

The Chemical Mechanism of MECCA
as applied for the
evaluation of development cycle 2 of MESSy

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The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs3

MECCA version: 2.5c2

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Selected reactions:

“((Tr && (G | Het) && !I) | | St)”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 134

Aqueous phase: 0

All species: 134

Number of reactions in selected mechanism:

Gas phase (Gnnn): 228

Aqueous phase (Annn): 0

Henry (Hnnn): 0

Photolysis (Jnnn): 70

Heterogeneous (HETnnn): 22

Equilibria (EQnn): 0

Dummy (Dnn): 0

All equations: 320

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

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11*EXP(55./temp)$	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34*((temp/300.)**(-2.4))*cair$	Sander et al. (2006)
G1002	StG	$O_3 + O(^1D) \rightarrow 2 O_2$	1.2E-10	Sander et al. (2006)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2 O_2$	$8.E-12*EXP(-2060./temp)$	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	$k_3rd(temp, cair, 4.4E-32, 1.3, 4.7E-11, 0.2, 0.6)$	Sander et al. (2006)
G2101	StG	$H + O_3 \rightarrow OH + O_2$	$1.4E-10*EXP(-470./temp)$	Sander et al. (2006)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	1.1E-10	Sander et al. (2006)
G2103	StG	$OH + O(^3P) \rightarrow H + O_2$	$2.2E-11*EXP(120./temp)$	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow LossOH + HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Sander et al. (2006)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH + O_2$	$3.E-11*EXP(200./temp)$	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow LossHO_2 + OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Sander et al. (2006)
G2108a	StG	$HO_2 + H \rightarrow 2 OH$	7.2E-11	Sander et al. (2006)
G2108b	StG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Sander et al. (2006)
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow LossO1D + 2 OH$	$1.63E-10*EXP(60./temp)$	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Sander et al. (2006)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Sander et al. (2006)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2 NO$	$6.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	$4.7E-11*EXP(20./temp)$	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2006)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	$2.1E-11*EXP(100./temp)$	Sander et al. (2006)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.1E-12*EXP(210./temp)$	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Sander et al. (2006)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12*EXP(220./temp)$	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_NO3_NO2/(2.7E-27*EXP(11000./temp))$	Sander et al. (2006)*

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

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

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

#	labels	reaction	rate coefficient	reference
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. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E-}14 \cdot \text{EXP}(390./\text{temp}) / (1.+26.2 \cdot \text{EXP}(-1130./\text{temp}))$	Sander et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Sander et al. (2006)*
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 \cdot \text{EXP}(2.03 \cdot \log(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2006)*
G4110	StTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$1.57\text{E-}13 + \text{cair} \cdot 3.54\text{E-}33$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{HO}_2$	$4.0\text{E-}13$	Sander et al. (2006)
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + .22 \text{HO}_2 + .12 \text{OH} + .23 \text{CO} + .54 \text{HCOOH} + .1 \text{H}_2$	$1.2\text{E-}14 \cdot \text{EXP}(-2630./\text{temp})$	Sander et al. (2006)*
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, 8.8E-12, 0.85, 0.6)	Sander et al. (2006)
G4203	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13 \cdot \text{EXP}(700./\text{temp})$	Sander et al. (2006)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{ProdRO}_2 + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E-}12 \cdot \text{EXP}(365./\text{temp})$	Sander et al. (2006)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Atkinson et al. (1999)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{HCHO} + \text{HO}_2 + .75 \text{CH}_3\text{CHO} + .25 \text{CH}_3\text{OH}$	$1.6\text{E-}13 \cdot \text{EXP}(195./\text{temp})$	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	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$4.4\text{E-}12 \cdot \text{EXP}(365./\text{temp})$	Atkinson et al. (2006)
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E-}12 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2006)
G4210	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$4.2\text{E-}14 \cdot \text{EXP}(855./\text{temp})$	Atkinson et al. (2006)
G4211a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$4.3\text{E-}13 \cdot \text{EXP}(1040./\text{temp}) / (1.+1./37. \cdot \text{EXP}(660./\text{temp}))$	Tyndall et al. (2001)
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E-}13 \cdot \text{EXP}(1040./\text{temp}) / (1.+37. \cdot \text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{ProdRO}_2 + \text{CH}_3\text{O}_2 + \text{NO}_2$	$8.1\text{E-}12 \cdot \text{EXP}(270./\text{temp})$	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. (2006)
G4214	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$4.\text{E-}12$	Canosa-Mas et al. (1996)
G4215a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9 \cdot 2.\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2006)
G4215b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO}$	$0.1 \cdot 2.\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2006)
G4216	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{HO}_2 + .18 \text{CH}_3\text{COOH}$	$4.9\text{E-}12 \cdot \text{EXP}(211./\text{temp})$	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)

