

# The Chemical Mechanism of MECCA

KPP version: 2.2.1\_rs5

MECCA version: 3.7f

Date: April 7, 2015.

Selected reactions:

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

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 164

Aqueous phase: 0

All species: 164

Number of reactions in selected mechanism:

Gas phase (Gnn): 218

Aqueous phase (Annn): 0

Henry (Hnnn): 0

Photolysis (Jnnn): 68

Aqueous phase photolysis (PHnnn): 0

Heterogeneous (HETnnn): 12

Equilibria (EQnnn): 0

Isotope exchange (DGNnnn): 0

Dummy (Dnnn): 0

All equations: 298

This document is part of the electronic supplement to our article

“The atmospheric chemistry box model CAABA/MECCA-3.0”

in Geosci. Model Dev. (2011), available at:

<http://www.geosci-model-dev.net>

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	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	$O_3 + O(^1D) \rightarrow 2.0 \text{ o3lossxo} + 2.0 \text{ LossO3O} + 2. \text{ LossO3} + 2 O_2$	$1.2E-10$	Sander et al. (2011)*
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2.0 \text{ LossO3O} + 2. \text{ LossO3} + 2 O_2$	$8.E-12*EXP(-2060./temp)$	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	$H + O_3 \rightarrow 1.0 \text{ o3lossxo} + \text{LossO3H} + 1. \text{ LossO3} + OH + O_2$	$1.4E-10*EXP(-470./temp)$	Sander et al. (2011)
G2102	UpStG	$H_2 + O(^1D) \rightarrow 1.0 \text{ o3lossxo} + \text{LossO3H} + 1. \text{ LossO3} + H + OH$	$1.2E-10$	Sander et al. (2011)
G2103	UpStG	$OH + O(^3P) \rightarrow \text{LossO3H} + 1. \text{ LossO3} + H + O_2$	$1.8E-11*EXP(180./temp)$	Sander et al. (2011)
G2104	UpStTrG	$OH + O_3 \rightarrow 1.0 \text{ o3lossoh} + 1.0 \text{ LossG2104} + \text{LossO3H} + \text{LossOH} + 1. \text{ LossO3} + HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	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	$HO_2 + O(^3P) \rightarrow 1.0 \text{ LossG2106} + \text{LossO3H} + 1. \text{ LossO3} + OH + O_2$	$3.E-11*EXP(200./temp)$	Sander et al. (2011)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow 1.0 \text{ o3lossho2} + 1.0 \text{ LossG2107} + \text{LossO3H} + \text{LossHO2} + 1. \text{ LossO3} + OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	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	$HO_2 + H \rightarrow \text{LossO3Hn} + 1. \text{ ProdO3} + O(^3P) + H_2O$	$1.6E-12$	Sander et al. (2011)
G2109	UpStTrG	$HO_2 + OH \rightarrow \text{lossho2oh} + H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Sander et al. (2011)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow \text{ho2lossHO2} + 1.0 \text{ LossG2110} + H_2O_2 + O_2$	$k\_H02\_H02$	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 1.0 \text{ o3lossxo} + \text{LossO3O} + \text{LossO1D} + 1. \text{ LossO3} + 2 OH$	$1.63E-10*EXP(60./temp)$	Sander et al. (2011)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$1.8E-12$	Sander et al. (2011)
G3100	UpStGN	$N + O_2 \rightarrow \text{LossO3Nn} + 1. \text{ ProdO3} + NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	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	$N_2O + O(^1D) \rightarrow 1.0 \text{ o3lossxo} + \text{noprodN2O} + \text{LossO3O} + 1. \text{ LossO3} + 2 NO$	$7.25E-11*EXP(20./temp)$	Sander et al. (2011)
G3102b	StGN	$N_2O + O(^1D) \rightarrow 1.0 \text{ o3lossxo} + \text{LossO3O} + 1. \text{ LossO3} + N_2 + O_2$	$4.63E-11*EXP(20./temp)$	Sander et al. (2011)

