

The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs5

MECCA version: 3.0

Date: September 9, 2011.

Selected reactions:

“Tr && (G || (Aa && Mb1)) && !I && !Hg”

Number of aerosol phases: 2

Number of species in selected mechanism:

Gas phase: 161

Aqueous phase: 62

All species: 223

Number of reactions in selected mechanism:

Gas phase (Gnnn): 310

Aqueous phase (Annn): 28

Henry (Hnnn): 74

Photolysis (Jnnn): 90

Heterogeneous (HETnnn): 0

Equilibria (EQnn): 56

Isotope exchange (DGnnn): 0

Dummy (Dnn): 2

All equations: 560

This document describes the chemistry mechanism used in the study
“Chemical Mechanism Solvers in Air Quality Models” by Zhang et
al. (2011)

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)
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)
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)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	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)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	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_NO3_NO2	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_NO3_NO2/(2.7E-27*EXP(11000./temp))$	Sander et al. (2006)*
G3200	TrGN	$NO + OH \rightarrow HONO$	$k_3rd(temp, cair, 7.0E-31, 2.6, 3.6E-11, 0.1, 0.6)$	Sander et al. (2006)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	$3.5E-12*EXP(250./temp)$	Sander et al. (2006)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	$k_3rd(temp, cair, 1.8E-30, 3.0, 2.8E-11, 0., 0.6)$	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	$3.5E-12$	Sander et al. (2006)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	$1.8E-11*EXP(-390./temp)$	Sander et al. (2006)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k_NO2_HO2/(2.1E-27*EXP(10900./temp))$	Sander et al. (2006)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	$1.3E-12*EXP(380./temp)$	Sander et al. (2006)
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	$1.7E-12*EXP(-710./temp)$	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow NH_2O + O_2$	$4.3E-12*EXP(-930./temp)$	Kohlmann and Poppe (1999)
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	$4.8E-07*EXP(-628./temp)*temp**(-1.32)$	Kohlmann and Poppe (1999)
G3212	TrGN	$NH_2 + HO_2 \rightarrow HNO + H_2O$	$9.4E-09*EXP(-356./temp)*temp**(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	$1.92E-12*((temp/298.)**(-1.5))$	Kohlmann and Poppe (1999)

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

#	labels	reaction	rate coefficient	reference
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)
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)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.*\text{R}02*9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1.+1./26.2 * \text{EXP}(1130./\text{temp}))$	Sander et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow 0.5 \text{HCHO} + 0.5 \text{CH}_3\text{OH} + 0.5 \text{O}_2$	$2.*\text{R}02*9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1.+26.2 * \text{EXP}(-1130./\text{temp}))$	Sander et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow 0.7 \text{CH}_3\text{O}_2 + 0.3 \text{HCHO} + 0.3 \text{OH} + \text{H}_2\text{O}$	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	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$4.0\text{E-}13$	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	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + 0.63 \text{CO} + 0.13 \text{HO}_2 + 0.23125 \text{HCOOH} + 0.13875 \text{HCHO} + 0.13875 \text{H}_2\text{O}_2 + 0.13 \text{OH}$	$1.2\text{E-}14 * \text{EXP}(-2630./\text{temp})$	Sander et al. (2006)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 1.0\text{E-}28, 4.5, 8.8\text{E-}12, 0.85, 0.6)$	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	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Atkinson et al. (1999)

