 10^7$		
S 11	$\text{HSO}_3^- + \text{NO}_3^- \longrightarrow \text{SO}_3^- + \text{NO}_3^- + \text{H}^+$	2	$1.4 \times 10^9$	-2000	
S 12	$\text{HSO}_3^- + \text{HNO}_4 \longrightarrow \text{HSO}_4^- + \text{NO}_3^- + \text{H}^+$	2	$3.1 \times 10^5$		
S 13	$\text{HSO}_3^- + \text{CH}_3\text{OOH} \xrightarrow{\text{H}^+} \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OH}$	3	$1.6 \times 10^7$	-3800	
S 14	$\text{SO}_3^{2-} + \text{CH}_3\text{OOH} \xrightarrow{\text{H}^+} \text{SO}_4^{2-} + \text{CH}_3\text{OH}$	3	$1.6 \times 10^7$	-3800	
S 15	$\text{HSO}_3^- + \text{HCHO} \longrightarrow \text{CH}_2\text{OHSO}_3^-$	2	$4.3 \times 10^{-1}$		
S 16	$\text{SO}_3^{2-} + \text{HCHO} \xrightarrow{\text{H}^+} \text{CH}_2\text{OHSO}_3^-$	2	$1.4 \times 10^4$		
S 17	$\text{CH}_2\text{OHSO}_3^- + \text{OH}^- \longrightarrow \text{SO}_3^{2-} + \text{HCHO}$	2	$3.6 \times 10^3$		
S 18	$\text{HSO}_3^- + \text{HSO}_5^- \xrightarrow{\text{H}^+} \text{SO}_4^{2-} + \text{SO}_4^{2-} + \text{H}^+ + \text{H}^+$	2	$7.1 \times 10^6$		
S 19	$\text{SO}_4^- + \text{OH} \longrightarrow \text{HSO}_5^-$	2	$1.0 \times 10^9$		
S 20	$\text{SO}_4^- + \text{HO}_2 \longrightarrow \text{SO}_4^{2-} + \text{H}^+$	2	$3.5 \times 10^9$		
S 21	$\text{SO}_4^- + \text{O}_2^- \longrightarrow \text{SO}_4^{2-}$	2	$3.5 \times 10^9$		
S 22	$\text{SO}_4^- + \text{H}_2\text{O} \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}$	2	$1.1 \times 10^1$	-1110	
S 23	$\text{SO}_4^- + \text{H}_2\text{O}_2 \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2$	2	$1.2 \times 10^7$		
S 24	$\text{SO}_4^- + \text{NO}_3^- \longrightarrow \text{SO}_4^{2-} + \text{NO}_3^-$	2	$5.0 \times 10^4$		
S 25	$\text{SO}_4^- + \text{HSO}_3^- \longrightarrow \text{SO}_3^- + \text{SO}_4^{2-} + \text{H}^+$	2	$8.0 \times 10^8$		
S 26	$\text{SO}_4^- + \text{SO}_3^{2-} \longrightarrow \text{SO}_3^- + \text{SO}_4^{2-}$	2	$4.6 \times 10^8$		
S 27	$\text{SO}_4^{2-} + \text{NO}_3^- \longrightarrow \text{NO}_3^- + \text{SO}_4^-$	2	$1.0 \times 10^5$		
S 28	$\text{SO}_5^- + \text{HSO}_3^- \longrightarrow \text{SO}_4^- + \text{SO}_4^{2-} + \text{H}^+$	2	$7.5 \times 10^4$		

