

# The Chemical Mechanism of MECCA

KPP version: 2.2.1\_rs5

MECCA version: 3.0

Date: April 15, 2011.

Selected reactions:  
"iAra"

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase: 197

Aqueous phase: 89

All species: 286

Number of reactions in selected mechanism:

Gas phase (Gnm): 378

Aqueous phase (Anm): 147

Henry (Hnm): 93

Photolysis (Jnm): 116

Heterogeneous (HETnm): 21

Equilibria (EQnm): 68

Isotope exchange (DGMnm): 0

Dummy (Dnm): 1

All equations: 826

This document is part of the electronic supplement to our article  
"The atmospheric chemistry box model CAABA/MECCA-3.0"  
in Geosci. Model Dev. (2011), available at:  
<http://www.geosci-model-dev.net>

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11*EXP(55./temp)$	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34*((temp/300.)**(-2.4))*cair$	Sander et al. (2006)
G1002	StG	$O_3 + O(^1D) \rightarrow 2 O_2$	1.2E-10	Sander et al. (2006)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2 O_2$	$8.E-12*EXP(-2060./temp)$	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	$k\_3rd(temp, cair, 4.4E-32, 1.3, 4.7E-11, 0.2, 0.6)$	Sander et al. (2006)
G2101	StG	$H + O_3 \rightarrow OH + O_2$	$1.4E-10*EXP(-470./temp)$	Sander et al. (2006)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	1.1E-10	Sander et al. (2006)
G2103	StG	$OH + O(^3P) \rightarrow H + O_2$	$2.2E-11*EXP(120./temp)$	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Sander et al. (2006)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH + O_2$	$3.E-11*EXP(200./temp)$	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Sander et al. (2006)
G2108a	StG	$HO_2 + H \rightarrow 2 OH$	7.2E-11	Sander et al. (2006)
G2108b	StG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Sander et al. (2006)
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$1.63E-10*EXP(60./temp)$	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Sander et al. (2006)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Sander et al. (2006)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2 NO$	$6.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	$4.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2006)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	$2.1E-11*EXP(100./temp)$	Sander et al. (2006)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.1E-12*EXP(210./temp)$	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Sander et al. (2006)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12*EXP(220./temp)$	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_N03_NO2	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k\_N03\_NO2/(2.7E-27*EXP(11000./temp))$	Sander et al. (2006)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6, 3.6\text{E-}11, 0.1, 0.6)$	Sander et al. (2006)
G3201	StTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.5\text{E-}12 * \text{EXP}(250./\text{temp})$	Sander et al. (2006)
G3202	StTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0, 2.8\text{E-}11, 0., 0.6)$	Sander et al. (2006)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$k_{\text{NO2\_HO2}}$	Sander et al. (2006)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E-}12$	Sander et al. (2006)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11 * \text{EXP}(-390./\text{temp})$	Sander et al. (2006)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$k_{\text{HNO3\_OH}}$	Sander et al. (2006)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$k_{\text{NO2\_HO2}} / (2.1\text{E-}27 * \text{EXP}(10900./\text{temp}))$	Sander et al. (2006)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E-}12 * \text{EXP}(380./\text{temp})$	Sander et al. (2006)
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E-}12 * \text{EXP}(-710./\text{temp})$	Kohlmann and Poppe (1999)
G3210	TrGN	$\text{NH}_2 + \text{O}_3 \rightarrow \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12 * \text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E-}07 * \text{EXP}(-628./\text{temp}) * \text{temp}^{**}(-1.32)$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E-}09 * \text{EXP}(-356./\text{temp}) * \text{temp}^{**}(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12 * ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11 * ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11 * ((\text{temp}/298.)^{**}(-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11 * ((\text{temp}/298.)^{**}(-2.0))$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{NH}_2 + \text{O}_2$	$1.2\text{E-}14$	Kohlmann and Poppe (1999)
G3218	TrGN	$\text{NH}_2\text{O} \rightarrow \text{NHOH}$	$1.3\text{E}3$	Kohlmann and Poppe (1999)
G3219	TrGN	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	$8.0\text{E-}11 * \text{EXP}(-500./\text{temp})$	Kohlmann and Poppe (1999)
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E-}12 * \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$	$1.0\text{E-}12 * \text{EXP}(-1000./\text{temp})$	Kohlmann and Poppe (1999)
G3222	TrGN	$\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$	$1.66\text{E-}12$	Kohlmann and Poppe (1999)
G3223	TrGN	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11 * \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14 * \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4100	StG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow .75 \text{CH}_3\text{O}_2 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	$1.5\text{E-}10$	Sander et al. (2006)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E-}20 * \text{EXP}(2.82 * \log(\text{temp}) - 987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$2.9\text{E-}12 * \text{EXP}(-345./\text{temp})$	Sander et al. (2006)
G4103	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$4.1\text{E-}13 * \text{EXP}(750./\text{temp})$	Sander et al. (2006)*
G4104	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E-}12 * \text{EXP}(300./\text{temp})$	Sander et al. (2006)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E-}12$	Atkinson et al. (2006)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.*\text{R02}*9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+1./26.2*\text{EXP}(1130./\text{temp}))$	Sander et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$2.*\text{R02}*9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+26.2*\text{EXP}(-1130./\text{temp}))$	Sander et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Sander et al. (2006)*
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18*\text{EXP}(2.03*\log(\text{temp})+636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13*\text{EXP}(-1900./\text{temp})$	Sander et al. (2006)*
G4110	StTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E}-13+\text{cair}*3.54\text{E}-33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	4.0E-13	Sander et al. (2006)
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + .63 \text{CO} + .13 \text{HO}_2 + 0.23125 \text{HCOOH} + 0.13875 \text{HCHO} + 0.13875 \text{H}_2\text{O}_2 + .13 \text{OH}$	$1.2\text{E}-14*\text{EXP}(-2630./\text{temp})$	Sander et al. (2006)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	k_3rd(temp, cair, 1.0E-28, 4.5, 8.8E-12, 0.85, 0.6)	Sander et al. (2006)
G4203	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E}-13*\text{EXP}(700./\text{temp})$	Sander et al. (2006)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E}-12*\text{EXP}(365./\text{temp})$	Sander et al. (2006)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	2.3E-12	Atkinson et al. (1999)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .98 \text{CH}_3\text{CHO} + .38 \text{HO}_2 + .02 \text{HOCH}_2\text{CH}_2\text{O}_2$	$3.1\text{E}-13*\text{R02}$	Rickard and Pascoe (2009)*
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .43 \text{C}_2\text{H}_5\text{O}_2 + .43 \text{H}_2\text{O} + .57 \text{CH}_3\text{CHO} + .57 \text{OH}$	$0.6*k_{\text{CH300H\_OH}} + 8.01\text{E}-12$	see note
G4208	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O}$	$4.4\text{E}-12*\text{EXP}(365./\text{temp})$	Atkinson et al. (2006)
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HNO}_3$	KN03AL	Sander et al. (2006)
G4210	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$4.2\text{E}-14*\text{EXP}(855./\text{temp})$	Atkinson et al. (2006)
G4211a	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OOH}$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+1./37.*\text{EXP}(660./\text{temp}))$	Tyndall et al. (2001)
G4211b	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+37.*\text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E}-12*\text{EXP}(270./\text{temp})$	Tyndall et al. (2001)
G4213	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3C03_NO2	Sander et al. (2006)
G4214	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4217	TrGC	$\text{CH}_3\text{C(O)OO} \rightarrow .7 \text{CH}_3\text{O}_2 + .7 \text{CO}_2 + .3 \text{CH}_3\text{COOH}$	$1.00\text{E}-11*\text{R02}$	Rickard and Pascoe (2009)
G4218	TrGC	$\text{CH}_3\text{C(O)OOH} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)*
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$9.50\text{E}-13*\text{EXP}(-650./\text{temp})$	Rickard and Pascoe (2009)
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2006)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4222	TrGC	$C_2H_2 + OH \rightarrow 0.636 \text{ GLYOX} + 0.636 \text{ OH} + 0.364 \text{ HCOOH} + 0.364 \text{ CO} + 0.364 \text{ HO}_2$	$k_{3rd}(\text{temp}, \text{cair}, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)$	Sander et al. (2006)
G4223	TrGC	$HOCH_2CHO + OH \rightarrow .8 \text{ HOCH}_2\text{CO}_3 + .2 \text{ GLYOX} + .2 \text{ HO}_2 + \text{H}_2\text{O}$	$1.00E-11$	Rickard and Pascoe (2009)
G4224	TrGNC	$HOCH_2CHO + NO_3 \rightarrow HOCH_2CO_3 + HNO_3$	KN03AL	Rickard and Pascoe (2009)
G4225	TrGC	$HOCH_2CO_3 \rightarrow .7 \text{ HCHO} + .7 \text{ CO}_2 + .7 \text{ HO}_2 + .3 \text{ HOCH}_2\text{CO}_2\text{H}$	$1.00E-11 * R02$	Rickard and Pascoe (2009)
G4226	TrGC	$HOCH_2CO_3 + HO_2 \rightarrow .71 \text{ HOCH}_2\text{CO}_3\text{H} + .29 \text{ HOCH}_2\text{CO}_2\text{H} + .29 \text{ O}_3$	KAPH02	Rickard and Pascoe (2009)
G4227	TrGNC	$HOCH_2CO_3 + NO \rightarrow NO_2 + HO_2 + HCHO + CO_2$	KAPNO	Rickard and Pascoe (2009)
G4228	TrGNC	$HOCH_2CO_3 + NO_2 \rightarrow PHAN$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G4229	TrGNC	$HOCH_2CO_3 + NO_3 \rightarrow NO_2 + HO_2 + HCHO + CO_2$	KR02N03*1.60	Rickard and Pascoe (2009)
G4230	TrGC	$HOCH_2CO_2H + OH \rightarrow HCHO + HO_2 + CO_2 + H_2O$	$2.73E-12$	Rickard and Pascoe (2009)
G4231	TrGC	$HOCH_2CO_3H + OH \rightarrow HOCH_2CO_3 + H_2O$	$6.19E-12$	Rickard and Pascoe (2009)
G4232	TrGNC	$PHAN \rightarrow HOCH_2CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G4233	TrGNC	$PHAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	$1.12E-12$	Rickard and Pascoe (2009)
G4234	TrGC	$GLYOX + OH \rightarrow 1.2 \text{ CO} + .6 \text{ HO}_2 + .4 \text{ HCOCO}_3 + \text{H}_2\text{O}$	$1.14E-11$	Rickard and Pascoe (2009)
G4235	TrGNC	$GLYOX + NO_3 \rightarrow 1.2 \text{ CO} + .6 \text{ HO}_2 + .4 \text{ HCOCO}_3 + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G4236	TrGC	$HCOCO_3 \rightarrow .7 \text{ CO} + .7 \text{ HO}_2 + .7 \text{ CO}_2 + .3 \text{ HCOCO}_2\text{H}$	$1.00E-11 * R02$	Rickard and Pascoe (2009)
G4237	TrGC	$HCOCO_3 + HO_2 \rightarrow .71 \text{ HCOCO}_3\text{H} + .29 \text{ HCOCO}_2\text{H} + .29 \text{ O}_3$	KAPH02	Rickard and Pascoe (2009)
G4238	TrGNC	$HCOCO_3 + NO \rightarrow HO_2 + CO + NO_2 + CO_2$	KAPNO	Rickard and Pascoe (2009)
G4239	TrGNC	$HCOCO_3 + NO_3 \rightarrow HO_2 + CO + NO_2 + CO_2$	KR02N03*1.60	Rickard and Pascoe (2009)
G4240	TrGC	$HCOCO_2H + OH \rightarrow CO + HO_2 + CO_2 + H_2O$	$1.23E-11$	Rickard and Pascoe (2009)
G4241	TrGC	$HCOCO_3H + OH \rightarrow HCOCO_3 + H_2O$	$1.58E-11$	Rickard and Pascoe (2009)
G4242	TrGC	$HOCH_2CH_2O_2 \rightarrow .6 \text{ HOCH}_2\text{CH}_2\text{O} + .2 \text{ HOCH}_2\text{CHO} + .2 \text{ ETHGLY}$	$2.00E-12 * R02$	Rickard and Pascoe (2009)
G4243	TrGNC	$HOCH_2CH_2O_2 + NO \rightarrow .24875 \text{ HO}_2 + .4975 \text{ HCHO} + .74625 \text{ HOCH}_2\text{CH}_2\text{O} + .995 \text{ NO}_2 + .005 \text{ ETHOHNO}_3$	KR02NO	Rickard and Pascoe (2009)*
G4244	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow \text{HYETHO}_2\text{H}$	$2.00E-13 * \text{EXP}(1250./\text{temp})$	Rickard and Pascoe (2009)
G4245	TrGNC	$\text{ETHOHNO}_3 + OH \rightarrow HOCH_2CHO + NO_2 + H_2O$	$8.40E-13$	Rickard and Pascoe (2009)
G4246a	TrGC	$\text{HYETHO}_2\text{H} + OH \rightarrow HOCH_2CH_2O_2 + H_2O$	$0.6 * k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)*
G4246b	TrGC	$\text{HYETHO}_2\text{H} + OH \rightarrow HOCH_2CHO + OH + H_2O$	$1.38E-11$	Rickard and Pascoe (2009)
G4247a	TrGC	$HOCH_2CH_2O \rightarrow HO_2 + HOCH_2CHO$	$6.00E-14 * \text{EXP}(-550./\text{temp}) * C(\text{ind}_02)$	Rickard and Pascoe (2009)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4247b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HCHO} + \text{HCHO}$	$9.50\text{E}13 \cdot \text{EXP}(-5988./\text{temp})$	Rickard and Pascoe (2009)
G4248	TrGC	$\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$7.70\text{E}-12$	Rickard and Pascoe (2009)
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .736 \text{ iC}_3\text{H}_7\text{O}_2 + .264 \text{ C}_2\text{H}_5\text{O}_2 + .264 \text{ CO}_2 + .264 \text{ HO}_2 + \text{H}_2\text{O}$	$1.55\text{E}-17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-61./\text{temp})$	Rickard and Pascoe (2009)*
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .28 \text{ CH}_3\text{O}_2 + .1 \text{ CH}_4 + .075 \text{ CH}_3\text{COOH} + .56 \text{ CO} + .075 \text{ HCOOH} + .09 \text{ H}_2\text{O}_2 + .28 \text{ HO}_2 + .2 \text{ CO}_2 + .545 \text{ CH}_3\text{CHO} + .545 \text{ HCHO} + .36 \text{ OH}$	$6.5\text{E}-15 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2006)*
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO2}$	$\text{k\_3rd}(\text{temp}, \text{cair}, 8.\text{E}-27, 3.5, 3.\text{E}-11, 0., 0.5)$	Atkinson et al. (1999)
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO3BO2}$	$4.6\text{E}-13 \cdot \text{EXP}(-1155./\text{temp})$	Atkinson et al. (1999)
G4304	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$1.9\text{E}-13 \cdot \text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G4305	TrGNC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow .96 \text{ CH}_3\text{COCH}_3 + .96 \text{ HO}_2 + .96 \text{ NO}_2 + .04 \text{ iC}_3\text{H}_7\text{ONO}_2$	$2.7\text{E}-12 \cdot \text{EXP}(360./\text{temp})$	Atkinson et al. (1999)
G4306	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{ HO}_2$	$4.\text{E}-14 \cdot \text{R02}$	Rickard and Pascoe (2009)*
G4307	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .27 \text{ iC}_3\text{H}_7\text{O}_2 + .73 \text{ CH}_3\text{COCH}_3 + .73 \text{ OH} + \text{H}_2\text{O}$	$1.66\text{E}-11 + 0.6 \cdot \text{k\_CH300H\_OH}$	Rickard and Pascoe (2009)*
G4311	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$(1.33\text{E}-13 + 3.82\text{E}-11 \cdot \text{EXP}(-2000./\text{temp}))$	Sander et al. (2006)
G4312	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E}-13 \cdot \text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12 \cdot \text{EXP}(300./\text{temp})$	Sander et al. (2006)
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .6 \text{ CH}_3\text{C}(\text{O})\text{OO} + .6 \text{ HCHO} + .2 \text{ MGLYOX} + .2 \text{ CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E}-13 \cdot \text{EXP}(500./\text{temp}) \cdot 2 \cdot \text{R02}$	Tyndall et al. (2001)
G4315a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	see note
G4315b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	$8.39\text{E}-12$	Rickard and Pascoe (2009)
G4316	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$3.\text{E}-12$	Atkinson et al. (1999)
G4317	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}$	$8.4\text{E}-13 \cdot \text{EXP}(830./\text{temp})$	Tyndall et al. (1995)
G4320	TrGNC	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E}-13 \cdot \text{EXP}(-230./\text{temp})$	Atkinson et al. (1999)
G4321	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)
G4322	TrGC	$\text{HYPROPO2} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	$8.80\text{E}-13 \cdot \text{R02}$	Rickard and Pascoe (2009)
G4323	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{HYPROPO2H}$	$\text{KR02HO2} \cdot 0.520$	Rickard and Pascoe (2009)
G4324	TrGNC	$\text{HYPROPO2} + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}$	Rickard and Pascoe (2009)
G4325	TrGNC	$\text{HYPROPO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)
G4326a	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{HYPROPO2}$	$1.90\text{E}-12 \cdot \text{EXP}(190./\text{temp})$	Rickard and Pascoe (2009)
G4326b	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$2.44\text{E}-11$	Rickard and Pascoe (2009)
G4327	TrGNC	$\text{PRONO3BO2} + \text{HO}_2 \rightarrow \text{PR2O2HNO3}$	$\text{KR02HO2} \cdot 0.520$	Rickard and Pascoe (2009)
G4328	TrGNC	$\text{PRONO3BO2} + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}$	Rickard and Pascoe (2009)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4329	TrGNC	PRONO3BO2 + NO <sub>3</sub> → NOA + HO <sub>2</sub> + NO <sub>2</sub>	KR02NO3	Rickard and Pascoe (2009)
G4330a	TrGNC	PR2O2HNO3 + OH → PRONO3BO2	1.90E-12*EXP(190./temp)	Rickard and Pascoe (2009)
G4330b	TrGNC	PR2O2HNO3 + OH → NOA + OH	3.47E-12	Rickard and Pascoe (2009)
G4331	TrGNC	MGLYOX + NO <sub>3</sub> → CH <sub>3</sub> C(O)OO + CO + HNO <sub>3</sub>	KN03AL*2.4	Rickard and Pascoe (2009)
G4332	TrGNC	NOA + OH → MGLYOX + NO <sub>2</sub>	1.30E-13	Rickard and Pascoe (2009)
G4333	TrGC	HOCH2COCHO + OH → HOCH <sub>2</sub> CO <sub>3</sub> + CO	1.44E-11	Rickard and Pascoe (2009)
G4334	TrGNC	HOCH2COCHO + NO <sub>3</sub> → HOCH <sub>2</sub> CO <sub>3</sub> + CO + HNO <sub>3</sub>	KN03AL*2.4	Rickard and Pascoe (2009)
G4335	TrGC	HOCH2COCO2H + OH → HOCH <sub>2</sub> CO <sub>3</sub> + CO <sub>2</sub>	2.89E-12	Rickard and Pascoe (2009)
G4400	TrGC	nC <sub>4</sub> H <sub>10</sub> + OH → LC <sub>4</sub> H <sub>9</sub> O <sub>2</sub> + H <sub>2</sub> O	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)*
G4401	TrGC	LC <sub>4</sub> H <sub>9</sub> O <sub>2</sub> → 0.254 CO <sub>2</sub> + 0.5552 MEK + 0.5552 HO <sub>2</sub> + 0.3178 CH <sub>3</sub> CHO + 0.4448 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	2.5E-13*RO2	Rickard and Pascoe (2009)*
G4402	TrGC	LC <sub>4</sub> H <sub>9</sub> O <sub>2</sub> + HO <sub>2</sub> → LC <sub>4</sub> H <sub>9</sub> OOH	KR02HO2*0.625	Rickard and Pascoe (2009)
G4403	TrGNC	LC <sub>4</sub> H <sub>9</sub> O <sub>2</sub> + NO → 0.9172 NO <sub>2</sub> + 0.233 CO <sub>2</sub> + 0.5092 MEK + 0.5092 HO <sub>2</sub> + 0.2915 CH <sub>3</sub> CHO + 0.408 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.0828 LC4H9NO3	KR02NO	Rickard and Pascoe (2009)*
G4404	TrGC	LC <sub>4</sub> H <sub>9</sub> OOH + OH → 0.2285796 LC <sub>4</sub> H <sub>9</sub> O <sub>2</sub> + 0.7117253 MEK + 0.1193902 CO <sub>2</sub> + 0.0596951 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.7714204 OH + H <sub>2</sub> O	2.636E-11	Rickard and Pascoe (2009)*
G4405	TrGC	MVK + O <sub>3</sub> → 0.28 CH <sub>3</sub> C(O)OO + 0.56 CO + 0.225 LCARBON + 0.075 HCOOH + 0.09 H <sub>2</sub> O <sub>2</sub> + 0.28 HO <sub>2</sub> + 0.1 CO <sub>2</sub> + 0.1 CH <sub>3</sub> CHO + 0.645 HCHO + 0.36 OH + 0.545 MGLYOX	7.51E-16*EXP(-1521./temp)	Rickard and Pascoe (2009)
G4406	TrGC	MVK + OH → LHMVKABO2	4.13E-12*EXP(452./temp)	Rickard and Pascoe (2009)
G4413	TrGC	MEK + OH → LMEKO2 + H <sub>2</sub> O	3.24E-18*temp*temp*EXP(414./temp)	Rickard and Pascoe (2009)*
G4414	TrGC	LMEKO2 + HO <sub>2</sub> → LMEKOOH	KR02HO2*0.625	Rickard and Pascoe (2009)
G4415	TrGNC	LMEKO2 + NO → 0.538 HCHO + 0.538 CO <sub>2</sub> + 0.459 HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + 0.079 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.462 CH <sub>3</sub> C(O)OO + 0.462 CH <sub>3</sub> CHO + NO <sub>2</sub>	KR02NO	Rickard and Pascoe (2009)*
G4416	TrGC	LMEKOOH + OH → 0.40851 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> + 0.350196 BIACET + 0.807212 OH + 0.048506 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.505522 CO <sub>2</sub> + 0.192788 LMEKO2 + H <sub>2</sub> O	3.786E-11	Rickard and Pascoe (2009)*
G4417	TrGNC	LC4H9NO3 + OH → 0.91423 MEK + 0.08577 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.17154 CO <sub>2</sub> + NO <sub>2</sub> + H <sub>2</sub> O	9.598E-13	Rickard and Pascoe (2009)*
G4418	TrGNC	MPAN + OH → CH <sub>3</sub> COCH <sub>2</sub> OH + CO + NO <sub>2</sub>	3.2E-11	Orlando et al. (2002)
G4419	TrGNC	MPAN → MACO3 + NO <sub>2</sub>	k_PAN_M	see note

