

Kinetic data for MANIC

February 5, 2009

supplemental material to:

D. Lowe, D. Topping, and G. McFiggans

Modelling multi-phase halogen chemistry in the remote marine boundary layer: investigation of the influence of aerosol size resolution on predicted gas- and condensed-phase chemistry.

Atmos. Chem. Phys. Discuss., 2009

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

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	3.2×10^{-11}	70	
O 2	$O^1D + N_2 \rightarrow O_3$	2	1.8×10^{-11}	110	
O 3	$O^1D + H_2O \rightarrow 2OH$	2	2.2×10^{-10}		
O 4	$OH + O_3 \rightarrow HO_2 + O_2$	2	1.7×10^{-12}	-940	
O 5	$OH + HO_2 \rightarrow H_2O + O_2$	2	4.8×10^{-11}	250	
O 6	$OH + H_2O_2 \rightarrow HO_2 + H_2O$	2	2.9×10^{-12}	-160	
O 7	$HO_2 + O_3 \rightarrow OH + 2O_2$	2	1.0×10^{-14}	-490	
O 8	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	2	2.3×10^{-13}	600	
O 9	$O_3 + hv \rightarrow O_2 + O^1D$	1	1		
O 10	$H_2O_2 + hv \rightarrow 2OH$	1	1		
N 1	$NO + OH \xrightarrow{M} HONO$	3	2		Sander et al. (2006)
N 2	$NO + HO_2 \rightarrow NO_2 + OH$	2	3.5×10^{-12}	250	
N 3	$NO + O_3 \rightarrow NO_2 + O_2$	2	3.0×10^{-12}	-1500	
N 4	$NO + NO_3 \rightarrow 2NO_2$	2	1.5×10^{-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	1.2×10^{-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		Sander et al. (2006)
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	4.0×10^{-12}		
N 12	$NO_3 + NO_3 \rightarrow NO_2 + NO_2 + O_2$	2	8.5×10^{-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	2.6×10^{-22}		
N 16	$N_2O_5 + hv \rightarrow NO_2 + NO_3$	1	1		
N 17	$HONO + OH \rightarrow NO_2$	2	1.8×10^{-11}		
N 18	$HONO + hv \rightarrow NO + OH$	1	1	-390	
N 19	$HNO_3 + hv \rightarrow NO_2 + OH$	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	1.3×10^{-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	2.4×10^{-12}	-1175	
C 3	$C_2H_6 + OH \longrightarrow C_2H_5O_2 + H_2O$	2	1.7×10^{-11}	-1232	
C 4	$C_2H_4 + OH \longrightarrow EO_2$	2	1.66×10^{-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	1.2×10^{-14}	-2633	
C 6	$HO_2 + CH_3OO \longrightarrow ROOH + O_2$	2	4.1×10^{-13}	750	
C 7	$HO_2 + C_2H_5O_2 \longrightarrow ROOH + O_2$	2	7.5×10^{-13}	700	
C 8	$HO_2 + CH_3CO_3 \longrightarrow ROOH + O_2$	2	4.5×10^{-13}	1000	
C 9	$CH_3OO + CH_3OO \longrightarrow 1.4 HCHO + 0.8 HO_2 + O_2$	2	1.5×10^{-13}	220	
C 10	$C_2H_5O_2 + NO \longrightarrow ALD + HO_2 + NO_2$	2	4.2×10^{-12}	180	
C 11	$2C_2H_5O_2 \longrightarrow 1.6 ALD + 1.2 HO_2$	2	5.00×10^{-14}		
C 12	$EO_2 + NO \longrightarrow NO_2 + 2 HCHO + O_2$	2	4.2×10^{-12}	180	
C 13	$EO_2 + EO_2 \longrightarrow 2.4 HCHO + 1.2 HO_2 + 0.4 ALD$	2	5.00×10^{-14}		
C 14	$HO_2 + EO_2 \longrightarrow ROOH + O_2$	2	3.00×10^{-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	1.00×10^{-11}	600	
C 18	$HCHO + HO_2 \longrightarrow HOCH_2O_2$	2	6.7×10^{-15}		
C 19	$HCHO + NO_3 \xrightarrow{O_2} HNO_3 + HO_2 + CO$	2	5.8×10^{-16}		
C 20	$ALD + OH \longrightarrow CH_3CO_3 + H_2O$	2	6.9×10^{-12}	250	
C 21	$ALD + NO_3 \longrightarrow HNO_3 + CH_3CO_3$	2	1.40×10^{-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	4.2×10^{-12}		
C 25	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \longrightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{O}_2$	2	2.00×10^{-12}		
C 26	$2\text{HOCH}_2\text{O}_2 \longrightarrow 2\text{HCOOH} + \text{HO}_2 + 2\text{O}_2$	2	1.00×10^{-13}		
C 27	$\text{HCOOH} + \text{OH} \xrightarrow{\text{O}_2} \text{HO}_2 + \text{H}_2\text{O} + \text{CO}_2$	2	4.0×10^{-13}		
C 28	$\text{CH}_3\text{CO}_3 + \text{NO}_2 \longrightarrow \text{PAN}$	2	4.70×10^{-12}		
C 29	$\text{PAN} \longrightarrow \text{CH}_3\text{CO}_3 + \text{NO}_2$	1	1.9×10^{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	4.2×10^{-12}	180	