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

#	labels	reaction	rate coefficient	reference
G4218	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$k_{\text{CH300H_OH}}$	see note
G4219	TrGNC	$\text{NACA} + \text{OH} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6\text{E-}12*\text{EXP}(270./\text{temp})$	see note
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2$	2.E-14	see note
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	$k_{\text{PAN_M}}$	Sander et al. (2006)*
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .82 \text{C}_3\text{H}_7\text{O}_2 + .18 \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65\text{E-}17*\text{temp}*\text{temp}*\text{EXP}(-87./\text{temp})$	Atkinson (2003)
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .04 \text{CH}_3\text{COCHO} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5\text{E-}15*\text{EXP}(-1900./\text{temp})$	Sander et al. (2006)*
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 8.\text{E-}27, 3.5, 3.\text{E-}11, 0., 0.5)$	Atkinson et al. (1999)
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{ONIT}$	$4.6\text{E-}13*\text{EXP}(-1155./\text{temp})$	Atkinson et al. (1999)
G4304	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	$k_{\text{PrO2_HO2}}$	Atkinson (1997)*
G4305	TrGNC	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow 0.96 \text{ProdRO2} + .96 \text{CH}_3\text{COCH}_3 + .96 \text{HO}_2 + .96 \text{NO}_2 + .04 \text{C}_3\text{H}_7\text{ONO}_2$	$k_{\text{PrO2_NO}}$	Atkinson et al. (1999)*
G4306	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{HCHO} + .8 \text{HO}_2 + .2 \text{CH}_3\text{OH}$	$k_{\text{PrO2_CH3O2}}$	Kirchner and Stockwell (1996)
G4307	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .3 \text{C}_3\text{H}_7\text{O}_2 + .7 \text{CH}_3\text{COCH}_3 + .7 \text{OH}$	$k_{\text{CH300H_OH}}$	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	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow 0.98 \text{ProdRO2} + .98 \text{CH}_3\text{CHO} + .98 \text{HCHO} + .98 \text{HO}_2 + .98 \text{NO}_2 + .02 \text{ONIT}$	$4.2\text{E-}12*\text{EXP}(180./\text{temp})$	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. (2006)
G4312	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E-}13*\text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{ProdRO2} + \text{NO}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO}$	$2.9\text{E-}12*\text{EXP}(300./\text{temp})$	Sander et al. (2006)
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{COCHO} + .5 \text{CH}_3\text{OH} + .3 \text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2 + .2 \text{CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E-}13*\text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4315	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow .3 \text{CH}_3\text{COCH}_2\text{O}_2 + .7 \text{CH}_3\text{COCHO} + .7 \text{OH}$	$k_{\text{CH300H_OH}}$	see note
G4316	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{CH}_3\text{COCHO} + \text{HO}_2$	$2.15\text{E-}12*\text{EXP}(305./\text{temp})$	Dillon et al. (2006)
G4317	TrGC	$\text{CH}_3\text{COCHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}$	$8.4\text{E-}13*\text{EXP}(830./\text{temp})$	Tyndall et al. (1995)
G4318	TrGNC	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	3.2E-11	Orlando et al. (2002)

