The Chemical Equations of MECCA-AERO

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Number of reactions in selected mechanism:

Aqueous phase (Annn):	132
Henry (Hnnn):	77
Equilibria (EQnn):	50

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Table 1: Henry's law coefficients

substance	$\dfrac{k_H^{\ominus}}{\text{M/atm}}$	$\dfrac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^1	4300.	Hanson et al. (1992)
HO_2	3.9×10^3	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^5$	6338.	Lind and Kok (1994)
NH_3	58.	4085.	Chameides (1984)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)[*]
NO_3	2.	2000.	Thomas et al. (1993)
HONO	4.9×10^1	4780.	Schwartz and White (1981)
HNO_3	$2.45\times10^6/1.5\times10^1$	8694.	Brimblecombe and Clegg (1989)[*]
HNO_4	1.2×10^4	6900.	Régimbal and Mozurkewich (1997)
CH_3O_2	6.	5600.	Jacob (1986)[*]
CH_3OOH	3.0×10^2	5322.	Lind and Kok (1994)
HCHO	7.0×10^3	6425.	Chameides (1984)
HCOOH	3.7×10^3	5700.	Chameides (1984)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^2	5862.	Huthwelker et al. (1995)
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)[*]
HOBr	9.3×10^1	5862.	Vogt et al. (1996)[*]
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
I_2	3.	4431.	Palmer et al. (1985)
IO	4.5×10^2	5862.	see note
HOI	4.5×10^2	5862.	Chatfield and Crutzen (1990)[*]
ICl	1.1×10^2	5600.	see note
IBr	2.4×10^1	5600.	see note
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
DMSO	$5.\times10^4$	6425.	De Bruyn et al. (1994)[*]

The temperature dependence of the Henry constants is:

$$K_H = K_H^\ominus \times \exp\left(\frac{-\Delta_{soln}H}{R}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right)$$

NO_2: The temperature dependence is from Chameides (1984).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

HBr: Calculated using the acidity constant from Lax (1969).

HOBr: This value was estimated by Vogt et al. (1996).

IO: Assumed to be the same as $K_H(HOI)$.

HOI: Lower limit.

ICl: Calculated using thermodynamic data from Wagman et al. (1982).

IBr: Calculated using thermodynamic data from Wagman et al. (1982).

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 2: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\dfrac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO_2	0.2	0.	DeMore et al. (1997)*
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NH_3	0.06	0.	DeMore et al. (1997)*
NO_2	0.0015	0.	Ponche et al. (1993)*
NO_3	0.04	0.	Rudich et al. (1996)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO_3	0.5	0.	Abbatt and Waschewsky (1998)*
HNO_4	0.1	0.	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO_2	0.01	2000.	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
BrCl	0.38	6546.	see note
I_2	0.01	2000.	see note
IO	0.5	2000.	see note
HOI	0.5	0.	see note
ICl	0.01	2000.	see note
IBr	0.01	2000.	see note
SO_2	0.11	0.	DeMore et al. (1997)
H_2SO_4	0.65	0.	Pöschl et al. (1998)*
DMSO	0.048	2578.	De Bruyn et al. (1994)

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta_{\mathrm{obs}}G}{RT}\right)$$
$$= \exp\left(\frac{-\Delta_{\mathrm{obs}}H}{RT} + \frac{\Delta_{\mathrm{obs}}S}{R}\right)$$

It can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R} \times \frac{1}{T} + \frac{-\Delta_{\mathrm{obs}}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right)\Big/\mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R}$$

If no data were available, a value of $\alpha = 0.01$, $\alpha = 0.1$, or $\alpha = 0.5$, and a temperature dependence of $-\Delta_{\mathrm{obs}}H/R = 2000$ K has been assumed.

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

HO_2: Value for aqueous salts at 293 K.

NH_3: Value measured at 295 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

HONO: Value measured between 247 and 297 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

HCHO: Value measured between 260 and 270 K.

CO_2: Estimate.

HCl: Temperature dependence derived from published data at 2 different temperatures

HOCl: Assumed to be the same as $\alpha(HOBr)$.

HBr: Temperature dependence derived from published data at 2 different temperatures

HOBr: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

BrCl: Assumed to be the same as $\alpha(Cl_2)$.

