

# The Chemical Mechanism of MECCA

KPP version: 2.2.1\_rs5

MECCA version: 3.6

Date: July 6, 2015.

Selected reactions:

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

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 155 (**160**)

Aqueous phase: 0

All species: 155 (**160**)

Number of reactions in selected mechanism:

Gas phase (Gnn): 224 (**231**)

Aqueous phase (Annn): 0

Henry (Hnn): 0

Photolysis (Jnn): 74 (**78**)

Aqueous phase photolysis (PHnn): 0

Heterogeneous (HETnnn): 12

Equilibria (EQnn): 0

Isotope exchange (DGnnn): 0

Dummy (Dnn): 0

All equations: 310 (**321**)

This document is part of the electronic supplement to our article  
“Earth System Chemistry Integrated Modeling (ESCiMo) with the  
Modular Earth Submodel System (MESSy, version 2.51)”  
in Geosci. Model Dev. Discuss. (2015), available at:  
<http://www.geosci-model-dev-discuss.net>

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11*EXP(55./temp)$	Sander et al. (2011)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34*((temp/300.)**(-2.4))*cair$	Sander et al. (2011)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2 \text{ LossO3O} + 2 \text{ LossO3} + 2 O_2$	$1.2E-10$	Sander et al. (2011)*
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2 \text{ LossO3O} + 2 \text{ LossO3} + 2 O_2$	$8.E-12*EXP(-2060./temp)$	Sander et al. (2011)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	$k\_3rd(temp, cair, 4.4E-32, 1.3, 7.5E-11, -0.2, 0.6)$	Sander et al. (2011)
G2101	UpStG	$H + O_3 \rightarrow \text{LossO3H} + \text{LossO3} + OH + O_2$	$1.4E-10*EXP(-470./temp)$	Sander et al. (2011)
G2102	UpStG	$H_2 + O(^1D) \rightarrow \text{LossO3H} + \text{LossO3} + H + OH$	$1.2E-10$	Sander et al. (2011)
G2103	UpStG	$OH + O(^3P) \rightarrow \text{LossO3H} + \text{LossO3} + H + O_2$	$1.8E-11*EXP(180./temp)$	Sander et al. (2011)
G2104	UpStTrG	$OH + O_3 \rightarrow \text{LossG2104} + \text{LossO3H} + \text{LossOH} + \text{LossO3} + HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Sander et al. (2011)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Sander et al. (2011)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow \text{LossG2106} + \text{LossO3H} + \text{LossO3} + OH + O_2$	$3.E-11*EXP(200./temp)$	Sander et al. (2011)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow \text{LossG2107} + \text{LossO3H} + \text{LossHO2} + \text{LossO3} + OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Sander et al. (2011)
G2108a	UpStG	$HO_2 + H \rightarrow 2 OH$	$7.2E-11$	Sander et al. (2011)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	$6.9E-12$	Sander et al. (2011)
G2108c	UpStG	$HO_2 + H \rightarrow \text{LossO3Hn} + \text{ProdO3} + O(^3P) + H_2O$	$1.6E-12$	Sander et al. (2011)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Sander et al. (2011)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow \text{LossG2110} + H_2O_2 + O_2$	$k\_H02\_H02$	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow \text{LossO3O} + \text{LossO1D} + \text{LossO3} + 2 OH$	$1.63E-10*EXP(60./temp)$	Sander et al. (2011)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$1.8E-12$	Sander et al. (2011)
G3100	UpStGN	$N + O_2 \rightarrow \text{LossO3Nn} + \text{ProdO3} + NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	Sander et al. (2011)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Sander et al. (2011)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow \text{LossO3O} + \text{LossO3} + 2 NO$	$7.25E-11*EXP(20./temp)$	Sander et al. (2011)
G3102b	StGN	$N_2O + O(^1D) \rightarrow \text{LossO3O} + \text{LossO3} + N_2 + O_2$	$4.63E-11*EXP(20./temp)$	Sander et al. (2011)
G3103	UpStTrGN	$NO + O_3 \rightarrow \text{LossG3103} + NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2011)
G3104	UpStGN	$NO + N \rightarrow \text{LossO3Nn} + \text{ProdO3} + O(^3P) + N_2$	$2.1E-11*EXP(100./temp)$	Sander et al. (2011)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow \text{LossG3105} + 2 \text{ LossO3N2} + 2 \text{ LossO3N} + 2 \text{ LossO3} + NO + O_2$	$5.1E-12*EXP(210./temp)$	Sander et al. (2011)
G3106	StTrGN	$NO_2 + O_3 \rightarrow \text{LossG3106} + NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Sander et al. (2011)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12*EXP(220./temp)$	Sander et al. (2011)

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

#	labels	reaction	rate coefficient	reference
G3108	StTrGN	$\text{NO}_3 + \text{NO} \rightarrow 2 \text{NO}_2$	$1.5\text{E-}11*\text{EXP}(170./\text{temp})$	Sander et al. (2011)
G3109	UpStTrGN	$\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	$\text{k\_NO3\_NO2}$	Sander et al. (2011)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$\text{k\_NO3\_NO2}/(2.7\text{E-}27*\text{EXP}(11000./\text{temp}))$	Sander et al. (2011)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$\text{k\_3rd}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6, 3.6\text{E-}11, 0.1, 0.6)$	Sander et al. (2011)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{LossG3201} + \text{ProdHO2} + \text{ProdO3} + \text{NO}_2 + \text{OH}$	$3.3\text{E-}12*\text{EXP}(270./\text{temp})$	Sander et al. (2011)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{LossG3202} + \text{HNO}_3$	$\text{k\_3rd}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0, 2.8\text{E-}11, 0., 0.6)$	Sander et al. (2011)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$\text{k\_NO2\_HO2}$	Sander et al. (2011)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{LossO3N} + \text{LossO3} + \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E-}12$	Sander et al. (2011)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{LossO3Nn} + \text{ProdO3} + \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11*\text{EXP}(-390./\text{temp})$	Sander et al. (2011)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{LossO3Nn} + \text{ProdO3} + \text{H}_2\text{O} + \text{NO}_3$	$\text{k\_HNO3\_OH}$	Sander et al. (2011)*
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. (2011)*
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. (2011)
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E-}12*\text{EXP}(-710./\text{temp})$	Kohlmann and Poppe (1999)
G3210	TrGN	$\text{NH}_2 + \text{O}_3 \rightarrow \text{LossO3} + \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12*\text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E-}07*\text{EXP}(-628./\text{temp})*\text{temp}**(-1.32)$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E-}09*\text{EXP}(-356./\text{temp})*\text{temp}**(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12*((\text{temp}/298.)*(-1.5))$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11*((\text{temp}/298.)*(-1.5))$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{LossO3} + \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11*((\text{temp}/298.)*(-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{LossO3} + \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11*((\text{temp}/298.)*(-2.0))$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{LossO3} + \text{NH}_2 + \text{O}_2$	$1.2\text{E-}14$	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	$\text{HNO} + \text{NO}_2 \rightarrow \text{LossO3} + \text{HONO} + \text{NO}$	$1.0\text{E-}12*\text{EXP}(-1000./\text{temp})$	Kohlmann and Poppe (1999)
G3222	TrGN	$\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$	$1.66\text{E-}12$	Kohlmann and Poppe (1999)
G3223	TrGN	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11*\text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14*\text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4100	UpStG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow \text{LossO3} + .75 \text{CH}_3\text{O}_2 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	$1.75\text{E-}10$	Sander et al. (2011)
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. (2011)