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

#	labels	reaction	rate coefficient	reference
G4319	TrGNC	MPAN \rightarrow MVKO2 + NO ₂	k_PAN_M	see note
G4320	TrGNC	C ₃ H ₇ ONO ₂ + OH \rightarrow CH ₃ COCH ₃ + NO ₂	6.2E-13*EXP(-230./temp)	Atkinson et al. (1999)
G4400	TrGC	C ₄ H ₁₀ + OH \rightarrow C ₄ H ₉ O ₂ + H ₂ O	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)
G4401	TrGC	C ₄ H ₉ O ₂ + CH ₃ O ₂ \rightarrow .88 CH ₃ COC ₂ H ₅ + .68 HCHO + 1.23 HO ₂ + .12 CH ₃ CHO + .12 C ₂ H ₅ O ₂ + .18 CH ₃ OH	k_Pr02_CH302	see note
G4402	TrGC	C ₄ H ₉ O ₂ + HO ₂ \rightarrow C ₄ H ₉ OOH	k_Pr02_H02	see note
G4403	TrGNC	C ₄ H ₉ O ₂ + NO \rightarrow ProdRO2 + .84 NO ₂ + .56 CH ₃ COC ₂ H ₅ + .56 HO ₂ + .28 C ₂ H ₅ O ₂ + .84 CH ₃ CHO + .16 ONIT	k_Pr02_NO	see note
G4404	TrGC	C ₄ H ₉ OOH + OH \rightarrow .15 C ₄ H ₉ O ₂ + .85 CH ₃ COC ₂ H ₅ + .85 OH + .85 H ₂ O	k_CH300H_OH	see note
G4405	TrGC	MVK + O ₃ \rightarrow .45 HCOOH + .9 CH ₃ COCHO + .1 CH ₃ C(O)OO + .19 OH + .22 CO + .32 HO ₂	.5*(1.36E-15*EXP(-2112./temp) + 7.51E-16*EXP(-1521./temp))	Pöschl et al. (2000)
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 ₂ \rightarrow MVKOOH	1.82E-13*EXP(1300./temp)	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO \rightarrow ProdRO2 + NO ₂ + .25 CH ₃ C(O)OO + .25 CH ₃ COCH ₂ OH + .75 HCHO + .25 CO + .75 HO ₂ + .5 CH ₃ COCHO	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO ₂ \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 ₃ O ₂ \rightarrow .5 CH ₃ COCHO + .375 CH ₃ COCH ₂ OH + .125 CH ₃ C(O)OO + 1.125 HCHO + .875 HO ₂ + .125 CO + .25 CH ₃ OH	2.E-12	von Kuhlmann (2001)
G4411	TrGC	MVKO2 + MVKO2 \rightarrow CH ₃ COCH ₂ OH + CH ₃ COCHO + .5 CO + .5 HCHO + HO ₂	2.E-12	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH \rightarrow MVKO2	3.E-11	Pöschl et al. (2000)
G4413	TrGC	CH ₃ COC ₂ H ₅ + OH \rightarrow MEKO2	1.3E-12*EXP(-25./temp)	Atkinson et al. (1999)
G4414	TrGC	MEKO2 + HO ₂ \rightarrow MEKOOH	k_Pr02_H02	see note
G4415	TrGNC	MEKO2 + NO \rightarrow 0.985 ProdRO2 + .985 CH ₃ CHO + .985 CH ₃ C(O)OO + .985 NO ₂ + .015 ONIT	k_Pr02_NO	see note
G4416	TrGC	MEKOOH + OH \rightarrow .8 MeCOCO + .8 OH + .2 MEKO2	k_CH300H_OH	see note
G4417	TrGNC	ONIT + OH \rightarrow CH ₃ COC ₂ H ₅ + NO ₂ + H ₂ O	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	ISOP + O ₃ \rightarrow .28 HCOOH + .65 MVK + .1 MVKO2 + .1 CH ₃ C(O)OO + .14 CO + .58 HCHO + .09 H ₂ O ₂ + .08 CH ₃ O ₂ + .25 OH + .25 HO ₂	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
G4501	TrGC	ISOP + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO ₃ → ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO ₂ → ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)*
G4504a	TrGNC	ISO2 + NO → .956 NO ₂ + .956 MVK + .956 HCHO + .956 HO ₂ + .044 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)*
G4505	TrGC	ISO2 + CH ₃ O ₂ → .5 MVK + 1.25 HCHO + HO ₂ + .25 CH ₃ COCHO + .25 CH ₃ COCH ₂ OH + .25 CH ₃ OH	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO ₂	2.E-12	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH	1.E-10	Pöschl et al. (2000)
G4508	TrGNC	ISON + OH → CH ₃ COCH ₂ OH + NACA	1.3E-11	Pöschl et al. (2000)
G6100	StTrGCl	Cl + O ₃ → ClO + O ₂	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	StGCl	ClO + O(³ P) → Cl + O ₂	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl ₂ + O ₂	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O ₂	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OCIO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl ₂ O ₂	k_C10_C10	Atkinson et al. (2007)
G6103	StTrGCl	Cl ₂ O ₂ → ClO + ClO	k_C10_C10/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6200	StGCl	Cl + H ₂ → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO ₂ → HCl + O ₂	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO ₂ → ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H ₂ O ₂ → HCl + HO ₂	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → .94 Cl + .94 HO ₂ + .06 HCl + .06 O ₂	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO ₂ → HOCl	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)
G6205	StTrGCl	HCl + OH → Cl + H ₂ O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH → ClO + H ₂ O	3.0E-12*EXP(-500./temp)	Sander et al. (2006)
G6300	StTrGNCl	ClO + NO → NO ₂ + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGNCl	ClO + NO ₂ → ClNO ₃	k_3rd_iupac(temp, cair, 1.6E-31, 3.4, 7.E-11, 0., 0.4)	Atkinson et al. (2007)
G6302	TrGCl	ClNO ₃ → ClO + NO ₂	6.918E-7*exp(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGNCl	ClNO ₃ + O(³ P) → ClO + NO ₃	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGNCl	ClNO ₃ + Cl → Cl ₂ + NO ₃	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH ₄ → HCl + CH ₃ O ₂	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO ₂	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH ₃ OOH → HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$3.3\text{E-}12 \cdot \text{EXP}(-115./\text{temp})$	Sander et al. (2006)
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 3 \text{Cl}$	$3.3\text{E-}10$	Sander et al. (2006)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{Cl}$	$1.65\text{E-}10$	see note
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	$2.4\text{E-}12 \cdot \text{EXP}(-1250./\text{temp})$	Sander et al. (2006)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{OH} + 3 \text{Cl}$	$3.\text{E-}10$	see note
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E-}12 \cdot \text{EXP}(-1520./\text{temp})$	Sander et al. (2006)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HCl}$	$k_{3rd_iupac}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$7.9\text{e-}11$	Atkinson et al. (2006)