Table 3: Continued

no	reaction	$n$	$k_0 [ (M^{1-n}) s^{-1} ]$	$-E_a/R [K]$	reference
S 29	$\text{SO}_5^- + \text{SO}_3^{2-} \rightarrow \text{SO}_4^- + \text{SO}_4^{2-}$	2	$9.4 \times 10^6$		
S 30	$\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{SO}_3^- + \text{HSO}_5^-$	2	$2.5 \times 10^4$		
S 31	$\text{SO}_5^- + \text{SO}_3^{2-} \xrightarrow{\text{H}^+} \text{SO}_3^- + \text{HSO}_5^-$	2	$3.6 \times 10^6$		
S 32	$\text{SO}_5^- + \text{O}_2^- \xrightarrow{\text{H}^+} \text{HSO}_5^- + \text{O}_2$	2	$2.3 \times 10^8$		
S 33	$\text{SO}_5^- + \text{SO}_5^- \rightarrow 2 \text{SO}_4^-$	2	$1.0 \times 10^8$	-2600	
S 34	$\text{DMS} + \text{O}_3 \rightarrow \text{O}_2 + \text{DMSO}$	2	$8.6 \times 10^8$		
S 35	$\text{DMS} + \text{OH} \rightarrow 0.5 \text{CH}_3\text{SO}_3^- + 0.5 \text{CH}_3\text{OO}$ $+ 0.5 \text{HSO}_4^- + \text{HCHO} + \text{H}^+$	2	$1.9 \times 10^{10}$		
S 36	$\text{DMSO} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2^- + \text{CH}_3\text{OO} + \text{H}^+$	2	$4.5 \times 10^9$		
S 37	$\text{CH}_3\text{SO}_2^- + \text{OH} \rightarrow \text{CH}_3\text{SO}_3^- + \text{H}_2\text{O} + \text{O}_2$	2	$1.2 \times 10^{10}$		
S 38	$\text{CH}_3\text{SO}_3^- + \text{OH} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OO}$	2	$1.2 \times 10^7$		
Cl 1	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl}^- + \text{H}^+$	2	$2.0 \times 10^9$		
Cl 2	$\text{Cl} + \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{ClOH}^-$	2	$1.8 \times 10^5$		
Cl 3	$\text{Cl} + \text{NO}_3^- \rightarrow \text{NO}_3 + \text{Cl}^-$	2	$1.0 \times 10^8$		
Cl 4	$\text{Cl} + \text{DOM} \rightarrow \text{Cl}^- + \text{HO}_2$	2	$5.0 \times 10^9$		
Cl 5	$\text{Cl} + \text{SO}_4^{2-} \rightarrow \text{SO}_4^- + \text{Cl}^-$	2	$2.1 \times 10^8$		
Cl 6	$\text{Cl} + \text{Cl} \rightarrow \text{Cl}_2$	2	$8.8 \times 10^7$		
Cl 7	$\text{Cl}^- + \text{OH} \rightarrow \text{ClOH}^-$	2	$4.2 \times 10^9$		
Cl 8	$\text{Cl}^- + \text{O}_3 \rightarrow \text{ClO}^- + \text{O}_2$	2	$3.0 \times 10^{-3}$		
Cl 9	$\text{Cl}^- + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{Cl}$	2	$9.3 \times 10^6$		
Cl 10	$\text{Cl}^- + \text{SO}_4^- \rightarrow \text{SO}_4^{2-} + \text{Cl}$	2	$2.5 \times 10^8$		
Cl 11	$\text{Cl}^- + \text{HSO}_5^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	2	$1.8 \times 10^{-3}$	-4330	
Cl 12	$\text{Cl}^- + \text{HOCl} + \text{H}^+ \rightarrow \text{Cl}_2$	3	$2.2 \times 10^4$	-7352	
Cl 13	$\text{Cl}_2 \rightarrow \text{Cl}^- + \text{HOCl} + \text{H}^+$	1	$2.2 \times 10^1$	-3508	
Cl 14	$\text{Cl}_2^- + \text{OH} \rightarrow \text{HOCl} + \text{Cl}^-$	2	$1.0 \times 10^9$	-8012	
Cl 15	$\text{Cl}_2^- + \text{OH}^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{OH}$	2	$4.0 \times 10^6$		
Cl 16	$\text{Cl}_2^- + \text{HO}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{O}_2$	2	$3.1 \times 10^9$		
Cl 17	$\text{Cl}_2^- + \text{O}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{HO}_2$	2	$6.0 \times 10^9$		
Cl 18	$\text{Cl}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{HO}_2$	2	$7.0 \times 10^5$	-3340	
Cl 19	$\text{Cl}_2^- + \text{NO}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{NO}_2$	2	$6.0 \times 10^7$		

