

# The Chemical Mechanism of MECCA

KPP version: 2.2.1\_rs3

MECCA version: 2.5h

Date: November 11, 2009.

Selected reactions:

“(Tr && (G || Het) && !Cl && !Br && !I) || St) && !Hg”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 75

Aqueous phase: 0

All species: 75

Number of reactions in selected mechanism:

Gas phase (Gnnn): 134

Aqueous phase (Annn): 0

Henry (Hnnn): 0

Photolysis (Jnnn): 44

Heterogeneous (HETnnn): 13

Equilibria (EQnn): 0

Dummy (Dnn): 0

All equations: 191

Further information can be found in the article “Technical Note:  
The new comprehensive atmospheric chemistry module MECCA” by  
R. Sander et al. (Atmos. Chem. Phys. **5**, 445-450, 2005), available at  
<http://www.atmos-chem-phys.net/5/445>.

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11*EXP(55./temp)$	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34*((temp/300.)**(-2.4))*cair$	Sander et al. (2006)
G1002	StG	$O_3 + O(^1D) \rightarrow 2 O_2$	$1.2E-10$	Sander et al. (2006)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2 O_2$	$8.E-12*EXP(-2060./temp)$	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	$k\_3rd(temp, cair, 4.4E-32, 1.3, 4.7E-11, 0.2, 0.6)$	Sander et al. (2006)
G2101	StG	$H + O_3 \rightarrow OH + O_2$	$1.4E-10*EXP(-470./temp)$	Sander et al. (2006)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	$1.1E-10$	Sander et al. (2006)
G2103	StG	$OH + O(^3P) \rightarrow H + O_2$	$2.2E-11*EXP(120./temp)$	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Sander et al. (2006)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH + O_2$	$3.E-11*EXP(200./temp)$	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Sander et al. (2006)
G2108a	StG	$HO_2 + H \rightarrow 2 OH$	$7.2E-11$	Sander et al. (2006)
G2108b	StG	$HO_2 + H \rightarrow H_2 + O_2$	$6.9E-12$	Sander et al. (2006)
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	$1.6E-12$	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$k\_H02\_H02$	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$1.63E-10*EXP(60./temp)$	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$1.8E-12$	Sander et al. (2006)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Sander et al. (2006)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2 NO$	$6.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	$4.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2006)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	$2.1E-11*EXP(100./temp)$	Sander et al. (2006)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.1E-12*EXP(210./temp)$	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Sander et al. (2006)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12*EXP(220./temp)$	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	$k\_N03\_N02$	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k\_N03\_N02/(2.7E-27*EXP(11000./temp))$	Sander et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G3200	TrG	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$\text{k\_3rd}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6, 3.6\text{E-}11, 0.1, 0.6)$	Sander et al. (2006)
G3201	StTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.5\text{E-}12 * \text{EXP}(250./\text{temp})$	Sander et al. (2006)
G3202	StTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$\text{k\_3rd}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0, 2.8\text{E-}11, 0., 0.6)$	Sander et al. (2006)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$\text{k\_NO2\_HO2}$	Sander et al. (2006)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E-}12$	Sander et al. (2006)
G3205	TrG	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11 * \text{EXP}(-390./\text{temp})$	Sander et al. (2006)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$\text{k\_HNO3\_OH}$	Sander et al. (2006)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$\text{k\_NO2\_HO2}/(2.1\text{E-}27 * \text{EXP}(10900./\text{temp}))$	Sander et al. (2006)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E-}12 * \text{EXP}(380./\text{temp})$	Sander et al. (2006)
G4100	StG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow .75 \text{CH}_3\text{O}_2 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	$1.5\text{E-}10$	Sander et al. (2006)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E-}20 * \text{EXP}(2.82 * \log(\text{temp}) - 987./\text{temp})$	Atkinson (2003)*