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

#	labels	reaction	rate coefficient	reference
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow 0.98 \text{ CH}_3\text{CHO} + 0.38 \text{ HO}_2 + 0.02 \text{ HOCH}_2\text{CH}_2\text{O}_2$	$3.1\text{E-}13*\text{R02}$	Rickard and Pascoe (2009)*
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow 0.43 \text{ C}_2\text{H}_5\text{O}_2 + 0.43 \text{ H}_2\text{O} + 0.57 \text{ CH}_3\text{CHO} + 0.57 \text{ OH}$	$0.6*k_{\text{CH300H_OH}} + 8.01\text{E-}12$	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	$\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$	$k_{\text{CH3C03_N02}}$	Sander et al. (2006)
G4214	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	$4.\text{E-}12$	Canosa-Mas et al. (1996)
G4217	TrGC	$\text{CH}_3\text{C(O)OO} \rightarrow 0.7 \text{ CH}_3\text{O}_2 + 0.7 \text{ CO}_2 + 0.3 \text{ CH}_3\text{COOH}$	$1.00\text{E-}11*\text{R02}$	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	$\text{PAN} \rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$	$k_{\text{PAN_M}}$	Sander et al. (2006)*
G4222	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow 0.636 \text{ GLYOX} + 0.636 \text{ OH} + 0.364 \text{ HCOOH} + 0.364 \text{ CO} + 0.364 \text{ HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 5.5\text{e-}30, 0.0, 8.3\text{e-}13, -2., 0.6)$	Sander et al. (2006)
G4223	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow 0.8 \text{ HOCH}_2\text{CO}_3 + 0.2 \text{ GLYOX} + 0.2 \text{ HO}_2 + \text{H}_2\text{O}$	$1.00\text{E-}11$	Rickard and Pascoe (2009)
G4224	TrGNC	$\text{HOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO}_3 + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G4225	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow 0.7 \text{ HCHO} + 0.7 \text{ CO}_2 + 0.7 \text{ HO}_2 + 0.3 \text{ HOCH}_2\text{CO}_2\text{H}$	$1.00\text{E-}11*\text{R02}$	Rickard and Pascoe (2009)
G4226	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 0.71 \text{ HOCH}_2\text{CO}_3\text{H} + 0.29 \text{ HOCH}_2\text{CO}_2\text{H} + 0.29 \text{ O}_3$	KAPH02	Rickard and Pascoe (2009)
G4227	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G4228	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G4229	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KRO2N03*1.60	Rickard and Pascoe (2009)
G4230	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$2.73\text{E-}12$	Rickard and Pascoe (2009)
G4231	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$6.19\text{E-}12$	Rickard and Pascoe (2009)
G4232	TrGNC	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G4233	TrGNC	$\text{PHAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$1.12\text{E-}12$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4234	TrGC	GLYOX + OH $\rightarrow$ 1.2 CO + 0.6 HO ₂ + 0.4 HCOCO ₃ + H ₂ O	1.14E-11	Rickard and Pascoe (2009)
G4235	TrGNC	GLYOX + NO ₃ $\rightarrow$ 1.2 CO + 0.6 HO ₂ + 0.4 HCOCO ₃ + HNO ₃	KN03AL	Rickard and Pascoe (2009)
G4236	TrGC	HCOCO ₃ $\rightarrow$ 0.7 CO + 0.7 HO ₂ + 0.7 CO ₂ + 0.3 HCOCO ₂ H	1.00E-11*R02	Rickard and Pascoe (2009)
G4237	TrGC	HCOCO ₃ + HO ₂ $\rightarrow$ 0.71 HCOCO ₃ H + 0.29 HCOCO ₂ H + 0.29 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 ₂ H + OH $\rightarrow$ CO + HO ₂ + CO ₂ + H ₂ O	1.23E-11	Rickard and Pascoe (2009)
G4241	TrGC	HCOCO ₃ H + OH $\rightarrow$ HCOCO ₃ + H ₂ O	1.58E-11	Rickard and Pascoe (2009)
G4242	TrGC	HOCH ₂ CH ₂ O ₂ $\rightarrow$ 0.6 HOCH ₂ CH ₂ O + 0.2 HOCH ₂ CHO + 0.2 ETHGLY	2.00E-12*R02	Rickard and Pascoe (2009)
G4243	TrGNC	HOCH ₂ CH ₂ O ₂ + NO $\rightarrow$ 0.24875 HO ₂ + 0.4975 HCHO + 0.74625 HOCH ₂ CH ₂ O + 0.995 NO ₂ + 0.005 ETHOHNO ₃	KR02N0	Rickard and Pascoe (2009)*
G4244	TrGC	HOCH ₂ CH ₂ O ₂ + HO ₂ $\rightarrow$ HYETHO2H	2.00E-13*EXP(1250./temp)	Rickard and Pascoe (2009)
G4245	TrGNC	ETHOHNO ₃ + OH $\rightarrow$ HOCH ₂ CHO + NO ₂ + H ₂ O	8.40E-13	Rickard and Pascoe (2009)
G4246a	TrGC	HYETHO2H + OH $\rightarrow$ HOCH ₂ CH ₂ O ₂ + H ₂ O	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G4246b	TrGC	HYETHO2H + OH $\rightarrow$ HOCH ₂ CHO + OH + H ₂ O	1.38E-11	Rickard and Pascoe (2009)
G4247a	TrGC	HOCH ₂ CH ₂ O $\rightarrow$ HO ₂ + HOCH ₂ CHO	6.00E-14*EXP(-550./temp)*C(ind_02)	Rickard and Pascoe (2009)
G4247b	TrGC	HOCH ₂ CH ₂ O $\rightarrow$ HO ₂ + HCHO + HCHO	9.50E13*EXP(-5988./temp)	Rickard and Pascoe (2009)
G4248	TrGC	ETHGLY + OH $\rightarrow$ HOCH ₂ CHO + HO ₂ + H ₂ O	7.70E-12	Rickard and Pascoe (2009)
G4300	TrGC	C ₃ H ₈ + OH $\rightarrow$ 0.736 iC ₃ H ₇ O ₂ + 0.264 C ₂ H ₅ O ₂ + 0.264 CO ₂ + 0.264 HO ₂ + H ₂ O	1.55E-17*temp*temp*EXP(-61./temp)	Rickard and Pascoe (2009)*
G4301	TrGC	C ₃ H ₆ + O ₃ $\rightarrow$ 0.28 CH ₃ O ₂ + 0.1 CH ₄ + 0.075 CH ₃ COOH + 0.56 CO + 0.075 HCOOH + 0.09 H ₂ O ₂ + 0.28 HO ₂ + 0.2 CO ₂ + 0.545 CH ₃ CHO + 0.545 HCHO + 0.36 OH	6.5E-15*EXP(-1900./temp)	Sander et al. (2006)*
G4302	TrGC	C ₃ H ₆ + OH $\rightarrow$ HYPROPO2	k_3rd(temp, cair, 8.E-27, 3.5, 3.E-11, 0., 0.5)	Atkinson et al. (1999)
G4303	TrGNC	C ₃ H ₆ + NO ₃ $\rightarrow$ PRONO3BO2	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	iC ₃ H ₇ O ₂ + HO ₂ $\rightarrow$ iC ₃ H ₇ OOH	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G4305	TrGNC	iC ₃ H ₇ O ₂ + NO $\rightarrow$ 0.96 CH ₃ COCH ₃ + 0.96 HO ₂ + 0.96 NO ₂ + 0.04 iC ₃ H ₇ ONO ₂	2.7E-12*EXP(360./temp)	Atkinson et al. (1999)
G4306	TrGC	iC ₃ H ₇ O ₂ $\rightarrow$ CH ₃ COCH ₃ + 0.8 HO ₂	4.E-14*R02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G4307	TrGC	$iC_3H_7OOH + OH \rightarrow 0.27 iC_3H_7O_2 + 0.73 CH_3COCH_3 + 0.73 OH + H_2O$	$1.66E-11 + 0.6*k_{CH300H_OH}$	Rickard and Pascoe (2009)*
G4311	TrGC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	$(1.33E-13+3.82E-11*EXP(-2000./temp))$	Sander et al. (2006)
G4312	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	$8.6E-13*EXP(700./temp)$	Tyndall et al. (2001)
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow CH_3C(O)OO + HCHO + NO_2$	$2.9E-12*EXP(300./temp)$	Sander et al. (2006)
G4314	TrGC	$CH_3COCH_2O_2 \rightarrow 0.6 CH_3C(O)OO + 0.6 HCHO + 0.2 MGLYOX + 0.2 CH_3COCH_2OH$	$7.5E-13*EXP(500./temp)*2.*R02$	Tyndall et al. (2001)
G4315a	TrGC	$CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2 + H_2O$	$0.6*k_{CH300H_OH}$	see note
G4315b	TrGC	$CH_3COCH_2O_2H + OH \rightarrow MGLYOX + OH + H_2O$	$8.39E-12$	Rickard and Pascoe (2009)
G4316	TrGC	$CH_3COCH_2OH + OH \rightarrow MGLYOX + HO_2 + H_2O$	$3.E-12$	Atkinson et al. (1999)
G4317	TrGC	$MGLYOX + OH \rightarrow CH_3C(O)OO + CO$	$8.4E-13*EXP(830./temp)$	Tyndall et al. (1995)
G4320	TrGNC	$iC_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	$6.2E-13*EXP(-230./temp)$	Atkinson et al. (1999)
G4321	TrGNC	$CH_3COCH_2O_2 + NO_3 \rightarrow CH_3C(O)OO + HCHO + NO_2$	KR02N03	Rickard and Pascoe (2009)
G4322	TrGC	$HYPPOPO_2 \rightarrow CH_3CHO + HCHO + HO_2$	$8.80E-13*R02$	Rickard and Pascoe (2009)
G4323	TrGC	$HYPPOPO_2 + HO_2 \rightarrow HYPPOPO_2H$	$KR02H02*0.520$	Rickard and Pascoe (2009)
G4324	TrGNC	$HYPPOPO_2 + NO \rightarrow CH_3CHO + HCHO + HO_2 + NO_2$	KR02N0	Rickard and Pascoe (2009)
G4325	TrGNC	$HYPPOPO_2 + NO_3 \rightarrow CH_3CHO + HCHO + HO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)
G4326a	TrGC	$HYPPOPO_2H + OH \rightarrow HYPPOPO_2$	$1.90E-12*EXP(190./temp)$	Rickard and Pascoe (2009)
G4326b	TrGC	$HYPPOPO_2H + OH \rightarrow CH_3COCH_2OH + OH$	$2.44E-11$	Rickard and Pascoe (2009)
G4327	TrGNC	$PRONO_3BO_2 + HO_2 \rightarrow PR_2O_2HNO_3$	$KR02H02*0.520$	Rickard and Pascoe (2009)
G4328	TrGNC	$PRONO_3BO_2 + NO \rightarrow NOA + HO_2 + NO_2$	KR02N0	Rickard and Pascoe (2009)
G4329	TrGNC	$PRONO_3BO_2 + NO_3 \rightarrow NOA + HO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)
G4330a	TrGNC	$PR_2O_2HNO_3 + OH \rightarrow PRONO_3BO_2$	$1.90E-12*EXP(190./temp)$	Rickard and Pascoe (2009)
G4330b	TrGNC	$PR_2O_2HNO_3 + OH \rightarrow NOA + OH$	$3.47E-12$	Rickard and Pascoe (2009)
G4331	TrGNC	$MGLYOX + NO_3 \rightarrow CH_3C(O)OO + CO + HNO_3$	$KN03AL*2.4$	Rickard and Pascoe (2009)
G4332	TrGNC	$NOA + OH \rightarrow MGLYOX + NO_2$	$1.30E-13$	Rickard and Pascoe (2009)
G4333	TrGC	$HOCH_2COCHO + OH \rightarrow HOCH_2CO_3 + CO$	$1.44E-11$	Rickard and Pascoe (2009)
G4334	TrGNC	$HOCH_2COCHO + NO_3 \rightarrow HOCH_2CO_3 + CO + HNO_3$	$KN03AL*2.4$	Rickard and Pascoe (2009)
G4335	TrGC	$HOCH_2COCO_2H + OH \rightarrow HOCH_2CO_3 + CO_2$	$2.89E-12$	Rickard and Pascoe (2009)
G4400	TrGC	$nC_4H_{10} + OH \rightarrow LC_4H_9O_2 + H_2O$	$1.81E-17*temp*temp*EXP(114./temp)$	Atkinson (2003)*
G4401	TrGC	$LC_4H_9O_2 \rightarrow 0.254 CO_2 + 0.5552 MEK + 0.5552 HO_2 + 0.3178 CH_3CHO + 0.4448 C_2H_5O_2$	$2.5E-13*R02$	Rickard and Pascoe (2009)*
G4402	TrGC	$LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$	$KR02H02*0.625$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4403	TrGNC	LC ₄ H ₉ O ₂ + NO → 0.9172 NO ₂ + 0.233 CO ₂ + 0.5092 MEK + 0.5092 HO ₂ + 0.2915 CH ₃ CHO + 0.408 C ₂ H ₅ O ₂ + 0.0828 LC ₄ H ₉ NO ₃	KR02NO	Rickard and Pascoe (2009)*