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

#	labels	reaction	rate coefficient	reference
G3103	UpStTrGN	$\text{NO} + \text{O}_3 \rightarrow 1.0 \text{ LossG3103} + \text{NO}_2 + \text{O}_2$	$3.5\text{E-}12\text{*EXP}(-1500./\text{temp})$	Sander et al. (2011)
G3104	UpStGN	$\text{NO} + \text{N} \rightarrow \text{LossO3Nn} + 1. \text{ ProdO3} + \text{O}(^3\text{P}) + \text{N}_2$	$2.1\text{E-}11\text{*EXP}(100./\text{temp})$	Sander et al. (2011)
G3105	UpStGN	$\text{NO}_2 + \text{O}(^3\text{P}) \rightarrow 1.0 \text{ LossG3105} + 2.0 \text{ LossO3N2} + 2.0 \text{ LossO3N} + 2. \text{ LossO3} + \text{NO} + \text{O}_2$	$5.1\text{E-}12\text{*EXP}(210./\text{temp})$	Sander et al. (2011)
G3106	StTrGN	$\text{NO}_2 + \text{O}_3 \rightarrow 1.0 \text{ LossG3106} + \text{NO}_3 + \text{O}_2$	$1.2\text{E-}13\text{*EXP}(-2450./\text{temp})$	Sander et al. (2011)
G3107	UpStGN	$\text{NO}_2 + \text{N} \rightarrow \text{N}_2\text{O} + \text{O}(^3\text{P})$	$5.8\text{E-}12\text{*EXP}(220./\text{temp})$	Sander et al. (2011)
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	$\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	k_N03_N02	Sander et al. (2011)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	k_N03_N02/(2.7E-27*EXP(11000./temp))	Sander et al. (2011)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	k_3rd(temp, cair, 7.0E-31, 2.6, 3.6E-11, 0.1, 0.6)	Sander et al. (2011)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow 1.0 \text{ o3prodho2} + 1.0 \text{ LossG3201} + \text{ProdHO2} + 1. \text{ ProdO3} + \text{NO}_2 + \text{OH}$	$3.3\text{E-}12\text{*EXP}(270./\text{temp})$	Sander et al. (2011)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{ohlossNO2} + 1.0 \text{ LossG3202} + \text{HNO}_3$	k_3rd(temp, cair, 1.8E-30, 3.0, 2.8E-11, 0., 0.6)	Sander et al. (2011)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	k_N02_H02	Sander et al. (2011)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow 1.0 \text{ o3lossno} + \text{LossO3N} + 1. \text{ LossO3} + \text{NO}_2 + \text{OH} + \text{O}_2$	3.5E-12	Sander et al. (2011)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow 1.0 \text{ o3prodho2} + \text{ohlossNO2} + \text{LossO3Nn} + 1. \text{ ProdO3} + \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11\text{*EXP}(-390./\text{temp})$	Sander et al. (2011)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow 1.0 \text{ o3prodho2} + \text{ohlossNO2} + \text{LossO3Nn} + 1. \text{ ProdO3} + \text{H}_2\text{O} + \text{NO}_3$	k_HN03_OH	Sander et al. (2011)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	k_N02_H02/(2.1E-27*EXP(10900./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	$\text{NH}_2 + \text{O}_3 \rightarrow 1. \text{ LossO3} + \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12\text{*EXP}(-930./\text{temp})$	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	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12\text{*}((\text{temp}/298.)\text{**}(-1.5))$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11\text{*}((\text{temp}/298.)\text{**}(-1.5))$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow 1. \text{ LossO3} + \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11\text{*}((\text{temp}/298.)\text{**}(-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow 1. \text{ LossO3} + \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11\text{*}((\text{temp}/298.)\text{**}(-2.0))$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow 1. \text{ LossO3} + \text{NH}_2 + \text{O}_2$	$1.2\text{E-}14$	Kohlmann and Poppe (1999)
G3218	TrGN	$\text{NH}_2\text{O} \rightarrow \text{NHOH}$	1.3E3	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)

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

#	labels	reaction	rate coefficient	reference
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E-}12 \cdot \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow 1. \text{ LossO3} + \text{HONO} + \text{NO}$	$1.0\text{E-}12 \cdot \text{EXP}(-1000./\text{temp})$	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	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11 \cdot \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14 \cdot \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4100	UpStG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 1. \text{ LossO3} + .75 \text{ CH}_3\text{O}_2 + .75 \text{ OH} + .25 \text{ HCHO} + .4 \text{ H} + .05 \text{ H}_2$	$1.75\text{E-}10$	Sander et al. (2011)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E-}20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp}) - 987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$2.9\text{E-}12 \cdot \text{EXP}(-345./\text{temp})$	Sander et al. (2011)
G4103	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{ho2loss} + \text{CH}_3\text{OOH} + \text{O}_2$	$4.1\text{E-}13 \cdot \text{EXP}(750./\text{temp})$	Sander et al. (2011)*
G4104	UpStTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{noprodro2} + \text{ProdMeO2} + 1. \text{ ProdO3} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E-}12 \cdot \text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow 1.0 \text{ o3lossno} + \text{LossO3N} + 1. \text{ LossO3} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E-}12$	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{ HCHO} + 2 \text{ HO}_2$	$9.5\text{E-}14 \cdot \text{EXP}(390./\text{temp}) / (1. + 1. / 26.2 \cdot \text{EXP}(1130./\text{temp}))$	Sander et al. (2011)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E-}14 \cdot \text{EXP}(390./\text{temp}) / (1. + 26.2 \cdot \text{EXP}(-1130./\text{temp}))$	Sander et al. (2011)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{ CH}_3\text{O}_2 + .3 \text{ HCHO} + .3 \text{ OH} + \text{H}_2\text{O}$	$k_{\text{CH3OOH\_OH}}$	Wallington et al.
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 \cdot \text{EXP}(2.03 \cdot \text{LOG}(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow 1.0 \text{ o3lossno} + \text{LossO3N} + 1. \text{ LossO3} + \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2011)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow 1.0 \text{ LossG4110} + \text{H} + \text{CO}_2$	$(1.57\text{E-}13 + \text{cair} \cdot 3.54\text{E-}33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$4.0\text{E-}13$	Sander et al. (2011)
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow 1.0 \text{ o3lossro} + \text{LossO3R} + 1. \text{ LossO3} + \text{HCHO} + .63 \text{ CO} + .13 \text{ HO}_2 + 0.23125 \text{ HCOOH} + 0.13875 \text{ HCHO} + 0.13875 \text{ H}_2\text{O}_2 + .13 \text{ OH}$	$1.2\text{E-}14 \cdot \text{EXP}(-2630./\text{temp})$	Sander et al. (2011)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 1.0\text{E-}28, 4.5, 7.5\text{E-}12, 0.85, 0.6)$	Sander et al. (2011)
G4203	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13 \cdot \text{EXP}(700./\text{temp})$	Sander et al. (2011)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1. \text{ ProdO3} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E-}12 \cdot \text{EXP}(365./\text{temp})$	Sander et al. (2011)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow 1.0 \text{ o3lossno} + 1. \text{ LossO3} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Wallington et al.