C 31	$\text{CH}_3\text{OO} + \text{NO} \xrightarrow{\text{O}_2} \text{HCHO} + \text{NO}_2 + \text{HO}_2$	2	3.0×10^{-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	3.8×10^{-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	1.3×10^{-12}		
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	1.12×10^{-11}	-250	Atkison 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			Atkison et al. (2006)
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	1.9×10^{-13}		
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	3.3×10^{-10}	520	
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	9.0×10^{-11}		
S 9	$\text{CH}_3\text{SCH}_3 + \text{BrO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{Br}$	2	2.54×10^{-14}	-2386	
S 10	$\text{CH}_3\text{SCH}_3 + \text{ClO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{Cl}$	2	9.5×10^{-15}	850	
S 11	$\text{CH}_3\text{SCH}_3 + \text{IO} \longrightarrow \text{CH}_3\text{SOCH}_3 + \text{I}$	2	1.4×10^{-14}		
S 12	$\text{CH}_3\text{SCH}_2\text{OO} + \text{NO} \longrightarrow \text{HCHO} + \text{CH}_3\text{S} + \text{NO}_2$	2	4.9×10^{-12}	263	
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	1.0×10^{-11}		
S 14	$\text{CH}_3\text{S} + \text{O}_3 \longrightarrow \text{CH}_3\text{SO} + \text{O}_2$	2	1.15×10^{-12}	432	
S 15	$\text{CH}_3\text{S} + \text{NO}_2 \longrightarrow \text{CH}_3\text{SO} + \text{NO}$	2	3.0×10^{-11}	210	
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	1.2×10^{-11}		
S 17	$\text{CH}_3\text{SO} + \text{O}_3 \xrightarrow{\text{O}_2} \text{CH}_3\text{SO}_2$	2	6.0×10^{-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	1.9×10^{13}		-8661
S 19	$CH_3SO_2 + NO_2 \rightarrow CH_3SO_3 + NO$	2	2.2×10^{-12}		
S 20	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	2	3×10^{-13}		
S 21	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	2	5×10^{-11}		
S 22	$CH_3SO_3 \xrightarrow{H_2O} CH_3OO + H_2SO_4$	1	1.36×10^{14}		-11071
S 23	$CH_3SOCH_3 + OH \rightarrow 0.95 CH_3SO_2H + 0.95 CH_3OO$ +0.05 DMSO ₂	2	8.7×10^{-11}		
S 24	$CH_3SO_2H + OH \rightarrow 0.95 CH_3SO_2 + 0.05 CH_3SO_3H$ +0.05 HO ₂ + H ₂ O	2	9×10^{-11}		
S 25	$CH_3SO_2H + NO_3 \rightarrow CH_3SO_2 + HNO_3$	2	1.0×10^{-13}		
Cl 1	$Cl + O_3 \rightarrow ClO + O_2$	2	2.8×10^{-11}		-250
Cl 2	$Cl + HO_2 \rightarrow HCl + O_2$	2	1.8×10^{-11}		170
Cl 3	$Cl + HO_2 \rightarrow ClO + OH$	2	4.1×10^{-11}		-450
Cl 4	$Cl + H_2O_2 \rightarrow HCl + HO_2$	2	1.1×10^{-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 ₂ O	2	1.6×10^{-10}		
Cl 6	$Cl + CH_4 \xrightarrow{O_2} HCl + CH_3OO$	2	9.6×10^{-12}		-1360
Cl 7	$Cl + C_2H_6 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	7.7×10^{-11}		-90
Cl 8	$Cl + C_2H_4 \xrightarrow{O_2} HCl + C_2H_5O_2$	2	1×10^{-10}		
Cl 9	$Cl + HCHO \xrightarrow{O_2} HCl + HO_2 + CO$	2	8.1×10^{-11}		
Cl 10	$Cl + ROOH \rightarrow CH_3OO + HCl$	2	5.7×10^{-11}		-30
Cl 11	$Cl + OCIO \rightarrow ClO + ClO$	2	3.2×10^{-11}		170
Cl 12	$Cl + ClONO_2 \rightarrow Cl_2 + NO_3$	2	6.5×10^{-12}		135
Cl 13	$ClO + OH \rightarrow Cl + HO_2$	2	7.4×10^{-12}		-270
Cl 14	$ClO + OH \rightarrow HCl + O_2$	2	6.0×10^{-13}		-230
Cl 15	$ClO + HO_2 \rightarrow HOCl + O_2$	2	2.2×10^{-12}		340
Cl 16	$ClO + CH_3OO \rightarrow Cl + HCHO + HO_2$	2	3.3×10^{-12}		-115
Cl 17	$ClO + NO \rightarrow Cl + NO_2$	2	6.2×10^{-12}		295
Cl 18	$ClO + NO_2 \xrightarrow{M} ClONO_2$	3 ₂			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	1.0×10^{-12}	Atkison et al. (2006)
Cl 20	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$	2	1.0×10^{-12}	-1590	
Cl 21	$\text{ClO} + \text{ClO} \rightarrow 2\text{Cl} + \text{O}_2$	2	3.0×10^{-11}	-2450	
Cl 22	$\text{ClO} + \text{ClO} \rightarrow \text{Cl} + \text{OCIO}$	2	3.5×10^{-13}	-1370	
Cl 23	$\text{OCIO} + \text{OH} \rightarrow \text{HOCl} + \text{O}_2$	2	4.5×10^{-13}	800	
Cl 24	$\text{OCIO} + \text{NO} \rightarrow \text{ClO} + \text{NO}_2$	2	1.1×10^{-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	3.0×10^{-12}	-500	