Table 3: Continued

no	reaction	$n$	$k_0 [M^{1-n}] s^{-1}$	$-E_a/R [K]$	reference
Cl 20	$\text{Cl}_2^- + \text{CH}_3\text{OOH} \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{CH}_3\text{OO}$	2	$7.0 \times 10^5$		-3340
Cl 21	$\text{Cl}_2^- + \text{DOM} \rightarrow \text{Cl}^- + \text{Cl}^- + \text{HO}_2$	2	$1.0 \times 10^6$		-1082
Cl 22	$\text{Cl}_2^- + \text{HSO}_3^- \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^- + \text{H}^+$	2	$4.7 \times 10^8$		
Cl 23	$\text{Cl}_2^- + \text{SO}_3^{2-} \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^-$	2	$6.2 \times 10^7$		
Cl 24	$\text{Cl}_2^- + \text{Cl}_2^- \rightarrow \text{Cl}_2 + 2\text{Cl}^-$	2	$6.2 \times 10^9$		
Cl 25	$\text{Cl}_2^- + \text{Cl} \rightarrow \text{Cl}^- + \text{Cl}_2$	2	$2.7 \times 10^9$		
Cl 26	$\text{Cl}_2^- + \text{DMS} \rightarrow 0.5\text{CH}_3\text{SO}_3^- + 0.5\text{CH}_3\text{OO} + 0.5\text{HSO}_4^-$ $+ \text{HCHO} + 2\text{Cl}^- + 2\text{H}^+$	2	$3.0 \times 10^9$		
Cl 27	$\text{ClOH}^- \rightarrow \text{Cl}^- + \text{OH}$	1	$6.0 \times 10^9$		
Cl 28	$\text{ClOH}^- + \text{H}^+ \rightarrow \text{Cl}$	2	$4.0 \times 10^{10}$		
Cl 29	$\text{HOCl} + \text{HO}_2 \rightarrow \text{Cl} + \text{O}_2$	2	$7.5 \times 10^6$		= Cl30
Cl 30	$\text{HOCl} + \text{O}_2^- \rightarrow \text{Cl} + \text{OH}^- + \text{O}_2$	2	$7.5 \times 10^6$		
Cl 31	$\text{HOCl} + \text{SO}_3^{2-} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	2	$7.6 \times 10^8$		= Cl31
Cl 32	$\text{HOCl} + \text{HSO}_3^- \rightarrow \text{Cl}^- + \text{HSO}_4^- + \text{H}^+$	2	$7.6 \times 10^8$		
Cl 33	$\text{Cl}_2 + \text{HO}_2 \rightarrow \text{Cl}_2^- + \text{H}^+ + \text{O}_2$	2	$1.0 \times 10^9$		
Cl 34	$\text{Cl}_2 + \text{O}_2^- \rightarrow \text{Cl}_2^- + \text{O}_2$	2	$1.0 \times 10^9$		= Cl33
Br 1	$\text{Br} + \text{OH}^- \rightarrow \text{BrOH}^-$	2	$1.3 \times 10^{10}$		
Br 2	$\text{Br} + \text{DOM} \rightarrow \text{Br}^- + \text{HO}_2$	2	$2.0 \times 10^8$		
Br 3	$\text{Br}^- + \text{OH} \rightarrow \text{BrOH}^-$	2	$1.1 \times 10^{10}$		
Br 4	$\text{Br}^- + \text{O}_3 \rightarrow \text{BrO}^-$	2	$2.1 \times 10^2$		-4450
Br 5	$\text{Br}^- + \text{NO}_3 \rightarrow \text{Br} + \text{NO}_3^-$	2	$3.8 \times 10^9$		
Br 6	$\text{Br}^- + \text{SO}_4^{2-} \rightarrow \text{Br} + \text{SO}_4^{2-}$	2	$2.1 \times 10^9$		
Br 7	$\text{Br}^- + \text{HSO}_5^- \rightarrow \text{HOBr} + \text{SO}_4^{2-}$	2	$1.0$		
Br 8	$\text{Br}^- + \text{HOBr} + \text{H}^+ \rightarrow \text{Br}_2$	3	$1.6 \times 10^{10}$		
Br 9	$\text{Br}_2 \rightarrow \text{Br}^- + \text{HOBr} + \text{H}^+$	1	$9.7 \times 10^1$		-5338
Br 10	$\text{Br}_2^- + \text{O}_2^- \rightarrow \text{Br}^- + \text{Br}^-$	2	$1.7 \times 10^8$		
Br 11	$\text{Br}_2^- + \text{HO}_2 \rightarrow \text{Br}_2 + \text{H}_2\text{O}_2 - \text{H}^+$	2	$4.4 \times 10^9$		
Br 12	$\text{Br}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{HO}_2$	2	$5.0 \times 10^2$		
Br 13	$\text{Br}_2^- + \text{Br}_2^- \rightarrow \text{Br}^- + \text{Br}^- + \text{Br}_2$	1	$1.9 \times 10^9$		
Br 14	$\text{Br}_2^- + \text{CH}_3\text{OOH} \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{CH}_3\text{OO}$	2	$1.0 \times 10^5$		