I_2: Estimate.

IO: Estimate.

HOI: Assumed to be the same as $\alpha(HOBr)$.

ICl: Estimate.

IBr: Estimate.

H_2SO_4: Value measured at 303 K.

Table 3: Henry's law equilibria

#	labels	reaction	rate coefficient	reference
H1000f	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	`k_exf(01,KPP_O2)`	see note
H1000b	TrAa01Sc	$O_2(aq) \rightarrow O_2$	`k_exb(01,KPP_O2)`	see note
H1001f	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	`k_exf(01,KPP_O3)`	see note
H1001b	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	`k_exb(01,KPP_O3)`	see note
H2100f	TrAa01Sc	$OH \rightarrow OH(aq)$	`k_exf(01,KPP_OH)`	see note
H2100b	TrAa01Sc	$OH(aq) \rightarrow OH$	`k_exb(01,KPP_OH)`	see note
H2101f	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	`k_exf(01,KPP_HO2)`	see note
H2101b	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	`k_exb(01,KPP_HO2)`	see note
H2102f	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	`k_exf(01,KPP_H2O2)`	see note
H2102b	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	`k_exb(01,KPP_H2O2)`	see note
H3101f	TrAa01NSc	$NO_2 \rightarrow NO_2(aq)$	`k_exf(01,KPP_NO2)`	see note
H3101b	TrAa01NSc	$NO_2(aq) \rightarrow NO_2$	`k_exb(01,KPP_NO2)`	see note
H3102f	TrAa01NSc	$NO_3 \rightarrow NO_3(aq)$	`k_exf(01,KPP_NO3)`	see note
H3102b	TrAa01NSc	$NO_3(aq) \rightarrow NO_3$	`k_exb(01,KPP_NO3)`	see note
H3200f	TrAa01NMblScScm	$NH_3 \rightarrow NH_3(aq)$	`k_exf(01,KPP_NH3)`	see note
H3200b	TrAa01NMblScScm	$NH_3(aq) \rightarrow NH_3$	`k_exb(01,KPP_NH3)`	see note
H3201	TrAa01MblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	`k_exf_N2O5(01) * C(KPP_H2O_a01)`	Behnke et al. (1994), Behnke et al. (1997)[*]
H3202f	TrAa01NSc	$HONO \rightarrow HONO(aq)$	`k_exf(01,KPP_HONO)`	see note
H3202b	TrAa01NSc	$HONO(aq) \rightarrow HONO$	`k_exb(01,KPP_HONO)`	see note
H3203f	TrAa01MblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	`k_exf(01,KPP_HNO3)`	see note
H3203b	TrAa01MblNScScm	$HNO_3(aq) \rightarrow HNO_3$	`k_exb(01,KPP_HNO3)`	see note
H3204f	TrAa01NSc	$HNO_4 \rightarrow HNO_4(aq)$	`k_exf(01,KPP_HNO4)`	see note
H3204b	TrAa01NSc	$HNO_4(aq) \rightarrow HNO_4$	`k_exb(01,KPP_HNO4)`	see note
H4100f	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	`k_exf(01,KPP_CO2)`	see note
H4100b	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	`k_exb(01,KPP_CO2)`	see note
H4101f	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	`k_exf(01,KPP_HCHO)`	see note
H4101b	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	`k_exb(01,KPP_HCHO)`	see note
H4102f	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	`k_exf(01,KPP_CH3O2)`	see note
H4102b	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	`k_exb(01,KPP_CH3O2)`	see note
H4103f	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	`k_exf(01,KPP_HCOOH)`	see note
H4103b	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	`k_exb(01,KPP_HCOOH)`	see note
H4104f	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	`k_exf(01,KPP_CH3OOH)`	see note
H4104b	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	`k_exb(01,KPP_CH3OOH)`	see note