Cl 27	$\text{HCl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	2	1.8×10^{-12}	-240	
Cl 28	$\text{ClNO}_2 + \text{OH} \rightarrow \text{HOCl} + \text{NO}_2$	2	2.4×10^{-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	1.2×10^{-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	1.7×10^{-11}	-800	
Br 2	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	2	7.7×10^{-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	5×10^{-14}		
Br 4	$\text{Br} + \text{HCHO} \xrightarrow{\text{O}_2} \text{HBr} + \text{CO} + \text{HO}_2$	2	1.7×10^{-11}	-800	
Br 5	$\text{Br} + \text{ROOH} \rightarrow \text{CH}_3\text{OO} + \text{HBr}$	2	2.66×10^{-12}	-1610	
Br 6	$\text{Br} + \text{NO}_2 \xrightarrow{M} \text{BrNO}_2$	3	2		
Br 7	$\text{Br} + \text{BrONO}_2 \rightarrow \text{Br}_2 + \text{NO}_3$	2	4.9×10^{-11}		
Br 8	$\text{BrO} + \text{OH} \rightarrow \text{Br} + \text{HO}_2$	2	1.8×10^{-11}	250	
Br 9	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	2	4.5×10^{-12}	500	
Br 10	$\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{HOBr} + \text{HCHO}$	2	4.1×10^{-12}		
Br 11	$\text{BrO} + \text{CH}_3\text{OO} \rightarrow \text{Br} + \text{HCHO} + \text{HO}_2$	2	1.6×10^{-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	1.5×10^{-14}		
Br 13	$BrO + NO \longrightarrow Br + NO_2$	2	8.7×10^{-12}		
Br 14	$BrO + NO_2 \xrightarrow{M} BrONO_2$	3			Sander et al. (2006)
Br 15	$BrO + BrO \longrightarrow 2Br + O_2$	2	2.4×10^{-12}		
Br 16	$BrO + BrO \longrightarrow Br_2 + O_2$	2	2.9×10^{-14}		
Br 17	$HBr + OH \longrightarrow Br + H_2O$	2	5.5×10^{-12}		
Br 18	$BrONO_2 \longrightarrow BrO + NO_2$	1			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	1.9×10^{-11}		
I 2	$I + HO_2 \longrightarrow HI + O_2$	2	1.5×10^{-11}		
I 3	$I + NO_2 \xrightarrow{M} INO_2$	3			M. Kanakidou, pers. comm.
I 4	$I + NO_3 \longrightarrow IO + NO_2$	2	4.5×10^{-10}		
I 5	$I + I \longrightarrow I_2$	2	2.99×10^{-11}		
I 6	$IO + HO_2 \longrightarrow HOI + O_2$	2	1.4×10^{-11}		
I 7	$IO + NO \longrightarrow I + NO_2$	2	7.15×10^{-12}		
I 8	$IO + NO_2 \xrightarrow{M} IONO_2$	3			
I 9	$IO + IO \longrightarrow OIO + I$	2	5.4×10^{-11}		
I 10	$OIO + OH \longrightarrow 0.5HOIO_2 + 0.5HOI$	2	2.0×10^{-10}		
I 11	$OIO + NO \longrightarrow NO_2 + IO$	2	5.1×10^{-13}		
I 12	$HI + OH \longrightarrow I + H_2O$	2	1.6×10^{-11}		
I 13	$HI + NO_3 \longrightarrow I + HNO_3$	2	1.3×10^{-12}		
I 14	$INO_2 \xrightarrow{M} I + NO_2$	2	2.4		
I 15	$INO_2 \xrightarrow{M} IO + NO_2$	2	1.1×10^{15}		
I 16	$I_2 + OH \longrightarrow I + HOI$	2	2.1×10^{-10}		
I 17	$I_2 + NO_3 \longrightarrow I + IONO_2$	2	1.5×10^{-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	4.3×10^{-12}	-	
I 19	$C_3H_7I + OH \rightarrow CH_3OO + I$	2	1.2×10^{-12}	-	
I 20	$IO + hv \xrightarrow{O_2} I + O_3$	1	1		Pechtl et al. (2006)
I 21	$OIO + hv \rightarrow I + O_2$	1	0		
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		
Hx 1	$Cl + CH_3I \rightarrow HCl + HCHO + I$	2	2.9×10^{-11}	-	
Hx 2	$Cl + BrCl \rightarrow Br + Cl_2$	2	1.5×10^{-11}	-	
Hx 3	$Cl + Br_2 \rightarrow BrCl + Br$	2	1.2×10^{-10}	-	
Hx 4	$I_2 + Cl \rightarrow I + ICl$	2	2.09×10^{-10}	-	
Hx 5	$Br + OClO \rightarrow BrO + ClO$	2	2.6×10^{-11}	-	
Hx 6	$Br + Cl_2 \rightarrow BrCl + Cl$	2	1.1×10^{-15}	-	
Hx 7	$Br + BrCl \rightarrow Br_2 + Cl$	2	3.3×10^{-15}	-	
Hx 8	$I_2 + Br \rightarrow I + IBr$	2	1.2×10^{-10}	-	
Hx 9	$I + BrO \rightarrow IO + Br$	2	1.2×10^{-11}	-	
Hx 10	$BrO + ClO \rightarrow Br + OCIO$	2	1.6×10^{-12}	430	
Hx 11	$BrO + ClO \rightarrow Br + Cl + O_2$	2	2.9×10^{-12}	220	
Hx 12	$BrO + ClO \rightarrow BrCl + O_2$	2	5.8×10^{-13}	170	
Hx 13	$IO + ClO \rightarrow 0.8I + 0.55OCIO + 0.45O_2 + 0.25Cl + 0.2ICl$	2	4.7×10^{-12}	280	
Hx 14	$IO + BrO \rightarrow Br + 0.8OIO + 0.2I + 0.2O_2$	2	1.5×10^{-11}	510	
Hx 15	$BrCl + hv \rightarrow Br + Cl$	1	1		
Hx 16	$ICl + hv \rightarrow I + Cl$	1	1		