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$2.9\text{E-}12 * \text{EXP}(-345./\text{temp})$	Sander et al. (2006)
G4103	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$4.1\text{E-}13 * \text{EXP}(750./\text{temp})$	Sander et al. (2006)*
G4104	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E-}12 * \text{EXP}(300./\text{temp})$	Sander et al. (2006)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E-}12$	Atkinson et al. (1999)
G4106a	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 1./26.2 * \text{EXP}(1130./\text{temp}))$	Sander et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 26.2 * \text{EXP}(-1130./\text{temp}))$	Sander et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	$\text{k\_CH300H\_OH}$	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	$\text{HCOOH} + \text{OH} \rightarrow \text{HO}_2$	$4.0\text{E-}13$	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)
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)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{HCHO} + \text{HO}_2 + .75 \text{CH}_3\text{CHO} + .25 \text{CH}_3\text{OH}$	$1.6\text{E-}13 * \text{EXP}(195./\text{temp})$	see note
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .3 \text{C}_2\text{H}_5\text{O}_2 + .7 \text{CH}_3\text{CHO} + .7 \text{OH}$	$\text{k\_CH300H\_OH}$	see note
G4208	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp})$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E}-12*\text{EXP}(-1900./\text{temp})$	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	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+1./37.*\text{EXP}(660./\text{temp}))$	Tyndall et al. (2001)
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+37.*\text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$8.1\text{E}-12*\text{EXP}(270./\text{temp})$	Tyndall et al. (2001)
G4213	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_PA_N02	Sander et al. (2006)
G4214	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4215a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9*2.\text{E}-12*\text{EXP}(500./\text{temp})$	Sander et al. (2006)
G4215b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO}$	$0.1*2.\text{E}-12*\text{EXP}(500./\text{temp})$	Sander et al. (2006)
G4216	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{HO}_2 + .18 \text{CH}_3\text{COOH}$	$4.9\text{E}-12*\text{EXP}(211./\text{temp})$	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow 2 \text{CH}_3\text{O}_2 + 2 \text{CO}_2 + \text{O}_2$	$2.5\text{E}-12*\text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4218	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	k_CH300H_OH	see note
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2$	2.E-14	see note
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2006)*
G4222	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{CH}_3\text{O}_2$	$\text{k\_3rd}(\text{temp}, \text{cair}, 5.5\text{e}-30, 0.0, 8.3\text{e}-13, -2., 0.6)$	Sander et al. (2006)
G4301a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5\text{E}-15*\text{EXP}(-1900./\text{temp})$	Sander et al. (2003)*
G4302a	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow .98 \text{CH}_3\text{CHO} + .98 \text{HCHO}$	$\text{k\_3rd}(\text{temp}, \text{cair}, 8.\text{E}-27, 3.5, 3.\text{E}-11, 0., 0.5)$	Atkinson et al. (1999)
G4311	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$1.33\text{E}-13+3.82\text{E}-11*\text{EXP}(-2000./\text{temp})$	Sander et al. (2006)
G4312a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$8.6\text{E}-13*\text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO}$	$2.9\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2006)
G4314a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{OH} + \text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2$	$7.5\text{E}-13*\text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4400a	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow 0.8 \text{CH}_3\text{C}(\text{O})\text{OO} + .85 \text{CH}_3\text{CHO} + .1 \text{HCHO}$	$1.81\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(114./\text{temp})$	Atkinson (2003)
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)
G6101	StGCl	$\text{ClO} + \text{O}(^3\text{P}) \rightarrow \text{Cl} + \text{O}_2$	$2.5\text{E}-11*\text{EXP}(110./\text{temp})$	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)