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4420	TrGC	LMEKO2 $\rightarrow$ 0.538 HCHO + 0.538 CO <sub>2</sub> + 0.459 HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + 0.079 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + 0.462 CH <sub>3</sub> C(O)OO + 0.462 CH <sub>3</sub> CHO	1.483E-12*R02	Rickard and Pascoe (2009)*
G4421	TrGC	MACR + OH $\rightarrow$ .57 MACO3 + .43 MACRO2	1.86E-11*EXP(175./temp)	Rickard and Pascoe (2009)
G4422	TrGC	MACR + O <sub>3</sub> $\rightarrow$ .59 MGLYOX + .41 CH <sub>3</sub> C(O)OO + .03375 HCOOH + .55625 HCHO + .82 CO + .12375 H <sub>2</sub> O <sub>2</sub> + .41 HO <sub>2</sub> + .82 OH	1.36E-15*EXP(-2112./temp)	Rickard and Pascoe (2009)
G4423	TrGNC	MACR + NO <sub>3</sub> $\rightarrow$ MACO3 + HNO <sub>3</sub>	KN03AL*2.0	Rickard and Pascoe (2009)
G4424	TrGC	MACO3 $\rightarrow$ .7 CH <sub>3</sub> C(O)OO + .7 HCHO + .7 CO <sub>2</sub> + .3 MACO2H	1.00E-11*R02	Rickard and Pascoe (2009)
G4425	TrGC	MACO3 + HO <sub>2</sub> $\rightarrow$ .71 MACO3H + .29 MACO2H + .29 O <sub>3</sub>	KAPH02	Rickard and Pascoe (2009)
G4426	TrGNC	MACO3 + NO $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + NO <sub>2</sub> + CO <sub>2</sub>	8.70E-12*EXP(290./temp)	Rickard and Pascoe (2009)
G4427	TrGNC	MACO3 + NO <sub>2</sub> $\rightarrow$ MPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G4428	TrGNC	MACO3 + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + NO <sub>2</sub> + CO <sub>2</sub>	KR02N03*1.60	Rickard and Pascoe (2009)
G4429	TrGC	MACRO2 $\rightarrow$ .7 CH <sub>3</sub> COCH <sub>2</sub> OH + .7 HCHO + .7 HO <sub>2</sub> + .3 MACROH	9.20E-14*R02	Rickard and Pascoe (2009)
G4430	TrGC	MACRO2 + HO <sub>2</sub> $\rightarrow$ MACROOH	KR02H02*0.625	Rickard and Pascoe (2009)
G4431	TrGNC	MACRO2 + NO $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G4432	TrGNC	MACRO2 + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G4433	TrGC	MACROOH + OH $\rightarrow$ MACRO2	2.82E-11	Rickard and Pascoe (2009)
G4434	TrGC	MACROH + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + HCHO + HO <sub>2</sub>	2.46E-11	Rickard and Pascoe (2009)
G4435	TrGC	MACO2H + OH $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + CO <sub>2</sub>	1.51E-11	Rickard and Pascoe (2009)
G4436	TrGC	MACO3H + OH $\rightarrow$ MACO3	1.87E-11	Rickard and Pascoe (2009)
G4437	TrGC	LHMKABO2 $\rightarrow$ 0.06 CO2H3CHO + 0.18 HO <sub>2</sub> + 0.18 HCHO + 0.18 MGLYOX + 0.42 CH <sub>3</sub> C(O)OO + .42 HOCH <sub>2</sub> CHO + .2 HO12CO3C4 + .14 BIACETOH	(.3*2.00E-12 + .7*8.80E-13)*R02	Rickard and Pascoe (2009)*
G4438	TrGC	LHMKABO2 + HO <sub>2</sub> $\rightarrow$ LHMKABOOH	KR02H02*0.625	Rickard and Pascoe (2009)
G4439	TrGNC	LHMKABO2 + NO $\rightarrow$ .3 MGLYOX + .7 HOCH <sub>2</sub> CHO + .7 CH <sub>3</sub> C(O)OO + .3 HCHO + .3 HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G4440	TrGNC	LHMKABO2 + NO <sub>3</sub> $\rightarrow$ .3 MGLYOX + .7 HOCH <sub>2</sub> CHO + .7 CH <sub>3</sub> C(O)OO + .3 HCHO + .3 HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*



Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4441	TrGC	LHMVKABOOH + OH → .3 CO2H3CHO + .7 BIACETOH + OH	4.496E-11	Rickard and Pascoe (2009)*
G4442	TrGC	MVKOH + OH → LMVKOHABO2	4.60E-12*EXP(452./temp)	Rickard and Pascoe (2009)
G4443	TrGC	MVKOH + O <sub>3</sub> → 0.56 CO + 0.545 HOCH2COCHO + 0.075 HOCH2COCO2H + 0.075 HCOOH + 0.09 H <sub>2</sub> O <sub>2</sub> + 0.28 HOCH <sub>2</sub> CO <sub>3</sub> + 0.28 HO <sub>2</sub> + 0.2 CO <sub>2</sub> + 0.545 HCHO + 0.36 OH + 0.1 HOCH <sub>2</sub> CHO	7.51E-16*EXP(-1521./temp)	Rickard and Pascoe (2009)
G4444	TrGC	LMVKOHABO2 → .7 HOCH <sub>2</sub> CHO + .7 HOCH <sub>2</sub> CO <sub>3</sub> + .3 HOCH2COCHO + .3 HCHO + .3 HO <sub>2</sub>	(0.3*2.00E-12+0.7*8.80E-13)*R02	Rickard and Pascoe (2009)*
G4445	TrGC	LMVKOHABO2 + HO <sub>2</sub> → LMVKOHABOOH	KR02H02*0.625	Rickard and Pascoe (2009)
G4446	TrGNC	LMVKOHABO2 + NO → .3 HOCH2COCHO + .3 HCHO + .3 HO <sub>2</sub> + .7 HOCH <sub>2</sub> CHO + .7 HOCH <sub>2</sub> CO <sub>3</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G4447	TrGNC	LMVKOHABO2 + NO <sub>3</sub> → .3 HOCH2COCHO + .3 HCHO + .3 HO <sub>2</sub> + .7 HOCH <sub>2</sub> CHO + .7 HOCH <sub>2</sub> CO <sub>3</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G4448	TrGC	LMVKOHABOOH + OH → .7 HO12CO3C4 + .3 CO2H3CHO + OH	5.98E-11	Rickard and Pascoe (2009)*
G4449	TrGC	CO2H3CHO + OH → CO2H3CO3	2.45E-11	Rickard and Pascoe (2009)
G4450	TrGNC	CO2H3CHO + NO <sub>3</sub> → CO2H3CO3 + HNO <sub>3</sub>	KN03AL*4.0	Rickard and Pascoe (2009)
G4451	TrGC	CO2H3CO3 → MGLYOX + HO <sub>2</sub> + CO <sub>2</sub>	1.00E-11*R02	Rickard and Pascoe (2009)
G4452	TrGC	CO2H3CO3 + HO <sub>2</sub> → CO2H3CO3H	KAPH02	Rickard and Pascoe (2009)
G4453	TrGNC	CO2H3CO3 + NO → MGLYOX + HO <sub>2</sub> + NO <sub>2</sub> + CO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G4454	TrGNC	CO2H3CO3 + NO <sub>3</sub> → MGLYOX + HO <sub>2</sub> + NO <sub>2</sub> + CO <sub>2</sub>	KR02N03*1.60	Rickard and Pascoe (2009)
G4455	TrGC	CO2H3CO3H + OH → CO2H3CO3	7.34E-12	Rickard and Pascoe (2009)
G4456	TrGC	HO12CO3C4 + OH → BIACETOH + HO <sub>2</sub>	1.88E-11	Rickard and Pascoe (2009)
G4500	TrGC	C <sub>5</sub> H <sub>8</sub> + O <sub>3</sub> → .051 CH <sub>3</sub> O <sub>2</sub> + .1575 CH <sub>3</sub> C(O)OO + .054 LHMVKABO2 + .522 CO + .06875 HCOOH + .11 H <sub>2</sub> O <sub>2</sub> + .32475 MACR + .1275 C <sub>3</sub> H <sub>6</sub> + .2625 HO <sub>2</sub> + .255 CO <sub>2</sub> + .74975 HCHO + .04125 MACO2H + .27 OH + .244 MVK	7.86E-15*EXP(-1913./temp)	Rickard and Pascoe (2009)
G4501	TrGC	C <sub>5</sub> H <sub>8</sub> + OH → .25 LISOPACO2 + .491 ISOPBO2 + .259 ISOPDO2	2.54E-11*EXP(410./temp)	Atkinson (1997)
G4509	TrGNC	C <sub>5</sub> H <sub>8</sub> + NO <sub>3</sub> → NISOPO2	3.03E-12*EXP(-446./temp)	Rickard and Pascoe (2009)
G4510	TrGC	LISOPACO2 → .9 LHC4ACCHO + .8 HO <sub>2</sub> + .1 ISOPAHO	2.4E-12*R02	Rickard and Pascoe (2009)
G4511	TrGC	LISOPACO2 + HO <sub>2</sub> → LISOPACOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4512	TrGNC	LISOPACO2 + NO → .892 LHC4ACCHO + .892 HO <sub>2</sub> + .892 NO <sub>2</sub> + .108 LISOPACNO3	KR02N0	Rickard and Pascoe (2009)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4513	TrGNC	LISOPACO2 + NO <sub>3</sub> → LHC4ACCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G4514	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH	1.07E-10	Rickard and Pascoe (2009)
G4515	TrGC	ISOPAOH + OH → LHC4ACCHO + HO <sub>2</sub>	9.30E-11	Rickard and Pascoe (2009)
G4516	TrGNC	LISOPACNO3 + OH → LHC4ACCHO + NO <sub>2</sub>	8.91E-11	Rickard and Pascoe (2009)
G4517	TrGC	ISOPBO2 → .6 MVK + .2 MVKOH + .6 HCHO + .6 HO <sub>2</sub> + .2 CH <sub>3</sub> O <sub>2</sub> + .2 ISOPBOH	8.E-13*R02	Rickard and Pascoe (2009)
G4518	TrGC	ISOPBO2 + HO <sub>2</sub> → ISOPBOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4519	TrGNC	ISOPBO2 + NO → .696 MVK + .232 MVKOH + .696 HCHO + .696 HO <sub>2</sub> + .232 CH <sub>3</sub> O <sub>2</sub> + .928 NO <sub>2</sub> + .072 ISOPBNO3	KR02N0	Rickard and Pascoe (2009)
G4520	TrGNC	ISOPBO2 + NO <sub>3</sub> → .75 MVK + .25 MVKOH + .75 HCHO + .75 HO <sub>2</sub> + .25 CH <sub>3</sub> O <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G4521	TrGC	ISOPBOOH + OH → ISOPBO2	4.2E-11	Rickard and Pascoe (2009)
G4522	TrGC	ISOPBOH + OH → .75 MVK + .25 MVKOH + .75 HCHO + .75 HO <sub>2</sub> + .25 CH <sub>3</sub> O <sub>2</sub>	3.85E-11	Rickard and Pascoe (2009)
G4523	TrGNC	ISOPBNO3 + OH → MVK + HCHO + NO <sub>2</sub>	3.55E-11	Rickard and Pascoe (2009)
G4524	TrGC	ISOPDO2 → .8 MACR + .8 HCHO + .8 HO <sub>2</sub> + .1 HCOC5 + .1 ISOPDOH	2.9E-12*R02	Rickard and Pascoe (2009)
G4525	TrGC	ISOPDO2 + HO <sub>2</sub> → ISOPDOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4526	TrGNC	ISOPDO2 + NO → .855 MACR + .855 HCHO + .855 HO <sub>2</sub> + .855 NO <sub>2</sub> + .145 ISOPDNO3	KR02N0	Rickard and Pascoe (2009)
G4527	TrGNC	ISOPDO2 + NO <sub>3</sub> → MACR + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G4528	TrGC	ISOPDOOH + OH → HCOC5 + OH	1.07E-10	Rickard and Pascoe (2009)
G4529	TrGC	ISOPDOH + OH → HCOC5 + HO <sub>2</sub>	7.38E-11	Rickard and Pascoe (2009)
G4530	TrGNC	ISOPDNO3 + OH → HCOC5 + NO <sub>2</sub>	6.1E-11	Rickard and Pascoe (2009)
G4531	TrGNC	NISOPO2 → .8 NC4CHO + .6 HO <sub>2</sub> + .2 LISOPACNO3	1.3E-12*R02	Rickard and Pascoe (2009)
G4532	TrGNC	NISOPO2 + HO <sub>2</sub> → NISOPOOH	.706*KR02H02	Rickard and Pascoe (2009)
G4533	TrGNC	NISOPO2 + NO → NC4CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G4534	TrGNC	NISOPO2 + NO <sub>3</sub> → NC4CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G4535	TrGNC	NISOPOOH + OH → NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G4536	TrGNC	NC4CHO + OH → LNISO3	4.16E-11	Rickard and Pascoe (2009)
G4537	TrGNC	NC4CHO + O <sub>3</sub> → .445 NO <sub>2</sub> + .89 CO + .075625 H <sub>2</sub> O <sub>2</sub> + .034375 HCOCO <sub>2</sub> H + .555 NOA + .445 HO <sub>2</sub> + .520625 GLYOX + .89 OH + .445 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
G4538	TrGNC	NC4CHO + NO <sub>3</sub> → LNISO3 + HNO <sub>3</sub>	KN03AL*4.25	Rickard and Pascoe (2009)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4539	TrGNC	$\text{LNISO3} + \text{HO}_2 \rightarrow \text{LNISOOH}$	$.5*.706*\text{KR02H02} + .5*\text{KAPH02}$	Rickard and Pascoe (2009)
G4540	TrGNC	$\text{LNISO3} + \text{NO} \rightarrow \text{NOA} + .5 \text{GLYOX} + .5 \text{CO} + \text{HO}_2 + \text{NO}_2 + .5 \text{CO}_2$	$.5*\text{KAPNO} + .5*\text{KR02NO}$	Rickard and Pascoe (2009)
G4541	TrGNC	$\text{LNISO3} + \text{NO}_3 \rightarrow \text{NOA} + .5 \text{GLYOX} + .5 \text{CO} + \text{HO}_2 + \text{NO}_2 + .5 \text{CO}_2$	$1.3*\text{KR02NO3}$	Rickard and Pascoe (2009)
G4542	TrGNC	$\text{LNISOOH} + \text{OH} \rightarrow \text{LNISO3}$	$2.65\text{E-11}$	Rickard and Pascoe (2009)
G4543	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow .52 \text{LC578O2} + .48 \text{LHC4ACCO3}$	$4.52\text{E-11}$	Rickard and Pascoe (2009)
G4544	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow .2225 \text{CH}_3\text{C(O)OO} + .89 \text{CO} + .0171875 \text{HOCH}_2\text{CO}_2\text{H} + .075625 \text{H}_2\text{O}_2 + .0171875 \text{HCOCO}_2\text{H} + .2775 \text{CH}_3\text{COCH}_2\text{OH} + .6675 \text{HO}_2 + .2603125 \text{GLYOX} + .2225 \text{HCHO} + .89 \text{OH} + .2603125 \text{HOCH}_2\text{CHO} + .5 \text{MGLYOX}$	$2.40\text{E-17}$	Rickard and Pascoe (2009)
G4545	TrGNC	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO3} + \text{HNO}_3$	$\text{KN03AL}*4.25$	Rickard and Pascoe (2009)
G4546	TrGC	$\text{LC578O2} \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{MGLYOX} + .5 \text{GLYOX} + .5 \text{HOCH}_2\text{CHO} + \text{HO}_2$	$9.20\text{E-14}*R02$	Rickard and Pascoe (2009)
G4547	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{LC578OOH}$	$\text{KR02H02}*0.706$	Rickard and Pascoe (2009)
G4548	TrGNC	$\text{LC578O2} + \text{NO} \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{MGLYOX} + .5 \text{GLYOX} + .5 \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02NO}$	Rickard and Pascoe (2009)
G4549	TrGNC	$\text{LC578O2} + \text{NO}_3 \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{MGLYOX} + .5 \text{GLYOX} + .5 \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02NO3}$	Rickard and Pascoe (2009)
G4550	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	$3.16\text{E-11}$	Rickard and Pascoe (2009)
G4551	TrGC	$\text{LHC4ACCO3} \rightarrow .3 \text{LHC4ACCO2H} + .35 \text{CH}_3\text{COCH}_2\text{OH} + .35 \text{HOCH}_2\text{CHO} + .35 \text{CH}_3\text{C(O)OO} + .35 \text{CO} + .35 \text{HO}_2 + .7 \text{CO}_2$	$1.00\text{E-11}*R02$	Rickard and Pascoe (2009)
G4552	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow .71 \text{LHC4ACCO3H} + .29 \text{LHC4ACCO2H} + .29 \text{O}_3$	$\text{KAPH02}$	Rickard and Pascoe (2009)
G4553	TrGNC	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{HOCH}_2\text{CHO} + .5 \text{CH}_3\text{C(O)OO} + .5 \text{CO} + .5 \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$\text{KAPNO}$	Rickard and Pascoe (2009)
G4554	TrGNC	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	$\text{k\_CH3C03\_NO2}$	Rickard and Pascoe (2009)
G4555	TrGNC	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{HOCH}_2\text{CHO} + .5 \text{CH}_3\text{C(O)OO} + .5 \text{CO} + .5 \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$1.6*\text{KR02NO3}$	Rickard and Pascoe (2009)
G4556	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{HOCH}_2\text{CHO} + .5 \text{CH}_3\text{C(O)OO} + .5 \text{CO} + .5 \text{HO}_2 + \text{CO}_2$	$2.52\text{E-11}$	Rickard and Pascoe (2009)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4557	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	2.88E-11	Rickard and Pascoe (2009)
G4558	TrGNC	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G4559	TrGNC	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	2.52E-11	Rickard and Pascoe (2009)
G4560	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	3.81E-11	Rickard and Pascoe (2009)
G4561	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3$	9.20E-14*R02	Rickard and Pascoe (2009)
G4562	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	KR02HO2*0.706	Rickard and Pascoe (2009)
G4563	TrGNC	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)
G4564	TrGNC	$\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)
G4565	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	9.7E-12	Rickard and Pascoe (2009)
G6100	StTrGCl	$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	StGCl	$\text{ClO} + \text{O}(^3\text{P}) \rightarrow \text{Cl} + \text{O}_2$	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow 2 \text{ Cl} + \text{O}_2$	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl} + \text{OClO}$	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	k_ClO_ClO/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6200	StGCl	$\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	$\text{Cl} + \text{HO}_2 \rightarrow \text{HCl} + \text{O}_2$	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	$\text{Cl} + \text{HO}_2 \rightarrow \text{ClO} + \text{OH}$	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	$\text{ClO} + \text{OH} \rightarrow .94 \text{ Cl} + .94 \text{ HO}_2 + .06 \text{ HCl} + .06 \text{ O}_2$	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)
G6205	StTrGCl	$\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	$\text{HOCl} + \text{OH} \rightarrow \text{ClO} + \text{H}_2\text{O}$	3.0E-12*EXP(-500./temp)	Sander et al. (2006)
G6300	StTrGNCl	$\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGNCl	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	k_3rd_iupac(temp, cair, 1.6E-31, 3.4, 7.E-11, 0., 0.4)	Atkinson et al. (2007)
G6302	TrGCl	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	6.918E-7*exp(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGNCl	$\text{ClNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{ClO} + \text{NO}_3$	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGNCl	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\text{O}_2$	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{HCl} + \text{OH}$	5.9E-11	Atkinson et al. (2006)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$3.3\text{E}-12 \cdot \text{EXP}(-115./\text{temp})$	Sander et al. (2006)
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 3 \text{Cl}$	$3.3\text{E}-10$	Sander et al. (2006)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{Cl}$	$1.65\text{E}-10$	see note
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	$2.4\text{E}-12 \cdot \text{EXP}(-1250./\text{temp})$	Sander et al. (2006)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{OH} + 3 \text{Cl}$	$3.\text{E}-10$	see note
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E}-12 \cdot \text{EXP}(-1520./\text{temp})$	Sander et al. (2006)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$k_{3\text{rd\_iupac}}(\text{temp}, \text{cair}, 1.85\text{E}-29, 3.3, 6.0\text{E}-10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$8.0\text{e}-11$	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$k_{3\text{rd\_iupac}}(\text{temp}, \text{cair}, 6.1\text{e}-30, 3.0, 2.0\text{e}-10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$8.3\text{E}-11 \cdot \text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
G6500	StGFCl	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + \text{Cl}$	$1.4\text{E}-10$	Sander et al. (2006)
G6501	StGFCl	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 2 \text{Cl}$	$2.3\text{E}-10$	Sander et al. (2006)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E}-11 \cdot \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E}-11 \cdot \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	$2.7\text{E}-12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E}-14 \cdot \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E}-12 \cdot \text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E}-12 \cdot \text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7203	StGBr	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E}-10 \cdot \text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E}-11 \cdot \text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGBr	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	$4.9\text{E}-11$	Orlando and Tyndall (1996)
G7301	StTrGNBr	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.7\text{E}-12 \cdot \text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGNBr	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	$k_{\text{BrO\_NO2}}$	Atkinson et al. (2007)*
G7303	TrGBr	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO\_NO2}} / (5.44\text{E}-9 \cdot \exp(14192./\text{temp}) \cdot 1.\text{E}6 \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm}2\text{Pa} \cdot N_{\text{A}}))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.6\text{E}-12 \cdot \text{EXP}(-1600./\text{temp})$	Kondo and Benson (1984)
G7402a	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{HCHO}$	$G7402a_{\text{yield}} \cdot 5.7\text{E}-12$	Aranda et al. (1997)
G7402b	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{Br} + \text{HCHO} + \text{HO}_2$	$(1. - G7402a_{\text{yield}}) \cdot 5.7\text{E}-12$	Aranda et al. (1997)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.35\text{E}-12 \cdot \text{EXP}(-1300./\text{temp})$	Sander et al. (2006)
G7404	TrGCBBr	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HBr}$	$2.8\text{E}-13 \cdot \text{EXP}(224./\text{temp}) / (1. + 1.13\text{E}24 \cdot \text{EXP}(-3200./\text{temp}) / C(\text{ind}_{02}))$	Atkinson et al. (2006)*