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

#	labels	reaction	rate coefficient	reference
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. (2011)*
G4104	UpStTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{ProdMeO2} + \text{ProdO3} + \text{HCHO} + \text{NO}_2$ $+ \text{HO}_2$	$2.8\text{E-}12*\text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{LossO3N} + \text{LossO3} + \text{HCHO} + \text{HO}_2 +$ $\text{NO}_2$	1.3E-12	Atkinson et al. (2006)
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. (2011)
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. (2011)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Sander et al. (2011)*
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	$\text{HCHO} + \text{NO}_3 \rightarrow \text{LossO3N} + \text{LossO3} + \text{HNO}_3 + \text{CO} +$ $\text{HO}_2$	$3.4\text{E-}13*\text{EXP}(-1900./\text{temp})$	Sander et al. (2011)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{LossG4110} + \text{H} + \text{CO}_2$	$(1.57\text{E-}13+\text{cair}*3.54\text{E-}33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	4.0E-13	Sander et al. (2011)
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	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{LossO3R} + \text{LossO3} + \text{HCHO} + .63 \text{CO} +$ .13 $\text{HO}_2 + 0.23125 \text{HCOOH} + 0.13875 \text{HCHO} + 0.13875$ $\text{H}_2\text{O}_2 + .13 \text{OH}$	$1.2\text{E-}14*\text{EXP}(-2630./\text{temp})$	Sander et al. (2011)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow .6666667 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 1.0E-28, 4.5, 7.5E-12, 0.85, 0.6)	Sander et al. (2011)
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. (2011)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{ProdRO2} + \text{ProdO3} + \text{CH}_3\text{CHO} + \text{HO}_2$ $+ \text{NO}_2$	$2.6\text{E-}12*\text{EXP}(365./\text{temp})$	Sander et al. (2011)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{LossO3} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	2.3E-12	Atkinson et al. (1999)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{HCHO} + \text{HO}_2 + .75 \text{CH}_3\text{CHO}$ $+ .25 \text{CH}_3\text{OH}$	$1.6\text{E-}13*\text{EXP}(195./\text{temp})$	see note
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .3 \text{C}_2\text{H}_5\text{O}_2 + .7 \text{CH}_3\text{CHO} + .7 \text{OH}$	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)
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{LossO3N} + \text{LossO3} + \text{CH}_3\text{C}(\text{O})\text{OO}$ $+ \text{HNO}_3$	$1.4\text{E-}12*\text{EXP}(-1900./\text{temp})$	Sander et al. (2011)
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)

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

#	labels	reaction	rate coefficient	reference
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{ProdO3} + \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E-}13 \cdot \text{EXP}(1040./\text{temp}) / (1. + 37. \cdot \text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{ProdRO2} + \text{ProdO3} + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E-}12 \cdot \text{EXP}(270./\text{temp})$	Tyndall et al. (2001)
G4213	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_PA_NO2	Sander et al. (2011)
G4214	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{LossO3N} + \text{LossO3} + \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4215a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9 \cdot 2.0\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2011)
G4215b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO}$	$0.1 \cdot 2.0\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2011)
G4216	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{ CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{ HO}_2 + .18 \text{ CH}_3\text{COOH}$	$4.9\text{E-}12 \cdot \text{EXP}(211./\text{temp})$	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow 2 \text{ CH}_3\text{O}_2 + 2 \text{ CO}_2 + \text{O}_2$	$2.5\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4218	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	Rickard and Pascoe (2009)*
G4219	TrGNC	$\text{NACA} + \text{OH} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6\text{E-}12 \cdot \text{EXP}(270./\text{temp})$	see note
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$9.50\text{E-}13 \cdot \text{EXP}(-650./\text{temp})$	Rickard and Pascoe (2009)
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2011)*
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .82 \text{ iC}_3\text{H}_7\text{O}_2 + .18 \text{ C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-87./\text{temp})$	Atkinson (2003)
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{LossO3R} + \text{LossO3} + .57 \text{ HCHO} + .47 \text{ CH}_3\text{CHO} + .33 \text{ OH} + .26 \text{ HO}_2 + .07 \text{ CH}_3\text{O}_2 + .06 \text{ C}_2\text{H}_5\text{O}_2 + .23 \text{ CH}_3\text{C}(\text{O})\text{OO} + .04 \text{ MGLYOX} + .06 \text{ CH}_4 + .31 \text{ CO} + .22 \text{ HCOOH} + .03 \text{ CH}_3\text{OH}$	$6.5\text{E-}15 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2011)*
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 8.E-27, 3.5, 3.E-11, 0., 0.5)	Atkinson et al. (1999)
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{LossO3} + \text{LC4H9NO3}$	$4.6\text{E-}13 \cdot \text{EXP}(-1155./\text{temp})$	Atkinson et al. (1999)
G4304	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	k_Pr02_H02	Atkinson (1997)*
G4305	TrGNC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{ProdRO2} + \text{ProdO3} + .96 \text{ CH}_3\text{COCH}_3 + .96 \text{ HO}_2 + .96 \text{ NO}_2 + .04 \text{ iC}_3\text{H}_7\text{ONO}_2$	k_Pr02_NO	Atkinson et al. (1999)*
G4306	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{ HCHO} + .8 \text{ HO}_2 + .2 \text{ CH}_3\text{OH}$	k_Pr02_CH302	Kirchner and Stockwell (1996)
G4307	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .3 \text{ iC}_3\text{H}_7\text{O}_2 + .7 \text{ CH}_3\text{COCH}_3 + .7 \text{ OH}$	k_CH300H_OH	see note
G4308	TrGC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HO}_2 \rightarrow \text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH}$	$6.5\text{E-}13 \cdot \text{EXP}(650./\text{temp})$	Müller and Brasseur (1995)
G4309	TrGNC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow \text{ProdRO2} + \text{ProdO3} + .98 \text{ CH}_3\text{CHO} + .98 \text{ HCHO} + .98 \text{ HO}_2 + .98 \text{ NO}_2 + .02 \text{ LC4H9NO3}$	$4.2\text{E-}12 \cdot \text{EXP}(180./\text{temp})$	Müller and Brasseur (1995)*