Table 3: Continued

no	reaction	$n$	$k_0 [(M^{1-n}) s^{-1}]$	$-E_a/R [K]$	reference
Br 15	$\text{Br}_2^- + \text{DOM} \longrightarrow \text{Br}^- + \text{Br}^- + \text{HO}_2$	2	$1.0 \times 10^5$		
Br 16	$\text{Br}_2^- + \text{NO}_2^- \longrightarrow \text{Br}^- + \text{Br}^- + \text{NO}_2$	2	$1.7 \times 10^7$	-1720	
Br 17	$\text{Br}_2^- + \text{HSO}_3^- \longrightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{SO}_3^-$	2	$6.3 \times 10^7$	-782	
Br 18	$\text{Br}_2^- + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{Br}^- + \text{SO}_3^-$	2	$2.2 \times 10^8$	-650	
Br 19	$\text{Br}_2^- + \text{DMS} \longrightarrow 0.5\text{CH}_3\text{SO}_3^- + 0.5\text{CH}_3\text{OO} + 0.5\text{HSO}_4^-$ $+ \text{HCHO} + 2\text{Br}^- + 2\text{H}^+$	2	$3.2 \times 10^9$		
Br 20	$\text{BrOH}^- \longrightarrow \text{Br}^- + \text{OH}$	1	$3.3 \times 10^7$		
Br 21	$\text{BrOH}^- \longrightarrow \text{Br} + \text{OH}^-$	1	$4.2 \times 10^6$		
Br 22	$\text{BrOH}^- + \text{H}^+ \longrightarrow \text{Br}$	2	$4.4 \times 10^{10}$		
Br 23	$\text{BrOH}^- + \text{Br}^- \longrightarrow \text{Br}_2^- + \text{OH}^-$	2	$1.9 \times 10^8$		
Br 24	$\text{BrO}^- + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{SO}_4^{2-}$	2	$1.0 \times 10^8$		
Br 25	$\text{HOBr} + \text{HO}_2 \longrightarrow \text{Br} + \text{O}_2$	2	$1.0 \times 10^9$		
Br 26	$\text{HOBr} + \text{O}_2^- \longrightarrow \text{Br} + \text{OH}^- + \text{O}_2$	2	$3.5 \times 10^9$		
Br 27	$\text{HOBr} + \text{H}_2\text{O}_2 \longrightarrow \text{Br}^- + \text{H}^+ + \text{O}_2$	2	$1.2 \times 10^6$		
Br 28	$\text{HOBr} + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{HSO}_4^-$	2	$5.0 \times 10^9$		
Br 29	$\text{HOBr} + \text{HSO}_3^- \longrightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$	2	$5.0 \times 10^9$		= Br28
Br 30	$\text{Br}_2 + \text{HO}_2 \longrightarrow \text{Br}_2^- + \text{H}^+ + \text{O}_2$	2	$1.1 \times 10^8$		
Br 31	$\text{Br}_2 + \text{O}_2^- \longrightarrow \text{Br}_2^- + \text{O}_2$	2	$5.6 \times 10^9$		
I 1	$\text{HOI} + \text{I}^- + \text{H}^+ \longrightarrow \text{I}_2$	3	$4.4 \times 10^{12}$		
I 2	$\text{HOI} + \text{Cl}^- + \text{H}^+ \longrightarrow \text{ICl}$	3	$2.9 \times 10^{10}$		
I 3	$\text{ICl} \longrightarrow \text{HOI} + \text{Cl}^- + \text{H}^+$	1	$2.4 \times 10^6$		
I 4	$\text{HOI} + \text{Br}^- + \text{H}^+ \longrightarrow \text{IBr}$	3	$3.3 \times 10^{12}$		
I 5	$\text{IBr} \longrightarrow \text{HOI} + \text{H}^+ + \text{Br}^-$	1	$8.0 \times 10^5$		
I 6	$\text{HOCl} + \text{I}^- + \text{H}^+ \longrightarrow \text{ICI}$	3	$3.5 \times 10^{11}$		
I 7	$\text{HOBr} + \text{I}^- \longrightarrow \text{IBr} + \text{OH}^-$	2	$5.0 \times 10^9$		
I 8	$\text{IO}_2^- + \text{H}_2\text{O}_2 \longrightarrow \text{IO}_3^-$	2	$6.0 \times 10^1$		
I 9	$\text{IO} + \text{IO} \longrightarrow \text{HOI} + \text{IO}_2^- + \text{H}^+$	2	$1.5 \times 10^9$		
I 10	$\text{I}^- + \text{O}_3 \xrightarrow{\text{H}^+} \text{HOI}$	2	$4.2 \times 10^9$		
I 11	$\text{HOI} + \text{Cl}_2 \longrightarrow \text{IO}_2^- + 2\text{Cl}^- + 3\text{H}^+$	2	$1.0 \times 10^6$		
I 12	$\text{HOI} + \text{HOCl} \longrightarrow \text{IO}_2^- + \text{Cl}^- + 2\text{H}^+$	2	$5.0 \times 10^5$		