Table 2: Continued

no	reaction	n	$A[(cm^{-3})^{1-n}s^{-1}]$	$-E_a/R [K]$	reference
Hx 17	$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$	1	1		

n is the order of the reaction.¹ Photolysis rates are calculated for summer mid-day, in the mid-latitudes, using the PAPER model (Brühl and Crutzen, 1989; Landgraf and Crutzen, 1998), this maximum rate is then sinusiodally scaled using the in-built subroutine from KPP (Damian et al., 2002).² 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 $\text{CH}_3\text{SCH}_2\text{OO}$, 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 $T_0 = 298\text{ K}$.

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	1.1×10^8		
O 2	$O_3 + O_2^- \rightarrow OH + OH^-$	2	1.5×10^9		
O 3	$OH + OH \rightarrow H_2O_2$	2	5.5×10^9		
O 4	$OH + HO_2 \rightarrow H_2O$	2	7.1×10^9		
O 5	$OH + O_2^- \rightarrow OH^-$	2	1.0×10^{10}		
O 6	$OH + H_2O_2 \rightarrow HO_2$	2	2.7×10^7	-1684	
O 7	$HO_2 + HO_2 \rightarrow H_2O_2$	2	9.7×10^5	-2500	
O 8	$HO_2 + O_2^- \xrightarrow{H^+} H_2O_2$	2	1.0×10^8	-900	
N 1	$HONO + OH \rightarrow NO_2$	2	1.0×10^{10}		
N 2	$HONO + H_2O_2 \xrightarrow{H^+} HNO_3 + H^+$	3	4.6×10^3		
N 3	$NO_3^- + OH^- \rightarrow NO_3^- + OH$	2	8.2×10^7	-6800	
N 4	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	2	1.0×10^8	-2700	
N 5	$NO_2 + HO_2 \rightarrow HNO_4$	2	1.8×10^9		
N 6	$NO_2^- + O_3 \rightarrow NO_3^- + O_2$	2	5.0×10^5	-6950	
N 7	$NO_2^- + OH \rightarrow NO_2 + OH^-$	2	1.0×10^{10}		
N 8	$NO_4^- \rightarrow NO_2^- + O_2$	1	8.0×10^{-1}		
C 1	$HCHO + OH \rightarrow HCOOH + HO_2$	2	7.7×10^8	-1020	
C 2	$HCOOH + OH \rightarrow HO_2 + CO_2$	2	1.1×10^8	-991	
C 3	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	2	3.1×10^9	-1240	
C 4	$CH_3OO + HO_2 \rightarrow CH_3OOH$	2	4.3×10^5		
C 5	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	2	5.0×10^7		
C 6	$CH_3OH + OH \rightarrow HCHO + HO_2$	2	9.7×10^8		
C 7	$CH_3OOH + OH \rightarrow CH_3OO$	2	2.7×10^7	-1715	
C 8	$CH_3OOH + OH \rightarrow HCHO + OH$	2	1.1×10^7	-1715	
C 9	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	2	6.5×10^8		
C 10	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	2	4.3×10^5		
C 11	$CO_3^- + HCOO^- \rightarrow 2HCO_3^- + HO_2$	2	1.5×10^5		
C 12	$HCO_3^- + OH \rightarrow CO_3^-$	2	8.5×10^6		
C 13	$DOM + OH \rightarrow HO_2$	2	5.0×10^9		

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	1.5×10^9		
S 2	$\text{HSO}_3^- + \text{O}_3 \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{O}_2$	2	3.7×10^5	-5500	
S 3	$\text{SO}_3^{2-} + \text{O}_3 \longrightarrow \text{SO}_4^{2-} + \text{O}_2$	2	1.5×10^9	-5300	
S 4	$\text{HSO}_3^- + \text{OH} \longrightarrow \text{SO}_3^-$	2	4.5×10^9		
S 5	$\text{SO}_3^- + \text{OH} \longrightarrow \text{SO}_3^- + \text{OH}^-$	2	5.5×10^9		
S 6	$\text{HSO}_3^- + \text{HO}_2 \longrightarrow \text{SO}_4^{2-} + \text{OH} + \text{H}^+$	2	3.0×10^3		
S 7	$\text{HSO}_3^- + \text{O}_2^- \longrightarrow \text{SO}_4^{2-} + \text{OH}$	2	3.0×10^3		
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	2.0×10^7		
S 10	$\text{SO}_3^{2-} + \text{NO}_2 \xrightarrow{\text{NO}_2} \text{SO}_4^{2-} + \text{HONO} + \text{HONO}$	2	2.0×10^7		
S 11	$\text{HSO}_3^- + \text{NO}_3^- \longrightarrow \text{SO}_3^- + \text{NO}_3^- + \text{H}^+$	2	1.4×10^9	-2000	
S 12	$\text{HSO}_3^- + \text{HNO}_4 \longrightarrow \text{HSO}_4^- + \text{NO}_3^- + \text{H}^+$	2	3.1×10^5		
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	1.6×10^7	-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	1.6×10^7	-3800	
S 15	$\text{HSO}_3^- + \text{HCHO} \longrightarrow \text{CH}_2\text{OHSO}_3^-$	2	4.3×10^{-1}		
S 16	$\text{SO}_3^{2-} + \text{HCHO} \xrightarrow{\text{H}^+} \text{CH}_2\text{OHSO}_3^-$	2	1.4×10^4		
S 17	$\text{CH}_2\text{OHSO}_3^- + \text{OH}^- \longrightarrow \text{SO}_3^{2-} + \text{HCHO}$	2	3.6×10^3		
S 18	$\text{HSO}_3^- + \text{HSO}_5^- \xrightarrow{\text{H}^+} \text{SO}_4^{2-} + \text{SO}_4^{2-} + \text{H}^+ + \text{H}^+$	2	7.1×10^6		
S 19	$\text{SO}_4^- + \text{OH} \longrightarrow \text{HSO}_5^-$	2	1.0×10^9		
S 20	$\text{SO}_4^- + \text{HO}_2 \longrightarrow \text{SO}_4^{2-} + \text{H}^+$	2	3.5×10^9		
S 21	$\text{SO}_4^- + \text{O}_2^- \longrightarrow \text{SO}_4^{2-}$	2	3.5×10^9		
S 22	$\text{SO}_4^- + \text{H}_2\text{O} \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}$	2	1.1×10^1	-1110	
S 23	$\text{SO}_4^- + \text{H}_2\text{O}_2 \longrightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2$	2	1.2×10^7		
S 24	$\text{SO}_4^- + \text{NO}_3^- \longrightarrow \text{SO}_4^{2-} + \text{NO}_3^-$	2	5.0×10^4		
S 25	$\text{SO}_4^- + \text{HSO}_3^- \longrightarrow \text{SO}_3^- + \text{SO}_4^{2-} + \text{H}^+$	2	8.0×10^8		
S 26	$\text{SO}_4^- + \text{SO}_3^{2-} \longrightarrow \text{SO}_3^- + \text{SO}_4^{2-}$	2	4.6×10^8		
S 27	$\text{SO}_4^{2-} + \text{NO}_3^- \longrightarrow \text{NO}_3^- + \text{SO}_4^-$	2	1.0×10^5		
S 28	$\text{SO}_5^- + \text{HSO}_3^- \longrightarrow \text{SO}_4^- + \text{SO}_4^{2-} + \text{H}^+$	2	7.5×10^4		