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

#	labels	reaction	rate coefficient	reference
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	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$	$k_{\text{ClO\_ClO}}$	Atkinson et al. (2007)
G6103	StTrGCl	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	$k_{\text{ClO\_ClO}}/(9.3\text{E-}28*\text{EXP}(8835./\text{temp}))$	Atkinson et al. (2007), Sander et al. (2006)*
G6200	StGCl	$\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$	$3.9\text{E-}11*\text{EXP}(-2310./\text{temp})$	Atkinson et al. (2007)
G6201a	StGCl	$\text{Cl} + \text{HO}_2 \rightarrow \text{HCl} + \text{O}_2$	$4.4\text{E-}11-7.5\text{E-}11*\text{EXP}(-620./\text{temp})$	Atkinson et al. (2007)
G6201b	StGCl	$\text{Cl} + \text{HO}_2 \rightarrow \text{ClO} + \text{OH}$	$7.5\text{E-}11*\text{EXP}(-620./\text{temp})$	Atkinson et al. (2007)
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)
G6203	StGCl	$\text{ClO} + \text{OH} \rightarrow .94 \text{ Cl} + .94 \text{ HO}_2 + .06 \text{ HCl} + .06 \text{ O}_2$	$7.3\text{E-}12*\text{EXP}(300./\text{temp})$	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl}$	$2.2\text{E-}12*\text{EXP}(340./\text{temp})$	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)
G6206	StGCl	$\text{HOCl} + \text{OH} \rightarrow \text{ClO} + \text{H}_2\text{O}$	$3.0\text{E-}12*\text{EXP}(-500./\text{temp})$	Sander et al. (2006)
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	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$k_{\text{3rd\_iupac}}(\text{temp}, \text{cair}, 1.6\text{E-}31, 3.4, 7.\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G6303	StGNCl	$\text{ClNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{ClO} + \text{NO}_3$	$4.5\text{E-}12*\text{EXP}(-900./\text{temp})$	Atkinson et al. (2007)
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)
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 3 \text{ Cl}$	$3.3\text{E-}10$	Sander et al. (2006)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{Cl}$	$1.65\text{E-}10$	see note
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	$2.4\text{E-}12*\text{EXP}(-1250./\text{temp})$	Sander et al. (2006)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{OH} + 3 \text{ Cl}$	$3.\text{E-}10$	see note
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{ Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Sander et al. (2006)
G6500	StGFCl	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + \text{Cl}$	$1.4\text{E-}10$	Sander et al. (2006)
G6501	StGFCl	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 2 \text{ Cl}$	$2.3\text{E-}10$	Sander et al. (2006)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E-}11*\text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E-}11*\text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E-}12*\text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E-}12*\text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E-}12*\text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7203	StGBr	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E-}10*\text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E-}11*\text{EXP}(240./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G7301	StTrGNBr	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.7\text{E-}12*\text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGNBr	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E-}12*\text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.35\text{E-}12*\text{EXP}(-1300./\text{temp})$	Sander et al. (2006)
G7603a	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$1.6\text{E-}12*\text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E-}12*\text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	$5.8\text{E-}13*\text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	k_3rd(temp, cair, 3.3E-31, 4.3, 1.6E-12, 0., 0.6)	Sander et al. (2006)
G9400a	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E-}11*\text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-}13*\text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{ SO}_2 + \text{HCHO} + .6 \text{ CH}_3\text{O}_2 + .4 \text{ HO}_2$ $+ .4 \text{ CH}_3\text{SO}_3\text{H}$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.9\text{E}13*\text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	5.E-11	Barone et al. (1995)

\*Notes:

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

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

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

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

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

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:

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

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

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

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

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

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

G2110: The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)*(1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

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

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

G3203: The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

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

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

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

G4107: The rate coefficient is: `k_CH3OOH_OH = 3.8E-12*EXP(200./temp)`.

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

G4206: The rate coefficient was calculated by von Kuhlmann (pers. comm. 2004) using self reactions of  $\text{CH}_3\text{OO}$  and  $\text{C}_2\text{H}_5\text{OO}$  from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: Same value as for G4107:  $\text{CH}_3\text{OOH} + \text{OH}$  assumed.

G4216: The value  $1.0\text{E}-11$  is from Atkinson et al. (1999), the temperature dependence from Kirchner and Stockwell (1996).

G4218: Same value as for G4107:  $\text{CH}_3\text{OOH} + \text{OH}$  assumed.

G4220: This is 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001).

G4221: The rate coefficient is: `k_PAN_M = k_PA_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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

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

G6402: The initial products are probably HCl and  $\text{CH}_2\text{OOH}$  (Atkinson et al., 2006). It is assumed that  $\text{CH}_2\text{OOH}$  dissociates into HCHO and OH.

G6405: Average of reactions with  $\text{CH}_3\text{Br}$  and  $\text{CH}_3\text{F}$  from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with  $\text{CH}_3\text{CF}_3$ ,  $\text{CH}_3\text{CClF}_2$ , and  $\text{CH}_3\text{CCl}_2\text{F}$  from Sander et al. (2006).