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

#	labels	reaction	rate coefficient	reference
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	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow 1.0 \text{o3lossno} + \text{LossO3N} + 1. \text{LossO3} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E}-12*\text{EXP}(-1900./\text{temp})$	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)
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow 1.0 \text{o3prodro2} + 1. \text{ProdO3} + \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+37.*\text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow 1.0 \text{o3prodro2} + \text{ProdRO2} + 1. \text{ProdO3} + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E}-12*\text{EXP}(270./\text{temp})$	Tyndall et al. (2001)
G4213	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{panprod} + \text{PAN}$	k_CH3C03_N02	Sander et al. (2011)*
G4214	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow 1.0 \text{o3lossno} + \text{LossO3N} + 1. \text{LossO3} + \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4215a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9*2.0\text{E}-12*\text{EXP}(500./\text{temp})$	Sander et al. (2011)
G4215b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO}$	$0.1*2.0\text{E}-12*\text{EXP}(500./\text{temp})$	Sander et al. (2011)
G4216	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{HO}_2 + .18 \text{CH}_3\text{COOH}$	$4.9\text{E}-12*\text{EXP}(211./\text{temp})$	Wallington et al., 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	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)
G4219	TrGNC	$\text{NACA} + \text{OH} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6\text{E}-12*\text{EXP}(270./\text{temp})$	Pöschl et al. (2000)
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{panloss} + \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$9.50\text{E}-13*\text{EXP}(-650./\text{temp})$	Rickard and Pascoe (2009)
G4221	TrGNC	$\text{PAN} \rightarrow \text{panloss} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2011)*
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .82 \text{iC}_3\text{H}_7\text{O}_2 + .18 \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(-87./\text{temp})$	Atkinson (2003)
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{LossO3R} + 1. \text{LossO3} + .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .04 \text{MGlyOX} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5\text{E}-15*\text{EXP}(-1900./\text{temp})$	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)	Wallington et al.
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow 1.0 \text{o3lossno} + 1. \text{LossO3} + \text{LC4H9NO3}$	$4.6\text{E}-13*\text{EXP}(-1155./\text{temp})$	Wallington et al.
G4304	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	k_PrO2_HO2	Atkinson (1997)