Table 3: Continued

no	reaction	$n$	$k_0 [(M^{1-n}) s^{-1}]$	$-E_a/R [K]$	reference
I 13	$\text{HOI} + \text{HOBr} \longrightarrow \text{IO}_2^- + \text{Br}^- + 2\text{H}^+$	2	$1.0 \times 10^6$		
I 14	$\text{IO}_2^- + \text{HOCl} \longrightarrow \text{IO}_3^- + \text{Cl}^- + \text{H}^+$	2	$1.5 \times 10^3$		
I 15	$\text{IO}_2^- + \text{HOBr} \longrightarrow \text{IO}_3^- + \text{Br}^- + \text{H}^+$	2	$1.0 \times 10^6$		
I 16	$\text{IO}_2^- + \text{HOI} \longrightarrow \text{IO}_3^- + \text{I}^- + \text{H}^+$	2	$6.0 \times 10^2$		
I 17	$\text{I}_2 + \text{HSO}_3^- \longrightarrow 2\text{I}^- + \text{HSO}_4^- + 2\text{H}^+$	2	$1.0 \times 10^6$		
Hx 1	$\text{Br}^- + \text{HOCl} + \text{H}^+ \longrightarrow \text{BrCl}$	3	$1.3 \times 10^6$		
Hx 2	$\text{Cl}^- + \text{HOBr} + \text{H}^+ \longrightarrow \text{BrCl}$	3	$2.3 \times 10^{10}$		
Hx 3	$\text{BrCl} \longrightarrow \text{Cl}^- + \text{HOBr} + \text{H}^+$	1	$3.0 \times 10^6$		
Hx 4	$\text{Br}^- + \text{ClO}^- + \text{H}^+ \longrightarrow \text{BrCl} + \text{OH}^-$	3	$3.7 \times 10^{10}$		
Hx 5	$\text{Cl}_2 + \text{Br}^- \longrightarrow \text{BrCl}_2^-$	2	$7.7 \times 10^9$		
Hx 6	$\text{BrCl}_2^- \longrightarrow \text{Cl}_2 + \text{Br}^-$	1	$1.83 \times 10^3$		
hv 1	$\text{O}_3 + h\nu \longrightarrow \text{OH} + \text{OH} + \text{O}_2$	1	1		
hv 2	$\text{H}_2\text{O}_2 + h\nu \longrightarrow \text{OH} + \text{OH} + \text{OH}$	1	1		
hv 3	$\text{NO}_3^- + h\nu \xrightarrow{\text{H}^+} \text{NO}_2 + \text{OH}$	1	1		
hv 4	$\text{NO}_2^- + h\nu \xrightarrow{\text{H}^+} \text{NO} + \text{OH}$	1	1		
hv 5	$\text{HOCl} + h\nu \longrightarrow \text{OH} + \text{Cl}$	1	1		
hv 6	$\text{Cl}_2 + h\nu \longrightarrow \text{Cl} + \text{Cl}$	1	1		
hv 7	$\text{HOBr} + h\nu \longrightarrow \text{OH} + \text{Br}$	1	1		
hv 8	$\text{Br}_2 + h\nu \longrightarrow \text{Br} + \text{Br}$	1	1		
hv 9	$\text{BrCl} + h\nu \longrightarrow \text{Cl} + \text{Br}$	1	1		