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	9.4×10^6		
S 30	$\text{SO}_5^- + \text{HSO}_3^- \rightarrow \text{SO}_3^- + \text{HSO}_5^-$	2	2.5×10^4		
S 31	$\text{SO}_5^- + \text{SO}_3^{2-} \xrightarrow{\text{H}^+} \text{SO}_3^- + \text{HSO}_5^-$	2	3.6×10^6		
S 32	$\text{SO}_5^- + \text{O}_2^- \xrightarrow{\text{H}^+} \text{HSO}_5^- + \text{O}_2$	2	2.3×10^8		
S 33	$\text{SO}_5^- + \text{SO}_5^- \rightarrow 2 \text{SO}_4^-$	2	1.0×10^8	-2600	
S 34	$\text{DMS} + \text{O}_3 \rightarrow \text{O}_2 + \text{DMSO}$	2	8.6×10^8		
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	1.9×10^{10}		
S 36	$\text{DMSO} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2^- + \text{CH}_3\text{OO} + \text{H}^+$	2	4.5×10^9		
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	1.2×10^{10}		
S 38	$\text{CH}_3\text{SO}_3^- + \text{OH} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OO}$	2	1.2×10^7		
Cl 1	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl}^- + \text{H}^+$	2	2.0×10^9		
Cl 2	$\text{Cl} + \text{H}_2\text{O} \rightarrow \text{H}^+ + \text{ClOH}^-$	2	1.8×10^5		
Cl 3	$\text{Cl} + \text{NO}_3^- \rightarrow \text{NO}_3 + \text{Cl}^-$	2	1.0×10^8		
Cl 4	$\text{Cl} + \text{DOM} \rightarrow \text{Cl}^- + \text{HO}_2$	2	5.0×10^9		
Cl 5	$\text{Cl} + \text{SO}_4^{2-} \rightarrow \text{SO}_4^- + \text{Cl}^-$	2	2.1×10^8		
Cl 6	$\text{Cl} + \text{Cl} \rightarrow \text{Cl}_2$	2	8.8×10^7		
Cl 7	$\text{Cl}^- + \text{OH} \rightarrow \text{ClOH}^-$	2	4.2×10^9		
Cl 8	$\text{Cl}^- + \text{O}_3 \rightarrow \text{ClO}^- + \text{O}_2$	2	3.0×10^{-3}		
Cl 9	$\text{Cl}^- + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{Cl}$	2	9.3×10^6		
Cl 10	$\text{Cl}^- + \text{SO}_4^- \rightarrow \text{SO}_4^{2-} + \text{Cl}$	2	2.5×10^8		
Cl 11	$\text{Cl}^- + \text{HSO}_5^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	2	1.8×10^{-3}	-4330	
Cl 12	$\text{Cl}^- + \text{HOCl} + \text{H}^+ \rightarrow \text{Cl}_2$	3	2.2×10^4	-7352	
Cl 13	$\text{Cl}_2 \rightarrow \text{Cl}^- + \text{HOCl} + \text{H}^+$	1	2.2×10^1	-3508	
Cl 14	$\text{Cl}_2^- + \text{OH} \rightarrow \text{HOCl} + \text{Cl}^-$	2	1.0×10^9	-8012	
Cl 15	$\text{Cl}_2^- + \text{OH}^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{OH}$	2	4.0×10^6		
Cl 16	$\text{Cl}_2^- + \text{HO}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{O}_2$	2	3.1×10^9		
Cl 17	$\text{Cl}_2^- + \text{O}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{HO}_2$	2	6.0×10^9		
Cl 18	$\text{Cl}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Cl}^- + \text{Cl}^- + \text{H}^+ + \text{HO}_2$	2	7.0×10^5	-3340	
Cl 19	$\text{Cl}_2^- + \text{NO}_2^- \rightarrow \text{Cl}^- + \text{Cl}^- + \text{NO}_2$	2	6.0×10^7		