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

#	labels	reaction	rate coefficient	reference
G4310	TrGC	$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH} + \text{OH} \rightarrow .5 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{OH} + \text{H}_2\text{O}$	$3.8\text{E}-12*\text{EXP}(200./\text{temp})$	Müller and Brasseur (1995)
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. (2011)
G4312	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E}-13*\text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{ProdO}_3 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{MGLYOX} + .5 \text{CH}_3\text{OH} + .3 \text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2 + .2 \text{CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E}-13*\text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4315	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow .3 \text{CH}_3\text{COCH}_2\text{O}_2 + .7 \text{MGLYOX} + .7 \text{OH}$	$\text{k\_CH300H\_OH}$	see note
G4316	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2$	$2.15\text{E}-12*\text{EXP}(305./\text{temp})$	Dillon et al. (2006)
G4317	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}$	$8.4\text{E}-13*\text{EXP}(830./\text{temp})$	Tyndall et al. (1995)
G4318	TrGNC	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$3.2\text{E}-11$	Orlando et al. (2002)
G4319	TrGNC	$\text{MPAN} \rightarrow \text{MVKO}_2 + \text{NO}_2$	$\text{k\_PAN\_M}$	see note
G4320	TrGNC	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E}-13*\text{EXP}(-230./\text{temp})$	Atkinson et al. (1999)
G4400	TrGC	$\text{nC}_4\text{H}_{10} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.81\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(114./\text{temp})$	Atkinson (2003)
G4401	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .88 \text{MEK} + .68 \text{HCHO} + 1.23 \text{HO}_2 + .12 \text{CH}_3\text{CHO} + .12 \text{C}_2\text{H}_5\text{O}_2 + .18 \text{CH}_3\text{OH}$	$\text{k\_PrO}_2\text{-CH302}$	see note
G4402	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	$\text{k\_PrO}_2\text{-H}_2\text{O}_2$	see note
G4403	TrGNC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{ProdO}_3 + .84 \text{NO}_2 + .56 \text{MEK} + .56 \text{HO}_2 + .28 \text{C}_2\text{H}_5\text{O}_2 + .28 \text{CH}_3\text{CHO} + .16 \text{LC}_4\text{H}_9\text{NO}_3$	$\text{k\_PrO}_2\text{-NO}$	see note
G4404	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow .15 \text{LC}_4\text{H}_9\text{O}_2 + .85 \text{MEK} + .85 \text{OH} + .85 \text{H}_2\text{O}$	$\text{k\_CH300H\_OH}$	see note
G4405	TrGC	$\text{MVK} + \text{O}_3 \rightarrow \text{LossO}_3\text{R} + \text{LossO}_3 + .45 \text{HCOOH} + .9 \text{MGLYOX} + .1 \text{CH}_3\text{C}(\text{O})\text{OO} + .19 \text{OH} + .22 \text{CO} + .32 \text{HO}_2$	$.5*(1.36\text{E}-15*\text{EXP}(-2112./\text{temp}) + 7.51\text{E}-16*\text{EXP}(-1521./\text{temp}))$	Pöschl et al. (2000)
G4406	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{MVKO}_2$	$.5*(4.1\text{E}-12*\text{EXP}(452./\text{temp}) + 1.9\text{E}-11*\text{EXP}(175./\text{temp}))$	Pöschl et al. (2000)
G4407	TrGC	$\text{MVKO}_2 + \text{HO}_2 \rightarrow \text{MVKOOH}$	$1.82\text{E}-13*\text{EXP}(1300./\text{temp})$	Pöschl et al. (2000)
G4408	TrGNC	$\text{MVKO}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{ProdO}_3 + \text{NO}_2 + .25 \text{CH}_3\text{C}(\text{O})\text{OO} + .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{HCHO} + .25 \text{CO} + .75 \text{HO}_2 + .5 \text{MGLYOX}$	$2.54\text{E}-12*\text{EXP}(360./\text{temp})$	Pöschl et al. (2000)
G4409	TrGNC	$\text{MVKO}_2 + \text{NO}_2 \rightarrow \text{MPAN}$	$.25*\text{k\_3rd}(\text{temp}, \text{cair}, 9.7\text{E}-29, 5.6, 9.3\text{E}-12, 1.5, 0.6)$	Pöschl et al. (2000)*

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

#	labels	reaction	rate coefficient	reference
G4410	TrGC	$\text{MVKO}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ MGLYOX} + .375 \text{ CH}_3\text{COCH}_2\text{OH} + .125 \text{ CH}_3\text{C(O)OO} + 1.125 \text{ HCHO} + .875 \text{ HO}_2 + .125 \text{ CO} + .25 \text{ CH}_3\text{OH}$	2.E-12	von Kuhlmann (2001)
G4411	TrGC	$\text{MVKO}_2 + \text{MVKO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{MGLYOX} + .5 \text{ CO} + .5 \text{ HCHO} + \text{HO}_2$	2.E-12	Pöschl et al. (2000)
G4412	TrGC	$\text{MVKOOH} + \text{OH} \rightarrow \text{MVKO}_2$	3.E-11	Pöschl et al. (2000)
G4413	TrGC	$\text{MEK} + \text{OH} \rightarrow \text{LMEKO}_2$	$1.3\text{E-}12*\text{EXP}(-25./\text{temp})$	Atkinson et al. (1999)
G4414	TrGC	$\text{LMEKO}_2 + \text{HO}_2 \rightarrow \text{LMEKOOH}$	k_PrO2_HO2	see note
G4415	TrGNC	$\text{LMEKO}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{ProdO}_3 + .985 \text{ CH}_3\text{CHO} + .985 \text{ CH}_3\text{C(O)OO} + .985 \text{ NO}_2 + .015 \text{ LC4H9NO}_3$	k_PrO2_NO	see note
G4416	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow .8 \text{ BIACET} + .8 \text{ OH} + .2 \text{ LMEKO}_2$	k_CH300H_OH	see note
G4417	TrGNC	$\text{LC4H9NO}_3 + \text{OH} \rightarrow \text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	$\text{C}_5\text{H}_8 + \text{O}_3 \rightarrow \text{LossO3R} + \text{LossO3} + .28 \text{ HCOOH} + .65 \text{ MVK} + .1 \text{ MVKO}_2 + .1 \text{ CH}_3\text{C(O)OO} + .14 \text{ CO} + .58 \text{ HCHO} + .09 \text{ H}_2\text{O}_2 + .08 \text{ CH}_3\text{O}_2 + .25 \text{ OH} + .25 \text{ HO}_2$	$7.86\text{E-}15*\text{EXP}(-1913./\text{temp})$	Pöschl et al. (2000)
G4501	TrGC	$\text{C}_5\text{H}_8 + \text{OH} \rightarrow \text{ISO}_2$	$2.54\text{E-}11*\text{EXP}(410./\text{temp})$	Pöschl et al. (2000)
G4502	TrGNC	$\text{C}_5\text{H}_8 + \text{NO}_3 \rightarrow \text{LossO3} + \text{ISON}$	$3.03\text{E-}12*\text{EXP}(-446./\text{temp})$	Pöschl et al. (2000)
G4503	TrGC	$\text{ISO}_2 + \text{HO}_2 \rightarrow \text{ISOOH}$	$2.22\text{E-}13*\text{EXP}(1300./\text{temp})$	Boyd et al. (2003)*
G4504a	TrGNC	$\text{ISO}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{ProdO}_3 + .956 \text{ NO}_2 + .956 \text{ MVK} + .956 \text{ HCHO} + .956 \text{ HO}_2 + .044 \text{ ISON}$	$2.54\text{E-}12*\text{EXP}(360./\text{temp})$	Pöschl et al. (2000)*
G4505	TrGC	$\text{ISO}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ MVK} + 1.25 \text{ HCHO} + \text{HO}_2 + .25 \text{ MGLYOX} + .25 \text{ CH}_3\text{COCH}_2\text{OH} + .25 \text{ CH}_3\text{OH}$	2.E-12	von Kuhlmann (2001)
G4506	TrGC	$\text{ISO}_2 + \text{ISO}_2 \rightarrow 2 \text{ MVK} + \text{HCHO} + \text{HO}_2$	2.E-12	Pöschl et al. (2000)
G4507	TrGC	$\text{ISOOH} + \text{OH} \rightarrow \text{MVK} + \text{OH}$	1.E-10	Pöschl et al. (2000)
G4508	TrGNC	$\text{ISON} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NACA}$	1.3E-11	Pöschl et al. (2000)
G6100	UpStTrGCl	$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	$2.8\text{E-}11*\text{EXP}(-250./\text{temp})$	Atkinson et al. (2007)
G6101	UpStGCl	$\text{ClO} + \text{O}(^3\text{P}) \rightarrow 2 \text{ LossO3Cl} + 2 \text{ LossO3} + \text{Cl} + \text{O}_2$	$2.5\text{E-}11*\text{EXP}(110./\text{temp})$	Atkinson et al. (2007)
G6102a	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow 2 \text{ LossO3} + \text{Cl}_2 + \text{O}_2$	$1.0\text{E-}12*\text{EXP}(-1590./\text{temp})$	Atkinson et al. (2007)
G6102b	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow 2 \text{ LossO3} + 2 \text{ Cl} + \text{O}_2$	$3.0\text{E-}11*\text{EXP}(-2450./\text{temp})$	Atkinson et al. (2007)
G6102c	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{LossO3} + \text{Cl} + \text{OCIO}$	$3.5\text{E-}13*\text{EXP}(-1370./\text{temp})$	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	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	$\text{k\_ClO\_ClO}/(1.72\text{E-}27*\text{EXP}(8649./\text{temp}))$	Atkinson et al. (2007), Sander et al. (2011)*
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)