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G7405	TrGCBBr	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$1.8\text{e-}11 \cdot \text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7406	TrGCBBr	$\text{Br} + \text{C}_2\text{H}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$6.35\text{e-}15 \cdot \text{EXP}(440./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Br}$	$1.35\text{E-}12 \cdot \text{EXP}(-600./\text{temp})$	Sander et al. (2006)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	Sander et al. (2006)*
G7600	TrGClBr	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	3.32E-15	Manion et al. (2010)
G7601	TrGClBr	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	1.10E-15	Dolson and Leone (1987)
G7602	TrGClBr	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E-}10 \cdot \text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$1.6\text{E-}12 \cdot \text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E-}12 \cdot \text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	$5.8\text{E-}13 \cdot \text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGClBr	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	1.45E-11	Clyne and Cruse (1972)
G7605	TrGClBr	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	see note
G7606	TrGClBr	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	see note
G7607	TrGClBr	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.4\text{E-}12 \cdot \text{EXP}(-920./\text{temp})$	Sander et al. (2006)*
G8100	TrGI	$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	$2.1\text{E-}11 \cdot \text{EXP}(-830./\text{temp})$	Atkinson et al. (2007)
G8102	TrGI	$\text{OIO} + \text{OIO} \rightarrow \text{I}_{\text{part}}$	5.E-11	von Glasow et al. (2002)*
G8103	TrGI	$\text{IO} + \text{IO} \rightarrow .38 \text{OIO} + 1.62 \text{I} + .62 \text{O}_2$	$5.4\text{E-}11 \cdot \text{EXP}(180./\text{temp})$	Atkinson et al. (2007)*
G8200	TrGI	$\text{I} + \text{HO}_2 \rightarrow \text{HI} + \text{O}_2$	$1.5\text{E-}11 \cdot \text{EXP}(-1090./\text{temp})$	Atkinson et al. (2007)
G8201	TrGI	$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	$1.4\text{E-}11 \cdot \text{EXP}(540./\text{temp})$	Atkinson et al. (2007)
G8202	TrGI	$\text{HI} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O}$	$1.6\text{E-}11 \cdot \text{EXP}(440./\text{temp})$	Atkinson et al. (2007)
G8203	TrGI	$\text{OIO} + \text{OH} \rightarrow \text{HIO}_3$	$2.2\text{E-}10 \cdot \text{EXP}(243./\text{temp})$	Plane et al. (2006)
G8204	TrGI	$\text{I}_2 + \text{OH} \rightarrow \text{HOI} + \text{I}$	2.1E-10	Atkinson et al. (2007)
G8300	TrGI	$\text{I} + \text{NO}_2 \rightarrow \text{INO}_2$	k_I_NO2	Atkinson et al. (2007)*
G8301	TrGI	$\text{I} + \text{NO}_3 \rightarrow \text{IO} + \text{NO}_2$	1.E-10	Dillon et al. (2008)
G8302	TrGI	$\text{IO} + \text{NO} \rightarrow \text{I} + \text{NO}_2$	$7.15\text{E-}12 \cdot \text{EXP}(300./\text{temp})$	Atkinson et al. (2007)
G8303	TrGI	$\text{IO} + \text{NO}_2 \rightarrow \text{INO}_3$	$k_{\text{3rd\_iupac}}(\text{temp}, \text{cair}, 7.7\text{E-}31, 5., 1.6\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G8304	TrGI	$\text{OIO} + \text{NO} \rightarrow \text{NO}_2 + \text{IO}$	$1.1\text{E-}12 \cdot \text{EXP}(542./\text{temp})$	Atkinson et al. (2007)
G8305	TrGI	$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	$k_{\text{I\_NO2}} / (3.7\text{E-}7 \cdot \exp(9568./\text{temp}) * 1.\text{E6} * R_{\text{gas}} * \text{temp} / (\text{atm}2\text{Pa} * N_{\text{A}}))$	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGI	$\text{INO}_3 \rightarrow \text{IO} + \text{NO}_2$	0.	see note
G8307	TrGI	$\text{I}_2 + \text{NO}_3 \rightarrow \text{I} + \text{INO}_3$	1.5E-12	Atkinson et al. (2007)
G8308	TrGI	$\text{IO} + \text{NO}_3 \rightarrow \text{OIO} + \text{NO}_2$	9.E-12	Dillon et al. (2008)
G8400	TrGI	$\text{C}_3\text{H}_7\text{I} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{I}$	1.22E-12	Carl and Crowley (2001)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G8401	TrGI	$\text{CH}_3\text{O}_2 + \text{IO} \rightarrow .4 \text{I} + .6 \text{OIO} + \text{HCHO} + \text{HO}_2$	2.E-12	Dillon et al. (2006b), Bale et al. (2005)*
G8402	TrGI	$\text{CH}_3\text{I} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{HCHO} + \text{IO}$	3.4E-17	Wayne et al. (1991)*
G8600	TrGClI	$\text{IO} + \text{ClO} \rightarrow .2 \text{ICl} + .25 \text{Cl} + .55 \text{OCIO} + .8 \text{I} + .45 \text{O}_2$	$4.7\text{E-12} \cdot \text{EXP}(280./\text{temp})$	Atkinson et al. (2007)
G8700	TrGBrI	$\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br}$	1.2E-11	Sander et al. (2006)
G8701	TrGBrI	$\text{IO} + \text{BrO} \rightarrow \text{Br} + .8 \text{OIO} + .2 \text{I} + .2 \text{O}_2$	$1.5\text{E-11} \cdot \text{EXP}(510./\text{temp})$	Atkinson et al. (2007)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{3\text{rd}}(\text{temp}, \text{cair}, 3.3\text{E-31}, 4.3, 1.6\text{E-12}, 0., 0.6)$	Sander et al. (2006)
G9400a	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E-11} \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-13} \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.8\text{E13} \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	5.E-11	Barone et al. (1995)
G9600	TrGSCl	$\text{DMS} + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCl} + \text{HCHO}$	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	$\text{DMS} + \text{Br} \rightarrow \text{CH}_3\text{SO}_2 + \text{HBr} + \text{HCHO}$	$9.\text{E-11} \cdot \text{EXP}(-2386./\text{temp})$	Jefferson et al. (1994)
G9701	TrGSBr	$\text{DMS} + \text{BrO} \rightarrow \text{DMSO} + \text{Br}$	4.4E-13	Ingham et al. (1999)
G9800	TrGSI	$\text{DMS} + \text{IO} \rightarrow \text{DMSO} + \text{I}$	$3.2\text{E-13} \cdot \text{EXP}(-925./\text{temp})$	Dillon et al. (2006a)
G10100	TrGHg	$\text{Hg} + \text{O}_3 \rightarrow \text{HgO} + \text{O}_2$	3.0E-20	Hall (1995)
G10200	TrGHg	$\text{Hg} + \text{OH} \rightarrow \text{HgO} + \text{H}$	$3.55\text{E-14} \cdot \text{EXP}(294./\text{temp})$	Pal and Ariya (2004)
G10201	TrGHg	$\text{Hg} + \text{H}_2\text{O}_2 \rightarrow \text{HgO} + \text{H}_2\text{O}$	8.5E-19	Tokos et al. (1998)*
G10600	TrGHgCl	$\text{Hg} + \text{Cl} \rightarrow \text{HgCl}$	1.0E-11	Ariya et al. (2002)
G10601	TrGHgCl	$\text{Hg} + \text{Cl}_2 \rightarrow \text{HgCl}_2$	2.6E-18	Ariya et al. (2002)
G10700	TrGHgBr	$\text{Hg} + \text{Br} \rightarrow \text{HgBr}$	3.0E-13	Donohoue et al. (2006)
G10701	TrGHgBr	$\text{HgBr} + \text{Br} \rightarrow \text{HgBr}_2$	3.0E-12	Calvert and Lindberg (2003)
G10702	TrGHgBr	$\text{Hg} + \text{Br}_2 \rightarrow \text{HgBr}_2$	9.0E-17	Ariya et al. (2002)
G10703	TrGHgBr	$\text{Hg} + \text{BrO} \rightarrow \text{HgO} + \text{Br}$	1.0E-15	Raofie and Ariya (2003)
G10704	TrGHgBr	$\text{HgBr} + \text{BrO} \rightarrow \text{BrHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10705	TrGHgClBr	$\text{HgCl} + \text{BrO} \rightarrow \text{ClHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10706	TrGHgClBr	$\text{HgBr} + \text{Cl} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)
G10707	TrGHgClBr	$\text{HgCl} + \text{Br} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)

\*Notes:

Rate coefficients for three-body reactions are defined via the function `k_3rd(T, M, k0300, n, kinf300, m, fc)`. In the code, the temperature  $T$  is called `temp` and the concentration of “air molecules”  $M$  is called `cair`. Using the auxiliary variables  $k_0(T)$ ,  $k_{\text{inf}}(T)$ , and  $k_{\text{ratio}}$ , `k_3rd` is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (1)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (2)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (3)$$

$$\mathbf{k\_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left( \frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right) \quad (4)$$

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (5)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (6)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \quad (8)$$

$$\mathbf{k\_3rd\_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left( \frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right) \quad (9)$$

G1002: The path leading to  $2 \text{ O}(^3\text{P}) + \text{O}_2$  results in a null cycle regarding odd oxygen and is neglected.

G2110: The rate coefficient is: `k_H02_H02 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)`

`*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

G3109: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp, cair, 2.E-30, 4.4, 1.4E-12, 0.7, 0.6)`.

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is: `k_NO2_H02 = k_3rd(temp, cair, 1.8E-31, 3.2, 4.7E-12, 1.4, 0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./ (6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)) )`

G3207: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4103: Sander et al. (2006) recommend a zero product yield for HCHO.

G4107: The rate coefficient is: `k_CH300H_OH = 3.8E-12*EXP(200./temp)`.

G4109: The same temperature dependence assumed as for  $\text{CH}_3\text{CHO} + \text{NO}_3$ .

G4201: The product distribution is from Rickard and Pascoe (2009), after substitution of the Criegee intermediate by its decomposition products.

G4206: The product  $\text{C}_2\text{H}_5\text{OH}$ , which reacts only with OH, is substituted by its degradation products  $\approx 0.1 \text{ HOCH}_2\text{CH}_2\text{O}_2 + 0.9 \text{ CH}_3\text{CHO} + 0.9 \text{ HO}_2$ .

G4207: The rate constant  $8.01\text{E-}12$  is for the H abstraction in alpha to the  $-\text{OOH}$  group (Rickard and Pascoe, 2009) and  $0.6 * \mathbf{k\_CH300H\_OH}$  is for the  $\text{C}_2\text{H}_5\text{O}_2$  channel. The branching ratios are calculated from the terms of the rate coefficient at 298 K.

G4218: The rate coefficient is the same as for the  $\text{CH}_3\text{O}_2$  channel in G4107 ( $\text{CH}_3\text{OOH} + \text{OH}$ ).

G4221: The rate coefficient `isk_PAN_M = k_CH3CO3_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G4243: Orlando et al. (1998) estimated that about 25% of the  $\text{HOCH}_2\text{CH}_2\text{O}$  in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are  $2 \text{ HCHO} + \text{HO}_2$ .

G4300: The product  $\text{NC3H7O2}$  is substituted with its degradation products  $\text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{HO}_2$ .

G4301: The product distribution is for terminal olefin carbons from Zaveri and Peters (1999).

G4304: The value for the generic  $\text{RO}_2 + \text{HO}_2$  reaction from Atkinson (1997) is used here.

G4306: The MCM (Rickard and Pascoe, 2009) products are  $0.2 \text{ IPROPOL} + 0.2 \text{ CH}_3\text{COCH}_3 + 0.6 \text{ IC3H7O}$ . IPROPOL and IC3H7O are substituted with their degradation products. We assume IPROPOL to be oxidized entirely to  $\text{CH}_3\text{COCH}_3 + \text{HO}_2$  by OH. IC3H7O +  $\text{O}_2$  produces the same products.

G4307: Analogous to G4207 for both rate coefficient and branching ratios.

G4400:  $\text{LC}_4\text{H}_9\text{O}_2$  represents  $0.127 \text{ NC4H9O2} + 0.873 \text{ SC4H9O2}$ .

G4401:  $\text{NC4H9O}$  and  $\text{SC4H9O}$  are substituted with  $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2$  and  $0.636 \text{ MEK} + \text{HO}_2$  and  $0.364 \text{ CH}_3\text{CHO} + \text{C}_2\text{H}_5\text{O}_2$ , respectively. The stoichiometric coefficients on the right side are weighted averages.

G4403: The alkyl nitrate yield is the weighted average yield for the two isomers forming from  $\text{NC4H9O2}$  and  $\text{SC4H9O2}$ .

G4404: The product distribution is the weighted average of the single isomer hydroperoxides. It is calculated from the rate constants of single channels and the ratio of the isomers  $\text{NC4H9O2}$  and  $\text{SC4H9O2}$ . The



overall rate constant for this reaction is calculated as weighted average of the channels rate constants. The relative weight of the products from NC4H9OOH and SC4H9OOH are then 0.0887 and 0.9113. The channels producing RO<sub>2</sub> are given the rate coefficient 0.6\*k<sub>CH3OOH\_OH</sub> as for G4107. For NC4H9OOH the products are 0.327 NC4H9O2 + 0.673 C3H7CHO + 0.673 OH. C3H7CHO is then substituted with 2 CO<sub>2</sub> + C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>. Hence, 0.327 NC4H9O2 + 1.346 CO<sub>2</sub> + 0.673 C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> + 0.673 OH. For SC4H9OOH the products are 0.219 SC4H9O2 + 0.781 MEK + 0.781 OH.

G4413: LMEKO2 represents 0.459 MEKAO2 + 0.462 MEKBO2 + 0.079 MEKCO2.

G4415: Alkyl nitrate formation is neglected. The products of MEKAO and MEKCO are substituted with HCHO + CO<sub>2</sub> + HOCH<sub>2</sub>CH<sub>2</sub>O<sub>2</sub> and HCHO + CO<sub>2</sub> + C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>.

G4416: LMEKOOH is assumed having the composition 0.459 MEKAOOH + 0.462 MEKBOOH + 0.079 MEKCOOH. MEKAOOH + OH gives 0.89 CO2C3CHO + 0.89 OH + 0.11 MEKAO2 + H<sub>2</sub>O. CO2C3CHO is substituted with CH<sub>3</sub>COCH<sub>2</sub>O<sub>2</sub> + CO<sub>2</sub> and the products become 0.89 CH<sub>3</sub>COCH<sub>2</sub>O<sub>2</sub> + 0.89 CO<sub>2</sub> + 0.89 OH + 0.11 MEKAO2 + H<sub>2</sub>O. MEKBOOH + OH gives 0.758 BIACET + 0.758 OH + 0.242 MEKBO2 + H<sub>2</sub>O. MEKCOOH + OH gives 0.614 EGLYOX + 0.614 OH + 0.386 MEKCO2 + H<sub>2</sub>O. EGLYOX is substituted with C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> + 2 CO<sub>2</sub> and the products become 0.614 C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> + 1.228 CO<sub>2</sub> + 0.614 OH + 0.386 MEKCO2 + H<sub>2</sub>O.

G4417: The rate coefficient is the combination of the ones for the two isomers weighted by the relative abundances for NC4H9NO3 and SC4H9NO3, respectively. Product distribution is calculated accordingly. NC4H9NO3 + OH gives C3H7CHO + NO<sub>2</sub> + H<sub>2</sub>O with C3H7CHO being substituted with 2 CO<sub>2</sub> + C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>. After substitution is obtained 2 CO<sub>2</sub> + C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> +

NO<sub>2</sub> + H<sub>2</sub>O. SC4H9NO3 + OH gives MEK + NO<sub>2</sub> + H<sub>2</sub>O For the product distribution NC4H9NO3 and SC4H9NO3 account for 0.08577 and 0.91423, respectively.

G4419: The same value as for PAN is assumed.

G4420: Products are as in G4415. Only the main channels for each isomer are considered. Rate constant is the weighted average for the isomers.

G4437: LHMVKABO2 is a lumped species of virtual composition 0.3 HVMVKA02 + 0.7 HVMVKBO2. The products are the weighted average for the permutation reactions of each single RO2 in the MCM (Rickard and Pascoe, 2009).

G4439: products are the weighted average for the decomposition of 0.3 HVMVKA0 + 0.7 HVMVKBO.

G4440: as for G4439

G4441: The rate coefficient and products are 30% for HVMVKA0OH and 70% for HVMVKBOOH.

G4444: LMVKOHABO2 is a lumped species of virtual composition 0.3 MVKOHAO2 + 0.7 MVKOHBO2. The products are the weighted average for the permutation reactions of each single RO2 in the MCM (Rickard and Pascoe, 2009).

G4446: products are the weighted average for the decomposition of 0.3 MVKOHAO + 0.7 MVKOHBO.

G4447: as for G4446

G4448: The rate coefficient and products are 30% for MVKOHAAOH and 70% for MVKOHBOOH.

G6103: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G6402: The initial products are probably HCl and CH<sub>2</sub>OOH (Atkinson et al., 2006). It is assumed that CH<sub>2</sub>OOH dissociates into HCHO and OH.

G6405: Average of reactions with CH<sub>3</sub>Br and CH<sub>3</sub>F from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with CH<sub>3</sub>CF<sub>3</sub>, CH<sub>3</sub>CClF<sub>2</sub>, and CH<sub>3</sub>CCl<sub>2</sub>F from Sander et al. (2006).

G6409: It is assumed that the reaction liberates all Cl atoms in the form of HCl.

G7302: The rate coefficient is:  $k_{BrO\_NO2} = k_{3rd}(temp, cair, 5.2E-31, 3.2, 6.9E-12, 2.9, 0.6)$ .

G7303: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (Orlando and Tyndall, 1996).

G7404: It is assumed that the reaction liberates all Br atoms in the form of HBr.

G7407: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7408: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7605: Same value as for G7408: CH<sub>2</sub>Br<sub>2</sub>+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

G7606: Same value as for G7408: CH<sub>2</sub>Br<sub>2</sub>+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

G7607: It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

G8102: It is assumed that the reaction produces new particles.

G8103: The yield of 38 % OIO is from Atkinson et al. (2007). It is assumed here that the remaining 62 % produce 2 I + O<sub>2</sub>.

G8300: The rate coefficient is:  $k_{I\_NO2} = k_{3rd\_iupac}(temp, cair, 3.E-31, 1., 6.6E-11, 0., 0.63)$ .

G8305: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (van den Bergh and Troe, 1976).

G8306: According to John Plane and John Crowley (pers. comm. 2007), the rate coefficient of  $1.1E15*EXP(-12060./temp)$  suggested by Atkinson et al. (2007) is wrong.

G8401: The rate coefficient is from Dillon et al. (2006b), the yield of I atoms is a lower limit given on page 2170 of Bale et al. (2005).

G8402: The products are from Nakano et al. (2005).

G8701: 80% Br + OIO production is from Atkinson et al. (2007). The remaining channels are assumed to produce Br + I + O<sub>2</sub>.

G9400: Addition path. The rate coefficient is:  $k_{DMS\_OH} = 1.0E-39*EXP(5820./temp)*C(ind\_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind\_O2))$ .