$n$  is the order of the reaction. The temperature dependence is  $k = k_0 \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$ , where  $T_0 = 298\text{ K}$ .

Table 4: Heterogeneous reactions

no	reaction	$k$	reference
H 1	$\text{N}_2\text{O}_5 \xrightarrow{\text{H}_2\text{O}} \text{HNO}_{3\text{aq}} + \text{HNO}_{3\text{aq}}$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	
H 2	$\text{N}_2\text{O}_5 \xrightarrow{\text{Cl}^-} \text{ClNO}_2 + \text{NO}_3^-$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}f(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	
H 3	$\text{N}_2\text{O}_5 \xrightarrow{\text{Br}^-} \text{BrNO}_2 + \text{NO}_3^-$	$\bar{k}_t(\text{N}_2\text{O}_5)w_{l,i}f(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	
H 4	$\text{ClONO}_2 \xrightarrow{\text{H}_2\text{O}} \text{HOCl}_{\text{aq}} + \text{HNO}_{3\text{aq}}$	$\bar{k}_t(\text{ClONO}_2)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	see note
H 5	$\text{ClONO}_2 \xrightarrow{\text{Cl}^-} \text{Cl}_{2\text{aq}} + \text{NO}_3^-$	$\bar{k}_t(\text{ClONO}_2)w_{l,i}(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	see note
H 6	$\text{ClONO}_2 \xrightarrow{\text{Br}^-} \text{BrCl}_{\text{aq}} + \text{NO}_3^-$	$\bar{k}_t(\text{ClONO}_2)w_{l,i}(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	see note
H 7	$\text{BrONO}_2 \xrightarrow{\text{H}_2\text{O}} \text{HOBr}_{\text{aq}} + \text{HNO}_{3\text{aq}}$	$\bar{k}_t(\text{BrONO}_2)w_{l,i}[\text{H}_2\text{O}]/\text{Het}_T$	see note
H 8	$\text{BrONO}_2 \xrightarrow{\text{Cl}^-} \text{BrCl}_{\text{aq}} + \text{NO}_3^-$	$\bar{k}_t(\text{BrONO}_2)w_{l,i}(\text{Cl}^-)[\text{Cl}^-]/\text{Het}_T$	see note
H 9	$\text{BrONO}_2 \xrightarrow{\text{Br}^-} \text{Br}_{2\text{aq}} + \text{NO}_3^-$	$\bar{k}_t(\text{BrONO}_2)w_{l,i}(\text{Br}^-)[\text{Br}^-]/\text{Het}_T$	see note
H 10	$\text{IONO}_2 \xrightarrow{\text{H}_2\text{O}} \text{HOI}_{\text{aq}} + \text{HNO}_{3\text{aq}}$	$\bar{k}_t(\text{IONO}_2)w_{l,i}$	
H 11	$\text{HI} \xrightarrow{\text{H}_2\text{O}} \text{H}^+ + \text{I}^-$	$\bar{k}_t(\text{HI})w_{l,i}$	
H 12	$\text{INO}_2 \xrightarrow{\text{H}_2\text{O}} \text{HOI}_{\text{aq}} + \text{HONO}_{\text{aq}}$	$\bar{k}_t(\text{INO}_2)w_{l,i}$	
H 13	$\text{OIO} \xrightarrow{\text{H}_2\text{O}} \text{HOI}_{\text{aq}} + \text{HO}_{2\text{aq}}$	$\bar{k}_t(\text{H}_2\text{O})w_{l,i}$	
H 14	$\text{HIO}_3 \xrightarrow{\text{H}_2\text{O}} \text{IO}_3^- + \text{H}^+$	$\bar{k}_t(\text{HIO}_3)w_{l,i}$	