G4404	TrGC	LC ₄ H ₉ OOH + OH → 0.2285796 LC ₄ H ₉ O ₂ + 0.7117253 MEK + 0.1193902 CO ₂ + 0.0596951 C ₂ H ₅ O ₂ + 0.7714204 OH + H ₂ O	2.636E-11	Rickard and Pascoe (2009)*
G4405	TrGC	MVK + O ₃ → 0.28 CH ₃ C(O)OO + 0.56 CO + 0.225 LCARBON + 0.075 HCOOH + 0.09 H ₂ O ₂ + 0.28 HO ₂ + 0.1 CO ₂ + 0.1 CH ₃ 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 ₂ O	3.24E-18*temp*temp*EXP(414./temp)	Rickard and Pascoe (2009)*
G4414	TrGC	LMEKO2 + HO ₂ → LMEKOOH	KR02H02*0.625	Rickard and Pascoe (2009)
G4415	TrGNC	LMEKO2 + NO → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G4416	TrGC	LMEKOOH + OH → 0.40851 CH ₃ COCH ₂ O ₂ + 0.350196 BIACET + 0.807212 OH + 0.048506 C ₂ H ₅ O ₂ + 0.505522 CO ₂ + 0.192788 LMEKO2 + H ₂ O	3.786E-11	Rickard and Pascoe (2009)*
G4417	TrGNC	LC ₄ H ₉ NO ₃ + OH → 0.91423 MEK + 0.08577 C ₂ H ₅ O ₂ + 0.17154 CO ₂ + NO ₂ + H ₂ O	9.598E-13	Rickard and Pascoe (2009)*
G4418	TrGNC	MPAN + OH → CH ₃ COCH ₂ OH + CO + NO ₂	3.2E-11	Orlando et al. (2002)
G4419	TrGNC	MPAN → MACO3 + NO ₂	k_PAN_M	see note
G4420	TrGC	LMEKO2 → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO	1.483E-12*R02	Rickard and Pascoe (2009)*
G4421	TrGC	MACR + OH → 0.57 MACO3 + 0.43 MACRO2	1.86E-11*EXP(175./temp)	Rickard and Pascoe (2009)
G4422	TrGC	MACR + O ₃ → 0.59 MGLYOX + 0.41 CH ₃ C(O)OO + 0.03375 HCOOH + 0.55625 HCHO + 0.82 CO + 0.12375 H ₂ O ₂ + 0.41 HO ₂ + 0.82 OH	1.36E-15*EXP(-2112./temp)	Rickard and Pascoe (2009)
G4423	TrGNC	MACR + NO ₃ → MACO3 + HNO ₃	KN03AL*2.0	Rickard and Pascoe (2009)
G4424	TrGC	MACO3 → 0.7 CH ₃ C(O)OO + 0.7 HCHO + 0.7 CO ₂ + 0.3 MACO2H	1.00E-11*R02	Rickard and Pascoe (2009)
G4425	TrGC	MACO3 + HO ₂ → 0.71 MACO3H + 0.29 MACO2H + 0.29 O ₃	KAPH02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4426	TrGNC	$\text{MACO3} + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2 + \text{CO}_2$	$8.70\text{E-}12 * \text{EXP}(290./\text{temp})$	Rickard and Pascoe (2009)
G4427	TrGNC	$\text{MACO3} + \text{NO}_2 \rightarrow \text{MPAN}$	$k_ \text{CH3CO3_NO2}$	Rickard and Pascoe (2009)
G4428	TrGNC	$\text{MACO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2 + \text{CO}_2$	$\text{KR02N03} * 1.60$	Rickard and Pascoe (2009)
G4429	TrGC	$\text{MACRO2} \rightarrow 0.7 \text{CH}_3\text{COCH}_2\text{OH} + 0.7 \text{HCHO} + 0.7 \text{HO}_2$ + 0.3 MACROH	$9.20\text{E-}14 * \text{R02}$	Rickard and Pascoe (2009)
G4430	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACROOH}$	$\text{KR02H02} * 0.625$	Rickard and Pascoe (2009)
G4431	TrGNC	$\text{MACRO2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G4432	TrGNC	$\text{MACRO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4433	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{MACRO2}$	$2.82\text{E-}11$	Rickard and Pascoe (2009)
G4434	TrGC	$\text{MACROH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HCHO} + \text{HO}_2$	$2.46\text{E-}11$	Rickard and Pascoe (2009)
G4435	TrGC	$\text{MACO2H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO}_2$	$1.51\text{E-}11$	Rickard and Pascoe (2009)
G4436	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{MACO3}$	$1.87\text{E-}11$	Rickard and Pascoe (2009)
G4437	TrGC	$\text{LHMKABO2} \rightarrow 0.06 \text{CO2H3CHO} + 0.18 \text{HO}_2 + 0.18 \text{HCHO} + 0.18 \text{MGLYOX} + 0.42 \text{CH}_3\text{C}(\text{O})\text{OO} + 0.42 \text{HOCH}_2\text{CHO} + 0.2 \text{HO12CO3C4} + 0.14 \text{BIACETOH}$	$(.3 * 2.00\text{E-}12 + 0.7 * 8.80\text{E-}13) * \text{R02}$	Rickard and Pascoe (2009)*
G4438	TrGC	$\text{LHMKABO2} + \text{HO}_2 \rightarrow \text{LHMKABOOH}$	$\text{KR02H02} * 0.625$	Rickard and Pascoe (2009)
G4439	TrGNC	$\text{LHMKABO2} + \text{NO} \rightarrow 0.3 \text{MGLYOX} + 0.7 \text{HOCH}_2\text{CHO} + 0.7 \text{CH}_3\text{C}(\text{O})\text{OO} + 0.3 \text{HCHO} + 0.3 \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G4440	TrGNC	$\text{LHMKABO2} + \text{NO}_3 \rightarrow 0.3 \text{MGLYOX} + 0.7 \text{HOCH}_2\text{CHO} + 0.7 \text{CH}_3\text{C}(\text{O})\text{OO} + 0.3 \text{HCHO} + 0.3 \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G4441	TrGC	$\text{LHMKABOOH} + \text{OH} \rightarrow 0.3 \text{CO2H3CHO} + 0.7 \text{BIACETOH} + \text{OH}$	$4.496\text{E-}11$	Rickard and Pascoe (2009)*
G4442	TrGC	$\text{MVKOH} + \text{OH} \rightarrow \text{LMVKOHABO2}$	$4.60\text{E-}12 * \text{EXP}(452./\text{temp})$	Rickard and Pascoe (2009)
G4443	TrGC	$\text{MVKOH} + \text{O}_3 \rightarrow 0.56 \text{CO} + 0.545 \text{HOCH}_2\text{COCHO} + 0.075 \text{HOCH}_2\text{COCO2H} + 0.075 \text{HCOOH} + 0.09 \text{H}_2\text{O}_2 + 0.28 \text{HOCH}_2\text{CO}_3 + 0.28 \text{HO}_2 + 0.2 \text{CO}_2 + 0.545 \text{HCHO} + 0.36 \text{OH} + 0.1 \text{HOCH}_2\text{CHO}$	$7.51\text{E-}16 * \text{EXP}(-1521./\text{temp})$	Rickard and Pascoe (2009)
G4444	TrGC	$\text{LMVKOHABO2} \rightarrow 0.7 \text{HOCH}_2\text{CHO} + 0.7 \text{HOCH}_2\text{CO}_3 + 0.3 \text{HOCH}_2\text{COCHO} + 0.3 \text{HCHO} + 0.3 \text{HO}_2$	$(0.3 * 2.00\text{E-}12 + 0.7 * 8.80\text{E-}13) * \text{R02}$	Rickard and Pascoe (2009)*
G4445	TrGC	$\text{LMVKOHABO2} + \text{HO}_2 \rightarrow \text{LMVKOHABOOH}$	$\text{KR02H02} * 0.625$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4446	TrGNC	LMVKOHABO2 + NO $\rightarrow$ 0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO ₂ + 0.7 HOCH ₂ CHO + 0.7 HOCH ₂ CO ₃ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G4447	TrGNC	LMVKOHABO2 + NO ₃ $\rightarrow$ 0.3 HOCH2COCHO + 0.3 HCHO + 0.3 HO ₂ + 0.7 HOCH ₂ CHO + 0.7 HOCH ₂ CO ₃ + NO ₂	KR02NO3	Rickard and Pascoe (2009)*
G4448	TrGC	LMVKOHABOOH + OH $\rightarrow$ 0.7 HO12CO3C4 + 0.3 CO2H3CHO + OH	5.98E-11	Rickard and Pascoe (2009)*
G4449	TrGC	CO2H3CHO + OH $\rightarrow$ CO2H3CO3	2.45E-11	Rickard and Pascoe (2009)
G4450	TrGNC	CO2H3CHO + NO ₃ $\rightarrow$ CO2H3CO3 + HNO ₃	KN03AL*4.0	Rickard and Pascoe (2009)
G4451	TrGC	CO2H3CO3 $\rightarrow$ MGLYOX + HO ₂ + CO ₂	1.00E-11*R02	Rickard and Pascoe (2009)
G4452	TrGC	CO2H3CO3 + HO ₂ $\rightarrow$ CO2H3CO3H	KAPH02	Rickard and Pascoe (2009)
G4453	TrGNC	CO2H3CO3 + NO $\rightarrow$ MGLYOX + HO ₂ + NO ₂ + CO ₂	KAPNO	Rickard and Pascoe (2009)
G4454	TrGNC	CO2H3CO3 + NO ₃ $\rightarrow$ MGLYOX + HO ₂ + NO ₂ + CO ₂	KR02NO3*1.60	Rickard and Pascoe (2009)
G4455	TrGC	CO2H3CO3H + OH $\rightarrow$ CO2H3CO3	7.34E-12	Rickard and Pascoe (2009)
G4456	TrGC	HO12CO3C4 + OH $\rightarrow$ BIACETOH + HO ₂	1.88E-11	Rickard and Pascoe (2009)
G4500	TrGC	C ₅ H ₈ + O ₃ $\rightarrow$ 0.051 CH ₃ O ₂ + 0.1575 CH ₃ C(O)OO + 0.054 LHMVKABO2 + 0.522 CO + 0.06875 HCOOH + 0.11 H ₂ O ₂ + 0.32475 MACR + 0.1275 C ₃ H ₆ + 0.2625 HO ₂ + 0.255 CO ₂ + 0.74975 HCHO + 0.04125 MACO2H + 0.27 OH + 0.244 MVK	7.86E-15*EXP(-1913./temp)	Rickard and Pascoe (2009)
G4501	TrGC	C ₅ H ₈ + OH $\rightarrow$ 0.25 LISOPACO2 + 0.491 ISOPBO2 + 0.259 ISOPDO2	2.54E-11*EXP(410./temp)	Atkinson (1997)
G4509	TrGNC	C ₅ H ₈ + NO ₃ $\rightarrow$ NISOPO2	3.03E-12*EXP(-446./temp)	Rickard and Pascoe (2009)
G4510	TrGC	LISOPACO2 $\rightarrow$ 0.9 LHC4ACCHO + 0.8 HO ₂ + 0.1 ISOPA0H	2.4E-12*R02	Rickard and Pascoe (2009)
G4511	TrGC	LISOPACO2 + HO ₂ $\rightarrow$ LISOPACOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4512	TrGNC	LISOPACO2 + NO $\rightarrow$ 0.892 LHC4ACCHO + 0.892 HO ₂ + 0.892 NO ₂ + 0.108 LISOPACNO3	KR02NO	Rickard and Pascoe (2009)
G4513	TrGNC	LISOPACO2 + NO ₃ $\rightarrow$ LHC4ACCHO + HO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G4514	TrGC	LISOPACOOH + OH $\rightarrow$ LHC4ACCHO + OH	1.07E-10	Rickard and Pascoe (2009)
G4515	TrGC	ISOPA0H + OH $\rightarrow$ LHC4ACCHO + HO ₂	9.30E-11	Rickard and Pascoe (2009)
G4516	TrGNC	LISOPACNO3 + OH $\rightarrow$ LHC4ACCHO + NO ₂	8.91E-11	Rickard and Pascoe (2009)
G4517	TrGC	ISOPBO2 $\rightarrow$ 0.6 MVK + 0.2 MVKOH + 0.6 HCHO + 0.6 HO ₂ + 0.2 CH ₃ O ₂ + 0.2 ISOPBOH	8.E-13*R02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4518	TrGC	ISOPBO2 + HO ₂ → ISOPBOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4519	TrGNC	ISOPBO2 + NO → 0.696 MVK + 0.232 MVKOH + 0.696 HCHO + 0.696 HO ₂ + 0.232 CH ₃ O ₂ + 0.928 NO ₂ + 0.072 ISOPBNO3	KR02NO	Rickard and Pascoe (2009)
G4520	TrGNC	ISOPBO2 + NO ₃ → 0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO ₂ + 0.25 CH ₃ O ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G4521	TrGC	ISOPBOOH + OH → ISOPBO2	4.2E-11	Rickard and Pascoe (2009)
G4522	TrGC	ISOPBOH + OH → 0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO ₂ + 0.25 CH ₃ O ₂	3.85E-11	Rickard and Pascoe (2009)
G4523	TrGNC	ISOPBNO3 + OH → MVK + HCHO + NO ₂	3.55E-11	Rickard and Pascoe (2009)
G4524	TrGC	ISOPDO2 → 0.8 MACR + 0.8 HCHO + 0.8 HO ₂ + 0.1 HCOC5 + 0.1 ISOPDOH	2.9E-12*R02	Rickard and Pascoe (2009)
G4525	TrGC	ISOPDO2 + HO ₂ → ISOPDOOH	0.706*KR02H02	Rickard and Pascoe (2009)
G4526	TrGNC	ISOPDO2 + NO → 0.855 MACR + 0.855 HCHO + 0.855 HO ₂ + 0.855 NO ₂ + 0.145 ISOPDNO3	KR02NO	Rickard and Pascoe (2009)
G4527	TrGNC	ISOPDO2 + NO ₃ → MACR + HCHO + HO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G4528	TrGC	ISOPDOOH + OH → HCOC5 + OH	1.07E-10	Rickard and Pascoe (2009)