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

#	labels	reaction	rate coefficient	reference
G6201b	StGCl	$\text{Cl} + \text{HO}_2 \rightarrow \text{LossO3Cl} + \text{ProdO3} + \text{ClO} + \text{OH}$	$7.5\text{E-}11 * \text{EXP}(-620./\text{temp})$	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	$\text{ClO} + \text{OH} \rightarrow \text{LossO3Cl} + \text{LossO3} + .94 \text{ Cl} + .94 \text{ HO}_2 + .06 \text{ HCl} + .06 \text{ O}_2$	$7.3\text{E-}12 * \text{EXP}(300./\text{temp})$	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	$2.2\text{E-}12 * \text{EXP}(340./\text{temp})$	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)
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. (2011)
G6300	UpStTrGNCl	$\text{ClO} + \text{NO} \rightarrow \text{LossO3Cl} + \text{LossO3Nn} + \text{NO}_2 + \text{Cl}$	$6.2\text{E-}12 * \text{EXP}(295./\text{temp})$	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	TrGNCl	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	$6.918\text{E-}7 * \text{exp}(-10909./\text{temp}) * \text{cair}$	Anderson and Fahey (1990)
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	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{LossO3Cl} + \text{LossO3} + \text{HO}_2 + \text{Cl} + \text{HCHO}$	$3.3\text{E-}12 * \text{EXP}(-115./\text{temp})$	Sander et al. (2011)
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow 4.0 \text{ ProdLCl} + \text{ClO} + 3 \text{ Cl}$	$3.3\text{E-}10$	Sander et al. (2011)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{ProdLCl} + \text{LossO3Cl} + \text{LossO3} + \text{OH} + \text{Cl}$	$1.65\text{E-}10$	see note
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{ProdLCl} + \text{H}_2\text{O} + \text{Cl}$	$2.4\text{E-}12 * \text{EXP}(-1250./\text{temp})$	Sander et al. (2011)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 3 \text{ ProdLCl} + \text{LossO3Cl} + \text{LossO3} + \text{OH} + 3 \text{ Cl}$	$3.\text{E-}10$	see note
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 3 \text{ ProdLCl} + \text{H}_2\text{O} + 3 \text{ Cl}$	$1.64\text{E-}12 * \text{EXP}(-1520./\text{temp})$	Sander et al. (2011)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HCl}$	$\text{k\_3rd\_iupac}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$8.0\text{e-}11$	Atkinson et al. (2006)
G6500	StGFCl	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow 2 \text{ ProdLCl} + \text{ClO} + \text{Cl}$	$1.4\text{E-}10$	Sander et al. (2011)
G6501	StGFCl	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow 3 \text{ ProdLCl} + \text{ClO} + 2 \text{ Cl}$	$2.3\text{E-}10$	Sander et al. (2011)
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	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow 2 \text{ LossO3Br} + 2 \text{ LossO3} + \text{Br} + \text{O}_2$	$1.9\text{E-}11 * \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{ LossO3Br} + 2 \text{ LossO3} + 2 \text{ Br} + \text{O}_2$	$2.7\text{E-}12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{ LossO3Br} + 2 \text{ LossO3} + \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14 * \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E-}12 * \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)



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

#	labels	reaction	rate coefficient	reference
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	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{LossO3Br} + \text{LossO3} + \text{OH} + \text{BrO}$	$1.2\text{E}-10*\text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{ProdO3} + \text{HOBr} + \text{Br}$	$2.0\text{E}-11*\text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGNBr	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	$4.9\text{E}-11$	Orlando and Tyndall (1996)
G7301	StTrGNBr	$\text{BrO} + \text{NO} \rightarrow \text{LossO3Br} + \text{LossO3Nn} + \text{Br} + \text{NO}_2$	$8.7\text{E}-12*\text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGNBr	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	$k_{\text{BrO\_NO2}}$	Atkinson et al. (2007)*
G7303	TrGNBr	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO\_NO2}}/(5.44\text{E}-9*\text{exp}(14192./\text{temp})$ $*1.\text{E6}*R_{\text{gas}}*\text{temp}/(\text{atm2Pa}*N_{\text{A}}))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E}-12*\text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.6\text{E}-12*\text{EXP}(-1600./\text{temp})$	Kondo and Benson (1984)
G7402a	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{HCHO}$	$\text{G7402a\_yield}*5.7\text{E}-12$	Aranda et al. (1997)
G7402b	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{LossO3Br} + \text{LossO3} + \text{Br} + \text{HCHO} + \text{HO}_2$	$(1.-\text{G7402a\_yield})*5.7\text{E}-12$	Aranda et al. (1997)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{ProdLBr} + \text{H}_2\text{O} + \text{Br}$	$2.35\text{E}-12*\text{EXP}(-1300./\text{temp})$	Sander et al. (2011)
G7404	TrGCB	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HBr}$	$2.8\text{E}-13*\text{EXP}(224./\text{temp})/(1.+$ $1.13\text{E}24*\text{EXP}(-3200./\text{temp})/\text{C}(\text{ind\_02}))$	Atkinson et al. (2006)*
G7405	TrGCB	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$1.8\text{E}-11*\text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow 3 \text{ ProdSBr} + \text{H}_2\text{O} + 3 \text{ Br}$	$1.35\text{E}-12*\text{EXP}(-600./\text{temp})$	Sander et al. (2011)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow 2 \text{ ProdSBr} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E}-12*\text{EXP}(-840./\text{temp})$	Sander et al. (2011)*
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	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E}-10*\text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{LossO3} + \text{Br} + \text{OClO}$	$1.6\text{E}-12*\text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{LossO3Br} + \text{LossO3Cl} + 2 \text{ LossO3} + \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E}-12*\text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{LossO3Br} + \text{LossO3Cl} + 2 \text{ LossO3} + \text{BrCl} + \text{O}_2$	$5.8\text{E}-13*\text{EXP}(170./\text{temp})$	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	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{ProdSBr} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E}-12*\text{EXP}(-840./\text{temp})$	see note
G7606	TrGClBr	$\text{CHClBr}_2 + \text{OH} \rightarrow 2 \text{ ProdSBr} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E}-12*\text{EXP}(-840./\text{temp})$	see note
G7607	TrGClBr	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{ProdSBr} + \text{H}_2\text{O} + \text{Br}$	$2.4\text{E}-12*\text{EXP}(-920./\text{temp})$	Sander et al. (2011)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{LossO3} + \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0.,$ $0.6)$	Sander et al. (2011)
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)*