G6500	StGFCl	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + \text{Cl}$	$1.4\text{E-}10$	Sander et al. (2006)
G6501	StGFCl	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 2 \text{Cl}$	$2.3\text{E-}10$	Sander et al. (2006)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E-}11 \cdot \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{RG7101} + \text{Br} + \text{O}_2$	$1.9\text{E-}11 \cdot \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	$2.7\text{E-}12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14 \cdot \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E-}12 \cdot \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E-}12 \cdot \text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E-}12 \cdot \text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7203	StGBr	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E-}10 \cdot \text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E-}11 \cdot \text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGBr	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	$4.9\text{E-}11$	Orlando and Tyndall (1996)
G7301	StTrGNBr	$\text{BrO} + \text{NO} \rightarrow \text{RG7301} + \text{Br} + \text{NO}_2$	$8.7\text{E-}12 \cdot \text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGNBr	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	$k_{\text{BrO_NO2}}$	Atkinson et al. (2007)*
G7303	TrGBr	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO_NO2}} / (5.44\text{E-}9 \cdot \exp(14192./\text{temp}) \cdot 1.\text{E6} \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm}2\text{Pa} \cdot N_{\text{A}}))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E-}12 \cdot \text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.66\text{E-}12 \cdot \text{EXP}(-1610./\text{temp})$	Mallard et al. (1993)
G7402a	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{HCHO}$	$0.8/1.1 \cdot 5.7\text{E-}12$	Aranda et al. (1997)
G7402b	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{Br} + \text{HCHO} + \text{HO}_2$	$0.3/1.1 \cdot 5.7\text{E-}12$	Aranda et al. (1997)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.35\text{E-}12 \cdot \text{EXP}(-1300./\text{temp})$	Sander et al. (2006)
G7404	TrGCBBr	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HBr}$	$2.8\text{E-}13 \cdot \text{EXP}(224./\text{temp}) / (1.+1.13\text{E+}24 \cdot \text{EXP}(-3200./\text{temp}) / C(\text{ind}_{02}))$	Atkinson et al. (2006)
G7405	TrGCCl	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$1.8\text{e-}11 \cdot \text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Br}$	$1.35\text{E-}12 \cdot \text{EXP}(-600./\text{temp})$	Sander et al. (2006)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	Sander et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G7600	TrGBrCl	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	3.3E-15	Mallard et al. (1993)
G7601	TrGClBr	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	1.1E-15	Mallard et al. (1993)
G7602	TrGClBr	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	1.2E-10	Mallard et al. (1993)
G7603a	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGClBr	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G7604	TrGClBr	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	1.5E-11	Mallard et al. (1993)
G7605	TrGBr	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	2.0E-12*EXP(-840./temp)	see note
G7606	TrGBr	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + 2 \text{Br}$	2.0E-12*EXP(-840./temp)	see note
G7607	TrGBr	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	2.4E-12*EXP(-920./temp)	Sander et al. (2006)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	k_3rd(temp, cair, 3.3E-31, 4.3, 1.6E-12, 0., 0.6)	Sander et al. (2006)
G9400a	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2004)*
G9400b	TrGS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
G9402	TrGS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	1.9E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	5.E-11	Barone et al. (1995)
G9600	TrGSCl	$\text{DMS} + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCl} + \text{HCHO}$	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	$\text{DMS} + \text{Br} \rightarrow \text{CH}_3\text{SO}_2 + \text{HBr} + \text{HCHO}$	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	$\text{DMS} + \text{BrO} \rightarrow \text{DMSO} + \text{Br}$	2.54E-14*EXP(850./temp)	Ingham et al. (1999)
G10600	TrGHgCl	$\text{Hg} + \text{Cl} \rightarrow \text{HgCl}$	1.0E-11	Ariya et al. (2002)
G10601	TrGHgCl	$\text{Hg} + \text{Cl}_2 \rightarrow \text{HgCl}_2$	2.6E-18	Ariya et al. (2002)
G10700	TrGHgBr	$\text{Hg} + \text{Br} \rightarrow \text{HgBr}$	3.0E-13	Donohoue et al. (2006)
G10701	TrGHgBr	$\text{HgBr} + \text{Br} \rightarrow \text{HgBr}_2$	3.0E-12	Calvert and Lindberg (2003)
G10702	TrGHgBr	$\text{Hg} + \text{Br}_2 \rightarrow \text{HgBr}_2$	9.0E-17	Ariya et al. (2002)
G10703	TrGHgBr	$\text{Hg} + \text{BrO} \rightarrow \text{HgO} + \text{Br}$	1.0E-15	Raofie and Ariya (2003)
G10704	TrGHgBr	$\text{HgBr} + \text{BrO} \rightarrow \text{BrHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10705	TrGHgClBr	$\text{HgCl} + \text{BrO} \rightarrow \text{ClHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10706	TrGHgClBr	$\text{HgBr} + \text{Cl} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)
G10707	TrGHgClBr	$\text{HgCl} + \text{Br} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)