G10201: Upper limit.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_02)	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	jx(ip_01D)	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	jx(ip_03P)	see note
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	jx(ip_N20)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	jx(ip_NO)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO20)	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	jx(ip_NO02)	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	see note
J3104b	StGNJ	$N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$	jx(ip_NO3N00)	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HN03)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HN04)	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH300H)	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	jx(ip_CO2)	see note
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31 H + 0.69 H_2 + 1.155 H_2O$	jx(ip_CH4)	see note
J4200	TrG CJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)*
J4201	TrG CJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrG CJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3C03H)	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	see note
J4205	TrG CJ	$HOCH_2CHO + h\nu \rightarrow HO_2 + HCHO + HO_2 + CO$	jx(ip_HOCH2CHO)	see note
J4206	TrG CJ	$HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$	jx(ip_CH300H)	Rickard (2009)* and Pascoe
J4207	TrG CJ	$PHAN + h\nu \rightarrow HOCH_2CO_3 + NO_2$	jx(ip_PAN)	see note
J4208	TrG CJ	$GLYOX + h\nu \rightarrow 2 CO + 2 HO_2$	jx(ip_GLYOX)	see note
J4209	TrGNCJ	$HCOCO_2H + h\nu \rightarrow 2 HO_2 + CO + CO_2$	jx(ip_MGLYOX)	Rickard (2009)* and Pascoe
J4210	TrGNCJ	$HCOCO_3H + h\nu \rightarrow HO_2 + CO + OH + CO_2$	(jx(ip_CH300H)+jx(ip_HOCH2CHO))	Rickard (2009)* and Pascoe

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4211	TrGCJ	$\text{HYETHO2H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4212	TrGCJ	$\text{ETHOHNO3} + h\nu \rightarrow \text{HO}_2 + 2 \text{HCHO} + \text{NO}_2$	J_IC3H7N03	see note
J4300	TrGCJ	$\text{iC}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	von Kuhlmann (2001)*
J4301	TrGCJ	$\text{CH}_3\text{COCH}_3 + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{CH}_3\text{O}_2$	$\text{jx(ip\_CH3COCH3)}$	see note
J4302	TrGCJ	$\text{CH}_3\text{COCH}_2\text{OH} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{HO}_2$	J_ACETOL	see note
J4303	TrGCJ	$\text{MGLYOX} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO} + \text{HO}_2$	$\text{jx(ip\_MGLYOX)}$	see note
J4304	TrGCJ	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{OH}$	$\text{jx(ip\_CH300H)+J\_ACETOL}$	Rickard and Pascoe (2009)*
J4306	TrGNCJ	$\text{iC}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	J_IC3H7N03	von Kuhlmann et al. (2003)*
J4307	TrGCJ	$\text{NOA} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{NO}_2$	J_IC3H7N03+jx(ip\_CH3COCH3)	see note
J4308	TrGCJ	$\text{HOCH}_2\text{COCO}_2\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}_2$	$\text{jx(ip\_MGLYOX)}$	Rickard and Pascoe (2009)*
J4309	TrGCJ	$\text{HYPROPO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4310	TrGNCJ	$\text{PR}_2\text{O}_2\text{HNO}_3 + h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4311	TrGCJ	$\text{HOCH}_2\text{COCHO} + h\nu \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx(ip\_MGLYOX)}$	Rickard and Pascoe (2009)*
J4400	TrGCJ	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + 0.254 \text{CO}_2 + 0.5552 \text{MEK} + 0.5552 \text{HO}_2 + 0.3178 \text{CH}_3\text{CHO} + 0.4448 \text{C}_2\text{H}_5\text{O}_2$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4401	TrGCJ	$\text{MVK} + h\nu \rightarrow .5 \text{C}_3\text{H}_6 + .5 \text{CH}_3\text{C(O)OO} + .5 \text{HCHO} + \text{CO} + .5 \text{HO}_2$	$\text{jx(ip\_MVK)}$	see note
J4403	TrGCJ	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{C}_2\text{H}_5\text{O}_2$	$0.42*\text{jx(ip\_CHOH)}$	von Kuhlmann et al. (2003)*
J4404	TrGCJ	$\text{LMEKOOH} + h\nu \rightarrow 0.538 \text{HCHO} + 0.538 \text{CO}_2 + 0.459 \text{HOCH}_2\text{CH}_2\text{O}_2 + 0.079 \text{C}_2\text{H}_5\text{O}_2 + 0.462 \text{CH}_3\text{C(O)OO} + 0.462 \text{CH}_3\text{CHO} + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4405	TrGCJ	$\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C(O)OO}$	$2.15*\text{jx(ip\_MGLYOX)}$	see note
J4406	TrGNCJ	$\text{LC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + 0.254 \text{CO}_2 + 0.5552 \text{MEK} + 0.5552 \text{HO}_2 + 0.3178 \text{CH}_3\text{CHO} + 0.4448 \text{C}_2\text{H}_5\text{O}_2$	J_IC3H7N03	see note
J4407	TrGNCJ	$\text{MPAN} + h\nu \rightarrow \text{MACO}_3 + \text{NO}_2$	$\text{jx(ip\_PAN)}$	see note
J4408	TrGCJ	$\text{LMVKOHABOOH} + h\nu \rightarrow .3 \text{HOCH}_2\text{COCHO} + .3 \text{HCHO} + .3 \text{HO}_2 + .7 \text{HOCH}_2\text{CHO} + .7 \text{HOCH}_2\text{CO}_3 + \text{OH}$	$\text{J\_ACETOL+jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4409	TrGCJ	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4410	TrGCJ	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 + \text{HCOCO}_3\text{H}$	J_ACETOL	Rickard (2009)* and Pascoe
J4411	TrGCJ	$\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O})\text{OO} + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MACR})$	see note
J4412	TrGCJ	$\text{MACROOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4413	TrGCJ	$\text{MACROOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{OH}$	$2.77 * \text{jx}(\text{ip\_HOCH}_2\text{CHO})$	see note
J4414	TrGCJ	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$2.77 * \text{jx}(\text{ip\_HOCH}_2\text{CHO})$	see note
J4415	TrGCJ	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4416	TrGCJ	$\text{LHMVKABOOH} + h\nu \rightarrow .3 \text{MGLYOX} + .7 \text{CH}_3\text{C}(\text{O})\text{OO} + .7 \text{HOCH}_2\text{CHO} + .3 \text{HCHO} + .3 \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4417	TrGCJ	$\text{MVKOH} + h\nu \rightarrow .5 \text{HCHO} + .5 \text{HO}_2 + .5 \text{HOCH}_2\text{CO}_3 + \text{CO} + 1.5 \text{LCARBON}$	$\text{jx}(\text{ip\_MVK})$	Rickard (2009)* and Pascoe
J4418	TrGCJ	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard (2009)* and Pascoe
J4419	TrGCJ	$\text{HO}_2\text{C}_3\text{C}_4 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HOCH}_2\text{CHO} + \text{HO}_2$	J_ACETOL	Rickard (2009)* and Pascoe
J4420	TrGCJ	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HOCH}_2\text{CO}_3$	$2.15 * \text{jx}(\text{ip\_MGLYOX})$	see note
J4502	TrGCJ	$\text{LISOPACOOH} + h\nu \rightarrow \text{LHC}_4\text{ACCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4503	TrGNCJ	$\text{LISOPACNO}_3 + h\nu \rightarrow \text{LHC}_4\text{ACCHO} + \text{HO}_2 + \text{NO}_2$	$0.59 * \text{J\_IC3H7N03}$	see note
J4504	TrGCJ	$\text{ISOPBOOH} + h\nu \rightarrow .75 \text{MVK} + .25 \text{MVKOH} + .75 \text{HCHO} + .75 \text{HO}_2 + .25 \text{CH}_3\text{O}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4505	TrGNCJ	$\text{ISOPBNO}_3 + h\nu \rightarrow .75 \text{MVK} + .25 \text{MVKOH} + .75 \text{HCHO} + .75 \text{HO}_2 + .25 \text{CH}_3\text{O}_2 + \text{NO}_2$	$2.84 * \text{J\_IC3H7N03}$	see note
J4506	TrGCJ	$\text{ISOPDOOH} + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4507	TrGNCJ	$\text{ISOPDNO}_3 + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7N03	see note
J4508	TrGNCJ	$\text{NISOPOOH} + h\nu \rightarrow \text{NC}_4\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard (2009)* and Pascoe
J4509	TrGNCJ	$\text{NC}_4\text{CHO} + h\nu \rightarrow \text{NOA} + 2 \text{CO} + 2 \text{HO}_2$	$\text{jx}(\text{ip\_MACR})$	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4510	TrGNcJ	$\text{LNISOOH} + h\nu \rightarrow \text{NOA} + \text{OH} + .5 \text{GLYOX} + .5 \text{CO} + \text{HO}_2 + .5 \text{CO}_2$	$\text{jx(ip\_CH300H)}$	Taraborrelli et al. (2009)*
J4511	TrGCJ	$\text{LHC4ACCHO} + h\nu \rightarrow .5 \text{LHC4ACCO3} + .25 \text{CH}_3\text{COCH}_2\text{OH} + .25 \text{HOCH}_2\text{CHO} + .25 \text{CH}_3\text{C(O)OO} + .75 \text{CO} + 1.25 \text{HO}_2$	$\text{jx(ip\_MACR)}$	Rickard and Pascoe (2009)*
J4512	TrGCJ	$\text{LC578OOH} + h\nu \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{MGLYOX} + .5 \text{GLYOX} + .5 \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Taraborrelli et al. (2009)*
J4513	TrGCJ	$\text{LHC4ACCO3H} + h\nu \rightarrow .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{HOCH}_2\text{CHO} + .5 \text{CH}_3\text{C(O)OO} + .5 \text{CO} + .5 \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J4514	TrGNcJ	$\text{LC5PAN1719} + h\nu \rightarrow .5 \text{MACROH} + .5 \text{HO12CO3C4} + \text{CO} + \text{NO}_2$	$\text{jx(ip\_PAN)}$	see note
J4515	TrGCJ	$\text{HCOC5} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{HOCH}_2\text{CO}_3$	$0.5*\text{jx(ip\_MVK)}$	see note
J4516	TrGCJ	$\text{C59OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3 + \text{OH}$	$\text{J\_ACETOL}+\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)*
J6000	StTrGClJ	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$\text{jx(ip\_Cl2)}$	see note
J6100	StTrGClJ	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2 \text{Cl}$	$1.4*\text{jx(ip\_Cl2O2)}$	see note
J6101	StTrGClJ	$\text{OClO} + h\nu \rightarrow \text{ClO} + \text{O}(^3\text{P})$	$\text{jx(ip\_OClO)}$	see note
J6200	StGClJ	$\text{HCl} + h\nu \rightarrow \text{Cl} + \text{H}$	$\text{jx(ip\_HCl)}$	see note
J6201	StTrGClJ	$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$	$\text{jx(ip\_HOCl)}$	see note
J6300	TrGNClJ	$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$	$\text{jx(ip\_ClNO2)}$	see note
J6301a	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	$\text{jx(ip\_ClNO3)}$	see note
J6301b	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$\text{jx(ip\_ClON02)}$	see note
J6400	StGClJ	$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3\text{O}_2$	$\text{jx(ip\_CH3Cl)}$	see note
J6401	StGClJ	$\text{CCl}_4 + h\nu \rightarrow 4 \text{Cl}$	$\text{jx(ip\_CCl4)}$	see note
J6402	StGCClJ	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3 \text{Cl}$	$\text{jx(ip\_CH3CCl3)}$	see note
J6500	StGFClJ	$\text{CFCl}_3 + h\nu \rightarrow 3 \text{Cl}$	$\text{jx(ip\_CFCl3)}$	see note
J6501	StGFClJ	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2 \text{Cl}$	$\text{jx(ip\_CF2Cl2)}$	see note
J7000	StTrGBrJ	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	$\text{jx(ip\_Br2)}$	see note
J7100	StTrGBrJ	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	$\text{jx(ip\_BrO)}$	see note
J7200	StTrGBrJ	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	$\text{jx(ip\_HOBr)}$	see note
J7300	TrGNBrJ	$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$	$\text{jx(ip\_BrNO2)}$	see note
J7301	StTrGNBrJ	$\text{BrNO}_3 + h\nu \rightarrow 0.29 \text{Br} + 0.29 \text{NO}_3 + 0.71 \text{BrO} + 0.71 \text{NO}_2$	$\text{jx(ip\_BrNO3)}$	see note
J7400	StGBrJ	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$	$\text{jx(ip\_CH3Br)}$	see note
J7401	TrGBrJ	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2 \text{Br}$	$\text{jx(ip\_CH2Br2)}$	see note
J7402	TrGBrJ	$\text{CHBr}_3 + h\nu \rightarrow 3 \text{Br}$	$\text{jx(ip\_CHBr3)}$	see note
J7500	StGFBrJ	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$	$\text{jx(ip\_CF3Br)}$	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_BrCl})$	see note
J7601	StGFBrJ	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CF2ClBr})$	see note
J7602	TrGClBrJ	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CH2ClBr})$	see note
J7603	TrGClBrJ	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{Br} + 2 \text{Cl}$	$\text{jx}(\text{ip\_CHCl2Br})$	see note
J7604	TrGClBrJ	$\text{CHClBr}_2 + h\nu \rightarrow 2 \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CHClBr2})$	see note
J8000	TrGIJ	$\text{I}_2 + h\nu \rightarrow \text{I} + \text{I}$	$\text{jx}(\text{ip\_I2})$	see note
J8100	TrGIJ	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}({}^3\text{P})$	$\text{jx}(\text{ip\_IO})$	see note
J8200	TrGIJ	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	$\text{jx}(\text{ip\_HOI})$	see note
J8300	TrGNIJ	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$	$\text{jx}(\text{ip\_INO2})$	see note
J8301	TrGNIJ	$\text{INO}_3 + h\nu \rightarrow \text{I} + \text{NO}_3$	$\text{jx}(\text{ip\_INO3})$	see note
J8400	TrGIJ	$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2 \text{I} + 2 \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_CH2I2})$	see note
J8401	TrGIJ	$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_CH3I})$	see note
J8402	TrGIJ	$\text{C}_3\text{H}_7\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_C3H7I})$	see note
J8403	TrGIClJ	$\text{CH}_2\text{ClI} + h\nu \rightarrow \text{I} + \text{Cl} + 2 \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_CH2ClI})$	see note
J8600	TrGCIIJ	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	$\text{jx}(\text{ip\_ICl})$	see note
J8700	TrGBrIJ	$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$	$\text{jx}(\text{ip\_IBr})$	see note
PH3200_a01	TrAa01NJ	$\text{NO}_3^-(\text{aq}) + h\nu \rightarrow \text{NO}_2(\text{aq}) + \text{OH}(\text{aq}) - \text{H}^+(\text{aq})$	$\text{xaer}(01)*\text{jx}(\text{ip\_NO2}) * 1.4\text{E}-4$	see note
PH10200_a01	TrAa01HgJ	$\text{Hg}(\text{OH})_2(\text{aq}) + h\nu \rightarrow \text{Hg}(\text{aq})$	$\text{xaer}(01)*6\text{E}-5*\text{jx}(\text{ip\_NO2})$	see note

\*Notes:

J-values are calculated with an external module and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:

$\text{J}(11) \rightarrow \text{jx}(\text{ip\_COH2})$   
 $\text{J}(12) \rightarrow \text{jx}(\text{ip\_CHOH})$   
 $\text{J}(15) \rightarrow \text{jx}(\text{ip\_HOCH2CHO})$   
 $\text{J}(18) \rightarrow \text{jx}(\text{ip\_MACR})$   
 $\text{J}(22) \rightarrow \text{jx}(\text{ip\_ACETOL})$   
 $\text{J}(23)+\text{J}(24) \rightarrow \text{jx}(\text{ip\_MVK})$   
 $\text{J}(31)+\text{J}(32)+\text{J}(33) \rightarrow \text{jx}(\text{ip\_GLYOX})$   
 $\text{J}(34) \rightarrow \text{jx}(\text{ip\_MGLYOX})$   
 $\text{J}(41) \rightarrow \text{jx}(\text{ip\_CH3OOH})$

$\text{J}(53) \rightarrow \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J}(54) \rightarrow \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J}(55) \rightarrow \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J}(56)+\text{J}(57) \rightarrow \text{jx}(\text{ip\_NOA})$

J4207: It is assumed that J(PHAN) is the same as J(PAN).

J4212: It is assumed that J(ETHOHNO3) is the same as J( $\text{iC}_3\text{H}_7\text{ONO}_2$ ).

J4302: Following von Kuhlmann et al. (2003), we use  $\text{J}(\text{CH}_3\text{COCH}_2\text{OH}) = 0.11*\text{jx}(\text{ip\_CHOH})$ . As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999).