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

#	labels	reaction	rate coefficient	reference
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	$k_{\text{DMS\_OH}}$	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{LossO3} + \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-}13*\text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow 0.6 \text{ ProdO3} + .6 \text{ SO}_2 + \text{HCHO} + .6 \text{ CH}_3\text{O}_2 + .4 \text{ HO}_2 + .4 \text{ CH}_3\text{SO}_3\text{H}$	$1.\text{E-}10$	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{ProdO3} + \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.8\text{E}13*\text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{LossO3} + \text{CH}_3\text{SO}_3$	$3.\text{E-}13$	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5.\text{E-}11$	Barone et al. (1995)
G9600	TrGSCl	$\text{DMS} + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCl} + \text{HCHO}$	$3.3\text{E-}10$	Atkinson et al. (2004)
G9700	TrGSBr	$\text{DMS} + \text{Br} \rightarrow \text{CH}_3\text{SO}_2 + \text{HBr} + \text{HCHO}$	$9.\text{E-}11*\text{EXP}(-2386./\text{temp})$	Jefferson et al. (1994)
G9701	TrGSBr	$\text{DMS} + \text{BrO} \rightarrow \text{LossO3} + \text{DMSO} + \text{Br}$	$4.4\text{E-}13$	Ingham et al. (1999)
G01Diag	StTrG	$\text{O}_3(\text{s}) \rightarrow \text{LO}_3(\text{s})$	$k_{\text{O3s}}$	Roelofs and Lelieveld (1997)*
G9100	TrStGS	$\text{SO} + \text{O}_2 \rightarrow 2 \text{ ProdO3} + \text{SO}_2 + \text{O}(^3\text{P})$	$1.25\text{e-}13*\text{exp}(-2190/\text{temp})$	Sander et al. (2011)*
G9101	TrStGS	$\text{SO} + \text{O}_3 \rightarrow \text{SO}_2 + \text{O}_2$	$3.4\text{e-}12*\text{exp}(-1100/\text{temp})$	Sander et al. (2011)*
G9102	TrStGS	$\text{S} + \text{O}_2 \rightarrow \text{ProdO3} + \text{SO} + \text{O}(^3\text{P})$	$2.3\text{e-}12$	Sander et al. (2011)*
G9201	TrStGS	$\text{SH} + \text{O}_2 \rightarrow \text{OH} + \text{SO}$	$4.\text{e-}19$	Sander et al. (2011)*
G9202	TrStGS	$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$	$8.5\text{e-}41*\text{exp}(6540./\text{temp})*\text{C}(\text{ind\_H2O})$	Sander et al. (2003)*
G9406	TrStGS	$\text{OCS} + \text{OH} \rightarrow \text{SH} + \text{CO}_2$	$1.1\text{e-}13*\text{exp}(-1200./\text{temp})$	Sander et al. (2011)*
G9407	TrStGS	$\text{OCS} + \text{O}(^3\text{P}) \rightarrow \text{LossO3} + \text{CO} + \text{SO}$	$2.1\text{e-}11*\text{exp}(-2200./\text{temp})$	Sander et al. (2011)*
G10G6501	StGFCI	$(\text{CFCl}_3)_\text{c} + \text{O}(^1\text{D}) \rightarrow \text{O}(^1\text{D})$	$2.3\text{E-}10$	Sander et al. (2011)*
G12G6500	StGFCI	$(\text{CF}_2\text{Cl}_2)_\text{c} + \text{O}(^1\text{D}) \rightarrow \text{O}(^1\text{D})$	$1.4\text{E-}10$	Sander et al. (2011)*
G14G3102a	UpStGN	$(\text{N}_2\text{O})_\text{c} + \text{O}(^1\text{D}) \rightarrow \text{O}(^1\text{D})$	$7.25\text{E-}11*\text{EXP}(20./\text{temp})$	Sander et al. (2011)*
G15G3102b	StGN	$(\text{N}_2\text{O})_\text{c} + \text{O}(^1\text{D}) \rightarrow \text{O}(^1\text{D}) + \dots$	$4.63\text{E-}11*\text{EXP}(20./\text{temp})$	Sander et al. (2011)*
G17G6407	StGCCl	$(\text{CH}_3\text{CCl}_3)_\text{c} + \text{O}(^1\text{D}) \rightarrow \text{O}(^1\text{D})$	$3.\text{E-}10$	see note
G18G6408	StTrGCCl	$(\text{CH}_3\text{CCl}_3)_\text{c} + \text{OH} \rightarrow \text{OH}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Sander et al. (2011)*

\*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:

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

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

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

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

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

G10G6501, G12G6500, G14G3102a, G15G3102b, G17G6407, and G18G6408 are “diagnostic” reactions. They are identical to the corresponding reactions without prefix Gxy (xy=10,12,14,15,17,18). The diagnostic

species with index “*c*” are kept constant by Newtonian relaxation (MESSy submodel TNUDGE) in the lowest model layer and react in the same way, however non-competing for the reaction partners, as the corresponding prognostic species without index “*c*”.

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  $\text{CH}_3\text{CHO} + \text{NO}_3$ . At 298 K,  $k = 5.8 \times 10^{-16}$ .

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

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

G4207: The rate constant  $8.01\text{E-}12$  is for the H abstraction in alpha to the  $-\text{OOH}$  group (Rickard and Pascoe, 2009) and  $0.6*\text{k\_CH3OOH\_OH}$  is for the  $\text{C}_2\text{H}_5\text{O}_2$  channel. The branching ratios are calculated from the terms of the rate coefficient at 298 K.

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

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

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

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

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

G4401:  $\text{NC}_4\text{H}_9\text{O}$  and  $\text{SC}_4\text{H}_9\text{O}$  are substituted with  $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2$  and  $0.636 \text{ MEK} + \text{HO}_2$  and  $0.364 \text{ CH}_3\text{CHO} + \text{C}_2\text{H}_5\text{O}_2$ , respectively. The stoichiometric coefficients on the right side are weighted averages.

G4403: The alkyl nitrate yield is the weighted average yield for the two isomers forming from  $\text{NC}_4\text{H}_9\text{O}_2$  and  $\text{SC}_4\text{H}_9\text{O}_2$ .