*Notes:

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

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

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

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

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

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

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

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

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

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

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

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

G2110: The rate coefficient is: `k_H02_H02 = (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_H02 = k_3rd(temp, cair, 1.8E-31, 3.2, 4.7E-12, 1.4, 0.6)`.

G3206: The rate coefficient is: `k_HN03_OH = 2.4E-14 * EXP(460./temp) + 1./ (1./ (6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)))`

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

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

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

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

G4201: The product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998)).

G4206: The rate coefficient was calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH_3OO and $\text{C}_2\text{H}_5\text{OO}$ from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

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

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

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

G4219: According to Pöschl et al. (2000), the same value as for $\text{CH}_3\text{CHO} + \text{OH}$ can be assumed.

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

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

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

G4304: The rate coefficient is: `k_Pr02_H02 = 1.9E-13*EXP(1300./temp)`. Value for generic $\text{RO}_2 + \text{HO}_2$ reaction from Atkinson (1997) is used.

G4305: The rate coefficient is: `k_Pr02_NO = 2.7E-12*EXP(360./temp)`.

G4307: Same value as for G4107: $\text{CH}_3\text{OOH} + \text{OH}$ assumed.

G4309: The products are from von Kuhlmann (2001).

G4315: Same value as for G4107: $\text{CH}_3\text{OOH} + \text{OH}$ assumed.

G4319: Same value as for PAN assumed.

G4401: Same value as for propyl group assumed (`k_Pr02_CH302`).

G4402: Same value as for propyl group assumed (`k_Pr02_H02`).

G4403: Same value as for propyl group assumed (`k_Pr02_NO`).

G4404: Same value as for G4107: $\text{CH}_3\text{OOH} + \text{OH}$ assumed.

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

G4414: Same value as for propyl group assumed (k_{PrO2_H02}).

G4415: Same value as for propyl group assumed (k_{PrO2_N0}).

G4416: Same value as for G4107: $CH_3OOH+OH$ assumed.

G4417: Value for $C_4H_9ONO_2$ used here.

G4503: Same temperature dependence assumed as for other RO_2+HO_2 reactions.