For a definition of  $\bar{k}_t$  and  $w_{l,i}$  see Sander (1999).  $\text{Het}_T = [\text{H}_2\text{O}] + f(\text{Cl}^-)[\text{Cl}^-] + f(\text{Br}^-)[\text{Br}^-]$ , with  $f(\text{Cl}^-) = 5.0 \times 10^2$  and  $f(\text{Br}^-) = 3.0 \times 10^5$ . H4–H9: the total rate is determined by  $\bar{k}_t$ , the distribution among the different reaction paths was assumed to be the same as for reactions H1–H3.

Table 5: Aqueous phase equilibrium constants

no	reaction	$m$	$n$	$K_0 [M^{n-m}]$	$-\Delta H/R[K]$	reference
EQ 1	$\text{CO}_{2\text{aq}} \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	1	2	$4.3 \times 10^{-7}$	-913	
EQ 2	$\text{NH}_{3\text{aq}} \rightleftharpoons \text{OH}^- + \text{NH}_4^+$	1	2	$1.7 \times 10^{-5}$	-4325	
EQ 3	$\text{H}_2\text{O}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1	2	$1.0 \times 10^{-14}$	-6716	
EQ 4	$\text{HCOO}\text{H}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1	2	$1.8 \times 10^{-4}$		
EQ 5	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	1	2	$6.0 \times 10^{-8}$	1120	
EQ 6	$\text{H}_2\text{SO}_{4\text{aq}} \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1	2	$1.0 \times 10^3$		
EQ 7	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1	2	$1.2 \times 10^{-2}$	1120	
EQ 8	$\text{HO}_{2\text{aq}} \rightleftharpoons \text{O}_2^- + \text{H}^+$	1	2	$1.6 \times 10^{-5}$		
EQ 9	$\text{SO}_{2\text{aq}} \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1	2	$1.7 \times 10^{-2}$	2090	
EQ 10	$\text{Cl}_2^- \rightleftharpoons \text{Cl}_{\text{aq}} + \text{Cl}^+$	1	2	$5.2 \times 10^{-6}$		
EQ 11	$\text{HOCl}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	1	2	$3.2 \times 10^{-8}$		
EQ 12	$\text{HBr}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1	2	$1.0 \times 10^9$		
EQ 13	$\text{Br}_2^- \rightleftharpoons \text{Br}_{\text{aq}} + \text{Br}^-$	1	2	$9.1 \times 10^{-6}$		
EQ 14	$\text{HOB}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	1	2	$2.3 \times 10^{-9}$	-3091	
EQ 15	$\text{BrCl}_{\text{aq}} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	2	1	3.8		
EQ 16	$\text{BrCl}_{\text{aq}} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	2	1	$1.8 \times 10^4$		
EQ 17	$\text{Br}_{2\text{aq}} + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	2	1	1.3		
EQ 18	$\text{HNO}_{3\text{aq}} \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	1	2	$1.5 \times 10^1$		
EQ 19	$\text{HCl}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1	2	$1.7 \times 10^6$		
EQ 20	$\text{HONO}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	1	2	$5.1 \times 10^{-4}$	-1260	
EQ 21	$\text{HNO}_{4\text{aq}} \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1	2	$1.0 \times 10^{-5}$	8700	
EQ 22	$\text{ICl}_{\text{aq}} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	2	1	$7.7 \times 10^1$		
EQ 23	$\text{IBr}_{\text{aq}} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2	1	$2.9 \times 10^2$		
EQ 24	$\text{ICl}_{\text{aq}} + \text{Br}^- \rightleftharpoons \text{IClBr}^-$	2	1	$1.8 \times 10^4$		
EQ 25	$\text{IBr}_{\text{aq}} + \text{Cl}^- \rightleftharpoons \text{IClBr}^-$	2	1	1.3		

The temperature dependence is  $K = K_0 \times \exp\left(\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$ , where  $T_0 = 298\text{ K}$ .