J4306: Following von Kuhlmann et al. (2003), we use  $\text{J}(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7*\text{jx}(\text{ip\_PAN})$ .

J4307: NOA contains the chromophores of both  $\text{CH}_3\text{COCH}_3$  and a nitrate group. It is assumed here that the J values are additive, i.e.:  $\text{J}(\text{NOA}) = \text{J}(\text{CH}_3\text{COCH}_3) + \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$ .

J4406: It is assumed that J(LC4H9NO3) is the same as J( $\text{iC}_3\text{H}_7\text{ONO}_2$ ).

J4407: It is assumed that J(MPAN) is the same as J(PAN).

J4405: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4413: It is assumed that J(MACROOH) is 2.77 times larger than J( $\text{HOCH}_2\text{CHO}$ ), consistent with the pho-

tolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4414: It is assumed that  $J(\text{MACROH})$  is 2.77 times larger than  $J(\text{HOCH}_2\text{CHO})$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4420: It is assumed that  $J(\text{BIACETOH})$  is 2.15 times larger than  $J(\text{MGLYOX})$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4503: It is assumed that  $J(\text{LISOPACNO}_3) = 0.59 \times J(\text{iC}_3\text{H}_7\text{ONO}_2)$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4505: It is assumed that  $J(\text{ISOPBNO}_3) = 2.84 \times J(\text{iC}_3\text{H}_7\text{ONO}_2)$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4509: It is assumed that  $J(\text{NC}_4\text{CHO})$  is the same as  $J(\text{MACR})$ .

J4514: It is assumed that  $J(\text{LC5PAN1719})$  is the same as  $J(\text{PAN})$ .

J4515: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that  $J(\text{HCOC5})$  is half as large as  $J(\text{MVK})$ .

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder

et al. (1990) and the  $\text{Cl}_2\text{O}_2$  formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed  $\text{Cl}_2\text{O}_2/\text{ClO}$  ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the  $\text{Cl}_2\text{O}_2$  formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

J7301: The quantum yields are from Sander et al. (2003).



Table 3: Henry’s law coefficients

substance	$k_H^\ominus$ M/atm	$-\Delta_{\text{soln}}H/R$ K	reference
O <sub>2</sub>	$1.3 \times 10^{-3}$	1500.	Wilhelm et al. (1977)
O <sub>3</sub>	$1.2 \times 10^{-2}$	2560.	Chameides (1984)
OH	$3.0 \times 10^1$	4300.	Hanson et al. (1992)
HO <sub>2</sub>	$3.9 \times 10^3$	5900.	Hanson et al. (1992)
H <sub>2</sub> O <sub>2</sub>	$1. \times 10^5$	6338.	Lind and Kok (1994)
NH <sub>3</sub>	58.	4085.	Chameides (1984)
NO	$1.9 \times 10^{-3}$	1480.	Schwartz and White (1981)
NO <sub>2</sub>	$7.0 \times 10^{-3}$	2500.	Lee and Schwartz (1981)*
NO <sub>3</sub>	2.	2000.	Thomas et al. (1993)
N <sub>2</sub> O <sub>5</sub>	BIG	0.	see note
HONO	$4.9 \times 10^1$	4780.	Schwartz and White (1981)
HNO <sub>3</sub>	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO <sub>4</sub>	$1.2 \times 10^4$	6900.	Régimbal and Mozurkewich (1997)
CH <sub>3</sub> O <sub>2</sub>	6.	5600.	Jacob (1986)*
CH <sub>3</sub> OOH	$3.0 \times 10^2$	5322.	Lind and Kok (1994)
CO <sub>2</sub>	$3.1 \times 10^{-2}$	2423.	Chameides (1984)
HCHO	$7.0 \times 10^3$	6425.	Chameides (1984)
HCOOH	$3.7 \times 10^3$	5700.	Chameides (1984)
CH <sub>3</sub> COOH	$4.1 \times 10^3$	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	6.	5600.	see note
CH <sub>3</sub> CHO	$1.29 \times 10^1$	5890.	Sander et al. (2006)
CH <sub>3</sub> COCH <sub>3</sub>	28.1	5050.	Sander et al. (2006)
Cl <sub>2</sub>	$9.2 \times 10^{-2}$	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	$6.7 \times 10^2$	5862.	Huthwelker et al. (1995)
ClNO <sub>3</sub>	BIG	0.	see note
Br <sub>2</sub>	$7.7 \times 10^{-1}$	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	$9.3 \times 10^1$	5862.	Vogt et al. (1996)*
BrNO <sub>3</sub>	BIG	0.	see note
BrCl	$9.4 \times 10^{-1}$	5600.	Bartlett and Margerum (1999)
I <sub>2</sub>	3.	4431.	Palmer et al. (1985)

Table 3: Henry’s law coefficients (... continued)

substance	$k_{\text{H}}^{\ominus}$ M/atm	$-\frac{\Delta_{\text{soln}}H}{R}$ K	reference
IO	$4.5 \times 10^2$	5862.	see note
OIO	BIG	0.	see note
I <sub>2</sub> O <sub>2</sub>	BIG	0.	see note
HI	BIG	0.	see note
HOI	$4.5 \times 10^2$	5862.	Chatfield and Crutzen (1990)*
HIO <sub>3</sub>	BIG	0.	see note
INO <sub>2</sub>	BIG	0.	see note
INO <sub>3</sub>	BIG	0.	see note
ICl	$1.1 \times 10^2$	5600.	see note
IBr	$2.4 \times 10^1$	5600.	see note
SO <sub>2</sub>	1.2	3120.	Chameides (1984)
H <sub>2</sub> SO <sub>4</sub>	$1. \times 10^{11}$	0.	see note
CH <sub>3</sub> SO <sub>3</sub> H	BIG	0.	see note
DMS	$5.4 \times 10^{-1}$	3500.	Staudinger and Roberts (2001)
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*
Hg	0.13	0.	Schroeder and Munthe (1998)
HgO	$3.2 \times 10^6$	0.	Shon et al. (2005)
HgCl <sub>2</sub>	$2.4 \times 10^7$	0.	Shon et al. (2005)
HgBr <sub>2</sub>	$2.4 \times 10^7$	0.	see note
ClHgBr	$2.4 \times 10^7$	0.	see note
BrHgOBr	$2.4 \times 10^7$	0.	see note
ClHgOBr	$2.4 \times 10^7$	0.	see note

\*Notes:

The value “BIG” corresponds to virtually infinite solubility which is represented in the model using a very large but arbitrary number.

The temperature dependence of the Henry constants is:

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

where  $\Delta_{\text{soln}}H$  = molar enthalpy of dissolution [J/mol] and  $R = 8.314$  J/(molK).

NO<sub>2</sub>: The temperature dependence is from Chameides (1984).

HNO<sub>3</sub>: Calculated using the acidity constant from Davis and de Bruin (1964).

CH<sub>3</sub>O<sub>2</sub>: This value was estimated by Jacob (1986).

C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>: Assumed to be the same as  $K_{\text{H}}(\text{CH}_3\text{O}_2)$ .

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  $K_{\text{H}}(\text{HOI})$ .

HOI: Lower limit.

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

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

H<sub>2</sub>SO<sub>4</sub>: To account for the very high Henry’s law coefficient of H<sub>2</sub>SO<sub>4</sub>, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

HgBr<sub>2</sub>: Assumed to be the same as for HgCl<sub>2</sub>.

ClHgBr: Assumed to be the same as for HgCl<sub>2</sub>.

BrHgOBr: Assumed to be the same as for HgCl<sub>2</sub>.

ClHgOBr: Assumed to be the same as for HgCl<sub>2</sub>.

Table 4: Accommodation coefficients

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{K}$	reference
O <sub>2</sub>	0.01	2000.	see note
O <sub>3</sub>	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO <sub>2</sub>	0.5	(default)	Thornton and Abbatt (2005)
H <sub>2</sub> O <sub>2</sub>	0.077	3127.	Worsnop et al. (1989)
NH <sub>3</sub>	0.06	(default)	DeMore et al. (1997)*
NO	$5.0 \times 10^{-5}$	(default)	Saastad et al. (1993)*
NO <sub>2</sub>	0.0015	(default)	Ponche et al. (1993)*
NO <sub>3</sub>	0.04	(default)	Rudich et al. (1996)*
N <sub>2</sub> O <sub>5</sub>	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO <sub>3</sub>	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO <sub>4</sub>	(default)	(default)	DeMore et al. (1997)*
CH <sub>3</sub> O <sub>2</sub>	0.01	2000.	see note
CH <sub>3</sub> OOH	0.0046	3273.	Magi et al. (1997)
CO <sub>2</sub>	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH <sub>3</sub> COOH	$2.0 \times 10^{-2}$	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	(default)	(default)	see note
CH <sub>3</sub> CHO	$3.0 \times 10^{-2}$	(default)	see note
CH <sub>3</sub> COCH <sub>3</sub>	$3.72 \times 10^{-3}$	6395.	Davidovits et al. (1995)
Cl <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
ClNO <sub>3</sub>	0.108	(default)	Deiber et al. (2004)*
Br <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
BrNO <sub>3</sub>	0.063	(default)	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
I <sub>2</sub>	0.01	2000.	see note
IO	0.5	2000.	see note

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{\text{K}}$	reference
OIO	0.01	(default)	see note
I <sub>2</sub> O <sub>2</sub>	(default)	2000.	see note
HI	0.036	4130.	Schweitzer et al. (2000)*
HOI	0.5	(default)	see note
HIO <sub>3</sub>	0.01	(default)	see note
INO <sub>2</sub>	(default)	2000.	see note
INO <sub>3</sub>	(default)	2000.	see note
ICl	0.018	2000.	Braban et al. (2007)
IBr	0.018	2000.	see note
SO <sub>2</sub>	0.11	(default)	DeMore et al. (1997)
H <sub>2</sub> SO <sub>4</sub>	0.65	(default)	Pöschl et al. (1998)*
CH <sub>3</sub> SO <sub>3</sub> H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)
Hg	(default)	(default)	see note
HgO	(default)	(default)	see note
HgCl <sub>2</sub>	(default)	(default)	see note
HgBr <sub>2</sub>	(default)	(default)	see note
ClHgBr	(default)	(default)	see note
BrHgOBr	(default)	(default)	see note
ClHgOBr	(default)	(default)	see note

\*Notes:

If no data are available, the following default values are used:

$$\alpha^\ominus = 0.1$$

$$-\Delta_{\text{obs}}H/R = 0 \text{ K}$$

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

$$\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta_{\text{obs}}G}{RT}\right)$$

$$= \exp\left(\frac{-\Delta_{\text{obs}}H}{RT} + \frac{\Delta_{\text{obs}}S}{R}\right)$$

where  $\Delta_{\text{obs}}G$  is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and  $\Delta_{\text{obs}}H$  and  $\Delta_{\text{obs}}S$  are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

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

and further:

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

O<sub>2</sub>: Estimate.

O<sub>3</sub>: Value measured at 292 K.

OH: Value measured at 293 K.

NH<sub>3</sub>: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO<sub>2</sub>: Value measured at 298 K.

NO<sub>3</sub>: Value is a lower limit, measured at 273 K.

N<sub>2</sub>O<sub>5</sub>: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO<sub>3</sub>: Value measured at room temperature. Abbatt and Waschewsky (1998) say  $\gamma > 0.2$ . Here  $\alpha = 0.5$  is used.

HNO<sub>4</sub>: Value measured at 200 K for water ice.

CH<sub>3</sub>O<sub>2</sub>: Estimate.

CO<sub>2</sub>: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>: Estimate.

CH<sub>3</sub>CHO: Using the same estimate as in the CAPRAM 2.4 model ([http://projects.tropos.de/capram/capram\\_24.html](http://projects.tropos.de/capram/capram_24.html)).

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

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

ClNO<sub>3</sub>: Value measured at 274.5 K.

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.

BrNO<sub>3</sub>: Value measured at 273 K.

BrCl: Assumed to be the same as  $\alpha(\text{Cl}_2)$ .

I<sub>2</sub>: Estimate.

IO: Estimate.

OIO: Estimate.

I<sub>2</sub>O<sub>2</sub>: Estimate.

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

HOI: Assumed to be the same as  $\alpha(\text{HOBr})$ . See also Mössinger and Cox (2001) and Holmes et al. (2001).

HIO<sub>3</sub>: Estimate.

INO<sub>2</sub>: Estimate.

INO<sub>3</sub>: Estimate.

IBr: Assumed to be the same as  $\alpha(\text{ICl})$ .

H<sub>2</sub>SO<sub>4</sub>: Value measured at 303 K.

Hg: Estimate.

HgO: Estimate.

HgCl<sub>2</sub>: Estimate.

HgBr<sub>2</sub>: Estimate.

ClHgBr: Estimate.

BrHgOBr: Estimate.

ClHgOBr: Estimate.

Table 5: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
H1000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{O2})$	see note
H1000b_a01	TrAa01Sc	$O_2(aq) \rightarrow O_2$	$k_{\text{exb}}(01, \text{ind}_{O2})$	see note
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{O3})$	see note
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(01, \text{ind}_{O3})$	see note
H2100f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	$k_{\text{exf}}(01, \text{ind}_{OH})$	see note
H2100b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	$k_{\text{exb}}(01, \text{ind}_{OH})$	see note
H2101f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{HO2})$	see note
H2101b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	$k_{\text{exb}}(01, \text{ind}_{HO2})$	see note
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{H2O2})$	see note
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(01, \text{ind}_{H2O2})$	see note
H3101f_a01	TrAa01NSc	$NO_2 \rightarrow NO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{NO2})$	see note
H3101b_a01	TrAa01NSc	$NO_2(aq) \rightarrow NO_2$	$k_{\text{exb}}(01, \text{ind}_{NO2})$	see note
H3102f_a01	TrAa01NSc	$NO_3 \rightarrow NO_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{NO3})$	see note
H3102b_a01	TrAa01NSc	$NO_3(aq) \rightarrow NO_3$	$k_{\text{exb}}(01, \text{ind}_{NO3})$	see note
H3200f_a01	TrAa01NMblScScm	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{NH3})$	see note
H3200b_a01	TrAa01NMblScScm	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(01, \text{ind}_{NH3})$	see note
H3201_a01	TrAa01MblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf}}_{N2O5}(01)*C(\text{ind}_{H2O\_a01})$	Behnke et al. (1994), Behnke et al. (1997)*
H3202f_a01	TrAa01NSc	$HONO \rightarrow HONO(aq)$	$k_{\text{exf}}(01, \text{ind}_{HONO})$	see note
H3202b_a01	TrAa01NSc	$HONO(aq) \rightarrow HONO$	$k_{\text{exb}}(01, \text{ind}_{HONO})$	see note
H3203f_a01	TrAa01MblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{HNO3})$	see note
H3203b_a01	TrAa01MblNScScm	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(01, \text{ind}_{HNO3})$	see note
H3204f_a01	TrAa01NSc	$HNO_4 \rightarrow HNO_4(aq)$	$k_{\text{exf}}(01, \text{ind}_{HNO4})$	see note
H3204b_a01	TrAa01NSc	$HNO_4(aq) \rightarrow HNO_4$	$k_{\text{exb}}(01, \text{ind}_{HNO4})$	see note
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{CO2})$	see note
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(01, \text{ind}_{CO2})$	see note
H4101f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCHO})$	see note
H4101b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	$k_{\text{exb}}(01, \text{ind}_{HCHO})$	see note
H4102f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	$k_{\text{exf}}(01, \text{ind}_{CH3O2})$	see note
H4102b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	$k_{\text{exb}}(01, \text{ind}_{CH3O2})$	see note
H4103f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCOOH})$	see note
H4103b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	$k_{\text{exb}}(01, \text{ind}_{HCOOH})$	see note
H4104f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{CH3OOH})$	see note
H4104b_a01	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	$k_{\text{exb}}(01, \text{ind}_{CH3OOH})$	see note