G4504: Yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).

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

G6402: The initial products are probably HCl and CH_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

G6405: Average of reactions with CH_3Br and CH_3F from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with CH_3CF_3 , CH_3CClF_2 , and CH_3CCl_2F from Sander et al. (2006).

G7302: The rate coefficient is: $k_{BrO_N02} = k_{3rd(temp, cair, 5.2E-31, 3.2, 6.9E-12, 2.9, 0.6)}$.

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

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_2Br_2+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_2Br_2+OH assumed. It is assumed that the reaction liberates all Br atoms but not Cl. The fate of the carbon atom is currently not considered.

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

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

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_02)	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	jx(ip_01D)	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	jx(ip_03P)	see note
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H20)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	jx(ip_N20)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	jx(ip_NO)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO20)	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	jx(ip_NO02)	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	see note
J3104b	StGNJ	$N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$	jx(ip_NO3N00)	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HNO3)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HNO4)	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH300H)	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	jx(ip_CO2)	see note
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31 H + 0.69 H_2 + 1.155 H_2O$	jx(ip_CH4)	see note
J4200	TrGJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	see note
J4201	TrGJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrGJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	jx(ip_PAA)	see note
J4203	TrGNJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	see note
J4204	TrGNJ	$PAN + h\nu \rightarrow .6 CH_3C(O)OO + .6 NO_2 + .4 CH_3O_2 + .4 NO_3 + .4 CO_2$	jx(ip_PAN)	see note
J4300	TrGJ	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH300H)	see note
J4301	TrGJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	see note
J4302	TrGJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note
J4303	TrGJ	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_CH3COCHO)	see note
J4304	TrGJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	jx(ip_CH300H)	see note
J4305	TrGNJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	jx(ip_PAN)	see note
J4306	TrGNJ	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*jx(ip_PAN)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4400	TrGCJ	$C_4H_9OOH + h\nu \rightarrow OH + .67 CH_3COC_2H_5 + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	$jx(ip_CH300H)$	see note
J4401	TrGCJ	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	$0.019*jx(ip_COH2)+.015*jx(ip_CH3COCHO)$	see note
J4402	TrGCJ	$MVKOOH + h\nu \rightarrow OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 CH_3C(O)OO + .25 CO$	$jx(ip_CH300H)$	see note
J4403	TrGCJ	$CH_3COC_2H_5 + h\nu \rightarrow CH_3C(O)OO + C_2H_5O_2$	$0.42*jx(ip_CHOH)$	see note
J4404	TrGCJ	$MEKOOH + h\nu \rightarrow CH_3C(O)OO + CH_3CHO + OH$	$jx(ip_CH300H)$	see note
J4405	TrGCJ	$MeCOCO + h\nu \rightarrow 2 CH_3C(O)OO$	$2.15*jx(ip_CH3COCHO)$	see note
J4406	TrGN CJ	$ONIT + h\nu \rightarrow NO_2 + .67 CH_3COC_2H_5 + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	$3.7*jx(ip_PAN)$	see note
J4500	TrGCJ	$ISOOH + h\nu \rightarrow MVK + HCHO + HO_2 + OH$	$jx(ip_CH300H)$	see note
J4501	TrGN CJ	$ISON + h\nu \rightarrow MVK + HCHO + NO_2 + HO_2$	$3.7*jx(ip_PAN)$	see note
J6000	StTrGClJ	$Cl_2 + h\nu \rightarrow Cl + Cl$	$jx(ip_Cl2)$	see note
J6100	StTrGClJ	$Cl_2O_2 + h\nu \rightarrow 2 Cl$	$1.4*jx(ip_Cl2O2)$	see note
J6101	StTrGClJ	$OCIO + h\nu \rightarrow ClO + O(^3P)$	$jx(ip_OC10)$	see note
J6200	StGClJ	$HCl + h\nu \rightarrow Cl + H$	$jx(ip_HCl)$	see note
J6201	StTrGClJ	$HOCl + h\nu \rightarrow OH + Cl$	$jx(ip_HOCl)$	see note
J6300	TrGNClJ	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	$jx(ip_ClNO2)$	see note
J6301a	StTrGNClJ	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	$jx(ip_ClNO3)$	see note
J6301b	StTrGNClJ	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	$jx(ip_ClON02)$	see note
J6400	StGClJ	$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$	$jx(ip_CH3Cl)$	see note
J6401	StGClJ	$CCl_4 + h\nu \rightarrow 4 Cl$	$jx(ip_CC14)$	see note
J6402	StGCclJ	$CH_3CCl_3 + h\nu \rightarrow 3 Cl$	$jx(ip_CH3CC13)$	see note
J6500	StGFClJ	$CFCl_3 + h\nu \rightarrow 3 Cl$	$jx(ip_CFC13)$	see note
J6501	StGFClJ	$CF_2Cl_2 + h\nu \rightarrow 2 Cl$	$jx(ip_CF2Cl2)$	see note
J7000	StTrGBrJ	$Br_2 + h\nu \rightarrow Br + Br$	$jx(ip_Br2)$	see note
J7100	TrGBrJ	$BrO + h\nu \rightarrow RJ7100 + Br + O(^3P)$	$jx(ip_Br0)$	see note
J7200	StTrGBrJ	$HOBr + h\nu \rightarrow Br + OH$	$jx(ip_HOBr)$	see note
J7300	TrGNBrJ	$BrNO_2 + h\nu \rightarrow Br + NO_2$	$jx(ip_BrNO2)$	see note
J7301	StTrGNBrJ	$BrNO_3 + h\nu \rightarrow 0.29 Br + 0.29 NO_3 + 0.71 BrO + 0.71 NO_2$	$jx(ip_BrNO3)$	see note
J7400	StGBrJ	$CH_3Br + h\nu \rightarrow Br + CH_3O_2$	$jx(ip_CH3Br)$	see note
J7401	TrGBrJ	$CH_2Br_2 + h\nu \rightarrow 2 Br$	$jx(ip_CH2Br2)$	see note
J7402	TrGBrJ	$CHBr_3 + h\nu \rightarrow 3 Br$	$jx(ip_CHBr3)$	see note
J7500	StGFBrJ	$CF_3Br + h\nu \rightarrow Br$	$jx(ip_CF3Br)$	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGClBrJ	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_BrCl)	see note
J7601	StGFBrJ	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_CF2ClBr)	see note
J7602	TrGClBrJ	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_CH2ClBr)	see note
J7603	TrGClBrJ	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{Br} + 2 \text{Cl}$	jx(ip_CHCl2Br)	see note
J7604	TrGClBrJ	$\text{CHClBr}_2 + h\nu \rightarrow 2 \text{Br} + \text{Cl}$	jx(ip_CHClBr2)	see note
J8401a	TrGJ	$\text{CH}_3\text{I} + h\nu \rightarrow \text{CH}_3\text{O}_2$	JX(ip_CH3I)	see note
J9002	StGSJ	$\text{SF}_6 + h\nu \rightarrow \text{products}$	JX(ip_SF6)	see note