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	7.0×10^5	-3340	
Cl 21	$\text{Cl}_2^- + \text{DOM} \rightarrow \text{Cl}^- + \text{Cl}^- + \text{HO}_2$	2	1.0×10^6	-1082	
Cl 22	$\text{Cl}_2^- + \text{HSO}_3^- \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^- + \text{H}^+$	2	4.7×10^8		
Cl 23	$\text{Cl}_2^- + \text{SO}_3^{2-} \rightarrow \text{SO}_3^- + \text{Cl}^- + \text{Cl}^-$	2	6.2×10^7		
Cl 24	$\text{Cl}_2^- + \text{Cl}_2^- \rightarrow \text{Cl}_2 + 2\text{Cl}^-$	2	6.2×10^9		
Cl 25	$\text{Cl}_2^- + \text{Cl} \rightarrow \text{Cl}^- + \text{Cl}_2$	2	2.7×10^9		
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	3.0×10^9		
Cl 27	$\text{ClOH}^- \rightarrow \text{Cl}^- + \text{OH}$	1	6.0×10^9		
Cl 28	$\text{ClOH}^- + \text{H}^+ \rightarrow \text{Cl}$	2	4.0×10^{10}		
Cl 29	$\text{HOCl} + \text{HO}_2 \rightarrow \text{Cl} + \text{O}_2$	2	7.5×10^6	= Cl30	
Cl 30	$\text{HOCl} + \text{O}_2^- \rightarrow \text{Cl} + \text{OH}^- + \text{O}_2$	2	7.5×10^6		
Cl 31	$\text{HOCl} + \text{SO}_3^{2-} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	2	7.6×10^8	= Cl31	
Cl 32	$\text{HOCl} + \text{HSO}_3^- \rightarrow \text{Cl}^- + \text{HSO}_4^- + \text{H}^+$	2	7.6×10^8		
Cl 33	$\text{Cl}_2 + \text{HO}_2 \rightarrow \text{Cl}_2^- + \text{H}^+ + \text{O}_2$	2	1.0×10^9		
Cl 34	$\text{Cl}_2 + \text{O}_2^- \rightarrow \text{Cl}_2^- + \text{O}_2$	2	1.0×10^9	= Cl33	
Br 1	$\text{Br} + \text{OH}^- \rightarrow \text{BrOH}^-$	2	1.3×10^{10}		
Br 2	$\text{Br} + \text{DOM} \rightarrow \text{Br}^- + \text{HO}_2$	2	2.0×10^8		
Br 3	$\text{Br}^- + \text{OH} \rightarrow \text{BrOH}^-$	2	1.1×10^{10}		
Br 4	$\text{Br}^- + \text{O}_3 \rightarrow \text{BrO}^-$	2	2.1×10^2	-4450	
Br 5	$\text{Br}^- + \text{NO}_3 \rightarrow \text{Br} + \text{NO}_3^-$	2	3.8×10^9		
Br 6	$\text{Br}^- + \text{SO}_4^{2-} \rightarrow \text{Br} + \text{SO}_4^{2-}$	2	2.1×10^9		
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	1.6×10^{10}		
Br 9	$\text{Br}_2 \rightarrow \text{Br}^- + \text{HOBr} + \text{H}^+$	1	9.7×10^1	-5338	
Br 10	$\text{Br}_2^- + \text{O}_2^- \rightarrow \text{Br}^- + \text{Br}^-$	2	1.7×10^8		
Br 11	$\text{Br}_2^- + \text{HO}_2 \rightarrow \text{Br}_2 + \text{H}_2\text{O}_2 - \text{H}^+$	2	4.4×10^9	7457	
Br 12	$\text{Br}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{HO}_2$	2	5.0×10^2		
Br 13	$\text{Br}_2^- + \text{Br}_2^- \rightarrow \text{Br}^- + \text{Br}^- + \text{Br}_2$	1	1.9×10^9		
Br 14	$\text{Br}_2^- + \text{CH}_3\text{OOH} \rightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{CH}_3\text{OO}$	2	1.0×10^5		