Table 5: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
H6000f_a01	TrAa01ClMblSc	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_Cl2})$	see note
H6000b_a01	TrAa01ClMblSc	$\text{Cl}_2(\text{aq}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(01, \text{ind\_Cl2})$	see note
H6200f_a01	TrAa01ClMblScScm	$\text{HCl} \rightarrow \text{HCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HCl})$	see note
H6200b_a01	TrAa01ClMblScScm	$\text{HCl}(\text{aq}) \rightarrow \text{HCl}$	$k_{\text{exb}}(01, \text{ind\_HCl})$	see note
H6201f_a01	TrAa01ClMblSc	$\text{HOCl} \rightarrow \text{HOCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HOCl})$	see note
H6201b_a01	TrAa01ClMblSc	$\text{HOCl}(\text{aq}) \rightarrow \text{HOCl}$	$k_{\text{exb}}(01, \text{ind\_HOCl})$	see note
H6300_a01	TrAa01ClMblN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{aq}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_N2O5}}(01) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a01	TrAa01ClMblN	$\text{ClNO}_3 \rightarrow \text{HOCl}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf\_ClNO3}}(01) * C(\text{ind\_H2O\_a01})$	see note
H6302_a01	TrAa01ClMblN	$\text{ClNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{Cl}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_ClNO3}}(01) * 5.E2$	see note
H7000f_a01	TrAa01BrMblSc	$\text{Br}_2 \rightarrow \text{Br}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_Br2})$	see note
H7000b_a01	TrAa01BrMblSc	$\text{Br}_2(\text{aq}) \rightarrow \text{Br}_2$	$k_{\text{exb}}(01, \text{ind\_Br2})$	see note
H7200f_a01	TrAa01BrMblScScm	$\text{HBr} \rightarrow \text{HBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HBr})$	see note
H7200b_a01	TrAa01BrMblScScm	$\text{HBr}(\text{aq}) \rightarrow \text{HBr}$	$k_{\text{exb}}(01, \text{ind\_HBr})$	see note
H7201f_a01	TrAa01BrMblSc	$\text{HOBr} \rightarrow \text{HOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HOBr})$	see note
H7201b_a01	TrAa01BrMblSc	$\text{HOBr}(\text{aq}) \rightarrow \text{HOBr}$	$k_{\text{exb}}(01, \text{ind\_HOBr})$	see note
H7300_a01	TrAa01BrMblN	$\text{N}_2\text{O}_5 + \text{Br}^-(\text{aq}) \rightarrow \text{BrNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_N2O5}}(01) * 3.E5$	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a01	TrAa01BrMblN	$\text{BrNO}_3 \rightarrow \text{HOBr}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf\_BrNO3}}(01) * C(\text{ind\_H2O\_a01})$	see note
H7302_a01	TrAa01BrMblN	$\text{BrNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{Br}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_BrNO3}}(01) * 3.E5$	see note
H7600f_a01	TrAa01ClBrMblSc	$\text{BrCl} \rightarrow \text{BrCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_BrCl})$	see note
H7600b_a01	TrAa01ClBrMblSc	$\text{BrCl}(\text{aq}) \rightarrow \text{BrCl}$	$k_{\text{exb}}(01, \text{ind\_BrCl})$	see note
H7601_a01	TrAa01ClBrMblN	$\text{ClNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{BrCl}(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_ClNO3}}(01) * 3.E5$	see note
H7602_a01	TrAa01ClBrMblN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl}(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf\_BrNO3}}(01) * 5.E2$	see note
H8000f_a01	TrAa01ISc	$\text{I}_2 \rightarrow \text{I}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_I2})$	see note
H8000b_a01	TrAa01ISc	$\text{I}_2(\text{aq}) \rightarrow \text{I}_2$	$k_{\text{exb}}(01, \text{ind\_I2})$	see note
H8100f_a01	TrAa01IMblSc	$\text{IO} \rightarrow \text{IO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_IO})$	see note
H8100b_a01	TrAa01IMblSc	$\text{IO}(\text{aq}) \rightarrow \text{IO}$	$k_{\text{exb}}(01, \text{ind\_IO})$	see note
H8101_a01	TrAa01I	$\text{OIO} \rightarrow \text{HOI}(\text{aq}) + \text{HO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_OIO})$	see note
H8102_a01	TrAa01I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI}(\text{aq}) + \text{H}^+(\text{aq}) + \text{IO}_2^-(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_I2O2})$	see note
H8200f_a01	TrAa01IMblSc	$\text{HOI} \rightarrow \text{HOI}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HOI})$	see note
H8200b_a01	TrAa01IMblSc	$\text{HOI}(\text{aq}) \rightarrow \text{HOI}$	$k_{\text{exb}}(01, \text{ind\_HOI})$	see note
H8201_a01	TrAa01IMblSc	$\text{HI} \rightarrow \text{H}^+(\text{aq}) + \text{I}^-(\text{aq})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see note

Table 5: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
H8202_a01	TrAa01ISc	$\text{HIO}_3 \rightarrow \text{IO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{mt}}(\text{HIO}_3) \cdot \text{lwc}$	see note
H8300_a01	TrAa01I	$\text{INO}_2 \rightarrow \text{HOI}(\text{aq}) + \text{HONO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_INO2})$	see note
H8301_a01	TrAa01IMbl	$\text{INO}_3 \rightarrow \text{HOI}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_INO3})$	see note
H8600f_a01	TrAa01CIIMblSc	$\text{ICl} \rightarrow \text{ICl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_ICl})$	see note
H8600b_a01	TrAa01CIIMblSc	$\text{ICl}(\text{aq}) \rightarrow \text{ICl}$	$k_{\text{exb}}(01, \text{ind\_ICl})$	see note
H8700f_a01	TrAa01BrIMblSc	$\text{IBr} \rightarrow \text{IBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_IBr})$	see note
H8700b_a01	TrAa01BrIMblSc	$\text{IBr}(\text{aq}) \rightarrow \text{IBr}$	$k_{\text{exb}}(01, \text{ind\_IBr})$	see note
H9100f_a01	TrAa01SMblScScm	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_SO2})$	see note
H9100b_a01	TrAa01SMblScScm	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(01, \text{ind\_SO2})$	see note
H9200_a01	TrAa01SMblScScm	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$\text{xnom7sulf} * k_{\text{exf}}(01, \text{ind\_H2SO4})$	see note
H9400f_a01	TrAa01S	$\text{DMSO} \rightarrow \text{DMSO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_DMSO})$	see note
H9400b_a01	TrAa01S	$\text{DMSO}(\text{aq}) \rightarrow \text{DMSO}$	$k_{\text{exb}}(01, \text{ind\_DMSO})$	see note
H9401_a01	TrAa01SMbl	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_CH3SO3H})$	see note
H9402f_a01	TrAa01S	$\text{DMS} \rightarrow \text{DMS}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_DMS})$	see note
H9402b_a01	TrAa01S	$\text{DMS}(\text{aq}) \rightarrow \text{DMS}$	$k_{\text{exb}}(01, \text{ind\_DMS})$	see note
H10000f_a01	TrAa01Hg	$\text{Hg} \rightarrow \text{Hg}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_Hg})$	see note
H10000b_a01	TrAa01Hg	$\text{Hg}(\text{aq}) \rightarrow \text{Hg}$	$k_{\text{exb}}(01, \text{ind\_Hg})$	see note
H10100f_a01	TrAa01Hg	$\text{HgO} \rightarrow \text{HgO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HgO})$	see note
H10100b_a01	TrAa01Hg	$\text{HgO}(\text{aq}) \rightarrow \text{HgO}$	$k_{\text{exb}}(01, \text{ind\_HgO})$	see note
H10600f_a01	TrAa01HgCl	$\text{HgCl}_2 \rightarrow \text{HgCl}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HgCl2})$	see note
H10600b_a01	TrAa01HgCl	$\text{HgCl}_2(\text{aq}) \rightarrow \text{HgCl}_2$	$k_{\text{exb}}(01, \text{ind\_HgCl2})$	see note
H10700f_a01	TrAa01HgBr	$\text{HgBr}_2 \rightarrow \text{HgBr}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_HgBr2})$	see note
H10700b_a01	TrAa01HgBr	$\text{HgBr}_2(\text{aq}) \rightarrow \text{HgBr}_2$	$k_{\text{exb}}(01, \text{ind\_HgBr2})$	see note
H10701f_a01	TrAa01HgClBr	$\text{ClHgBr} \rightarrow \text{ClHgBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_ClHgBr})$	see note
H10701b_a01	TrAa01HgClBr	$\text{ClHgBr}(\text{aq}) \rightarrow \text{ClHgBr}$	$k_{\text{exb}}(01, \text{ind\_ClHgBr})$	see note
H10702f_a01	TrAa01HgBr	$\text{BrHgOBr} \rightarrow \text{BrHgOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_BrHgOBr})$	see note
H10702b_a01	TrAa01HgBr	$\text{BrHgOBr}(\text{aq}) \rightarrow \text{BrHgOBr}$	$k_{\text{exb}}(01, \text{ind\_BrHgOBr})$	see note
H10703f_a01	TrAa01HgClBr	$\text{ClHgOBr} \rightarrow \text{ClHgOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind\_ClHgOBr})$	see note
H10703b_a01	TrAa01HgClBr	$\text{ClHgOBr}(\text{aq}) \rightarrow \text{ClHgOBr}$	$k_{\text{exb}}(01, \text{ind\_ClHgOBr})$	see note

\*Notes:

The forward ( $k_{\text{exf}}$ ) and backward ( $k_{\text{exb}}$ ) rate coefficients are calculated in the file `messy_mecca_aero.f90`

using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry’s law constants in subroutine `mecca_aero_henry`.

$k_{\text{mt}}$  = mass transfer coefficient

$\text{lwc}$  = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302,



H7601, H7602: For uptake of X (X = N<sub>2</sub>O<sub>5</sub>, ClNO<sub>3</sub>, or BrNO<sub>3</sub>) and subsequent reaction with H<sub>2</sub>O, Cl<sup>-</sup>, and Br<sup>-</sup>, we define:

$$k_{\text{exf}}(\text{X}) = \frac{k_{\text{mt}}(\text{X}) \times \text{LWC}}{[\text{H}_2\text{O}] + 5 \times 10^2 [\text{Cl}^-] + 3 \times 10^5 [\text{Br}^-]}$$

The total uptake rate of X is only determined by  $k_{\text{mt}}$ . The factors only affect the branching between hydrolysis and the halide reactions. The factor  $5 \times 10^2$  was chosen such that the chloride reaction dominates over hydrolysis at about  $[\text{Cl}^-] > 0.1 \text{ M}$  (see Fig. 3 in

Behnke et al. (1997)), i.e. when the ratio  $[\text{H}_2\text{O}]/[\text{Cl}^-]$  is less than  $5 \times 10^2$ . The ratio  $5 \times 10^2 / 3 \times 10^5$  was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2 \text{HNO}_3$	<code>khet_St(ihs_N2O5_H2O)</code>	see note
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^-(\text{aq}) + 2 \text{H}^+(\text{aq})$	<code>khet_Tr(iht_N2O5)</code>	see note
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see note
HET420	StHetNCl	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see note
HET421	StHetNCl	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H2O)</code>	see note
HET422	StHetNCl	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N2O5_HCl)</code>	see note
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see note
HET520	StHetNBr	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H2O)</code>	see note
HET540	StHetNClBr	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see note
HET541	StHetNClBr	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see note
HET542	StHetClBr	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see note
HET543	StHetClBr	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HCl)</code>	see note
HET1001	StTrHetHg	$\text{Hg} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_Hg) + khet_St(ihs_Hg)</code>	see note
HET1002	StTrHetHg	$\text{HgO} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1003	StTrHetHg	$\text{HgCl} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1004	StTrHetHg	$\text{HgCl}_2 \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1005	StTrHetHg	$\text{HgBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1006	StTrHetHg	$\text{HgBr}_2 \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1007	StTrHetHg	$\text{ClHgBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1008	StTrHetHg	$\text{BrHgOBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1009	StTrHetHg	$\text{ClHgOBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note

\*Notes:

Heterogeneous reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see [www.messy-interface.org](http://www.messy-interface.org) for details)

Table 7: Acid-base and other equilibria

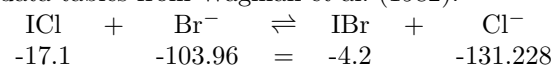
#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ20_a01	TrAa01Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a01	TrAa01MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a01	TrAa01MblNScScm	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ31_a01	TrAa01NSc	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a01	TrAa01MblNScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a01	TrAa01NSc	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ40_a01	TrAa01MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a01	TrAa01ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ60_a01	TrAa01Cl	$\text{Cl}_2 \rightleftharpoons \text{Cl} + \text{Cl}^-$	7.3E-6		Yu (2004)
EQ61_a01	TrAa01ClMblScScm	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a01	TrAa01ClSc	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ70_a01	TrAa01Br	$\text{Br}_2 \rightleftharpoons \text{Br} + \text{Br}^-$	2.54E-6	-2256	Liu et al. (2002)
EQ71_a01	TrAa01BrMblScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ72_a01	TrAa01BrSc	$\text{HOBr} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ73_a01	TrAa01ClBrMbl	$\text{BrCl} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01ClBrMbl	$\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01ClBrMbl	$\text{Br}_2 + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01ClBrMbl	$\text{Br}^- + \text{Cl}_2 \rightleftharpoons \text{BrCl}_2^-$	4.2E6	14072	Wang et al. (1994)
EQ80_a01	TrAa01ClIMblSc	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ81_a01	TrAa01BrIMblSc	$\text{IBr} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2.9E2		Troy and Margerum (1991)
EQ82_a01	TrAa01ClBrIMblSc	$\text{ICl} + \text{Br}^- \rightleftharpoons \text{IBr} + \text{Cl}^-$	3.3E2		see note
EQ90_a01	TrAa01SMblScScm	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01SMblScScm	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01SMblScScm	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01SMblScScm	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ100_a01	TrAa01Hg	$\text{Hg}^{2+} + \text{OH}^- \rightleftharpoons \text{HgOH}^+$	4.0E10		Ammann and Pöschl (2007)
EQ101_a01	TrAa01Hg	$\text{HgOH}^+ + \text{OH}^- \rightleftharpoons \text{Hg}(\text{OH})_2$	1.58E11		Ammann and Pöschl (2007)
EQ102_a01	TrAa01HgCl	$\text{Hg}^{2+} + \text{Cl}^- \rightleftharpoons \text{HgCl}^+$	5.8E6		Ammann and Pöschl (2007)
EQ103_a01	TrAa01HgCl	$\text{HgCl}^+ + \text{Cl}^- \rightleftharpoons \text{HgCl}_2$	2.5E6		Ammann and Pöschl (2007)
EQ104_a01	TrAa01HgCl	$\text{HgOH}^+ + \text{Cl}^- \rightleftharpoons \text{Hg}(\text{OH})\text{Cl}$	2.69E7		Ammann and Pöschl (2007)
EQ105_a01	TrAa01HgBr	$\text{Hg}^{2+} + \text{Br}^- \rightleftharpoons \text{HgBr}^+$	1.1E9		Raofie and Ariya (2004)
EQ106_a01	TrAa01HgBr	$\text{HgBr}^+ + \text{Br}^- \rightleftharpoons \text{HgBr}_2$	2.5E8		Raofie and Ariya (2004)
EQ107_a01	TrAa01HgS	$\text{Hg}^{2+} + \text{SO}_3^{2-} \rightleftharpoons \text{HgSO}_3$	2.E13		van Loon et al. (2001)
EQ108_a01	TrAa01HgS	$\text{HgSO}_3 + \text{SO}_3^{2-} \rightleftharpoons \text{Hg}(\text{SO}_3)_2^{2-}$	1.E10		van Loon et al. (2001)

\*Notes:

EQ40: For  $pK_a(\text{CO}_2)$ , see also Dickson and Millero (1987).