*Notes:

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

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the Cl_2O_2 formation rate coefficient by

Sander et al. (2003) can approximately reproduce the observed $\text{Cl}_2\text{O}_2/\text{ClO}$ ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the Cl_2O_2 formation rate is about 5 to 15 % less than the value by Sander

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

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

Table 3: Henry's law coefficients

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
O ₂	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O ₃	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^1	4300.	Hanson et al. (1992)
HO ₂	3.9×10^3	5900.	Hanson et al. (1992)
H ₂ O ₂	$1. \times 10^5$	6338.	Lind and Kok (1994)
NH ₃	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO ₂	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO ₃	2.	2000.	Thomas et al. (1993)
HONO	4.9×10^1	4780.	Schwartz and White (1981)
HNO ₃	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO ₄	1.2×10^4	6900.	Régimbal and Mozurkewich (1997)
CH ₃ O ₂	6.	5600.	Jacob (1986)*
CH ₃ OOH	3.0×10^2	5322.	Lind and Kok (1994)
HCHO	7.0×10^3	6425.	Chameides (1984)
HCOOH	3.7×10^3	5700.	Chameides (1984)
CO ₂	3.1×10^{-2}	2423.	Chameides (1984)
Cl ₂	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^2	5862.	Huthwelker et al. (1995)
Br ₂	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	9.3×10^1	5862.	Vogt et al. (1996)*
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO ₂	1.2	3120.	Chameides (1984)
H ₂ SO ₄	$1. \times 10^{11}$	0.	see note
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*
Hg	0.13	0.	Schroeder and Munthe (1998)
HgO	3.2×10^6	0.	Shon et al. (2005)
HgCl ₂	2.4×10^7	0.	Shon et al. (2005)
HgBr ₂	2.4×10^7	0.	see note
ClHgBr	2.4×10^7	0.	see note
BrHgOBr	2.4×10^7	0.	see note

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

substance	k_{H}^{\ominus} M/atm	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
ClHgOBr	2.4×10^7	0.	see note

*Notes:

The temperature dependence of the Henry constants is:

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

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

NO₂: The temperature dependence is from Chameides

(1984).