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	1.0×10^5		
Br 16	$\text{Br}_2^- + \text{NO}_2^- \longrightarrow \text{Br}^- + \text{Br}^- + \text{NO}_2$	2	1.7×10^7	-1720	
Br 17	$\text{Br}_2^- + \text{HSO}_3^- \longrightarrow \text{Br}^- + \text{Br}^- + \text{H}^+ + \text{SO}_3^-$	2	6.3×10^7	-782	
Br 18	$\text{Br}_2^- + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{Br}^- + \text{SO}_3^-$	2	2.2×10^8	-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	3.2×10^9		
Br 20	$\text{BrOH}^- \longrightarrow \text{Br}^- + \text{OH}$	1	3.3×10^7		
Br 21	$\text{BrOH}^- \longrightarrow \text{Br} + \text{OH}^-$	1	4.2×10^6		
Br 22	$\text{BrOH}^- + \text{H}^+ \longrightarrow \text{Br}$	2	4.4×10^{10}		
Br 23	$\text{BrOH}^- + \text{Br}^- \longrightarrow \text{Br}_2^- + \text{OH}^-$	2	1.9×10^8		
Br 24	$\text{BrO}^- + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{SO}_4^{2-}$	2	1.0×10^8		
Br 25	$\text{HOBr} + \text{HO}_2 \longrightarrow \text{Br} + \text{O}_2$	2	1.0×10^9		
Br 26	$\text{HOBr} + \text{O}_2^- \longrightarrow \text{Br} + \text{OH}^- + \text{O}_2$	2	3.5×10^9		
Br 27	$\text{HOBr} + \text{H}_2\text{O}_2 \longrightarrow \text{Br}^- + \text{H}^+ + \text{O}_2$	2	1.2×10^6		
Br 28	$\text{HOBr} + \text{SO}_3^{2-} \longrightarrow \text{Br}^- + \text{HSO}_4^-$	2	5.0×10^9		
Br 29	$\text{HOBr} + \text{HSO}_3^- \longrightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$	2	5.0×10^9		= Br28
Br 30	$\text{Br}_2 + \text{HO}_2 \longrightarrow \text{Br}_2^- + \text{H}^+ + \text{O}_2$	2	1.1×10^8		
Br 31	$\text{Br}_2 + \text{O}_2^- \longrightarrow \text{Br}_2^- + \text{O}_2$	2	5.6×10^9		
I 1	$\text{HOI} + \text{I}^- + \text{H}^+ \longrightarrow \text{I}_2$	3	4.4×10^{12}		
I 2	$\text{HOI} + \text{Cl}^- + \text{H}^+ \longrightarrow \text{ICl}$	3	2.9×10^{10}		
I 3	$\text{ICl} \longrightarrow \text{HOI} + \text{Cl}^- + \text{H}^+$	1	2.4×10^6		
I 4	$\text{HOI} + \text{Br}^- + \text{H}^+ \longrightarrow \text{IBr}$	3	3.3×10^{12}		
I 5	$\text{IBr} \longrightarrow \text{HOI} + \text{H}^+ + \text{Br}^-$	1	8.0×10^5		
I 6	$\text{HOCl} + \text{I}^- + \text{H}^+ \longrightarrow \text{ICI}$	3	3.5×10^{11}		
I 7	$\text{HOBr} + \text{I}^- \longrightarrow \text{IBr} + \text{OH}^-$	2	5.0×10^9		
I 8	$\text{IO}_2^- + \text{H}_2\text{O}_2 \longrightarrow \text{IO}_3^-$	2	6.0×10^1		
I 9	$\text{IO} + \text{IO} \longrightarrow \text{HOI} + \text{IO}_2^- + \text{H}^+$	2	1.5×10^9		
I 10	$\text{I}^- + \text{O}_3 \xrightarrow{\text{H}^+} \text{HOI}$	2	4.2×10^9		
I 11	$\text{HOI} + \text{Cl}_2 \longrightarrow \text{IO}_2^- + 2\text{Cl}^- + 3\text{H}^+$	2	1.0×10^6		
I 12	$\text{HOI} + \text{HOCl} \longrightarrow \text{IO}_2^- + \text{Cl}^- + 2\text{H}^+$	2	5.0×10^5		

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	1.0×10^6		
I 14	$\text{IO}_2^- + \text{HOCl} \longrightarrow \text{IO}_3^- + \text{Cl}^- + \text{H}^+$	2	1.5×10^3		
I 15	$\text{IO}_2^- + \text{HOBr} \longrightarrow \text{IO}_3^- + \text{Br}^- + \text{H}^+$	2	1.0×10^6		
I 16	$\text{IO}_2^- + \text{HOI} \longrightarrow \text{IO}_3^- + \text{I}^- + \text{H}^+$	2	6.0×10^2		
I 17	$\text{I}_2 + \text{HSO}_3^- \longrightarrow 2\text{I}^- + \text{HSO}_4^- + 2\text{H}^+$	2	1.0×10^6		
Hx 1	$\text{Br}^- + \text{HOCl} + \text{H}^+ \longrightarrow \text{BrCl}$	3	1.3×10^6		
Hx 2	$\text{Cl}^- + \text{HOBr} + \text{H}^+ \longrightarrow \text{BrCl}$	3	2.3×10^{10}		
Hx 3	$\text{BrCl} \longrightarrow \text{Cl}^- + \text{HOBr} + \text{H}^+$	1	3.0×10^6		
Hx 4	$\text{Br}^- + \text{ClO}^- + \text{H}^+ \longrightarrow \text{BrCl} + \text{OH}^-$	3	3.7×10^{10}		
Hx 5	$\text{Cl}_2 + \text{Br}^- \longrightarrow \text{BrCl}_2^-$	2	7.7×10^9		
Hx 6	$\text{BrCl}_2^- \longrightarrow \text{Cl}_2 + \text{Br}^-$	1	1.83×10^3		
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	4.3×10^{-7}	-913	
EQ 2	$\text{NH}_{3\text{aq}} \rightleftharpoons \text{OH}^- + \text{NH}_4^+$	1	2	1.7×10^{-5}	-4325	
EQ 3	$\text{H}_2\text{O}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1	2	1.0×10^{-14}	-6716	
EQ 4	$\text{HCOO}\text{H}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1	2	1.8×10^{-4}		
EQ 5	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	1	2	6.0×10^{-8}	1120	
EQ 6	$\text{H}_2\text{SO}_{4\text{aq}} \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1	2	1.0×10^3		
EQ 7	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1	2	1.2×10^{-2}	1120	
EQ 8	$\text{HO}_{2\text{aq}} \rightleftharpoons \text{O}_2^- + \text{H}^+$	1	2	1.6×10^{-5}		
EQ 9	$\text{SO}_{2\text{aq}} \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1	2	1.7×10^{-2}	2090	
EQ 10	$\text{Cl}_2^- \rightleftharpoons \text{Cl}_{\text{aq}} + \text{Cl}^+$	1	2	5.2×10^{-6}		
EQ 11	$\text{HOCl}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	1	2	3.2×10^{-8}		
EQ 12	$\text{HBr}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1	2	1.0×10^9		
EQ 13	$\text{Br}_2^- \rightleftharpoons \text{Br}_{\text{aq}} + \text{Br}^-$	1	2	9.1×10^{-6}		
EQ 14	$\text{HOBr}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	1	2	2.3×10^{-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	1.8×10^4		
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	1.5×10^1		
EQ 19	$\text{HCl}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1	2	1.7×10^6		
EQ 20	$\text{HONO}_{\text{aq}} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	1	2	5.1×10^{-4}	-1260	
EQ 21	$\text{HNO}_{4\text{aq}} \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1	2	1.0×10^{-5}	8700	
EQ 22	$\text{ICl}_{\text{aq}} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	2	1	7.7×10^1		
EQ 23	$\text{IBr}_{\text{aq}} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2	1	2.9×10^2		
EQ 24	$\text{ICl}_{\text{aq}} + \text{Br}^- \rightleftharpoons \text{IClBr}^-$	2	1	1.8×10^4		
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	α_0^0	reference
O ₃	1.2×10^{-2}	2560		0.002	
O ₂	1.3×10^{-3}	1500		0.01	estimated by Pechtl et al. (2006)
OH	3.0×10^1	4300		0.01	
HO ₂	3.9×10^3	5900		0.2	
H ₂ O ₂	1.0×10^5	6338		0.077	
NO ₂	6.4×10^{-3}	2500		0.0015	
NO ₃	2.0	2000		0.04	
N ₂ O ₅	∞	—		0.03	Behnke et al. (1997), see note estimated by Allan et al. (1999), see note
				0.003	
HONO	4.9×10^1	4780		0.04	
HNO ₃	1.7×10^5	8694		0.5	
HNO ₄	1.2×10^4	6900		0.1	
NH ₃	5.8×10^1	4085		0.06	
CH ₃ OO	6.0	= HO ₂		0.01	
ROOH	3.0×10^2	5322		0.0046	
HCHO	7.0×10^3	6425		0.04	
HCOOH	3.7×10^3	5700		0.014	
CO ₂	3.1×10^{-2}	2423		0.01	
HCl	1.2	9001		0.074	
HOCl	6.7×10^2	5862		0.074 = HOBr	
ClONO ₂	∞	—		0.1	
Cl ₂	9.1×10^{-2}	2500		0.038	
HBr	1.3	10239		0.031	
HOBr	9.3×10^1	= HOCl		0.5	
BrONO ₂	∞	—		0.8	
Br ₂	7.6×10^{-1}	4094		0.038	
BrCl	9.4×10^{-1}	5600		= Cl ₂	
DMSO	5.0×10^4	= HCHO		0.048	
DMSO ₂	∞	—		0.03	
SO ₂	1.2	3120		0.11	