Table 3: Henry's law equilibria

#	labels	reaction	rate coefficient	reference
H6000f	TrAa01ClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	`k_exf(01,KPP_Cl2)`	see note
H6000b	TrAa01ClMblSc	$Cl_2(aq) \rightarrow Cl_2$	`k_exb(01,KPP_Cl2)`	see note
H6200f	TrAa01ClMblScScm	$HCl \rightarrow HCl(aq)$	`k_exf(01,KPP_HCl)`	see note
H6200b	TrAa01ClMblScScm	$HCl(aq) \rightarrow HCl$	`k_exb(01,KPP_HCl)`	see note
H6201f	TrAa01ClMblSc	$HOCl \rightarrow HOCl(aq)$	`k_exf(01,KPP_HOCl)`	see note
H6201b	TrAa01ClMblSc	$HOCl(aq) \rightarrow HOCl$	`k_exb(01,KPP_HOCl)`	see note
H6300	TrAa01ClMblN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	`k_exf_N2O5(01) * 5.E2`	Behnke et al. (1994), Behnke et al. (1997)[*]
H6301	TrAa01ClMblN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	`k_exf_ClNO3(01) * C(KPP_H2O_a01)`	see note
H6302	TrAa01ClMblN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	`k_exf_ClNO3(01) * 5.E2`	see note
H7000f	TrAa01BrMblSc	$Br_2 \rightarrow Br_2(aq)$	`k_exf(01,KPP_Br2)`	see note
H7000b	TrAa01BrMblSc	$Br_2(aq) \rightarrow Br_2$	`k_exb(01,KPP_Br2)`	see note
H7200f	TrAa01BrMblScScm	$HBr \rightarrow HBr(aq)$	`k_exf(01,KPP_HBr)`	see note
H7200b	TrAa01BrMblScScm	$HBr(aq) \rightarrow HBr$	`k_exb(01,KPP_HBr)`	see note
H7201f	TrAa01BrMblSc	$HOBr \rightarrow HOBr(aq)$	`k_exf(01,KPP_HOBr)`	see note
H7201b	TrAa01BrMblSc	$HOBr(aq) \rightarrow HOBr$	`k_exb(01,KPP_HOBr)`	see note
H7300	TrAa01BrMblN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	`k_exf_N2O5(01) * 3.E5`	Behnke et al. (1994), Behnke et al. (1997)[*]
H7301	TrAa01BrMblN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	`k_exf_BrNO3(01) * C(KPP_H2O_a01)`	see note
H7302	TrAa01BrMblN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	`k_exf_BrNO3(01) * 3.E5`	see note
H7600f	TrAa01ClBrMblSc	$BrCl \rightarrow BrCl(aq)$	`k_exf(01,KPP_BrCl)`	see note
H7600b	TrAa01ClBrMblSc	$BrCl(aq) \rightarrow BrCl$	`k_exb(01,KPP_BrCl)`	see note
H7601	TrAa01ClBrMblN	$ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	`k_exf_ClNO3(01) * 3.E5`	see note
H7602	TrAa01ClBrMblN	$BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	`k_exf_BrNO3(01) * 5.E2`	see note
H8000f	TrAa01ISc	$I_2 \rightarrow I_2(aq)$	`k_exf(01,KPP_I2)`	see note
H8000b	TrAa01ISc	$I_2(aq) \rightarrow I_2$	`k_exb(01,KPP_I2)`	see note
H8100f	TrAa01IMblSc	$IO \rightarrow IO(aq)$	`k_exf(01,KPP_IO)`	see note
H8100b	TrAa01IMblSc	$IO(aq) \rightarrow IO$	`k_exb(01,KPP_IO)`	see note
H8101	TrAa01I	$OIO \rightarrow HOI(aq) + HO_2(aq)$	`k_exf(01,KPP_OIO)`	see note
H8102	TrAa01I	$I_2O_2 \rightarrow HOI(aq) + H^+(aq) + IO_2^-(aq)$	`k_exf(01,KPP_I2O2)`	see note
H8200f	TrAa01IMblSc	$HOI \rightarrow HOI(aq)$	`k_exf(01,KPP_HOI)`	see note
H8200b	TrAa01IMblSc	$HOI(aq) \rightarrow HOI$	`k_exb(01,KPP_HOI)`	see note
H8201	TrAa01IMblSc	$HI \rightarrow H^+(aq) + I^-(aq)$	$k_{mt}(HI) \cdot lwc$	see note