G7302: The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

G9400: Addition path. The rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_02)	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	jx(ip_01D)	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	jx(ip_03P)	see note
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	jx(ip_N20)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_N02)	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	jx(ip_NO)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_N020)	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	jx(ip_N002)	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	see note
J3104b	StGNJ	$N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$	jx(ip_N03N00)	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HN03)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HN04)	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH300H)	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	jx(ip_CO2)	see note
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31 H + 0.69 H_2 + 1.155 H_2O$	jx(ip_CH4)	see note
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	jx(ip_PAA)	see note
J4204	TrGN CJ	$PAN + h\nu \rightarrow .6 CH_3C(O)OO + .6 NO_2 + .4 CH_3O_2 + .4 NO_3 + .4 CO_2$	jx(ip_PAN)	see note
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3C0CH3)	see note
J6000	StTrGClJ	$Cl_2 + h\nu \rightarrow Cl + Cl$	jx(ip_Cl2)	see note
J6100	StTrGClJ	$Cl_2O_2 + h\nu \rightarrow 2 Cl$	1.4*jx(ip_Cl202)	see note
J6101	StTrGClJ	$OClo + h\nu \rightarrow ClO + O(^3P)$	jx(ip_OCl0)	see note
J6200	StGClJ	$HCl + h\nu \rightarrow Cl + H$	jx(ip_HCl)	see note
J6201	StTrGClJ	$HOCl + h\nu \rightarrow OH + Cl$	jx(ip_HOCl)	see note
J6301a	StTrGNClJ	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	jx(ip_ClN03)	see note
J6301b	StTrGNClJ	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	jx(ip_ClON02)	see note
J6400	StGClJ	$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$	jx(ip_CH3Cl)	see note



Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6401	StGClJ	$\text{CCl}_4 + h\nu \rightarrow 4 \text{ Cl}$	jx(ip_CCl4)	see note
J6402	StGCClJ	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3 \text{ Cl}$	jx(ip_CH3CCl3)	see note
J6500	StGFClJ	$\text{CFCl}_3 + h\nu \rightarrow 3 \text{ Cl}$	jx(ip_CFC13)	see note
J6501	StGFClJ	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2 \text{ Cl}$	jx(ip_CF2Cl2)	see note
J7200	StTrGBrJ	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	jx(ip_HOBr)	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
J7400	StGBrJ	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$	jx(ip_CH3Br)	see note
J7500	StGFBBrJ	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$	jx(ip_CF3Br)	see note
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_BrCl)	see note
J7601	StGFBBrJ	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_CF2ClBr)	see note
J9002	StGSJ	$\text{SF}_6 + h\nu \rightarrow \text{products}$	JX(ip_SF6)	see note

\*Notes:

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

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the  $\text{Cl}_2\text{O}_2$  formation rate coefficient by

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

et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

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

Table 3: Henry’s law coefficients

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
O <sub>2</sub>	$1.3 \times 10^{-3}$	1500.	Wilhelm et al. (1977)
O <sub>3</sub>	$1.2 \times 10^{-2}$	2560.	Chameides (1984)
OH	$3.0 \times 10^1$	4300.	Hanson et al. (1992)
HO <sub>2</sub>	$3.9 \times 10^3$	5900.	Hanson et al. (1992)
H <sub>2</sub> O <sub>2</sub>	$1. \times 10^5$	6338.	Lind and Kok (1994)
NO	$1.9 \times 10^{-3}$	1480.	Schwartz and White (1981)
NO <sub>2</sub>	$7.0 \times 10^{-3}$	2500.	Lee and Schwartz (1981)*
NO <sub>3</sub>	2.	2000.	Thomas et al. (1993)
HONO	$4.9 \times 10^1$	4780.	Schwartz and White (1981)
HNO <sub>3</sub>	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO <sub>4</sub>	$1.2 \times 10^4$	6900.	Régimbal and Mozurkewich (1997)
CH <sub>3</sub> O <sub>2</sub>	6.	5600.	Jacob (1986)*
CH <sub>3</sub> OOH	$3.0 \times 10^2$	5322.	Lind and Kok (1994)
HCHO	$7.0 \times 10^3$	6425.	Chameides (1984)
HCOOH	$3.7 \times 10^3$	5700.	Chameides (1984)
CO <sub>2</sub>	$3.1 \times 10^{-2}$	2423.	Chameides (1984)
Cl <sub>2</sub>	$9.2 \times 10^{-2}$	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	$6.7 \times 10^2$	5862.	Huthwelker et al. (1995)
Br <sub>2</sub>	$7.7 \times 10^{-1}$	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	$9.3 \times 10^1$	5862.	Vogt et al. (1996)*
BrCl	$9.4 \times 10^{-1}$	5600.	Bartlett and Margerum (1999)
SO <sub>2</sub>	1.2	3120.	Chameides (1984)
H <sub>2</sub> SO <sub>4</sub>	$1. \times 10^{11}$	0.	see note
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*

\*Notes:

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  $R = 8.314 \text{ J/(mol K)}$ .