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

#	labels	reaction	rate coefficient	reference
G4305	TrGNC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodho2} + \text{ProdRO2} + 1. \text{ ProdO3}$ $+ .96 \text{ CH}_3\text{COCH}_3 + .96 \text{ HO}_2 + .96 \text{ NO}_2 + .04 \text{ iC}_3\text{H}_7\text{ONO}_2$	$k_{\text{PrO2\_NO}}$	Wallington et al.
G4306	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{ HCHO} + .8 \text{ HO}_2$ $+ .2 \text{ CH}_3\text{OH}$	$k_{\text{PrO2\_CH3O2}}$	Kirchner and Stockwell (1996)
G4307	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .3 \text{ iC}_3\text{H}_7\text{O}_2 + .7 \text{ CH}_3\text{COCH}_3 + .7$ $\text{OH}$	$k_{\text{CH300H\_OH}}$	see note*
G4308	TrGC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HO}_2 \rightarrow \text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH}$	$6.5\text{E-}13*\text{EXP}(650./\text{temp})$	Müller and Brasseur (1995)
G4309	TrGNC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2}$ $+ 1. \text{ ProdO3} + .98 \text{ CH}_3\text{CHO} + .98 \text{ HCHO} + .98 \text{ HO}_2 +$ $.98 \text{ NO}_2 + .02 \text{ LC4H9NO3}$	$4.2\text{E-}12*\text{EXP}(180./\text{temp})$	Müller and Brasseur (1995)
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	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1.$ $\text{ProdO3} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{NO}_2$	$2.9\text{E-}12*\text{EXP}(300./\text{temp})$	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	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow .3 \text{ CH}_3\text{COCH}_2\text{O}_2 + .7$ $\text{MGLYOX} + .7 \text{ OH}$	$k_{\text{CH300H\_OH}}$	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)
G4320	TrGNC	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13*\text{EXP}(-230./\text{temp})$	Wallington et al.
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	$\text{LC}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .88 \text{ MEK} + .68 \text{ HCHO} + 1.23 \text{ HO}_2$ $+ .12 \text{ CH}_3\text{CHO} + .12 \text{ C}_2\text{H}_5\text{O}_2 + .18 \text{ CH}_3\text{OH}$	$k_{\text{PrO2\_CH3O2}}$	see note*
G4402	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	$k_{\text{PrO2\_HO2}}$	see note*
G4403	TrGNC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1. \text{ ProdO3}$ $+ .84 \text{ NO}_2 + .56 \text{ MEK} + .56 \text{ HO}_2 + .28 \text{ C}_2\text{H}_5\text{O}_2 + .28$ $\text{CH}_3\text{CHO} + .16 \text{ LC4H9NO3}$	$k_{\text{PrO2\_NO}}$	see note*
G4404	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow .15 \text{ LC}_4\text{H}_9\text{O}_2 + .85 \text{ MEK} + .85 \text{ OH}$ $+ .85 \text{ H}_2\text{O}$	$k_{\text{CH300H\_OH}}$	see note*
G4405	TrGC	$\text{MVK} + \text{O}_3 \rightarrow 1.0 \text{ o3lossro} + \text{LossO3R} + 1. \text{ LossO3} + .45$ $\text{HCOOH} + .9 \text{ MGLYOX} + .1 \text{ CH}_3\text{C}(\text{O})\text{OO} + .19 \text{ OH} +$ $.22 \text{ CO} + .32 \text{ HO}_2$	$.5*(1.36\text{E-}15*\text{EXP}(-2112./\text{temp})$ $+7.51\text{E-}16*\text{EXP}(-1521./\text{temp}))$	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
G4406	TrGC	MVK + OH $\rightarrow$ MVKO2	.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))	Pöschl et al. (2000)
G4407	TrGC	MVKO2 + HO <sub>2</sub> $\rightarrow$ MVKOOH	1.82E-13*EXP(1300./temp)	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO $\rightarrow$ 1.0 o3prodro2 + ProdRO2 + 1. ProdO3 + NO <sub>2</sub> + .25 CH <sub>3</sub> C(O)OO + .25 CH <sub>3</sub> COCH <sub>2</sub> OH + .75 HCHO + .25 CO + .75 HO <sub>2</sub> + .5 MGLYOX	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO <sub>2</sub> $\rightarrow$ MPAN	.25*k_3rd(temp, cair, 9.7E-29, 5.6, 9.3E-12, 1.5, 0.6)	Pöschl et al. (2000)
G4410	TrGC	MVKO2 + CH <sub>3</sub> O <sub>2</sub> $\rightarrow$ .5 MGLYOX + .375 CH <sub>3</sub> COCH <sub>2</sub> OH + .125 CH <sub>3</sub> C(O)OO + 1.125 HCHO + .875 HO <sub>2</sub> + .125 CO + .25 CH <sub>3</sub> OH	2.E-12	von Kuhlmann (2001)
G4411	TrGC	MVKO2 + MVK $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + MGLYOX + .5 CO + .5 HCHO + HO <sub>2</sub>	2.E-12	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH $\rightarrow$ MVKO2	3.E-11	Pöschl et al. (2000)
G4413	TrGC	MEK + OH $\rightarrow$ LMEKO2	1.3E-12*EXP(-25./temp)	Wallington et al.
G4414	TrGC	LMEKO2 + HO <sub>2</sub> $\rightarrow$ LMEKOOH	k_PrO2_HO2	see note*
G4415	TrGNC	LMEKO2 + NO $\rightarrow$ 1.0 o3prodro2 + ProdRO2 + 1. ProdO3 + .985 CH <sub>3</sub> CHO + .985 CH <sub>3</sub> C(O)OO + .985 NO <sub>2</sub> + .015 LC4H9NO3	k_PrO2_NO	see note*
G4416	TrGC	LMEKOOH + OH $\rightarrow$ .8 BIACET + .8 OH + .2 LMEKO2	k_CH300H_OH	see note*
G4417	TrGNC	LC4H9NO3 + OH $\rightarrow$ MEK + NO <sub>2</sub> + H <sub>2</sub> O	1.7E-12	Wallington et al.
G4418	TrGNC	MPAN + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + NO <sub>2</sub>	3.2E-11	Orlando et al. (2002)
G4419	TrGNC	MPAN $\rightarrow$ MVKO2 + NO <sub>2</sub>	k_PAN_M	see note*
G4500	TrGC	C <sub>5</sub> H <sub>8</sub> + O <sub>3</sub> $\rightarrow$ LossO3R + 1. LossO3 + .28 HCOOH + .65 MVK + .1 MVKO2 + .1 CH <sub>3</sub> C(O)OO + .14 CO + .58 HCHO + .09 H <sub>2</sub> O <sub>2</sub> + .08 CH <sub>3</sub> O <sub>2</sub> + .25 OH + .25 HO <sub>2</sub>	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)
G4501	TrGC	C <sub>5</sub> H <sub>8</sub> + OH $\rightarrow$ ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	C <sub>5</sub> H <sub>8</sub> + NO <sub>3</sub> $\rightarrow$ 1.0 o3lossno + 1. LossO3 + ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO <sub>2</sub> $\rightarrow$ ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)
G4504	TrGNC	ISO2 + NO $\rightarrow$ 1.0 o3prodro2 + ProdRO2 + 1. ProdO3 + .956 NO <sub>2</sub> + .956 MVK + .956 HCHO + .956 HO <sub>2</sub> + .044 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4505	TrGC	ISO2 + CH <sub>3</sub> O <sub>2</sub> $\rightarrow$ .5 MVK + 1.25 HCHO + HO <sub>2</sub> + .25 MGLYOX + .25 CH <sub>3</sub> COCH <sub>2</sub> OH + .25 CH <sub>3</sub> OH	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 $\rightarrow$ 2 MVK + HCHO + HO <sub>2</sub>	2.E-12	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
G4507	TrGC	ISOOH + OH $\rightarrow$ MVK + OH	1.E-10	Pöschl et al. (2000)
G4508	TrGNC	ISON + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + NACA	1.3E-11	Pöschl et al. (2000)
G6100	UpStTrGCl	Cl + O <sub>3</sub> $\rightarrow$ ClO + O <sub>2</sub>	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + O( <sup>3</sup> P) $\rightarrow$ 2.0 LossO3Cl + 2. LossO3 + Cl + O <sub>2</sub>	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO $\rightarrow$ 2. LossO3 + Cl <sub>2</sub> + O <sub>2</sub>	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO $\rightarrow$ 2. LossO3 + 2 Cl + O <sub>2</sub>	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO $\rightarrow$ 1. LossO3 + Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO $\rightarrow$ Cl <sub>2</sub> O <sub>2</sub>	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	Cl <sub>2</sub> O <sub>2</sub> $\rightarrow$ ClO + ClO	k_ClO_ClO/(1.72E-27*EXP(8649./temp))	Atkinson et al. (2007), Sander et al. (2011)*
G6200	StGCl	Cl + H <sub>2</sub> $\rightarrow$ HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO <sub>2</sub> $\rightarrow$ HCl + O <sub>2</sub>	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO <sub>2</sub> $\rightarrow$ LossO3Cln + 1. ProdO3 + ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H <sub>2</sub> O <sub>2</sub> $\rightarrow$ HCl + HO <sub>2</sub>	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH $\rightarrow$ LossO3Cl + 1. LossO3 + .94 Cl + .94 HO <sub>2</sub> + .06 HCl + .06 O <sub>2</sub>	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO <sub>2</sub> $\rightarrow$ HOCl + O <sub>2</sub>	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH $\rightarrow$ Cl + H <sub>2</sub> O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH $\rightarrow$ ClO + H <sub>2</sub> O	3.0E-12*EXP(-500./temp)	Sander et al. (2011)
G6300	UpStTrGNCl	ClO + NO $\rightarrow$ 1.0 LossO3Cl + LossO3Nn + NO <sub>2</sub> + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGNCl	ClO + NO <sub>2</sub> $\rightarrow$ ClNO <sub>3</sub>	k_3rd_iupac(temp, cair, 1.6E-31, 3.4, 7.E-11, 0., 0.4)	Atkinson et al. (2007)
G6302	TrGNCl	ClNO <sub>3</sub> $\rightarrow$ ClO + NO <sub>2</sub>	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGNCl	ClNO <sub>3</sub> + O( <sup>3</sup> P) $\rightarrow$ ClO + NO <sub>3</sub>	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGNCl	ClNO <sub>3</sub> + Cl $\rightarrow$ Cl <sub>2</sub> + NO <sub>3</sub>	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH <sub>4</sub> $\rightarrow$ HCl + CH <sub>3</sub> O <sub>2</sub>	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO $\rightarrow$ HCl + CO + HO <sub>2</sub>	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH <sub>3</sub> OOH $\rightarrow$ HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH <sub>3</sub> O <sub>2</sub> $\rightarrow$ 1.0 o3lossro + LossO3Cl + 1. LossO3 + HO <sub>2</sub> + Cl + HCHO	3.3E-12*EXP(-115./temp)	Sander et al. (2011)
G6404	StGCl	CCl <sub>4</sub> + O( <sup>1</sup> D) $\rightarrow$ 4.0 ProdLCl + ClO + 3 Cl	3.3E-10	Sander et al. (2011)
G6405	StGCl	CH <sub>3</sub> Cl + O( <sup>1</sup> D) $\rightarrow$ 1.0 o3lossxo + 1.0 ProdLCl + LossO3Cl + 1. LossO3 + OH + Cl	1.65E-10	see note*
G6406	StGCl	CH <sub>3</sub> Cl + OH $\rightarrow$ 1.0 ProdLCl + H <sub>2</sub> O + Cl	2.4E-12*EXP(-1250./temp)	Sander et al. (2011)