Table 6: Continued

species	K_H^0 [M/atm]	$-\Delta_{soln}H/R$ [K]	reference	α^0	reference
H_2SO_4	∞	—		0.65	
$\text{CH}_3\text{SO}_2\text{H}$	∞	—	assumed by Pechtl et al. (2006)	0.0002	
$\text{CH}_3\text{SO}_3\text{H}$	∞	—	assumed by Pechtl et al. (2006)	0.076	
HI	∞	—		0.036	
IO	4.5×10^2	$= \text{HOI}$		0.5	
HOI	4.5×10^2	$= \text{HOCl}$		HOBr	
INO_2	∞	—		0.2	
IONO_2	∞	—		0.2	
I_2	3.0	4431		0.01	
ICl	1.1×10^2	$= \text{BrCl}$		0.01	
IBr	2.4×10^1	$= \text{BrCl}$		0.01	
OIO	∞	—	estimated by Pechtl et al. (2006)	1	estimated by Pechtl et al. (2006)
HIO_3	∞	—		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 N_2O_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

- Allan, B. J., Carslaw, N., Coe, H., Burgess, R. A., and Plane, J. M. C.: Observations of the Nitrate Radical in the Marine Boundary Layer, *Journal of Atmospheric Chemistry*, 33, 129–154, 1999.
- Atkison, R., Cox, R. A., Crowley, J. N., R. F. Hampson, J., Hynes, R. G., Jenkin, M. E., Kerr, J. A., Rossi, M. J., and Troe, J.: Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, URL <http://www.iupac-kinetic.ch.cam.ac.uk>, 2006.
- Behnke, W., George, C., Scheer, V., and Zetzsch, C.: Production and decay of ClNO₂ from the reaction of gaseous N₂O₅ with NaCl solution: Bulk and aerosol experiments, *Journal of Geophysical Research*, 102, 3795–3804, 1997.
- Brühl, C. and Crutzen, P. J.: On the disproportionate role of tropospheric ozone as a filter against solar UV-B radiation, *Geophysical Research Letters*, 16, 703–706, 1989.
- Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G. R.: The Kinetic PreProcessor KPP — A Software Environment for Solving Chemical Kinetics, *Computers and Chemical Engineering*, 26, 1567–1579, 2002.
- Jayne, J. T., Pöschl, U., min Chen, Y., Dai, D., Molina, L. T., Worsnop, D. R., Kolb, C. E., and Molina, M. J.: Pressure and Temperature Dependence of the Gas-Phase Reaction of SO₃ with H₂O and the Heterogeneous Reaction of SO₂ with H₂O/H₂SO₄ Surfaces, *Journal of Physical Chemistry A*, 101, 10 000–10 011, 1997.
- Landgraf, J. and Crutzen, P. J.: An efficient method for online calculations of photolysis and heating rates, *Journal of Atmospheric Science*, 55, 863–878, 1998.
- Pechtl, S., Lovejoy, E. R., Burkholder, J. B., and von Glasow, R.: Modeling the possible role of iodine oxides in atmospheric new particle formations, *Atmospheric Chemistry and Physics*, 6, 505–523, 2006.
- Sander, R.: Modeling atmospheric chemistry: interactions between gas-phase species and liquid cloud/aerosol particles, *Surveys in Geophysics*, 20, 1–31, 1999.
- Sander, S. P., Friedl, R. R., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Kurylo, M. J., Molina, M. J., Moortgat, G. K., Keller-Rudek, H., Finlayson-Pitts, B. J., Wine, P. H., Huie, R. E., and Orkin, V. L.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation number 15, JPL Publication 06-02, Pasadena, 2006.