G4404: The product distribution is the weighted average of the single isomer hydroperoxides. It is calculated from the rate constants of single channels and the ratio of the isomers  $\text{NC}_4\text{H}_9\text{O}_2$  and  $\text{SC}_4\text{H}_9\text{O}_2$ . The overall rate constant for this reaction is calculated as weighted average of the channels rate constants. The relative weight of the products from  $\text{NC}_4\text{H}_9\text{OOH}$  and  $\text{SC}_4\text{H}_9\text{OOH}$  are then 0.0887 and 0.9113. The

channels producing  $\text{RO}_2$  are given the rate coefficient  $0.6 \cdot k_{\text{CH300H\_OH}}$  as for G4107. For  $\text{NC4H9OOH}$  the products are  $0.327 \text{ NC4H9O2} + 0.673 \text{ C3H7CHO} + 0.673 \text{ OH}$ .  $\text{C3H7CHO}$  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  $\text{SC4H9OOH}$  the products are  $0.219 \text{ SC4H9O2} + 0.781 \text{ MEK} + 0.781 \text{ OH}$ .

G4415: Alkyl nitrate formation is neglected. The products of  $\text{MEKAO}$  and  $\text{MEKCO}$  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:  $\text{LMEKOOH}$  is assumed having the composition  $0.459 \text{ MEKAOOH} + 0.462 \text{ MEKBOOH} + 0.079 \text{ MEKCOOH}$ .  $\text{MEKAOOH} + \text{OH}$  gives  $0.89 \text{ CO2C3CHO} + 0.89 \text{ OH} + 0.11 \text{ MEKAO2} + \text{H}_2\text{O}$ .  $\text{CO2C3CHO}$  is substituted with  $\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$  and the products become  $0.89 \text{ CH}_3\text{COCH}_2\text{O}_2 + 0.89 \text{ CO}_2 + 0.89 \text{ OH} + 0.11 \text{ MEKAO2} + \text{H}_2\text{O}$ .  $\text{MEKBOOH} + \text{OH}$  gives  $0.758 \text{ BIACET} + 0.758 \text{ OH} + 0.242 \text{ MEKBO2} + \text{H}_2\text{O}$ .  $\text{MEKCOOH} + \text{OH}$  gives  $0.614 \text{ EGLYOX} + 0.614 \text{ OH} + 0.386 \text{ MEKCO2} + \text{H}_2\text{O}$ .  $\text{EGLYOX}$  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  $\text{NC4H9NO3}$  and  $\text{SC4H9NO3}$ , respectively. Product distribution is calculated accordingly.  $\text{NC4H9NO3} + \text{OH}$  gives  $\text{C3H7CHO} + \text{NO}_2 + \text{H}_2\text{O}$  with

$\text{C3H7CHO}$  being substituted with  $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2$ . After substitution is obtained  $2 \text{ CO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 + \text{H}_2\text{O}$ .  $\text{SC4H9NO3} + \text{OH}$  gives  $\text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$ . For the product distribution  $\text{NC4H9NO3}$  and  $\text{SC4H9NO3}$  account for 0.08577 and 0.91423, respectively.

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

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

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).

G6409: It is assumed that the reaction liberates all Cl atoms in the form of  $\text{HCl}$ .

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  $\text{HBr}$ .

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:  $\text{CH}_2\text{Br}_2 + \text{OH}$  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:  $\text{CH}_2\text{Br}_2 + \text{OH}$  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.

G9100: Only in “aero” and “aecl” sensitivity studies.

G9101: Only in “aero” and “aecl” sensitivity studies.

G9102: Only in “aero” and “aecl” sensitivity studies.

G9201: Only in “aero” and “aecl” sensitivity studies.

G9202: Only in “aero” and “aecl” sensitivity studies.

G9406: Only in “aero” and “aecl” sensitivity studies.

G9400: Addition path. The rate coefficient is:  $k_{\text{DMS\_OH}} = 1.0\text{E-}39 \cdot \text{EXP}(5820./\text{temp}) \cdot \text{C}(\text{ind\_02}) / (1. + 5.0\text{E-}30 \cdot \text{EXP}(6280./\text{temp}) \cdot \text{C}(\text{ind\_02}))$ .