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

#	labels	reaction	rate coefficient	reference
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 3.0 \text{ ProdLCl} +$ $\text{LossO3Cl} + 1. \text{ LossO3} + \text{OH} + 3 \text{ Cl}$	3.E-10	see note*
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 3.0 \text{ ProdLCl} + \text{H}_2\text{O} + 3 \text{ Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Sander et al. (2011)
G6409a	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	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow 2.0 \text{ ProdLCl} + \text{ClO} + \text{Cl}$	$1.4\text{E-}10$	Sander et al. (2011)
G6501	StGFCl	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow 3.0 \text{ ProdLCl} + \text{ClO} + 2 \text{ Cl}$	$2.3\text{E-}10$	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	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow 2.0 \text{ LossO3Br} + 2. \text{ LossO3} + \text{Br} + \text{O}_2$	$1.9\text{E-}11*\text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2.0 \text{ LossO3Br} + 2. \text{ LossO3} + 2 \text{ Br} + \text{O}_2$	$2.7\text{E-}12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2.0 \text{ LossO3Br} + 2. \text{ LossO3} + \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14*\text{EXP}(840./\text{temp})$	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)
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	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{LossO3Br} + 1. \text{ LossO3} + \text{OH} + \text{BrO}$	$1.2\text{E-}10*\text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow 1. \text{ ProdO3} + \text{HOBr} + \text{Br}$	$2.0\text{E-}11*\text{EXP}(240./\text{temp})$	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	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	$\text{k\_BrO\_NO2}$	Atkinson et al. (2007)*
G7303	TrGNBr	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$\text{k\_BrO\_NO2}/(5.44\text{E-}9*\text{EXP}(14192./\text{temp})$ $*1.\text{E6}*R_{\text{gas}}*\text{temp}/(\text{atm}2\text{Pa}*N_A))$	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	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow 1.0 \text{ o3lossro} + \text{LossO3Br} + 1. \text{ LossO3} +$ $\text{Br} + \text{HCHO} + \text{HO}_2$	$(1.-\text{G7402a\_yield})*5.7\text{E-}12$	Aranda et al. (1997)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow 1.0 \text{ ProdLBr} + \text{H}_2\text{O} + \text{Br}$	$2.35\text{E-}12*\text{EXP}(-1300./\text{temp})$	Sander et al. (2011)
G7404a	TrGCBBr	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HBr}$	$2.8\text{E-}13*\text{EXP}(224./\text{temp})/(1.+$ $1.13\text{E}24*\text{EXP}(-3200./\text{temp})/\text{C}(\text{ind\_02}))$	Atkinson et al. (2006)
G7405	TrGCBBr	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$1.8\text{e-}11*\text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow 3.0 \text{ ProdSBr} + \text{H}_2\text{O} + 3 \text{ Br}$	$1.35\text{E-}12*\text{EXP}(-600./\text{temp})$	Sander et al. (2011)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow 2.0 \text{ ProdSBr} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	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)