NO<sub>2</sub>: The temperature dependence is from Chameides (1969).  
(1984).

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

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

HBr: Calculated using the acidity constant from Lax

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

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

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{K}$	reference
O <sub>2</sub>	0.01	2000.	see note
O <sub>3</sub>	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO <sub>2</sub>	0.5	0.	Thornton and Abbatt (2005)
H <sub>2</sub> O <sub>2</sub>	0.077	3127.	Worsnop et al. (1989)
NO	$5.0 \times 10^{-5}$	0.	Saastad et al. (1993)*
NO <sub>2</sub>	0.0015	0.	Ponche et al. (1993)*
NO <sub>3</sub>	0.04	0.	Rudich et al. (1996)*
N <sub>2</sub> O <sub>5</sub>	0.1	0.	DeMore et al. (1997)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO <sub>3</sub>	0.5	0.	Abbatt and Waschewsky (1998)*
HNO <sub>4</sub>	0.1	0.	DeMore et al. (1997)*
CH <sub>3</sub> O <sub>2</sub>	0.01	2000.	see note
CH <sub>3</sub> OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO <sub>2</sub>	0.01	2000.	see note
Cl <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
ClNO <sub>3</sub>	0.108	0.	Deiber et al. (2004)*
Br <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
BrNO <sub>3</sub>	0.063	0.	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO <sub>2</sub>	0.11	0.	DeMore et al. (1997)
H <sub>2</sub> SO <sub>4</sub>	0.65	0.	Pöschl et al. (1998)*
CH <sub>3</sub> SO <sub>3</sub> H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)

\*Notes:

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:

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

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

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

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

OH: Value measured at 293 K.

NO: Value measured between 193 and 243 K.

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

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

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

HONO: Value measured between 247 and 297 K.

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

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

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

HCHO: Value measured between 260 and 270 K.

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

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

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

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

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

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

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

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

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

Table 5: Henry’s law equilibria

#	labels	reaction	rate coefficient	reference
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\*Notes:

The forward (**k<sub>exf</sub>**) and backward (**k<sub>exb</sub>**) rate coefficients are calculated in the file **messy\_mecca\_aero.f90** using the accommodation coefficients in subroutine **mecca\_aero\_alpha** and Henry’s law constants in subroutine **mecca\_aero\_henry**.

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

lwc = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of  $X$  ( $= \text{N}_2\text{O}_5, \text{ClNO}_3, \text{BrNO}_3$ ) and subsequent reaction with  $\text{H}_2\text{O}$ ,  $\text{Cl}^-$ , and  $\text{Br}^-$ , we define  $k_{\text{exf}}(X) = k_{\text{mt}}(X) \times lwc / ([\text{H}_2\text{O}] + 5.0E2[\text{Cl}^-] + 3.0E5[\text{Br}^-])$ .

H6301, H6302, H7601: The total uptake is determined by  $k_{\text{mt}}(\text{ClNO}_3)$ . The relative rates are assumed to be the same as for  $\text{N}_2\text{O}_5$  (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by  $k_{\text{mt}}(\text{BrNO}_3)$ . The relative rates are assumed to be the same as for  $\text{N}_2\text{O}_5$  (H3201, H6300, H7300).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2 \text{HNO}_3$	<code>khet_St(ihs_N205_H20)</code>	see note
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^-(\text{aq}) + 2 \text{H}^+(\text{aq})$	<code>khet_Tr(iht_N205)</code>	see note
HET202	TrHetN	$\text{HNO}_3 \rightarrow \text{NO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	<code>khet_Tr(iht_HNO3)</code>	see note
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see note
HET420	StHetNCl	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see note
HET421	StHetNCl	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H20)</code>	see note
HET422	StHetNCl	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N205_HCl)</code>	see note
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see note
HET520	StHetNBr	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H20)</code>	see note
HET540	StHetNClBr	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see note
HET541	StHetNClBr	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see note
HET542	StHetClBr	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see note
HET543	StHetClBr	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HCl)</code>	see note

\*Notes:

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

Table 7: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
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\*Notes:

Table 8: Aqueous phase reactions

#	labels	reaction	$k_0$ [ $M^{1-n}s^{-1}$ ]	$-E_a/R[K]$	reference
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\*Notes:



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