G9407: Only in “aero” and “aecl” sensitivity studies.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow 2. \text{ProdO3} + O(^3P) + O(^3P)$	jx(ip_02)	see note
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	jx(ip_01D)	see note
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	jx(ip_03P)	see note
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	see note
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	see note
J3100	UpStGNJ	$N_2O + h\nu \rightarrow \text{ProdO3} + O(^1D) + N_2$	jx(ip_N20)	see note
J3101	UpStTrGNJ	$NO_2 + h\nu \rightarrow \text{LossJ3101} + NO + O(^3P)$	jx(ip_N02)	see note
J3102a	UpStGNJ	$NO + h\nu \rightarrow \text{ProdO3} + N + O(^3P)$	jx(ip_N0)	see note
J3103a	UpStTrGNJ	$NO_3 + h\nu \rightarrow \text{LossJ3103a} + NO_2 + O(^3P)$	jx(ip_N020)	see note
J3103b	UpStTrGNJ	$NO_3 + h\nu \rightarrow 2 \text{LossO3N} + 2. \text{LossO3} + NO + O_2$	jx(ip_N002)	see note
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	see note
J3200	TrGNJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HN03)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow 0.333 \text{ProdO3} + .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	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_CH0H)	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow \text{ProdO3} + CO + O(^3P)$	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)	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_CH3C03H)	see note
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	$0.19*jx(ip\_CH0H)$	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	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	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	$0.074*jx(ip\_CH0H)$	see note
J4303	TrGCJ	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	see note
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HCHO + OH$	jx(ip_CH300H)	see note
J4305	TrGNCJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	jx(ip_PAN)	see note
J4306	TrGNCJ	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	$3.7*jx(ip\_PAN)$	see note
J4400	TrGCJ	$LC_4H_9OOH + h\nu \rightarrow OH + .67 \text{MEK} + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	jx(ip_CH300H)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4401	TrGCJ	$\text{MVK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO} + \text{HO}_2$	$0.019 * \text{jx}(\text{ip\_C0H2}) + 0.015 * \text{jx}(\text{ip\_MGLY0X})$	see note
J4402	TrGCJ	$\text{MVKOOH} + h\nu \rightarrow \text{OH} + .5 \text{ MGLY0X} + .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ HCHO} + .75 \text{ HO}_2 + .25 \text{ CH}_3\text{C}(\text{O})\text{OO} + .25 \text{ CO}$	$\text{jx}(\text{ip\_CH300H})$	see note
J4403	TrGCJ	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2$	$0.42 * \text{jx}(\text{ip\_CH0H})$	see note
J4404	TrGCJ	$\text{LMEKOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CHO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	see note
J4405	TrGCJ	$\text{BIACET} + h\nu \rightarrow 2 \text{ CH}_3\text{C}(\text{O})\text{OO}$	$2.15 * \text{jx}(\text{ip\_MGLY0X})$	see note
J4406	TrGNCJ	$\text{LC4H9NO3} + h\nu \rightarrow \text{NO}_2 + .67 \text{ MEK} + .67 \text{ HO}_2 + .33 \text{ C}_2\text{H}_5\text{O}_2 + .33 \text{ CH}_3\text{CHO}$	$3.7 * \text{jx}(\text{ip\_PAN})$	see note
J4500	TrGCJ	$\text{ISOOH} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	see note
J4501	TrGNCJ	$\text{ISON} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$3.7 * \text{jx}(\text{ip\_PAN})$	see note
J6000	StTrGClJ	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$\text{jx}(\text{ip\_Cl2})$	see note
J6100	StTrGClJ	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2. \text{ LossO3} + 2 \text{ Cl}$	$\text{jx}(\text{ip\_Cl202})$	see note
J6101	StTrGClJ	$\text{OClO} + h\nu \rightarrow \text{ProdO3} + \text{ClO} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip\_0Cl0})$	see note
J6200	StGClJ	$\text{HCl} + h\nu \rightarrow \text{Cl} + \text{H}$	$\text{jx}(\text{ip\_HCl})$	see note
J6201	StTrGClJ	$\text{HOCl} + h\nu \rightarrow \text{LossO3Cl} + \text{LossO3} + \text{OH} + \text{Cl}$	$\text{jx}(\text{ip\_H0Cl})$	see note
J6300	TrGNClJ	$\text{ClNO}_2 + h\nu \rightarrow \text{ProdO3} + \text{Cl} + \text{NO}_2$	$\text{jx}(\text{ip\_ClNO2})$	see note
J6301a	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	$\text{jx}(\text{ip\_ClNO3})$	see note
J6301b	StTrGNClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$\text{jx}(\text{ip\_ClON02})$	see note
J6400	StGClJ	$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{ProdLCl} + \text{Cl} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_CH3Cl})$	see note
J6401	StGClJ	$\text{CCl}_4 + h\nu \rightarrow 4 \text{ ProdLCl} + 4 \text{ Cl}$	$\text{jx}(\text{ip\_CC14})$	see note
J6402	StGCClJ	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3 \text{ ProdLCl} + 3 \text{ Cl}$	$\text{jx}(\text{ip\_CH3CC13})$	see note
J6500	StGFClJ	$\text{CFCl}_3 + h\nu \rightarrow 3 \text{ ProdLCl} + 3 \text{ Cl}$	$\text{jx}(\text{ip\_CFC13})$	see note
J6501	StGFClJ	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2 \text{ ProdLCl} + 2 \text{ Cl}$	$\text{jx}(\text{ip\_CF2Cl2})$	see note
J7000	StTrGBrJ	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	$\text{jx}(\text{ip\_Br2})$	see note
J7100	StTrGBrJ	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip\_Br0})$	see note
J7200	StTrGBrJ	$\text{HOBr} + h\nu \rightarrow \text{LossO3Br} + \text{LossO3} + \text{Br} + \text{OH}$	$\text{jx}(\text{ip\_H0Br})$	see note
J7300	TrGNBrJ	$\text{BrNO}_2 + h\nu \rightarrow \text{ProdO3} + \text{Br} + \text{NO}_2$	$\text{jx}(\text{ip\_BrNO2})$	see note
J7301	StTrGNBrJ	$\text{BrNO}_3 + h\nu \rightarrow 0.85 \text{ Br} + 0.85 \text{ NO}_3 + 0.15 \text{ BrO} + 0.15 \text{ NO}_2$	$\text{jx}(\text{ip\_BrNO3})$	see note
J7400	StGBrJ	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{ProdLBr} + \text{Br} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_CH3Br})$	see note
J7401	TrGBrJ	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2 \text{ ProdSBr} + 2 \text{ Br}$	$\text{jx}(\text{ip\_CH2Br2})$	see note
J7402	TrGBrJ	$\text{CHBr}_3 + h\nu \rightarrow 3 \text{ ProdSBr} + 3 \text{ Br}$	$\text{jx}(\text{ip\_CHBr3})$	see note
J7500	StGFBrJ	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{ProdLBr} + \text{Br}$	$\text{jx}(\text{ip\_CF3Br})$	see note
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_BrCl})$	see note
J7601	StGFBrJ	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{ProdLBr} + \text{ProdLCl} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CF2ClBr})$	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7602	TrGClBrJ	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{ProdSBr} + \text{ProdSCl} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CH2ClBr})$	see note
J7603	TrGClBrJ	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{ProdSBr} + 2 \text{ProdSCl} + \text{Br} + 2 \text{Cl}$	$\text{jx}(\text{ip\_CHCl2Br})$	see note
J7604	TrGClBrJ	$\text{CHClBr}_2 + h\nu \rightarrow 2 \text{ProdSBr} + \text{ProdSCl} + 2 \text{Br} + \text{Cl}$	$\text{jx}(\text{ip\_CHClBr2})$	see note
J8401a	TrGJ	$\text{CH}_3\text{I} + h\nu \rightarrow \text{CH}_3\text{O}_2$	$\text{JX}(\text{ip\_CH3I})$	see note
J9000	TrStGSJ	$\text{OCS} + h\nu \rightarrow \text{CO} + \text{S}$	$\text{JX}(\text{ip\_OCS})$	see note
J9001	TrStGSJ	$\text{SO}_2 + h\nu \rightarrow \text{SO} + \text{O}(^3\text{P})$	$60.*\text{JX}(\text{ip\_OCS})$	see note
J9002	TrStGSJ	$\text{SO}_3 + h\nu \rightarrow \text{SO}_2 + \text{O}(^3\text{P})$	$\text{JX}(\text{ip\_SO3})$	see note
J9003	TrStGSJ	$\text{H}_2\text{SO}_4 + h\nu \rightarrow \text{SO}_3 + \text{H}_2\text{O}$	$\text{JX}(\text{ip\_H2SO4})$	see note
J11J6500	StGFClJ	$(\text{CFCl}_3)_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_CFC13})$	see note
J13J6501	StGFClJ	$(\text{CF}_2\text{Cl}_2)_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_CF2Cl2})$	see note
J16J3100	UpStGNJ	$(\text{N}_2\text{O})_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_N2O})$	see note
J19J6402	StGCClJ	$(\text{CH}_3\text{CCl}_3)_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_CH3CCl3})$	see note
J20J7601	StGFBrJ	$(\text{CF}_2\text{ClBr})_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_CF2ClBr})$	see note
J21J7500	StGFBrJ	$(\text{CF}_3\text{Br})_c + h\nu \rightarrow \dots$	$\text{jx}(\text{ip\_CF3Br})$	see note

\*Notes:

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

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

$\text{J}(11) \rightarrow \text{jx}(\text{ip\_COH2})$   
 $\text{J}(12) \rightarrow \text{jx}(\text{ip\_CHOH})$   
 $\text{J}(15) \rightarrow \text{jx}(\text{ip\_HOCH2CHO})$   
 $\text{J}(18) \rightarrow \text{jx}(\text{ip\_MACR})$   
 $\text{J}(22) \rightarrow \text{jx}(\text{ip\_ACETOL})$   
 $\text{J}(23)+\text{J}(24) \rightarrow \text{jx}(\text{ip\_MVK})$   
 $\text{J}(31)+\text{J}(32)+\text{J}(33) \rightarrow \text{jx}(\text{ip\_GLYOX})$   
 $\text{J}(34) \rightarrow \text{jx}(\text{ip\_MGLYOX})$   
 $\text{J}(41) \rightarrow \text{jx}(\text{ip\_CH3OOH})$   
 $\text{J}(53) \rightarrow \text{J}(\text{iC}_3\text{H}_7\text{ONO}_2)$

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

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

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

J11J6500, J13J6501, J16J3100, J19J6402, J20J7601, and J21J7500 are “diagnostic” reactions. They are identical to the corresponding reactions without prefix Jxy (xy=11,13,16,19,20,21). The diagnostic species with index “c” are kept constant by Newtonian relaxation (MESSy submodel TNUDGE) in the lowest model layer and photolyse in the same way as the corresponding prognostic species without index “c”.