G4529	TrGC	ISOPDOH + OH → HCOC5 + HO ₂	7.38E-11	Rickard and Pascoe (2009)
G4530	TrGNC	ISOPDNO3 + OH → HCOC5 + NO ₂	6.1E-11	Rickard and Pascoe (2009)
G4531	TrGNC	NISOP02 → 0.8 NC4CHO + 0.6 HO ₂ + 0.2 LISOPACNO3	1.3E-12*R02	Rickard and Pascoe (2009)
G4532	TrGNC	NISOP02 + HO ₂ → NISOP0OH	.706*KR02H02	Rickard and Pascoe (2009)
G4533	TrGNC	NISOP02 + NO → NC4CHO + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)
G4534	TrGNC	NISOP02 + NO ₃ → NC4CHO + HO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G4535	TrGNC	NISOP0OH + 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 ₃ → 0.445 NO ₂ + 0.89 CO + 0.075625 H ₂ O ₂ + 0.034375 HCOCO ₂ H + 0.555 NOA + 0.445 HO ₂ + 0.520625 GLYOX + 0.89 OH + 0.445 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
G4538	TrGNC	NC4CHO + NO ₃ → LNISO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G4539	TrGNC	LNISO3 + HO ₂ → LNISOOH	.5*.706*KR02H02 + 0.5*KAPH02	Rickard and Pascoe (2009)
G4540	TrGNC	LNISO3 + NO → NOA + 0.5 GLYOX + 0.5 CO + HO ₂ + NO ₂ + 0.5 CO ₂	0.5*KAPNO +0.5*KR02NO	Rickard and Pascoe (2009)
G4541	TrGNC	LNISO3 + NO ₃ → NOA + 0.5 GLYOX + 0.5 CO + HO ₂ + NO ₂ + 0.5 CO ₂	1.3*KR02NO3	Rickard and Pascoe (2009)
G4542	TrGNC	LNISOOH + OH → LNISO3	2.65E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4543	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow 0.52 \text{ LC578O2} + 0.48 \text{ LHC4ACCO3}$	$4.52\text{E-}11$	Rickard and Pascoe (2009)
G4544	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow 0.2225 \text{ CH}_3\text{C(O)OO} + 0.89 \text{ CO} + 0.0171875 \text{ HOCH}_2\text{CO}_2\text{H} + 0.075625 \text{ H}_2\text{O}_2 + 0.0171875 \text{ HCOCO}_2\text{H} + 0.2775 \text{ CH}_3\text{COCH}_2\text{OH} + 0.6675 \text{ HO}_2 + 0.2603125 \text{ GLYOX} + 0.2225 \text{ HCHO} + 0.89 \text{ OH} + 0.2603125 \text{ HOCH}_2\text{CHO} + 0.5 \text{ MGLYOX}$	$2.40\text{E-}17$	Rickard and Pascoe (2009)
G4545	TrGNC	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO3} + \text{HNO}_3$	KN03AL*4.25	Rickard and Pascoe (2009)
G4546	TrGC	$\text{LC578O2} \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ MGLYOX} + 0.5 \text{ GLYOX} + 0.5 \text{ HOCH}_2\text{CHO} + \text{HO}_2$	$9.20\text{E-}14*\text{R02}$	Rickard and Pascoe (2009)
G4547	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{LC578OOH}$	KR02H02*0.706	Rickard and Pascoe (2009)
G4548	TrGNC	$\text{LC578O2} + \text{NO} \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ MGLYOX} + 0.5 \text{ GLYOX} + 0.5 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G4549	TrGNC	$\text{LC578O2} + \text{NO}_3 \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ MGLYOX} + 0.5 \text{ GLYOX} + 0.5 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4550	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	$3.16\text{E-}11$	Rickard and Pascoe (2009)
G4551	TrGC	$\text{LHC4ACCO3} \rightarrow 0.3 \text{ LHC4ACCO2H} + 0.35 \text{ CH}_3\text{COCH}_2\text{OH} + 0.35 \text{ HOCH}_2\text{CHO} + 0.35 \text{ CH}_3\text{C(O)OO} + 0.35 \text{ CO} + 0.35 \text{ HO}_2 + 0.7 \text{ CO}_2$	$1.00\text{E-}11*\text{R02}$	Rickard and Pascoe (2009)
G4552	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 0.71 \text{ LHC4ACCO3H} + 0.29 \text{ LHC4ACCO2H} + 0.29 \text{ O}_3$	KAPH02	Rickard and Pascoe (2009)
G4553	TrGNC	$\text{LHC4ACCO3} + \text{NO} \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ HOCH}_2\text{CHO} + 0.5 \text{ CH}_3\text{C(O)OO} + 0.5 \text{ CO} + 0.5 \text{ HO}_2 + \text{NO}_2 + \text{CO}_2$	KAPN0	Rickard and Pascoe (2009)
G4554	TrGNC	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G4555	TrGNC	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ HOCH}_2\text{CHO} + 0.5 \text{ CH}_3\text{C(O)OO} + 0.5 \text{ CO} + 0.5 \text{ HO}_2 + \text{NO}_2 + \text{CO}_2$	$1.6*\text{KR02N03}$	Rickard and Pascoe (2009)
G4556	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ HOCH}_2\text{CHO} + 0.5 \text{ CH}_3\text{C(O)OO} + 0.5 \text{ CO} + 0.5 \text{ HO}_2 + \text{CO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)
G4557	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$2.88\text{E-}11$	Rickard and Pascoe (2009)
G4558	TrGNC	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G4559	TrGNC	$\text{LC5PAN1719} + \text{OH} \rightarrow 0.5 \text{ MACROH} + 0.5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4560	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	$3.81\text{E-}11$	Rickard and Pascoe (2009)
G4561	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3$	$9.20\text{E-}14*\text{R02}$	Rickard and Pascoe (2009)
G4562	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	$\text{KR02H02}*0.706$	Rickard and Pascoe (2009)
G4563	TrGNC	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G4564	TrGNC	$\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4565	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	$9.7\text{E-}12$	Rickard and Pascoe (2009)
G6100	StTrGCl	$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	$2.8\text{E-}11*\text{EXP}(-250./\text{temp})$	Atkinson et al. (2007)
G6102a	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$	$1.0\text{E-}12*\text{EXP}(-1590./\text{temp})$	Atkinson et al. (2007)
G6102b	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow 2 \text{Cl} + \text{O}_2$	$3.0\text{E-}11*\text{EXP}(-2450./\text{temp})$	Atkinson et al. (2007)
G6102c	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl} + \text{OClO}$	$3.5\text{E-}13*\text{EXP}(-1370./\text{temp})$	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	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	$\text{k_ClO_ClO}/(9.3\text{E-}28*\text{EXP}(8835./\text{temp}))$	Atkinson et al. (2007), Sander et al. (2006)*
G6202	StTrGCl	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	$1.1\text{E-}11*\text{EXP}(-980./\text{temp})$	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	$2.2\text{E-}12*\text{EXP}(340./\text{temp})$	Atkinson et al. (2007)
G6205	StTrGCl	$\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$	$1.7\text{E-}12*\text{EXP}(-230./\text{temp})$	Atkinson et al. (2007)
G6300	StTrGNCl	$\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$	$6.2\text{E-}12*\text{EXP}(295./\text{temp})$	Atkinson et al. (2007)
G6301	StTrGNCl	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 1.6\text{E-}31, 3.4, 7\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G6302	TrGCl	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	$6.918\text{E-}7*\text{exp}(-10909./\text{temp})*\text{cair}$	Anderson and Fahey (1990)
G6304	StTrGNCl	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	$6.2\text{E-}12*\text{EXP}(145./\text{temp})$	Atkinson et al. (2007)
G6400	StTrGCl	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\text{O}_2$	$6.6\text{E-}12*\text{EXP}(-1240./\text{temp})$	Atkinson et al. (2006)
G6401	StTrGCl	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$	$8.1\text{E-}11*\text{EXP}(-34./\text{temp})$	Atkinson et al. (2006)
G6402	StTrGCl	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{HCl} + \text{OH}$	$5.9\text{E-}11$	Atkinson et al. (2006)*
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$3.3\text{E-}12*\text{EXP}(-115./\text{temp})$	Sander et al. (2006)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Sander et al. (2006)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C(O)OO}$	$8.0\text{e-}11$	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 6.1\text{e-}30, 3.0, 2.0\text{e-}10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$8.3\text{E-}11*\text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E-}11*\text{EXP}(-800./\text{temp})$	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	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14*\text{EXP}(840./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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)
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	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO_NO2}} / (5.44\text{E-}9 \cdot \exp(14192./\text{temp}) \cdot 1.\text{E6} \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm2Pa} \cdot N_{\text{A}}))$	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)*
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	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	$3.32\text{E-}15$	Manion et al. (2010)
G7601	TrGClBr	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	$1.10\text{E-}15$	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	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	$1.45\text{E-}11$	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)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.3\text{E-}31, 4.3, 1.6\text{E-}12, 0., 0.6)$	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	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	$k_{\text{DMS_OH}}$	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)