EQ72: For  $pK_a(\text{HOBr})$ , 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):



$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

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

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

Table 8: Aqueous phase reactions

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A1000_a01	TrAa01Sc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9		Sehested et al. (1983)
A2100_a01	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A2101_a01	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A2102_a01	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A2103_a01	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A2104_a01	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A2105_a01	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A3100_a01	TrAa01NSc	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A3101_a01	TrAa01NSc	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A3102_a01	TrAa01NSc	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A3200_a01	TrAa01NSc	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A3201_a01	TrAa01NSc	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A3202_a01	TrAa01NSc	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A3203_a01	TrAa01NSc	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A3204_a01	TrAa01NSc	$HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$	4.6E3	-6800	Damschen and Martin (1983)
A4100_a01	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A4101_a01	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A4102_a01	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2 HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A4103_a01	TrAa01Sc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A4104_a01	TrAa01Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A4105_a01	TrAa01Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A4106_a01	TrAa01Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A4107_a01	TrAa01Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A4108_a01	TrAa01Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A4109_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8		Buxton et al. (1988)
A4110a_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715	Jacob (1986)
A4110b_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715	Jacob (1986)
A6000_a01	TrAa01Cl	$Cl + Cl \rightarrow Cl_2$	8.8E7		Wu et al. (1980)
A6001_a01	TrAa01Cl	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2 Cl^-$	3.5E9		Yu (2004)
A6100_a01	TrAa01Cl	$Cl^- + O_3 \rightarrow ClO^-$	3.0E-3		Hoigné et al. (1985)
A6101_a01	TrAa01Cl	$Cl_2 + O_2^- \rightarrow Cl_2^-$	1.0E9		Bjergbakke et al. (1981)
A6102_a01	TrAa01Cl	$Cl_2^- + O_2^- \rightarrow 2 Cl^-$	1.0E9		Jacobi (1996)*
A6200_a01	TrAa01Cl	$Cl \rightarrow H^+ + ClOH^-$	1.8E5		Yu (2004)
A6201_a01	TrAa01Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A6202_a01	TrAa01Cl	$Cl^- + OH^- \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a01	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a01	TrAa01ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a01	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a01	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a01	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a01	TrAa01ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a01	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH^-$	6.0E9		Yu (2004)
A6210_a01	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a01	TrAa01Cl	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a01	TrAa01Cl	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a01	TrAa01Cl	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a01	TrAa01Cl	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A7000_a01	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2 Br^- + Br_2$	1.9E9		Ross et al. (1992)
A7100_a01	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A7101_a01	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A7102_a01	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2 Br^-$	1.7E8		Wagner and Strehlow (1987)
A7200_a01	TrAa01Br	$Br^- + OH^- \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)
A7201_a01	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A7202_a01	TrAa01BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7203_a01	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A7204_a01	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2 Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A7205_a01	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A7206_a01	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999)
A7207_a01	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A7208_a01	TrAa01BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7209a_a01	TrAa01Br	$BrOH^- \rightarrow Br^- + OH^-$	3.3E7		Zehavi and Rabani (1972)
A7209b_a01	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A7210_a01	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A7300_a01	TrAa01Br	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A7301_a01	TrAa01Br	$Br_2^- + NO_2^- \rightarrow 2 Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A7400_a01	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2 Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*
A7601_a01	TrAa01Br	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A7602_a01	TrAa01ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A7603_a01	TrAa01ClBrMbl	$\text{HOBr} + \text{Cl}^- + \text{H}^+ \rightarrow \text{BrCl}$	2.3E10		see note
A7604_a01	TrAa01ClBrMbl	$\text{BrCl} \rightarrow \text{Cl}^- + \text{HOBr} + \text{H}^+$	3.0E6		Liu and Margerum (2001)
A8100_a01	TrAa01IMbl	$\text{I}^- + \text{O}_3 \rightarrow \text{HOI} + \text{OH}^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a01	TrAa01IMbl	$\text{IO} + \text{IO} \rightarrow \text{HOI} + \text{IO}_2^- + \text{H}^+$	1.5E9		Buxton et al. (1986)
A8200_a01	TrAa01IMbl	$\text{IO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{IO}_3^-$	6.0E1		Furrow (1987)
A8201_a01	TrAa01I	$\text{HOI} + \text{IO}_2^- \rightarrow \text{IO}_3^- + \text{I}^- + \text{H}^+$	6.0E2		Chinake and Simoyi (1996)
A8202_a01	TrAa01IMbl	$\text{HOI} + \text{I}^- + \text{H}^+ \rightarrow \text{I}_2$	4.4E12		Eigen and Kustin (1962)
A8203_a01	TrAa01IMbl	$\text{IO}_2^- + \text{I}^- + \text{H}^+ \rightarrow 2 \text{HOI} + \text{OH}^-$	2.0E10		Edblom et al. (1987)
A8600_a01	TrAa01ClIMbl	$\text{ICl} \rightarrow \text{HOI} + \text{Cl}^- + \text{H}^+$	2.4E6		Wang et al. (1989)
A8601_a01	TrAa01ClIMbl	$\text{I}^- + \text{HOCl} + \text{H}^+ \rightarrow \text{ICl}$	3.5E11		Nagy et al. (1988)
A8602_a01	TrAa01ClI	$\text{IO}_2^- + \text{HOCl} \rightarrow \text{IO}_3^- + \text{Cl}^- + \text{H}^+$	1.5E3		Lengyel et al. (1996)
A8603_a01	TrAa01ClIMbl	$\text{HOI} + \text{Cl}^- + \text{H}^+ \rightarrow \text{ICl}$	2.9E10		Wang et al. (1989)
A8604_a01	TrAa01ClI	$\text{HOI} + \text{Cl}_2 \rightarrow \text{IO}_2^- + 2 \text{Cl}^- + 3\text{H}^+$	1.0E6		Lengyel et al. (1996)
A8605_a01	TrAa01ClI	$\text{HOI} + \text{HOCl} \rightarrow \text{IO}_2^- + \text{Cl}^- + 2 \text{H}^+$	5.0E5		Citri and Epstein (1988)
A8606_a01	TrAa01ClI	$\text{ICl} + \text{I}^- \rightarrow \text{I}_2 + \text{Cl}^-$	1.1E9		Margerum et al. (1986)
A8700_a01	TrAa01BrIMbl	$\text{IBr} \rightarrow \text{HOI} + \text{H}^+ + \text{Br}^-$	8.0E5		Troy et al. (1991)
A8701_a01	TrAa01BrIMbl	$\text{I}^- + \text{HOBr} \rightarrow \text{IBr} + \text{OH}^-$	5.0E9		Troy and Margerum (1991)
A8702_a01	TrAa01BrI	$\text{IO}_2^- + \text{HOBr} \rightarrow \text{IO}_3^- + \text{Br}^- + \text{H}^+$	1.0E6		Chinake and Simoyi (1996)
A8703_a01	TrAa01BrIMbl	$\text{HOI} + \text{Br}^- + \text{H}^+ \rightarrow \text{IBr}$	3.3E12		Troy et al. (1991)
A8704_a01	TrAa01BrI	$\text{HOI} + \text{HOBr} \rightarrow \text{IO}_2^- + \text{Br}^- + 2 \text{H}^+$	1.0E6		Chinake and Simoyi (1996)
A8705_a01	TrAa01ClI	$\text{IBr} + \text{I}^- \rightarrow \text{I}_2 + \text{Br}^-$	2.0E9		Faria et al. (1993)
A9100_a01	TrAa01SSc	$\text{SO}_3^- + \text{O}_2 \rightarrow \text{SO}_5^-$	1.5E9		Huie and Neta (1987)
A9101_a01	TrAa01SMblScScm	$\text{SO}_3^{2-} + \text{O}_3 \rightarrow \text{SO}_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a01	TrAa01SSc	$\text{SO}_4^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a01	TrAa01SSc	$\text{SO}_4^- + \text{SO}_3^{2-} \rightarrow \text{SO}_3^- + \text{SO}_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a01	TrAa01SSc	$\text{SO}_5^- + \text{O}_2^- \rightarrow \text{HSO}_5^- + \text{OH}^-$	2.3E8		Buxton et al. (1996)
A9105_a01	TrAa01S	$\text{SO}_5^- + \text{SO}_3^{2-} \rightarrow .72 \text{SO}_4^- + .72 \text{SO}_4^{2-} + .28 \text{SO}_3^- + .28 \text{HSO}_5^- + .28 \text{OH}^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A9106_a01	TrAa01S	$\text{SO}_5^- + \text{SO}_5^- \rightarrow \text{O}_2 + \text{SO}_4^{2-}$	1.0E8		Ross et al. (1992)*
A9200_a01	TrAa01SSc	$\text{SO}_3^{2-} + \text{OH}^- \rightarrow \text{SO}_3^- + \text{OH}^-$	5.5E9		Buxton et al. (1988)
A9201_a01	TrAa01SSc	$\text{SO}_4^- + \text{OH}^- \rightarrow \text{HSO}_5^-$	1.0E9		Jiang et al. (1992)
A9202_a01	TrAa01SSc	$\text{SO}_4^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.5E9		Jiang et al. (1992)
A9203_a01	TrAa01SSc	$\text{SO}_4^- + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}^-$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a01	TrAa01SSc	$\text{SO}_4^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2$	1.2E7		Wine et al. (1989)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9205_a01	TrAa01SSc	$\text{HSO}_3^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-} + \text{OH}^-$	3.0E3		see note
A9206_a01	TrAa01SMblScScm	$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a01	TrAa01SSc	$\text{HSO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^-$	4.5E9		Buxton et al. (1988)
A9208_a01	TrAa01SSc	$\text{HSO}_3^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{OH}^- + \text{H}^+$	3.0E3		see note
A9209_a01	TrAa01SMblScScm	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a01	TrAa01SSc	$\text{HSO}_3^- + \text{SO}_4^- \rightarrow \text{SO}_3^- + \text{SO}_4^{2-} + \text{H}^+$	8.0E8		Huie and Neta (1987)
A9211_a01	TrAa01S	$\text{HSO}_3^- + \text{SO}_5^- \rightarrow .75 \text{SO}_4^- + .75 \text{SO}_4^{2-} + .75 \text{H}^+ + .25 \text{SO}_3^- + .25 \text{HSO}_5^-$	1.0E5		Huie and Neta (1987)
A9212_a01	TrAa01SSc	$\text{HSO}_3^- + \text{HSO}_5^- + \text{H}^+ \rightarrow 2 \text{HSO}_4^- + \text{H}^+$	7.1E6		Betterton and Hoffmann (1988)
A9300_a01	TrAa01SSc	$\text{SO}_3^{2-} + \text{NO}_2 \rightarrow \text{SO}_4^{2-} + 2 \text{HONO} - \text{NO}_2$	2.0E7		Clifton et al. (1988)
A9301_a01	TrAa01SSc	$\text{SO}_4^- + \text{NO}_3^- \rightarrow \text{SO}_4^{2-} + \text{NO}_3$	5.0E4		Exner et al. (1992)
A9302_a01	TrAa01SSc	$\text{SO}_4^{2-} + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{SO}_4^-$	1.0E5		Logager et al. (1993)
A9303_a01	TrAa01SSc	$\text{HSO}_3^- + \text{NO}_2 \rightarrow \text{HSO}_4^- + 2 \text{HONO} - \text{NO}_2$	2.0E7		Clifton et al. (1988)
A9304_a01	TrAa01SSc	$\text{HSO}_3^- + \text{NO}_3 \rightarrow \text{SO}_3^- + \text{NO}_3^- + \text{H}^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a01	TrAa01SSc	$\text{HSO}_3^- + \text{HNO}_4 \rightarrow \text{HSO}_4^- + \text{NO}_3^- + \text{H}^+$	3.1E5		Warneck (1999)
A9400_a01	TrAa01SSc	$\text{SO}_3^{2-} + \text{HCHO} \rightarrow \text{CH}_2\text{OHSO}_3^- + \text{OH}^-$	1.4E4		Boyce and Hoffmann (1984)
A9401_a01	TrAa01SSc	$\text{SO}_3^{2-} + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A9402_a01	TrAa01SSc	$\text{HSO}_3^- + \text{HCHO} \rightarrow \text{CH}_2\text{OHSO}_3^-$	4.3E-1		Boyce and Hoffmann (1984)
A9403_a01	TrAa01SSc	$\text{HSO}_3^- + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{HSO}_4^- + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A9404_a01	TrAa01SSc	$\text{CH}_2\text{OHSO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^{2-} + \text{HCHO}$	3.6E3		Seinfeld and Pandis (1998)
A9600_a01	TrAa01SCL	$\text{SO}_3^{2-} + \text{Cl}_2^- \rightarrow \text{SO}_3^- + 2 \text{Cl}^-$	6.2E7		Jacobi et al. (1996)
A9601_a01	TrAa01SCLMbl	$\text{SO}_3^{2-} + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a01	TrAa01SCL	$\text{SO}_4^- + \text{Cl}^- \rightarrow \text{SO}_4^{2-} + \text{Cl}$	2.5E8		Buxton et al. (1999a)
A9603_a01	TrAa01SCL	$\text{SO}_4^{2-} + \text{Cl} \rightarrow \text{SO}_4^- + \text{Cl}^-$	2.1E8		Buxton et al. (1999a)
A9604_a01	TrAa01SCL	$\text{HSO}_3^- + \text{Cl}_2^- \rightarrow \text{SO}_3^- + 2 \text{Cl}^- + \text{H}^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a01	TrAa01SCLMbl	$\text{HSO}_3^- + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^- + \text{H}^+$	7.6E8		see note
A9606_a01	TrAa01SCL	$\text{HSO}_5^- + \text{Cl}^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9700_a01	TrAa01SBr	$\text{SO}_3^{2-} + \text{Br}_2^- \rightarrow 2 \text{Br}^- + \text{SO}_3^-$	2.2E8	-649	Shoute et al. (1991)
A9701_a01	TrAa01SBr	$\text{SO}_3^{2-} + \text{BrO}^- \rightarrow \text{Br}^- + \text{SO}_4^{2-}$	1.0E8		Troy and Margerum (1991)
A9702_a01	TrAa01SBrMbl	$\text{SO}_3^{2-} + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^-$	5.0E9		Troy and Margerum (1991)
A9703_a01	TrAa01SBr	$\text{SO}_4^- + \text{Br}^- \rightarrow \text{Br} + \text{SO}_4^{2-}$	2.1E9		Jacobi (1996)
A9704_a01	TrAa01SBr	$\text{HSO}_3^- + \text{Br}_2^- \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{SO}_3^-$	6.3E7	-782	Shoute et al. (1991)
A9705_a01	TrAa01SBrMbl	$\text{HSO}_3^- + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$	5.0E9		see note
A9706_a01	TrAa01SBr	$\text{HSO}_5^- + \text{Br}^- \rightarrow \text{HOBr} + \text{SO}_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)



Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A9800_a01	TrAa01SI	$HSO_3^- + I_2 \rightarrow 2 I^- + HSO_4^- + 2 H^+$	1.7E9		Yiin and Margerum (1990)
A10100_a01	TrAa01Hg	$Hg + O_3 \rightarrow HgO + O_2$	4.7E7		Munthe (1992)
A10200_a01	TrAa01Hg	$HgO + H^+ \rightarrow Hg^{2+} + OH^-$	1.0E10		Pleijel and Munthe (1995)
A10201_a01	TrAa01Hg	$Hg + OH \rightarrow Hg^+ + OH^-$	2.0E9		Lin and Pehkonen (1997)
A10202_a01	TrAa01Hg	$Hg^+ + OH \rightarrow Hg^{2+} + OH^-$	1.0E10		Lin and Pehkonen (1997)
A10203_a01	TrAa01Hg	$Hg^{2+} + HO_2 \rightarrow Hg^+ + O_2 + H^+$	1.7E4		Enami et al. (2007)
A10204_a01	TrAa01Hg	$Hg^+ + HO_2 \rightarrow Hg + O_2 + H^+$	1.0E10		Lin and Pehkonen (1997)*
A10600_a01	TrAa01HgCl	$Hg + HOCl \rightarrow Hg^{2+} + Cl^- + OH^-$	2.09E6		Lin and Pehkonen (1998)
A10601_a01	TrAa01HgCl	$Hg + ClO^- \rightarrow Hg^{2+} + Cl^- + OH^-$	1.99E6		Lin and Pehkonen (1998)*
A10700_a01	TrAa01HgBr	$Hg + HOBr \rightarrow Hg^{2+} + Br^- + OH^-$	0.279		Wang and Pehkonen (2004)
A10701_a01	TrAa01HgBr	$Hg + BrO^- \rightarrow Hg^{2+} + Br^- + OH^-$	0.273		Wang and Pehkonen (2004)*
A10702_a01	TrAa01HgBr	$Hg + Br_2 \rightarrow Hg^{2+} + 2 Br^-$	0.196		Wang and Pehkonen (2004)
A10900_a01	TrAa01HgS	$HgSO_3 \rightarrow Hg + HSO_4^- + H^+$	0.0106		van Loon et al. (2000)

\*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  $SO_4^{2-}$ , 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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