Table 3: Henry's law equilibria

#	labels	reaction	rate coefficient	reference
H8202	TrAa01ISc	$HIO_3 \rightarrow IO_3^-(aq) + H^+(aq)$	$k_{mt}(HIO_3) \cdot lwc$	see note
H8300	TrAa01I	$INO_2 \rightarrow HOI(aq) + HONO(aq)$	`k_exf(01,KPP_INO2)`	see note
H8301	TrAa01IMbl	$INO_3 \rightarrow HOI(aq) + HNO_3(aq)$	`k_exf(01,KPP_INO3)`	see note
H8600f	TrAa01ClIMblSc	$ICl \rightarrow ICl(aq)$	`k_exf(01,KPP_ICl)`	see note
H8600b	TrAa01ClIMblSc	$ICl(aq) \rightarrow ICl$	`k_exb(01,KPP_ICl)`	see note
H8700f	TrAa01BrIMblSc	$IBr \rightarrow IBr(aq)$	`k_exf(01,KPP_IBr)`	see note
H8700b	TrAa01BrIMblSc	$IBr(aq) \rightarrow IBr$	`k_exb(01,KPP_IBr)`	see note
H9100f	TrAa01SMblScScm	$SO_2 \rightarrow SO_2(aq)$	`k_exf(01,KPP_SO2)`	see note
H9100b	TrAa01SMblScScm	$SO_2(aq) \rightarrow SO_2$	`k_exb(01,KPP_SO2)`	see note
H9200	TrAa01SMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	`xnom7sulf*k_exf(01,KPP_H2SO4)`	see note
H9400f	TrAa01S	$DMSO \rightarrow DMSO(aq)$	`k_exf(01,KPP_DMSO)`	see note
H9400b	TrAa01S	$DMSO(aq) \rightarrow DMSO$	`k_exb(01,KPP_DMSO)`	see note
H9401	TrAa01SMbl	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	`k_exf(01,KPP_CH3SO3H)`	see note

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca_mbl.f90` using the accommodation coefficients in subroutine `mecca_mbl_alpha` and Henry's law constants in subroutine `mecca_mbl_henry`.

k_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of X (= N_2O_5, $ClNO_3$, $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^-, we define $k_{exf}(X) = k_{mt}(X) \times lwc/([H_2O] + 5.0E2[Cl^-] + 3.0E5[Br^-])$.

H6301, H6302, H7601: The total uptake is determined by $k_{mt}(ClNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by $k_{mt}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 4: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ20	TrAa01Sc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21	TrAa01MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30	TrAa01MblNScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ31	TrAa01NSc	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32	TrAa01MblNScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ33	TrAa01NSc	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5		Warneck (1999)
EQ40	TrAa01MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41	TrAa01ScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4		Weast (1980)
EQ60	TrAa01Cl	$Cl_2^- \rightleftharpoons Cl + Cl^-$	5.2E-6		Jayson et al. (1973)
EQ61	TrAa01ClMblScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62	TrAa01ClSc	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8		Lax (1969)
EQ70	TrAa01Br	$Br_2^- \rightleftharpoons Br + Br^-$	2.54E-6	-2256	Liu et al. (2002)
EQ71	TrAa01BrMblScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ72	TrAa01BrSc	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ73	TrAa01ClBrMbl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ74	TrAa01ClBrMbl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ75	TrAa01ClBrMbl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ76	TrAa01ClBrMbl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ80	TrAa01ClIMblSc	$ICl + Cl^- \rightleftharpoons ICl_2^-$	7.7E1		Wang et al. (1989)
EQ81	TrAa01BrIMblSc	$IBr + Br^- \rightleftharpoons IBr_2^-$	2.9E2		Troy and Margerum (1991)
EQ82	TrAa01ClBrIMblSc	$ICl + Br^- \rightleftharpoons IBr + Cl^-$	3.3E2		see note
EQ90	TrAa01SMblScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91	TrAa01SMblScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92	TrAa01SMblScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93	TrAa01SMblScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)

*Notes:

EQ40: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

EQ72: For $pK_a(HOBr)$, see also Keller-Rudek et al. (1992).

EQ82: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):

ICl	+	Br$^-$	$\rightleftharpoons$	IBr	+	Cl$^-$
-17.1		-103.96	=	-4.2		-131.228
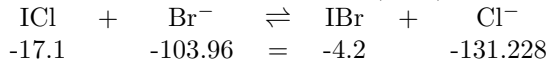
$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[\text{Cl}^-]/[\text{Br}^-]$ ratio equals 330.