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

#	labels	reaction	rate coefficient	reference
G7602	TrGClBr	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E}-10 \cdot \text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow 1. \text{ LossO3} + \text{Br} + \text{OClO}$	$1.6\text{E}-12 \cdot \text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{LossO3Br} + \text{LossO3Cl} + 2. \text{ LossO3} + \text{Br}$ $+ \text{Cl} + \text{O}_2$	$2.9\text{E}-12 \cdot \text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{LossO3Br} + \text{LossO3Cl} + 2. \text{ LossO3} + \text{BrCl}$ $+ \text{O}_2$	$5.8\text{E}-13 \cdot \text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGClBr	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	$1.45\text{E}-11$	Clyne and Cruse (1972)
G7605	TrGClBr	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow 1.0 \text{ ProdSBr} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E}-12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7606	TrGClBr	$\text{CHClBr}_2 + \text{OH} \rightarrow 2.0 \text{ ProdSBr} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E}-12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7607	TrGClBr	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow 1.0 \text{ ProdSBr} + \text{H}_2\text{O} + \text{Br}$	$2.4\text{E}-12 \cdot \text{EXP}(-920./\text{temp})$	Sander et al. (2011)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow 1. \text{ LossO3} + \text{H}_2\text{SO}_4 + \text{HO}_2$	$\text{k\_3rd}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0., 0.6)$	Sander et al. (2011)
G9400a	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E}-11 \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	$\text{k\_DMS\_OH}$	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow 1.0 \text{ o3lossro} + 1. \text{ LossO3} + \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E}-13 \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow 0.6 \text{ ProdO3} + .6 \text{ SO}_2 + \text{HCHO} + .6 \text{ CH}_3\text{O}_2 + .4 \text{ HO}_2 + .4 \text{ CH}_3\text{SO}_3\text{H}$	$1.\text{E}-10$	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow 1. \text{ ProdO3} + \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow 1.0 \text{ o3lossxo} + 1. \text{ LossO3} + \text{CH}_3\text{SO}_3$	$3.\text{E}-13$	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	$\text{DMS} + \text{Br} \rightarrow \text{CH}_3\text{SO}_2 + \text{HBr} + \text{HCHO}$	$9.\text{E}-11 \cdot \text{EXP}(-2386./\text{temp})$	Jefferson et al. (1994)
G9701	TrGSBr	$\text{DMS} + \text{BrO} \rightarrow 1. \text{ LossO3} + \text{DMSO} + \text{Br}$	$4.4\text{E}-13$	Ingham et al. (1999)
G01Diag	StTrG	$\text{O}_3(\text{s}) \rightarrow \text{LO}_3(\text{s})$	$\text{k\_O3s}$	Roelofs and Lelieveld (1997)

## General notes

### Three-body reactions

Rate coefficients for three-body reactions are defined via the function `k_3rd`( $T, M, k_0^{300}, n, k_{\text{inf}}^{300}, m, f_c$ ). 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 T. J. Wallington et al. (2014) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

### RO<sub>2</sub> self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as  $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \text{k\_CH302}} \times [\text{RO}_2]$  where  $k_{\text{self}}$  = second-order rate coefficient of the self reaction of the organic peroxy radical, `k_CH302` = second-order rate coefficient of the self reaction of  $\text{CH}_3\text{O}_2$ , and  $[\text{RO}_2]$  = sum of the concentrations of all organic peroxy radicals.

### Specific notes

G1002a: 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_H20))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

G3109: The rate coefficient is: `k_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  $\text{HCHO}$ .

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: Same value as for G4107

G4213: The rate coefficient is: `k_CH3CO3_NO2 = k_3rd(temp, cair, 9.7E-29, 5.6, 9.3E-12, 1.5, 0.6)`.

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.

G4307: Same value as for G4107

G4315: Same value as for G4107

G4401: Same value as for G4306

G4402: Same value as for G4304

G4403: Same value as for G4305

G4404: Same value as for G4107

G4414: Same value as for G4304

G4415: Same value as for G4305

G4416: Same value as for G4107

G4419: Same value as for G4221

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

G6204: At low temperatures, there may be a minor reaction channel leading to  $\text{O}_3 + \text{HCl}$ . See Finkbeiner et al. (1995) for details. It is neglected here.

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

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

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

**G7302:** The rate coefficient is:  $k_{\text{BrO}_2\text{NO}_2} = k_{\text{3rd}}(\text{temp}, \text{cair}, 5.2\text{E-}31, 3.2, 6.9\text{E-}12, 2.9, 0.6)$ .

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

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

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

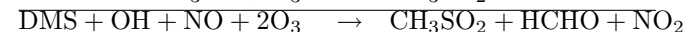
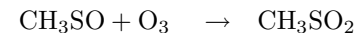
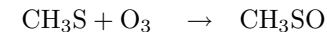
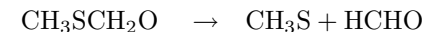
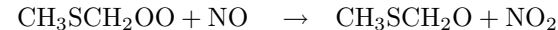
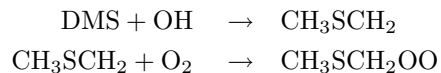
considered.

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

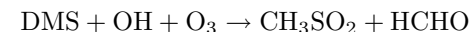
**G7606:** Same value as for G7408: CH<sub>2</sub>Br<sub>2</sub>+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

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

**G9400a:** For the abstraction path, the assumed reaction sequence (omitting H<sub>2</sub>O and O<sub>2</sub> as products) according to Yin et al. (1990) is:



Neglecting the effect on O<sub>3</sub> and NO<sub>x</sub>, the remaining reaction is:



**G9400b:** For the addition path, the rate coefficient is:  $k_{\text{DMS}_\text{OH}} = 1.0\text{E-}39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{ind}_2) / (1.+5.0\text{E-}30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{ind}_2))$ .