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

J4306: Following von Kuhlmann et al. (2003), we use

$\text{J}(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7*\text{jx}(\text{ip\_PAN})$ .

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

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

J7301: The quantum yields are recommended by Sander et al. (2011) for  $\lambda > 300\text{nm}$  and used here for the entire spectrum.

J9000: Only in “aero” and “aecl” sensitivity studies.

J9001: Only in “aero” and “aecl” sensitivity studies.

J9002: Only in “aero” and “aecl” sensitivity studies.

J9003: Only in “aero” and “aecl” sensitivity studies.

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)
H <sub>2</sub> O	BIG	0.	see note
NH <sub>3</sub>	58.	4085.	Chameides (1984)
NO	$1.9 \times 10^{-3}$	1480.	Schwartz and White (1981)
NO <sub>2</sub>	$7.0 \times 10^{-3}$	2500.	Lee and Schwartz (1981)*
NO <sub>3</sub>	2.	2000.	Thomas et al. (1993)
N <sub>2</sub> O <sub>5</sub>	BIG	0.	see note
HONO	$4.9 \times 10^1$	4780.	Schwartz and White (1981)
HNO <sub>3</sub>	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO <sub>4</sub>	$1.2 \times 10^4$	6900.	Régimbal and Mozurkewich (1997)
CH <sub>3</sub> OH	$2.20 \times 10^2$	5200.	Snider and Dawson (1985)
CH <sub>3</sub> O <sub>2</sub>	6.	5600.	Jacob (1986)*
CH <sub>3</sub> OOH	$3.0 \times 10^2$	5322.	Lind and Kok (1994)
CO <sub>2</sub>	$3.1 \times 10^{-2}$	2423.	Chameides (1984)
HCHO	$7.0 \times 10^3$	6425.	Chameides (1984)
HCOOH	$3.7 \times 10^3$	5700.	Chameides (1984)
CH <sub>3</sub> COOH	$4.1 \times 10^3$	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	6.	5600.	see note
CH <sub>3</sub> CHO	$1.29 \times 10^1$	5890.	Sander et al. (2006)
CH <sub>3</sub> COCH <sub>3</sub>	28.1	5050.	Sander et al. (2006)
MGLYOX	$3.70 \times 10^3$	7500.	Betterton and Hoffmann (1988)
Cl <sub>2</sub>	$9.2 \times 10^{-2}$	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	$6.7 \times 10^2$	5862.	Huthwelker et al. (1995)
ClNO <sub>3</sub>	BIG	0.	see note
Br <sub>2</sub>	$7.7 \times 10^{-1}$	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	$9.3 \times 10^1$	5862.	Vogt et al. (1996)*



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

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

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

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

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

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

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

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

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

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	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO <sub>2</sub>	0.5	(default)	Thornton and Abbatt (2005)
H <sub>2</sub> O <sub>2</sub>	0.077	3127.	Worsnop et al. (1989)
H <sub>2</sub> O	0.0	(default)	see note
NH <sub>3</sub>	0.06	(default)	DeMore et al. (1997)*
NO	$5.0 \times 10^{-5}$	(default)	Saastad et al. (1993)*
NO <sub>2</sub>	0.0015	(default)	Ponche et al. (1993)*
NO <sub>3</sub>	0.04	(default)	Rudich et al. (1996)*
N <sub>2</sub> O <sub>5</sub>	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO <sub>3</sub>	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO <sub>4</sub>	(default)	(default)	DeMore et al. (1997)*
CH <sub>3</sub> OH	(default)	(default)	see note
CH <sub>3</sub> O <sub>2</sub>	0.01	2000.	see note
CH <sub>3</sub> OOH	0.0046	3273.	Magi et al. (1997)
CO <sub>2</sub>	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH <sub>3</sub> COOH	$2.0 \times 10^{-2}$	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	(default)	(default)	see note
CH <sub>3</sub> CHO	$3.0 \times 10^{-2}$	(default)	see note
CH <sub>3</sub> COCH <sub>3</sub>	$3.72 \times 10^{-3}$	6395.	Davidovits et al. (1995)
MGLYOX	(default)	(default)	see note
Cl <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
ClNO <sub>3</sub>	0.108	(default)	Deiber et al. (2004)*
Br <sub>2</sub>	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
BrNO <sub>3</sub>	0.063	(default)	Deiber et al. (2004)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{\text{K}}$	reference
BrCl	0.038	6546.	see note
SO <sub>2</sub>	0.11	(default)	DeMore et al. (1997)
H <sub>2</sub> SO <sub>4</sub>	0.65	(default)	Pöschl et al. (1998)*
CH <sub>3</sub> SO <sub>3</sub> H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)

\*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):

$$\begin{aligned} \frac{\alpha}{1-\alpha} &= \exp\left(\frac{-\Delta_{\text{obs}}G}{RT}\right) \\ &= \exp\left(\frac{-\Delta_{\text{obs}}H}{RT} + \frac{\Delta_{\text{obs}}S}{R}\right) \end{aligned}$$

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:

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

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

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

OH: Value measured at 293 K.

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

NO: Value measured between 193 and 243 K.

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

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

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

HONO: Value measured between 247 and 297 K.

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

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

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

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

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

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

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

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

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

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

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

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

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

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

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

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

#	labels	reaction	rate coefficient	reference
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\*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 ( $X = \text{N}_2\text{O}_5$ ,  $\text{ClNO}_3$ , or  $\text{BrNO}_3$ ) and subsequent reaction with  $\text{H}_2\text{O}$ ,  $\text{Cl}^-$ , and  $\text{Br}^-$ , 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  $k_{\text{mt}}$ . The factors only affect the branching between hy-

drolysis and the halide reactions. The factor  $5 \times 10^2$  was chosen such that the chloride reaction dominates over hydrolysis at about  $[\text{Cl}^-] > 0.1 \text{ M}$  (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio  $[\text{H}_2\text{O}]/[\text{Cl}^-]$  is less than  $5 \times 10^2$ . The ratio  $5 \times 10^2 / 3 \times 10^5$  was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow \text{LossO3N} + 1. \text{ LossO3} + 2 \text{ HNO}_3$	<code>khet_St(ihs_N205_H20)</code>	see note
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 3. \text{ LossO3} + 2 \text{ NO}_3^-(\text{aq}) + 2 \text{ H}^+(\text{aq})$	<code>khet_Tr(iht_N205)</code>	see note
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{LossO3Cl} + 1. \text{ LossO3} + \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see note
HET420	StHetNCl	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{LossO3Cl} + 1. \text{ LossO3} + \text{Cl}_2 + \text{HNO}_3$	<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	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow 2. \text{ LossO3} + \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N205_HCl)</code>	see note
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{LossO3Br} + 1. \text{ LossO3} + \text{Br}_2 + \text{H}_2\text{O}$	<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	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{LossO3Cl} + 1. \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see note
HET541	StHetNClBr	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{LossO3Br} + 1. \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see note
HET542	StHetClBr	$\text{HOCl} + \text{HBr} \rightarrow \text{LossO3Cl} + 1. \text{ LossO3} + \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see note
HET543	StHetClBr	$\text{HOBr} + \text{HCl} \rightarrow \text{LossO3Br} + 1. \text{ LossO3} + \text{BrCl} + \text{H}_2\text{O}$	<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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