Table 5: Aqueous phase reactions

#	labels	reaction	$k_0\ [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A1000	TrAa01Sc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9		Sehested et al. (1983)
A2100	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A2101	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A2102	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A2103	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A2104	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A2105	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A3100	TrAa01NSc	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A3101	TrAa01NSc	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A3102	TrAa01NSc	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A3200	TrAa01NSc	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A3201	TrAa01NSc	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A3202	TrAa01NSc	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A3203	TrAa01NSc	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A3204	TrAa01NSc	$HONO + H_2O_2 \rightarrow HNO_3$	4.6E3	-6800	Damschen and Martin (1983)
A4100	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A4101	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A4102	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2\ HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A4103	TrAa01Sc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A4104	TrAa01Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A4105	TrAa01Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A4106	TrAa01Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A4107	TrAa01Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A4108	TrAa01Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A4109	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8		Buxton et al. (1988)
A4110a	TrAa01Sc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715	Jacob (1986)
A4110b	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715	Jacob (1986)
A6000	TrAa01Cl	$Cl + Cl \rightarrow Cl_2$	8.8E7		Wu et al. (1980)
A6001	TrAa01Cl	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2Cl^-$	1.8E9		Jacobi et al. (1999)
A6100	TrAa01Cl	$Cl^- + O_3 \rightarrow ClO^-$	3.0E-3		Hoigné et al. (1985)
A6101	TrAa01Cl	$Cl_2 + O_2^- \rightarrow Cl_2^-$	1.0E9		Bjergbakke et al. (1981)
A6102	TrAa01Cl	$Cl_2^- + O_2^- \rightarrow 2\ Cl^-$	1.0E9		Jacobi (1996)*
A6200	TrAa01Cl	$Cl + H_2O \rightarrow H^+ + ClOH^-$	1.3E3		Jayson et al. (1973)
A6201	TrAa01Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)

Table 5: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 \ [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A6202	TrAa01Cl	$Cl^- + OH \rightarrow ClOH^-$	4.3E9		Jayson et al. (1973)
A6203	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204	TrAa01ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2 \ Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208	TrAa01ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH$	6.1E9		Jayson et al. (1973)
A6210	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.1E10		Jayson et al. (1973)
A6300	TrAa01Cl	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301	TrAa01Cl	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302	TrAa01Cl	$Cl_2^- + NO_2^- \rightarrow 2 \ Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400	TrAa01Cl	$Cl_2^- + CH_3OOH \rightarrow 2 \ Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A7000	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2 \ Br^- + Br_2$	1.9E9		Ross et al. (1992)
A7100	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A7101	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A7102	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2 \ Br^-$	1.7E8		Wagner and Strehlow (1987)
A7200	TrAa01Br	$Br^- + OH \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)
A7201	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A7202	TrAa01BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7203	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A7204	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2 \ Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A7205	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A7206	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999)
A7207	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A7208	TrAa01BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7209a	TrAa01Br	$BrOH^- \rightarrow Br^- + OH$	3.3E7		Zehavi and Rabani (1972)
A7209b	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A7210	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A7300	TrAa01Br	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A7301	TrAa01Br	$Br_2^- + NO_2^- \rightarrow 2 \ Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A7400	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2 \ Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*
A7601	TrAa01Br	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A7602	TrAa01ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)