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

#	labels	reaction	rate coefficient	reference
G9402	TrGS	DMSO + OH $\rightarrow$ 0.6 SO ₂ + HCHO + 0.6 CH ₃ O ₂ + 0.4 HO ₂ + 0.4 CH ₃ SO ₃ H	1.E-10	Hynes and Wine (1996)
G9403	TrGS	CH ₃ SO ₂ $\rightarrow$ SO ₂ + CH ₃ O ₂	1.8E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	CH ₃ SO ₂ + O ₃ $\rightarrow$ CH ₃ SO ₃	3.E-13	Barone et al. (1995)
G9405	TrGS	CH ₃ SO ₃ + HO ₂ $\rightarrow$ CH ₃ SO ₃ H	5.E-11	Barone et al. (1995)
G9600	TrGSCl	DMS + Cl $\rightarrow$ CH ₃ SO ₂ + HCl + HCHO	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	DMS + Br $\rightarrow$ CH ₃ SO ₂ + HBr + HCHO	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	DMS + BrO $\rightarrow$ DMSO + Br	4.4E-13	Ingham et al. (1999)

*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_{ratio} , `k_3rd` is defined as:

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

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

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

$$\text{k_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right)} \quad (4)$$

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:

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

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

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

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

$$\text{k_3rd_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right)} \quad (9)$$

G2110: The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_`

H20)). 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_N03_N02 = 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_N02_H02 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

G3206: The rate coefficient is: `k_HN03_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 CH₃CHO+NO₃.

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

G4206: The product C₂H₅OH, which reacts only with OH, is substituted by its degradation products ≈ 0.1 HOCH₂CH₂O₂ + 0.9 CH₃CHO + 0.9 HO₂.

G4207: The rate constant $8.01\text{E-}12$ is for the H abstraction in alpha to the -OOH group (Rickard and Pascoe, 2009) and $0.6 \times \text{k_CH300H_OH}$ is for the C₂H₅O₂ 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 CH₃O₂ channel in G4107 (CH₃OOH+OH).

G4221: The rate coefficient `isk_PAN_M = k_CH3C03_N02/9.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 HOCH₂CH₂O in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + HO₂.

G4300: The product NC3H7O2 is substituted with its degradation products C₂H₅O₂ + CO₂ + HO₂.

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

G4304: The value for the generic RO₂ + HO₂ reaction from Atkinson (1997) is used here.

G4306: The MCM (Rickard and Pascoe, 2009) products are 0.2 IPROPOL + 0.2 CH₃COCH₃ + 0.6 IC3H7O. IPROPOL and IC3H7O are substituted with their degradation products. We assume IPROPOL to be oxidized entirely to CH₃COCH₃ + HO₂ by OH. IC3H7O + O₂ produces the same products.

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

G4400: LC₄H₉O₂ represents 0.127 NC4H9O2 + 0.873 SC4H9O2.

G4401: NC4H9O and SC4H9O are substituted with 2 CO₂ + C₂H₅O₂ and 0.636 MEK + HO₂ and 0.364 CH₃CHO + C₂H₅O₂, 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 NC4H9O2 and 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 NC4H9O2 and 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 RO₂ are given the rate coefficient $0.6 \cdot k_{\text{CH300H_OH}}$ as for G4107. For NC4H9OOH the products are $0.327 \text{ NC4H9O2} + 0.673 \text{ C3H7CHO} + 0.673 \text{ OH}$. C3H7CHO is then substituted with $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2$. Hence, $0.327 \text{ NC4H9O2} + 1.346 \text{ CO}_2 + 0.673 \text{ C}_2\text{H}_5\text{O}_2 + 0.673 \text{ OH}$. For SC4H9OOH the products are $0.219 \text{ SC4H9O2} + 0.781 \text{ MEK} + 0.781 \text{ OH}$.

G4413: LMEKO2 represents $0.459 \text{ MEKAO2} + 0.462 \text{ MEKBO2} + 0.079 \text{ MEKCO2}$.

G4415: Alkyl nitrate formation is neglected. The products of MEKAO and MEKCO are substituted with $\text{HCHO} + \text{CO}_2 + \text{HOCH}_2\text{CH}_2\text{O}_2$ and $\text{HCHO} + \text{CO}_2 + \text{C}_2\text{H}_5\text{O}_2$.

G4416: LMEKOOH is assumed having the composition $0.459 \text{ MEKAOOH} + 0.462 \text{ MEKBOOH} + 0.079 \text{ MEKCOOH}$. MEKAOOH + OH gives $0.89 \text{ CO2C3CHO} + 0.89 \text{ OH} + 0.11 \text{ MEKAO2} + \text{H}_2\text{O}$. CO2C3CHO is substituted with $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$ and the products become $0.89 \text{ CH}_3\text{COCH}_2\text{O}_2 + 0.89 \text{ CO}_2 + 0.89 \text{ OH} + 0.11 \text{ MEKAO2} + \text{H}_2\text{O}$. MEKBOOH + OH gives $0.758 \text{ BIACET} + 0.758 \text{ OH} + 0.242 \text{ MEKBO2} + \text{H}_2\text{O}$. MEKCOOH + OH gives $0.614 \text{ EGLYOX} + 0.614 \text{ OH} + 0.386 \text{ MEKCO2} + \text{H}_2\text{O}$. EGLYOX is substituted with $\text{C}_2\text{H}_5\text{O}_2 + 2 \text{ CO}_2$ and the products become $0.614 \text{ C}_2\text{H}_5\text{O}_2 + 1.228 \text{ CO}_2 + 0.614 \text{ OH} + 0.386 \text{ MEKCO2} + \text{H}_2\text{O}$.

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 + NO₂ + H₂O with

C3H7CHO being substituted with $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2$. After substitution is obtained $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 + \text{H}_2\text{O}$. SC4H9NO3 + OH gives MEK + NO₂ + H₂O 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 $0.3 \text{ HMMVKAO2} + 0.7 \text{ HMMVKBO2}$. 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 $0.3 \text{ HMMVKAO} + 0.7 \text{ HMMVKBO}$.

G4440: as for G4439

G4441: The rate coefficient and products are 30% for HMMVKAOOH and 70% for HMMVKBOOH.

G4444: LMKOHABO2 is a lumped species of virtual composition $0.3 \text{ MVMKOHAO2} + 0.7 \text{ MVMKOHBO2}$. 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 $0.3 \text{ MVMKOHAO} + 0.7 \text{ MVMKOHBO}$.

G4447: as for G4446

G4448: The rate coefficient and products are 30% for MVMKOHAOOH and 70% for MVMKOHBOOH.

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

G6402: The initial products are probably HCl and CH₂OOH (Atkinson et al., 2006). It is assumed that CH₂OOH dissociates into HCHO and OH.

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

G7302: The rate coefficient is: $k_{\text{BrO_NO2}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 5.2\text{E-}31, 3.2, 6.9\text{E-}12, 2.9, 0.6)$.

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: CH₂Br₂+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: CH₂Br₂+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.

G9400: Addition path. The rate coefficient is: $k_{\text{DMS_OH}} = 1.0\text{E-}39 \cdot \text{EXP}(5820./\text{temp}) \cdot \text{C}(\text{ind_02}) / (1. + 5.0\text{E-}30 \cdot \text{EXP}(6280./\text{temp}) \cdot \text{C}(\text{ind_02}))$.