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow o3prodo2 + 2. \text{ ProdO3} + O(^3P) + O(^3P)$	jx(ip_02)	Sander et al. (2014)
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	jx(ip_01D)	Sander et al. (2014)
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	jx(ip_03P)	Sander et al. (2014)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 \text{ OH}$	jx(ip_H202)	Sander et al. (2014)
J3100	UpStGNJ	$N_2O + h\nu \rightarrow 1.0 \text{ o3prodh2} + 1. \text{ ProdO3} + O(^1D) + N_2$	jx(ip_N20)	Sander et al. (2014)
J3101	UpStTrGNJ	$NO_2 + h\nu \rightarrow 1.0 \text{ LossJ3101} + NO + O(^3P)$	jx(ip_N02)	Sander et al. (2014)
J3102a	UpStGNJ	$NO + h\nu \rightarrow 1. \text{ ProdO3} + N + O(^3P)$	jx(ip_N0)	Sander et al. (2014)
J3103a	UpStTrGNJ	$NO_3 + h\nu \rightarrow 1.0 \text{ LossJ3103a} + NO_2 + O(^3P)$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGNJ	$NO_3 + h\nu \rightarrow 2.0 \text{ LossO3N} + 2. \text{ LossO3} + NO + O_2$	jx(ip_N002)	Sander et al. (2014)
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	Sander et al. (2014)
J3200	TrGNJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	Sander et al. (2014)
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HNO3)	Sander et al. (2014)
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow 0.333 \text{ o3prodh2} + 0.333 \text{ ProdO3} + .667 \text{ NO}_2 + .667 \text{ HO}_2 + .333 \text{ NO}_3 + .333 \text{ OH}$	jx(ip_HNO4)	Sander et al. (2014)
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH300H)	Sander et al. (2014)
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	Sander et al. (2014)
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	Sander et al. (2014)
J4102	StGJ	$CO_2 + h\nu \rightarrow 1. \text{ ProdO3} + CO + O(^3P)$	jx(ip_CO2)	Sander et al. (2014)
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31 \text{ H} + 0.69 \text{ H}_2 + 1.155 \text{ H}_2O$	jx(ip_CH4)	Sander et al. (2014)
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)	Sander et al. (2014)
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J4203	TrGNJCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	von Kuhlmann (2001)
J4204	TrGNJCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	Sander et al. (2014)
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)	Sander et al. (2014)
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note*
J4303	TrGCJ	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	Sander et al. (2014)
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HCHO + OH$	jx(ip_CH300H)	see note*
J4306	TrGNJCJ	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*jx(ip_PAN)	von Kuhlmann et al. (2003)*
J4400	TrGCJ	$LC_4H_9OOH + h\nu \rightarrow OH + .67 \text{ MEK} + .67 \text{ HO}_2 + .33 \text{ C}_2\text{H}_5\text{O}_2 + .33 \text{ CH}_3\text{CHO}$	jx(ip_CH300H)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4401	TrGCJ	$\text{MVK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO} + \text{HO}_2$	$0.019 \cdot \text{jx}(\text{ip\_COH2}) + 0.015 \cdot \text{jx}(\text{ip\_MGLYOX})$	Sander et al. (2014)
J4402	TrGCJ	$\text{MVKOOH} + h\nu \rightarrow \text{OH} + .5 \text{ MGLYOX} + .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ HCHO} + .75 \text{ HO}_2 + .25 \text{ CH}_3\text{C}(\text{O})\text{OO} + .25 \text{ CO}$	$\text{jx}(\text{ip\_CH300H})$	see note*
J4403	TrGCJ	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2$	$0.42 \cdot \text{jx}(\text{ip\_CHOH})$	von Kuhlmann et al. (2003)
J4404	TrGCJ	$\text{LMEKOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CHO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J4405	TrGCJ	$\text{BIACET} + h\nu \rightarrow 2 \text{ CH}_3\text{C}(\text{O})\text{OO}$	$2.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	see note*
J4406	TrGN CJ	$\text{LC4H9NO3} + h\nu \rightarrow \text{NO}_2 + .67 \text{ MEK} + .67 \text{ HO}_2 + .33 \text{ C}_2\text{H}_5\text{O}_2 + .33 \text{ CH}_3\text{CHO}$	$3.7 \cdot \text{jx}(\text{ip\_PAN})$	von Kuhlmann (2001)
J4407	TrGN CJ	$\text{MPAN} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$\text{jx}(\text{ip\_PAN})$	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	TrGN CJ	$\text{ISON} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$3.7 \cdot \text{jx}(\text{ip\_PAN})$	von Kuhlmann (2001)
J6000	StTrGClJ	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$\text{jx}(\text{ip\_Cl2})$	Sander et al. (2014)
J6100	StTrGClJ	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2. \text{ LossO3} + 2 \text{ Cl}$	$\text{jx}(\text{ip\_Cl202})$	Sander et al. (2014)
J6101	StTrGClJ	$\text{OCIO} + h\nu \rightarrow 1. \text{ ProdO3} + \text{ClO} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip\_OC10})$	Sander et al. (2014)
J6200	StGClJ	$\text{HCl} + h\nu \rightarrow \text{Cl} + \text{H}$	$\text{jx}(\text{ip\_HCl})$	Sander et al. (2014)
J6201	StTrGClJ	$\text{HOCl} + h\nu \rightarrow \text{LossO3Cl} + 1. \text{ LossO3} + \text{OH} + \text{Cl}$	$\text{jx}(\text{ip\_HOC1})$	Sander et al. (2014)
J6300	TrGN ClJ	$\text{ClNO}_2 + h\nu \rightarrow 1. \text{ ProdO3} + \text{Cl} + \text{NO}_2$	$\text{jx}(\text{ip\_ClNO2})$	Sander et al. (2014)
J6301a	StTrGN ClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	$\text{jx}(\text{ip\_ClNO3})$	Sander et al. (2014)
J6301b	StTrGN ClJ	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$\text{jx}(\text{ip\_ClON02})$	Sander et al. (2014)
J6400	StGClJ	$\text{CH}_3\text{Cl} + h\nu \rightarrow 1.0 \text{ ProdLCl} + \text{Cl} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_CH3Cl})$	Sander et al. (2014)
J6401	StGClJ	$\text{CCl}_4 + h\nu \rightarrow 4.0 \text{ ProdLCl} + 4 \text{ Cl}$	$\text{jx}(\text{ip\_CC14})$	Sander et al. (2014)
J6402	StGCClJ	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3.0 \text{ ProdLCl} + 3 \text{ Cl}$	$\text{jx}(\text{ip\_CH3CC13})$	Sander et al. (2014)
J6500	StGFClJ	$\text{CFCl}_3 + h\nu \rightarrow 3.0 \text{ ProdLCl} + 3 \text{ Cl}$	$\text{jx}(\text{ip\_CFC13})$	Sander et al. (2014)
J6501	StGFClJ	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2.0 \text{ ProdLCl} + 2 \text{ Cl}$	$\text{jx}(\text{ip\_CF2Cl2})$	Sander et al. (2014)
J7000	StTrGBrJ	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	$\text{jx}(\text{ip\_Br2})$	Sander et al. (2014)
J7100	StTrGBrJ	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip\_Br0})$	Sander et al. (2014)
J7200	StTrGBrJ	$\text{HOBr} + h\nu \rightarrow \text{LossO3Br} + 1. \text{ LossO3} + \text{Br} + \text{OH}$	$\text{jx}(\text{ip\_HOBr})$	Sander et al. (2014)
J7300	TrGNBrJ	$\text{BrNO}_2 + h\nu \rightarrow 1. \text{ ProdO3} + \text{Br} + \text{NO}_2$	$\text{jx}(\text{ip\_BrNO2})$	Sander et al. (2014)
J7301	StTrGNBrJ	$\text{BrNO}_3 + h\nu \rightarrow 0.85 \text{ Br} + 0.85 \text{ NO}_3 + 0.15 \text{ BrO} + 0.15 \text{ NO}_2$	$\text{jx}(\text{ip\_BrNO3})$	Sander et al. (2014)*
J7400	StGBrJ	$\text{CH}_3\text{Br} + h\nu \rightarrow 1.0 \text{ ProdLBr} + \text{Br} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip\_CH3Br})$	Sander et al. (2014)
J7401	TrGBrJ	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2.0 \text{ ProdSBr} + 2 \text{ Br}$	$\text{jx}(\text{ip\_CH2Br2})$	Sander et al. (2014)
J7402	TrGBrJ	$\text{CHBr}_3 + h\nu \rightarrow 3.0 \text{ ProdSBr} + 3 \text{ Br}$	$\text{jx}(\text{ip\_CHBr3})$	Sander et al. (2014)
J7500	StGFBrJ	$\text{CF}_3\text{Br} + h\nu \rightarrow 1.0 \text{ ProdLBr} + \text{Br}$	$\text{jx}(\text{ip\_CF3Br})$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx(ip\_BrCl)}$	Sander et al. (2014)
J7601	StGFBrJ	$\text{CF}_2\text{ClBr} + h\nu \rightarrow 1.0 \text{ ProdLBr} + 1.0 \text{ ProdLCl} + \text{Br} + \text{Cl}$	$\text{jx(ip\_CF2ClBr)}$	Sander et al. (2014)
J7602	TrGClBrJ	$\text{CH}_2\text{ClBr} + h\nu \rightarrow 1.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + \text{Br} + \text{Cl}$	$\text{jx(ip\_CH2ClBr)}$	Sander et al. (2014)
J7603	TrGClBrJ	$\text{CHCl}_2\text{Br} + h\nu \rightarrow 1.0 \text{ ProdSBr} + 2.0 \text{ ProdSCl} + \text{Br} + 2 \text{ Cl}$	$\text{jx(ip\_CHCl2Br)}$	Sander et al. (2014)
J7604	TrGClBrJ	$\text{CHClBr}_2 + h\nu \rightarrow 2.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + 2 \text{ Br} + \text{Cl}$	$\text{jx(ip\_CHClBr2)}$	Sander et al. (2014)
J8401a	TrGJ	$\text{CH}_3\text{I} + h\nu \rightarrow \text{CH}_3\text{O}_2$	$\text{JX(ip\_CH3I)}$	Sander et al. (2014)