Table 5: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0\ [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A7603	TrAa01ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604	TrAa01ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A8100	TrAa01IMbl	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A8101	TrAa01IMbl	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A8200	TrAa01IMbl	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A8201	TrAa01I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
A8202	TrAa01IMbl	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A8600	TrAa01ClIMbl	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601	TrAa01ClIMbl	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8602	TrAa01ClI	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A8603	TrAa01ClIMbl	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8604	TrAa01ClI	$HOI + Cl_2 \rightarrow IO_2^- + 2Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A8605	TrAa01ClI	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2\ H^+$	5.0E5		Citri and Epstein (1988)
A8700	TrAa01BrIMbl	$IBr \rightarrow HOI + H^+ + Br^-$	8.0E5		Troy et al. (1991)
A8701	TrAa01BrIMbl	$I^- + HOBr \rightarrow IBr + OH^-$	5.0E9		Troy and Margerum (1991)
A8702	TrAa01BrI	$IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$	1.0E6		Chinake and Simoyi (1996)
A8703	TrAa01BrIMbl	$HOI + Br^- + H^+ \rightarrow IBr$	3.3E12		Troy et al. (1991)
A8704	TrAa01BrI	$HOI + HOBr \rightarrow IO_2^- + Br^- + 2\ H^+$	1.0E6		Chinake and Simoyi (1996)
A9100	TrAa01SSc	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101	TrAa01SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102	TrAa01SSc	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103	TrAa01SSc	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104	TrAa01SSc	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105	TrAa01S	$SO_5^- + SO_3^{2-} \rightarrow .72\ SO_4^- + .72\ SO_4^{2-} + .28\ SO_3^- +$ .28 $HSO_5^- + .28\ OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A9106	TrAa01S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-}$	1.0E8		Ross et al. (1992)*
A9200	TrAa01SSc	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201	TrAa01SSc	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202	TrAa01SSc	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203	TrAa01SSc	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204	TrAa01SSc	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205	TrAa01SSc	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note
A9206	TrAa01SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207	TrAa01SSc	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)

Table 5: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0\ [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9208	TrAa01SSc	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note
A9209	TrAa01SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210	TrAa01SSc	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75\ SO_4^- + .75\ SO_4^{2-} + .75\ H^+ + .25\ SO_3^- + .25\ HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212	TrAa01SSc	$HSO_3^- + HSO_5^- \rightarrow 2\ SO_4^{2-} + 2\ H^+$	7.1E6		Betterton and Hoffmann (1988)
A9300	TrAa01SSc	$SO_3^{2-} + NO_2 \rightarrow SO_4^{2-} + 2\ HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9301	TrAa01SSc	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302	TrAa01SSc	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Logager et al. (1993)
A9303	TrAa01SSc	$HSO_3^- + NO_2 \rightarrow HSO_4^- + 2\ HONO - NO_2$	2.0E7		Clifton et al. (1988)
A9304	TrAa01SSc	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305	TrAa01SSc	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400	TrAa01SSc	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)
A9401	TrAa01SSc	$SO_3^{2-} + CH_3OOH \rightarrow SO_4^{2-} + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402	TrAa01SSc	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	4.3E-1		Boyce and Hoffmann (1984)
A9403	TrAa01SSc	$HSO_3^- + CH_3OOH \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404	TrAa01SSc	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600	TrAa01SCl	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2\ Cl^-$	6.2E7		Jacobi et al. (1996)
A9601	TrAa01SClMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602	TrAa01SCl	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603	TrAa01SCl	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604	TrAa01SCl	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2\ Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605	TrAa01SClMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9606	TrAa01SCl	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9700	TrAa01SBr	$SO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + SO_3^-$	2.2E8	-649	Shoute et al. (1991)
A9701	TrAa01SBr	$SO_3^{2-} + BrO^- \rightarrow Br^- + SO_4^{2-}$	1.0E8		Troy and Margerum (1991)
A9702	TrAa01SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9703	TrAa01SBr	$SO_4^- + Br^- \rightarrow Br + SO_4^{2-}$	2.1E9		Jacobi (1996)
A9704	TrAa01SBr	$HSO_3^- + Br_2^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	6.3E7	-782	Shoute et al. (1991)
A9705	TrAa01SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note
A9706	TrAa01SBr	$HSO_5^- + Br^- \rightarrow HOBr + SO_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)
A9800	TrAa01SI	$HSO_3^- + I_2 \rightarrow 2\ I^- + HSO_4^- + 2\ H^+$	1.0E6		Olsen and Epstein (1991)

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*Notes:

A6102: Jacobi (1996) found an upper limit of `6E9` and cite an upper limit from another study of `2E9`. Here, we set the rate coefficient to `1E9`.

A6301: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A7400: Assumed to be the same as for $Br_2^- + H_2O_2$.

A9105: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9106: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, we use SO_4^{2-} as a proxy. Note that this destroys the mass consistency for sulfur species.

A9205: D. Sedlak, pers. comm. (1993).

A9208: D. Sedlak, pers. comm. (1993).

A9605: assumed to be the same as for $SO_3^{2-} + HOCl$.

A9705: assumed to be the same as for $SO_3^{2-} + HOBr$.

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