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
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H2O2)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO2O)	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_N2O5)	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_HNO3)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow 0.667 NO_2 + 0.667 HO_2 + 0.333 NO_3 + 0.333 OH$	jx(ip_HNO4)	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
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)*
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3CO3H)	see note
J4204	TrGNJCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	see note
J4205	TrGCJ	$HOCH_2CHO + h\nu \rightarrow HO_2 + HCHO + HO_2 + CO$	jx(ip_HOCH2CHO)	see note
J4206	TrGCJ	$HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4207	TrGCJ	$PHAN + h\nu \rightarrow HOCH_2CO_3 + NO_2$	jx(ip_PAN)	see note
J4208	TrGCJ	$GLYOX + h\nu \rightarrow 2 CO + 2 HO_2$	jx(ip_GLYOX)	see note
J4209	TrGNJCJ	$HCOCO_2H + h\nu \rightarrow 2 HO_2 + CO + CO_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)*
J4210	TrGNJCJ	$HCOCO_3H + h\nu \rightarrow HO_2 + CO + OH + CO_2$	(jx(ip_CH300H)+jx(ip_HOCH2CHO))	Rickard and Pascoe (2009)*
J4211	TrGCJ	$HYETHO_2H + h\nu \rightarrow HOCH_2CH_2O + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4212	TrGCJ	$ETHOHNO_3 + h\nu \rightarrow HO_2 + 2 HCHO + NO_2$	J_IC3H7N03	see note
J4300	TrGCJ	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)*
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	see note
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	J_ACETOL	see note
J4303	TrGCJ	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4304	TrGCJ	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	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	$\text{NOA} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2$	$\text{J_IC3H7N03} + \text{jx}(\text{ip_CH3COCH3})$	see note
J4308	TrGCJ	$\text{HOCH}_2\text{COCO}_2\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)*
J4309	TrGCJ	$\text{HYPROPO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J4310	TrGNCJ	$\text{PR}_2\text{O}_2\text{HNO}_3 + h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J4311	TrGCJ	$\text{HOCH}_2\text{COCHO} + h\nu \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)*
J4400	TrGCJ	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + 0.254 \text{ CO}_2 + 0.5552 \text{ MEK} + 0.5552 \text{ HO}_2 + 0.3178 \text{ CH}_3\text{CHO} + 0.4448 \text{ C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J4401	TrGCJ	$\text{MVK} + h\nu \rightarrow 0.5 \text{ C}_3\text{H}_6 + 0.5 \text{ CH}_3\text{C}(\text{O})\text{OO} + 0.5 \text{ HCHO} + \text{CO} + 0.5 \text{ HO}_2$	$\text{jx}(\text{ip_MVK})$	see note
J4403	TrGCJ	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2$	$0.42 * \text{jx}(\text{ip_CHOH})$	von Kuhlmann et al. (2003)*
J4404	TrGCJ	$\text{LMEKOOH} + h\nu \rightarrow 0.538 \text{ HCHO} + 0.538 \text{ CO}_2 + 0.459 \text{ HOCH}_2\text{CH}_2\text{O}_2 + 0.079 \text{ C}_2\text{H}_5\text{O}_2 + 0.462 \text{ CH}_3\text{C}(\text{O})\text{OO} + 0.462 \text{ CH}_3\text{CHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J4405	TrGCJ	$\text{BIACET} + h\nu \rightarrow 2 \text{ CH}_3\text{C}(\text{O})\text{OO}$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	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	$\text{MPAN} + h\nu \rightarrow \text{MACO}_3 + \text{NO}_2$	$\text{jx}(\text{ip_PAN})$	see note
J4408	TrGCJ	$\text{LMVKOHABOOH} + h\nu \rightarrow 0.3 \text{ HOCH}_2\text{COCHO} + 0.3 \text{ HCHO} + 0.3 \text{ HO}_2 + 0.7 \text{ HOCH}_2\text{CHO} + 0.7 \text{ HOCH}_2\text{CO}_3 + \text{OH}$	$\text{J_ACETOL} + \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
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 and Pascoe (2009)*
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 and Pascoe (2009)*
J4411	TrGCJ	$\text{MACR} + h\nu \rightarrow 0.5 \text{ MACO}_3 + 0.5 \text{ CH}_3\text{C}(\text{O})\text{OO} + 0.5 \text{ HCHO} + 0.5 \text{ CO} + \text{HO}_2$	$\text{jx}(\text{ip_MACR})$	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference		
J4412	TrGCJ	MACROOH + $h\nu$ → CH ₃ COCH ₂ OH + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4413	TrGCJ	MACROOH + $h\nu$ → CH ₃ COCH ₂ OH + CO + HO ₂ + OH	2.77*jx(ip_H0CH2CH0)	see note		
J4414	TrGCJ	MACROH + $h\nu$ → CH ₃ COCH ₂ OH + CO + HO ₂ + HO ₂	2.77*jx(ip_H0CH2CH0)	see note		
J4415	TrGCJ	MACO3H + $h\nu$ → CH ₃ C(O)OO + HCHO + OH + CO ₂	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4416	TrGCJ	LHMKABOOH + $h\nu$ → 0.3 MGLYOX + 0.7 CH ₃ C(O)OO + 0.7 HOCH ₂ CHO + 0.3 HCHO + 0.3 HO ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4417	TrGCJ	MVKOH + $h\nu$ → 0.5 HCHO + 0.5 HO ₂ + 0.5 HOCH ₂ CO ₃ + CO + 1.5 LCARBON	jx(ip_MVK)	Rickard (2009)*	and	Pascoe
J4418	TrGCJ	CO2H3CHO + $h\nu$ → MGLYOX + CO + HO ₂ + HO ₂	jx(ip_H0CH2CH0)	Rickard (2009)*	and	Pascoe
J4419	TrGCJ	HO12CO3C4 + $h\nu$ → CH ₃ C(O)OO + HOCH ₂ CHO + HO ₂	J_ACETOL	Rickard (2009)*	and	Pascoe
J4420	TrGCJ	BIACETOH + $h\nu$ → CH ₃ C(O)OO + HOCH ₂ CO ₃	2.15*jx(ip_MGLYOX)	see note		
J4502	TrGCJ	LISOPACOOH + $h\nu$ → LHC4ACCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4503	TrGNCJ	LISOPACNO3 + $h\nu$ → LHC4ACCHO + HO ₂ + NO ₂	0.59*J_IC3H7N03	see note		
J4504	TrGCJ	ISOPBOOH + $h\nu$ → 0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO ₂ + 0.25 CH ₃ O ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4505	TrGNCJ	ISOPBNO3 + $h\nu$ → 0.75 MVK + 0.25 MVKOH + 0.75 HCHO + 0.75 HO ₂ + 0.25 CH ₃ O ₂ + NO ₂	2.84*J_IC3H7N03	see note		
J4506	TrGCJ	ISOPDOOH + $h\nu$ → MACR + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4507	TrGNCJ	ISOPDNO3 + $h\nu$ → MACR + HCHO + HO ₂ + NO ₂	J_IC3H7N03	see note		
J4508	TrGNCJ	NISOPOOH + $h\nu$ → NC4CHO + HO ₂ + OH	jx(ip_CH300H)	Rickard (2009)*	and	Pascoe
J4509	TrGNCJ	NC4CHO + $h\nu$ → NOA + 2 CO + 2 HO ₂	jx(ip_MACR)	see note		
J4510	TrGNCJ	LNISOOH + $h\nu$ → NOA + OH + 0.5 GLYOX + 0.5 CO + HO ₂ + 0.5 CO ₂	jx(ip_CH300H)	Taraborrelli et al. (2009)*		
J4511	TrGCJ	LHC4ACCHO + $h\nu$ → 0.5 LHC4ACCO3 + 0.25 CH ₃ COCH ₂ OH + 0.25 HOCH ₂ CHO + 0.25 CH ₃ C(O)OO + 0.75 CO + 1.25 HO ₂	jx(ip_MACR)	Rickard (2009)*	and	Pascoe
J4512	TrGCJ	LC578OOH + $h\nu$ → 0.5 CH ₃ COCH ₂ OH + 0.5 MGLYOX + 0.5 GLYOX + 0.5 HOCH ₂ CHO + HO ₂ + OH	jx(ip_CH300H)	Taraborrelli et al. (2009)*		

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4513	TrGCJ	$\text{LHC4ACCO3H} + h\nu \rightarrow 0.5 \text{ CH}_3\text{COCH}_2\text{OH} + 0.5 \text{ HOCH}_2\text{CHO} + 0.5 \text{ CH}_3\text{C(O)OO} + 0.5 \text{ CO} + 0.5 \text{ HO}_2 + \text{OH} + \text{CO}_2$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4514	TrGN CJ	$\text{LC5PAN1719} + h\nu \rightarrow 0.5 \text{ MACROH} + 0.5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	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	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	jx(ip_Cl2)	see note
J6100	StTrGClJ	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2 \text{ Cl}$	$1.4 * \text{jx(ip_Cl202)}$	see note
J6101	StTrGClJ	$\text{OClO} + h\nu \rightarrow \text{ClO} + \text{O}(^3\text{P})$	jx(ip_OClO)	see note
J6201	StTrGClJ	$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$	jx(ip_HOCl)	see note
J6300	TrGNClJ	$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$	jx(ip_ClNO2)	see note
J6301a	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	jx(ip_ClNO3)	see note
J6301b	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	jx(ip_ClON02)	see note
J7000	StTrGBrJ	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	jx(ip_Br2)	see note
J7100	StTrGBrJ	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	jx(ip_BrO)	see note
J7200	StTrGBrJ	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	jx(ip_HOBr)	see note
J7300	TrGNBrJ	$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$	jx(ip_BrNO2)	see note
J7301	StTrGNBrJ	$\text{BrNO}_3 + h\nu \rightarrow 0.29 \text{ Br} + 0.29 \text{ NO}_3 + 0.71 \text{ BrO} + 0.71 \text{ NO}_2$	jx(ip_BrNO3)	see note
J7401	TrGBrJ	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2 \text{ Br}$	jx(ip_CH2Br2)	see note
J7402	TrGBrJ	$\text{CHBr}_3 + h\nu \rightarrow 3 \text{ Br}$	jx(ip_CHBr3)	see note
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_BrCl)	see note
J7602	TrGClBrJ	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_CH2ClBr)	see note
J7603	TrGClBrJ	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{Br} + 2 \text{ Cl}$	jx(ip_CHCl2Br)	see note
J7604	TrGClBrJ	$\text{CHClBr}_2 + h\nu \rightarrow 2 \text{ Br} + \text{Cl}$	jx(ip_CHClBr2)	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:

$\text{J(11)} \rightarrow \text{jx(ip_COH2)}$

$\text{J(12)} \rightarrow \text{jx(ip_CHOH)}$

$\text{J(15)} \rightarrow \text{jx(ip_HOCH2CHO)}$

$\text{J(18)} \rightarrow \text{jx(ip_MACR)}$

$\text{J(22)} \rightarrow \text{jx(ip_ACETOL)}$

$\text{J(23)+J(24)} \rightarrow \text{jx(ip_MVK)}$

$\text{J(31)+J(32)+J(33)} \rightarrow \text{jx(ip_GLYOX)}$

$\text{J(34)} \rightarrow \text{jx(ip_MGLYOX)}$

$\text{J(41)} \rightarrow \text{jx(ip_CH300H)}$

$\text{J(53)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$

$\text{J(54)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$

$\text{J(55)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$

$\text{J(56)+J(57)} \rightarrow \text{jx(ip_NOA)}$

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

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

J4302: Following von Kuhlmann et al. (2003), we use $J(\text{CH}_3\text{COCH}_2\text{OH}) = 0.11 * jx(ip_CHOH)$. 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 $J(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7 * jx(ip_PAN)$.

J4307: NOA contains the chromophores of both CH_3COCH_3 and a nitrate group. It is assumed here that the J values are additive, i.e.: $J(\text{NOA}) = J(\text{CH}_3\text{COCH}_3) + J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J4406: It is assumed that $J(\text{LC4H9NO}_3)$ is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J4407: It is assumed that $J(\text{MPAN})$ is the same as $J(\text{PAN})$.

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

J4413: It is assumed that $J(\text{MACROOH})$ 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).

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 $J(\text{NC4CHO})$ 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 Cl_2O_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 Cl_2O_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 ₂	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O ₃	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^1	4300.	Hanson et al. (1992)
HO ₂	3.9×10^3	5900.	Hanson et al. (1992)
H ₂ O ₂	$1. \times 10^5$	6338.	Lind and Kok (1994)
NH ₃	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO ₂	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO ₃	2.	2000.	Thomas et al. (1993)
N ₂ O ₅	BIG	0.	see note
HONO	4.9×10^1	4780.	Schwartz and White (1981)
HNO ₃	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO ₄	1.2×10^4	6900.	Régimbal and Mozurkewich (1997)
CH ₃ O ₂	6.	5600.	Jacob (1986)*
CH ₃ OOH	3.0×10^2	5322.	Lind and Kok (1994)
CO ₂	3.1×10^{-2}	2423.	Chameides (1984)
HCHO	7.0×10^3	6425.	Chameides (1984)
HCOOH	3.7×10^3	5700.	Chameides (1984)
CH ₃ COOH	4.1×10^3	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
C ₂ H ₅ O ₂	6.	5600.	see note
CH ₃ CHO	1.29×10^1	5890.	Sander et al. (2006)
CH ₃ COCH ₃	28.1	5050.	Sander et al. (2006)
Cl ₂	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^2	5862.	Huthwelker et al. (1995)
ClNO ₃	BIG	0.	see note
Br ₂	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	9.3×10^1	5862.	Vogt et al. (1996)*
BrNO ₃	BIG	0.	see note
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO ₂	1.2	3120.	Chameides (1984)

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

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
H ₂ SO ₄	$1. \times 10^{11}$	0.	see note
CH ₃ SO ₃ H	BIG	0.	see note
DMS	5.4×10^{-1}	3500.	Staudinger and Roberts (2001)
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*

*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:

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

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

NO₂: The temperature dependence is from Chameides (1984).

HNO₃: Calculated using the acidity constant from Davis and de Bruin (1964).

CH₃O₂: This value was estimated by Jacob (1986).

C₂H₅O₂: Assumed to be the same as $K_H(\text{CH}_3\text{O}_2)$.

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

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

H₂SO₄: To account for the very high Henry’s law coefficient of H₂SO₄, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^\ominus$	$-\frac{\Delta_{\text{obs}}H/R}{K}$	reference
O ₂	0.01	2000.	see note
O ₃	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO ₂	0.5	(default)	Thornton and Abbatt (2005)
H ₂ O ₂	0.077	3127.	Worsnop et al. (1989)
NH ₃	0.06	(default)	DeMore et al. (1997)*
NO	5.0×10^{-5}	(default)	Saastad et al. (1993)*
NO ₂	0.0015	(default)	Ponche et al. (1993)*
NO ₃	0.04	(default)	Rudich et al. (1996)*
N ₂ O ₅	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO ₃	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO ₄	(default)	(default)	DeMore et al. (1997)*
CH ₃ O ₂	0.01	2000.	see note
CH ₃ OOH	0.0046	3273.	Magi et al. (1997)
CO ₂	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH ₃ COOH	2.0×10^{-2}	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
C ₂ H ₅ O ₂	(default)	(default)	see note
CH ₃ CHO	3.0×10^{-2}	(default)	see note
CH ₃ COCH ₃	3.72×10^{-3}	6395.	Davidovits et al. (1995)
Cl ₂	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
ClNO ₃	0.108	(default)	Deiber et al. (2004)*
Br ₂	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
BrNO ₃	0.063	(default)	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO ₂	0.11	(default)	DeMore et al. (1997)
H ₂ SO ₄	0.65	(default)	Pöschl et al. (1998)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{\text{K}}$	reference
CH ₃ SO ₃ H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)

*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:

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

O₂: Estimate.

O₃: Value measured at 292 K.

OH: Value measured at 293 K.

NH₃: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO₂: Value measured at 298 K.

NO₃: Value is a lower limit, measured at 273 K.

N₂O₅: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO₃: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO₄: Value measured at 200 K for water ice.

CH₃O₂: Estimate.

CO₂: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

C₂H₅O₂: Estimate.

CH₃CHO: Using the same estimate as in the CAPRAM 2.4 model (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 $\alpha(\text{HOBr})$.

ClNO₃: 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.

BrNO₃: Value measured at 273 K.

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

H₂SO₄: Value measured at 303 K.

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

#	labels	reaction	rate coefficient	reference
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
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
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)*
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
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
H6000f_a01	TrAa01ClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{Cl2})$	see note
H6000b_a01	TrAa01ClMblSc	$Cl_2(aq) \rightarrow Cl_2$	$k_{\text{exb}}(01, \text{ind}_{Cl2})$	see note
H6200f_a01	TrAa01ClMblScScm	$HCl \rightarrow HCl(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCl})$	see note
H6200b_a01	TrAa01ClMblScScm	$HCl(aq) \rightarrow HCl$	$k_{\text{exb}}(01, \text{ind}_{HCl})$	see note
H6201f_a01	TrAa01ClMblSc	$HOCl \rightarrow HOCl(aq)$	$k_{\text{exf}}(01, \text{ind}_{HOCl})$	see note
H6201b_a01	TrAa01ClMblSc	$HOCl(aq) \rightarrow HOCl$	$k_{\text{exb}}(01, \text{ind}_{HOCl})$	see note
H6300_a01	TrAa01ClMblN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	$k_{\text{exf_N2O5}}(01) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a01	TrAa01ClMblN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	$k_{\text{exf_ClNO3}}(01) * C(\text{ind}_{H2O_a01})$	see note
H6302_a01	TrAa01ClMblN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	$k_{\text{exf_ClNO3}}(01) * 5.E2$	see note
H7000f_a01	TrAa01BrMblSc	$Br_2 \rightarrow Br_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{Br2})$	see note
H7000b_a01	TrAa01BrMblSc	$Br_2(aq) \rightarrow Br_2$	$k_{\text{exb}}(01, \text{ind}_{Br2})$	see note
H7200f_a01	TrAa01BrMblScScm	$HBr \rightarrow HBr(aq)$	$k_{\text{exf}}(01, \text{ind}_{HBr})$	see note
H7200b_a01	TrAa01BrMblScScm	$HBr(aq) \rightarrow HBr$	$k_{\text{exb}}(01, \text{ind}_{HBr})$	see note
H7201f_a01	TrAa01BrMblSc	$HOBr \rightarrow HOBr(aq)$	$k_{\text{exf}}(01, \text{ind}_{HOBr})$	see note
H7201b_a01	TrAa01BrMblSc	$HOBr(aq) \rightarrow HOBr$	$k_{\text{exb}}(01, \text{ind}_{HOBr})$	see note
H7300_a01	TrAa01BrMblN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	$k_{\text{exf_N2O5}}(01) * 3.E5$	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a01	TrAa01BrMblN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	$k_{\text{exf_BrNO3}}(01) * C(\text{ind}_{H2O_a01})$	see note
H7302_a01	TrAa01BrMblN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	$k_{\text{exf_BrNO3}}(01) * 3.E5$	see note