Table 6: Henry Law coefficients

species	$K_H^0$ [M/atm]	$-\Delta_{soln} H / R$ [K]	reference	$\alpha_0^0$	reference
O <sub>3</sub>	$1.2 \times 10^{-2}$	2560		0.002	
O <sub>2</sub>	$1.3 \times 10^{-3}$	1500		0.01	estimated by Pechtl et al. (2006)
OH	$3.0 \times 10^1$	4300		0.01	
HO <sub>2</sub>	$3.9 \times 10^3$	5900		0.2	
H <sub>2</sub> O <sub>2</sub>	$1.0 \times 10^5$	6338		0.077	
NO <sub>2</sub>	$6.4 \times 10^{-3}$	2500		0.0015	
NO <sub>3</sub>	2.0	2000		0.04	
N <sub>2</sub> O <sub>5</sub>	$\infty$	—		0.03	Behnke et al. (1997), see note estimated by Allan et al. (1999), see note
				0.003	
HONO	$4.9 \times 10^1$	4780		0.04	
HNO <sub>3</sub>	$1.7 \times 10^5$	8694		0.5	
HNO <sub>4</sub>	$1.2 \times 10^4$	6900		0.1	
NH <sub>3</sub>	$5.8 \times 10^1$	4085		0.06	
CH <sub>3</sub> OO	6.0	= HO <sub>2</sub>		0.01	
ROOH	$3.0 \times 10^2$	5322		0.0046	
HCHO	$7.0 \times 10^3$	6425		0.04	
HCOOH	$3.7 \times 10^3$	5700		0.014	
CO <sub>2</sub>	$3.1 \times 10^{-2}$	2423		0.01	
HCl	1.2	9001		0.074	
HOCl	$6.7 \times 10^2$	5862		0.074 = HOBr	
ClONO <sub>2</sub>	$\infty$	—		0.1	
Cl <sub>2</sub>	$9.1 \times 10^{-2}$	2500		0.038	
HBr	1.3	10239		0.031	
HOBr	$9.3 \times 10^1$	= HOCl		0.5	
BrONO <sub>2</sub>	$\infty$	—		0.8	
Br <sub>2</sub>	$7.6 \times 10^{-1}$	4094		0.038	
BrCl	$9.4 \times 10^{-1}$	5600		= Cl <sub>2</sub>	
DMSO	$5.0 \times 10^4$	= HCHO		0.048	
DMSO <sub>2</sub>	$\infty$	—		0.03	
SO <sub>2</sub>	1.2	3120		0.11	

Table 6: Continued

species	$K_H^0$ [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	$\alpha^0$	reference
$\text{H}_2\text{SO}_4$	$\infty$	—		0.65	
$\text{CH}_3\text{SO}_2\text{H}$	$\infty$	—	assumed by Pechtl et al. (2006)	0.0002	
$\text{CH}_3\text{SO}_3\text{H}$	$\infty$	—	assumed by Pechtl et al. (2006)	0.076	
HI	$\infty$	—		0.036	
IO	$4.5 \times 10^2$	$= \text{HOI}$		0.5	
HOI	$4.5 \times 10^2$	$= \text{HOCl}$		HOBr	
$\text{INO}_2$	$\infty$	—		0.2	
$\text{IONO}_2$	$\infty$	—		0.2	
$\text{I}_2$	3.0	4431		0.01	
$\text{ICl}$	$1.1 \times 10^2$	$= \text{BrCl}$		0.01	
$\text{IBr}$	$2.4 \times 10^1$	$= \text{BrCl}$		0.01	
$\text{OIO}$	$\infty$	—	estimated by Pechtl et al. (2006)	1	estimated by Pechtl et al. (2006)
$\text{HIO}_3$	$\infty$	—		0.01	

The temperature dependence for the Henry Law constants is  $K_H = K_H^0 \times \exp\left(\frac{-\Delta_{soln}H}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$ , where  $T_0 = 298$  K.

No temperature dependence is considered for accommodation coefficients. Notes: The accommodation coefficient for  $\text{N}_2\text{O}_5$  is determined based on the composition of the condensed-phase. For the seasalt mode a value of 0.03 is used (Behnke et al., 1997), while the lower value of 0.003 is used for the non-seasalt mode (after estimations made by Allan et al., 1999).

## References

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