## General notes

J-values are calculated with an external module (e.g., JVAL) and then supplied to the MECCA chemistry.

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

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

$\text{J(41)} \rightarrow \text{jx(ip\_CH3OOH)}$   
 $\text{J(53)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J(54)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J(55)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2)$   
 $\text{J(56)+J(57)} \rightarrow \text{jx(ip\_NOA)}$

## Specific notes

J4302: It is assumed that  $\text{J}(\text{CH}_3\text{COCH}_2\text{OH})$  is 0.074 times that of J4101b.

J4304: It is assumed that  $\text{J}(\text{CH}_3\text{COCH}_2\text{O}_2\text{H})$  is the same as  $\text{J}(\text{CH}_3\text{OOH})$ .

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

J4402: It is assumed that  $\text{J}(\text{MVKOOH})$  is the same as  $\text{J}(\text{CH}_3\text{OOH})$ .

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).

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

J4500: It is assumed that  $\text{J}(\text{ISOOH})$  is the same as  $\text{J}(\text{CH}_3\text{OOH})$ .

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

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)*

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

## Specific notes

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)

## General notes

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

$$\alpha^\ominus = 0.1$$

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

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

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

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

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

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

and further:

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

## Specific notes

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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## General 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**.

For uptake of X (X = N<sub>2</sub>O<sub>5</sub>, ClNO<sub>3</sub>, or BrNO<sub>3</sub>) and

subsequent reaction with H<sub>2</sub>O, Cl<sup>−</sup>, and Br<sup>−</sup> in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

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

Here,  $k_{\text{mt}}$  = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by  $k_{\text{mt}}$ . The factors only affect

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

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 1.0 \text{ o3lossno} + \text{LossO3N} + 1. \text{ LossO3} + 2 \text{ HNO}_3$	<code>khet_St(ihs_N205_H20)</code>	see general notes*
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 general notes*
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 general notes*
HET420	StHetNCl	$\text{ClNO}_3 + \text{HCl} \rightarrow 1.0 \text{ o3lossno} + \text{LossO3Cl} + 1. \text{ LossO3} + \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see general notes*
HET421	StHetNCl	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H20)</code>	see general notes*
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 general notes*
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 general notes*
HET520	StHetNBr	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H20)</code>	see general notes*
HET540	StHetNClBr	$\text{ClNO}_3 + \text{HBr} \rightarrow 1.0 \text{ o3lossno} + \text{LossO3Cl} + 1. \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see general notes*
HET541	StHetNClBr	$\text{BrNO}_3 + \text{HCl} \rightarrow 1.0 \text{ o3lossno} + \text{LossO3Br} + 1. \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see general notes*
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 general notes*
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 general notes*

## General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA\_KHET) 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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**Specific notes**

Table 8: Aqueous phase reactions

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

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