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

#	labels	reaction	rate coefficient	reference
H7600f_a01	TrAa01ClBrMblSc	$\text{BrCl} \rightarrow \text{BrCl(aq)}$	$k_{\text{exf}}(01, \text{ind_BrCl})$	see note
H7600b_a01	TrAa01ClBrMblSc	$\text{BrCl(aq)} \rightarrow \text{BrCl}$	$k_{\text{exb}}(01, \text{ind_BrCl})$	see note
H7601_a01	TrAa01ClBrMblN	$\text{ClNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(01) * 3.E5$	see note
H7602_a01	TrAa01ClBrMblN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * 5.E2$	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
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
H1001f_a02	TrAa02MblScScm	$\text{O}_3 \rightarrow \text{O}_3(\text{aq})$	$k_{\text{exf}}(02, \text{ind_O3})$	see note
H1001b_a02	TrAa02MblScScm	$\text{O}_3(\text{aq}) \rightarrow \text{O}_3$	$k_{\text{exb}}(02, \text{ind_O3})$	see note
H2102f_a02	TrAa02MblScScm	$\text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2(\text{aq})$	$k_{\text{exf}}(02, \text{ind_H2O2})$	see note
H2102b_a02	TrAa02MblScScm	$\text{H}_2\text{O}_2(\text{aq}) \rightarrow \text{H}_2\text{O}_2$	$k_{\text{exb}}(02, \text{ind_H2O2})$	see note
H3200f_a02	TrAa02NMblScScm	$\text{NH}_3 \rightarrow \text{NH}_3(\text{aq})$	$k_{\text{exf}}(02, \text{ind_NH3})$	see note
H3200b_a02	TrAa02NMblScScm	$\text{NH}_3(\text{aq}) \rightarrow \text{NH}_3$	$k_{\text{exb}}(02, \text{ind_NH3})$	see note
H3201_a02	TrAa02MblNScScm	$\text{N}_2\text{O}_5 \rightarrow \text{HNO}_3(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf_N2O5}}(02) * \text{C}(\text{ind_H2O_a02})$	Behnke et al. (1994), Behnke et al. (1997)*
H3203f_a02	TrAa02MblNScScm	$\text{HNO}_3 \rightarrow \text{HNO}_3(\text{aq})$	$k_{\text{exf}}(02, \text{ind_HNO3})$	see note
H3203b_a02	TrAa02MblNScScm	$\text{HNO}_3(\text{aq}) \rightarrow \text{HNO}_3$	$k_{\text{exb}}(02, \text{ind_HNO3})$	see note
H4100f_a02	TrAa02MblScScm	$\text{CO}_2 \rightarrow \text{CO}_2(\text{aq})$	$k_{\text{exf}}(02, \text{ind_CO2})$	see note
H4100b_a02	TrAa02MblScScm	$\text{CO}_2(\text{aq}) \rightarrow \text{CO}_2$	$k_{\text{exb}}(02, \text{ind_CO2})$	see note
H6000f_a02	TrAa02ClMblSc	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{aq})$	$k_{\text{exf}}(02, \text{ind_Cl2})$	see note
H6000b_a02	TrAa02ClMblSc	$\text{Cl}_2(\text{aq}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(02, \text{ind_Cl2})$	see note
H6200f_a02	TrAa02ClMblScScm	$\text{HCl} \rightarrow \text{HCl(aq)}$	$k_{\text{exf}}(02, \text{ind_HCl})$	see note
H6200b_a02	TrAa02ClMblScScm	$\text{HCl(aq)} \rightarrow \text{HCl}$	$k_{\text{exb}}(02, \text{ind_HCl})$	see note
H6201f_a02	TrAa02ClMblSc	$\text{HOCl} \rightarrow \text{HOCl(aq)}$	$k_{\text{exf}}(02, \text{ind_HOCl})$	see note
H6201b_a02	TrAa02ClMblSc	$\text{HOCl(aq)} \rightarrow \text{HOCl}$	$k_{\text{exb}}(02, \text{ind_HOCl})$	see note
H6300_a02	TrAa02ClMblN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{aq}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_N2O5}}(02) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a02	TrAa02ClMblN	$\text{ClNO}_3 \rightarrow \text{HOCl(aq)} + \text{HNO}_3(\text{aq})$	$k_{\text{exf_ClNO3}}(02) * \text{C}(\text{ind_H2O_a02})$	see note
H6302_a02	TrAa02ClMblN	$\text{ClNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{Cl}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(02) * 5.E2$	see note
H7000f_a02	TrAa02BrMblSc	$\text{Br}_2 \rightarrow \text{Br}_2(\text{aq})$	$k_{\text{exf}}(02, \text{ind_Br2})$	see note
H7000b_a02	TrAa02BrMblSc	$\text{Br}_2(\text{aq}) \rightarrow \text{Br}_2$	$k_{\text{exb}}(02, \text{ind_Br2})$	see note

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

#	labels	reaction	rate coefficient	reference
H7200f_a02	TrAa02BrMblScScm	$\text{HBr} \rightarrow \text{HBr(aq)}$	$k_{\text{exf}}(\text{O2, ind_HBr})$	see note
H7200b_a02	TrAa02BrMblScScm	$\text{HBr(aq)} \rightarrow \text{HBr}$	$k_{\text{exb}}(\text{O2, ind_HBr})$	see note
H7201f_a02	TrAa02BrMblSc	$\text{HOBr} \rightarrow \text{HOBr(aq)}$	$k_{\text{exf}}(\text{O2, ind_HOBr})$	see note
H7201b_a02	TrAa02BrMblSc	$\text{HOBr(aq)} \rightarrow \text{HOBr}$	$k_{\text{exb}}(\text{O2, ind_HOBr})$	see note
H7300_a02	TrAa02BrMblN	$\text{N}_2\text{O}_5 + \text{Br}^-(\text{aq}) \rightarrow \text{BrNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_N2O5}}(\text{O2}) * 3.\text{E}5$	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a02	TrAa02BrMblN	$\text{BrNO}_3 \rightarrow \text{HOBr(aq)} + \text{HNO}_3(\text{aq})$	$k_{\text{exf_BrNO3}}(\text{O2}) * C(\text{ind_H2O_a02})$	see note
H7302_a02	TrAa02BrMblN	$\text{BrNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{Br}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(\text{O2}) * 3.\text{E}5$	see note
H7600f_a02	TrAa02ClBrMblSc	$\text{BrCl} \rightarrow \text{BrCl(aq)}$	$k_{\text{exf}}(\text{O2, ind_BrCl})$	see note
H7600b_a02	TrAa02ClBrMblSc	$\text{BrCl(aq)} \rightarrow \text{BrCl}$	$k_{\text{exb}}(\text{O2, ind_BrCl})$	see note
H7601_a02	TrAa02ClBrMblN	$\text{ClNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(\text{O2}) * 3.\text{E}5$	see note
H7602_a02	TrAa02ClBrMblN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(\text{O2}) * 5.\text{E}2$	see note
H9100f_a02	TrAa02SMblScScm	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(\text{O2, ind_SO2})$	see note
H9100b_a02	TrAa02SMblScScm	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(\text{O2, ind_SO2})$	see note
H9200_a02	TrAa02SMblScScm	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$x\text{nom7sulf} * k_{\text{exf}}(\text{O2, ind_H2SO4})$	see note
H9401_a02	TrAa02SMbl	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{exf}}(\text{O2, ind_CH3SO3H})$	see note

*Notes:

The forward (k_{exf}) and backward (k_{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_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of X (X = N_2O_5 , ClNO_3 , or BrNO_3) and subsequent reaction with H_2O , Cl^- , and Br^- , 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_{mt} . The factors only affect the branching between hy-

drolysis and the halide reactions. The factor 5×10^2 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 5×10^2 . 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
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*Notes:

Heterogeneous reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see 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
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)
EQ32_a01	TrAa01MblNScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ40_a01	TrAa01MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ61_a01	TrAa01ClMblScScm	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ71_a01	TrAa01BrMblScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
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)
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)
EQ21_a02	TrAa02MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a02	TrAa02MblNScScm	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ32_a02	TrAa02MblNScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ40_a02	TrAa02MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ61_a02	TrAa02ClMblScScm	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ71_a02	TrAa02BrMblScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ73_a02	TrAa02ClBrMbl	$\text{BrCl} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a02	TrAa02ClBrMbl	$\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a02	TrAa02ClBrMbl	$\text{Br}_2 + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.3	0	Wang et al. (1994)
EQ76_a02	TrAa02ClBrMbl	$\text{Br}^- + \text{Cl}_2 \rightleftharpoons \text{BrCl}_2^-$	4.2E6	14072	Wang et al. (1994)
EQ90_a02	TrAa02SMblScScm	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a02	TrAa02SMblScScm	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a02	TrAa02SMblScScm	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a02	TrAa02SMblScScm	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)

*Notes:

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

Table 8: Aqueous phase reactions

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A6204_a01	TrAa01ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6208_a01	TrAa01ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A7202_a01	TrAa01BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7208_a01	TrAa01BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7602_a01	TrAa01ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a01	TrAa01ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604_a01	TrAa01ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A9101_a01	TrAa01SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206_a01	TrAa01SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9209_a01	TrAa01SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9601_a01	TrAa01SCIMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9605_a01	TrAa01SCIMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9702_a01	TrAa01SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9705_a01	TrAa01SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note
A6204_a02	TrAa02ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6208_a02	TrAa02ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A7202_a02	TrAa02BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7208_a02	TrAa02BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7602_a02	TrAa02ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a02	TrAa02ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604_a02	TrAa02ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A9101_a02	TrAa02SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206_a02	TrAa02SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9209_a02	TrAa02SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9601_a02	TrAa02SCIMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9605_a02	TrAa02SCIMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9702_a02	TrAa02SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9705_a02	TrAa02SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note

*Notes:

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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