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

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

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

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

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

DMSO: Lower limit cited from another reference.

HgBr₂: Assumed to be the same as for HgCl₂

ClHgBr: Assumed to be the same as for HgCl₂

BrHgOBr: Assumed to be the same as for HgCl₂

ClHgOBr: Assumed to be the same as for HgCl₂

Table 4: Accommodation coefficients

substance	α^{\ominus}	$\frac{-\Delta_{\text{obs}}H/R}{K}$	reference
O ₂	0.01	2000.	see note
O ₃	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO ₂	0.5	0.	Thornton and Abbatt (2005)
H ₂ O ₂	0.077	3127.	Worsnop et al. (1989)
NH ₃	0.06	0.	DeMore et al. (1997)*
NO	5.0×10^{-5}	0.	Saastad et al. (1993)*
NO ₂	0.0015	0.	Ponche et al. (1993)*
NO ₃	0.04	0.	Rudich et al. (1996)*
N ₂ O ₅	0.1	0.	DeMore et al. (1997)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO ₃	0.5	0.	Abbatt and Waschewsky (1998)*
HNO ₄	0.1	0.	DeMore et al. (1997)*
CH ₃ O ₂	0.01	2000.	see note
CH ₃ OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO ₂	0.01	2000.	see note
Cl ₂	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
ClNO ₃	0.108	0.	Deiber et al. (2004)*
Br ₂	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
BrNO ₃	0.063	0.	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO ₂	0.11	0.	DeMore et al. (1997)
H ₂ SO ₄	0.65	0.	Pöschl et al. (1998)*
CH ₃ SO ₃ H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)
Hg	0.1	0.	see note
HgO	0.1	0.	see note
HgCl ₂	0.1	0.	see note

Table 4: Accommodation coefficients (... continued)

substance	α^\ominus	$\frac{-\Delta_{\text{obs}}H/R}{\text{K}}$	reference
HgBr ₂	0.1	0.	see note
ClHgBr	0.1	0.	see note
BrHgOBr	0.1	0.	see note
ClHgOBr	0.1	0.	see note

*Notes:

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:

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

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

O₂: Estimate.

O₃: Value measured at 292 K.

OH: Value measured at 293 K.

NH₃: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO₂: Value measured at 298 K.

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

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

HONO: Value measured between 247 and 297 K.

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

HNO₄: Value measured at 200 K for water ice.

CH₃O₂: Estimate.

HCHO: Value measured between 260 and 270 K.

CO₂: Estimate.

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

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

ClNO₃: Value measured at 274.5 K.

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

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

BrNO₃: Value measured at 273 K.

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

H₂SO₄: Value measured at 303 K.

Hg: Estimate.

HgO: Estimate.

HgCl₂: Estimate.

HgBr₂: Estimate.

ClHgBr: Estimate.

BrHgOBr: Estimate.

ClHgOBr: Estimate.

Table 5: Henry's law equilibria

#	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 ($= \text{N}_2\text{O}_5, \text{ClNO}_3, \text{BrNO}_3$) and subsequent reaction with H_2O , Cl^- , and Br^- , we define $k_{\text{exf}}(X) = k_{\text{mt}}(X) \times \text{lwc} / ([\text{H}_2\text{O}] + 5.0E2[\text{Cl}^-] + 3.0E5[\text{Br}^-])$.

H6301, H6302, H7601: The total uptake is determined

by $k_{\text{mt}}(\text{ClNO}_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by $k_{\text{mt}}(\text{BrNO}_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2 \text{HNO}_3$	<code>khet_St(ihs_N2O5_H2O)</code>	see note
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^- (\text{aq}) + 2 \text{H}^+ (\text{aq})$	<code>khet_Tr(iht_N2O5)</code>	see note
HET202	TrHetN	$\text{HNO}_3 \rightarrow \text{NO}_3^- (\text{aq}) + \text{H}^+ (\text{aq})$	<code>khet_Tr(iht_HNO3)</code>	see note
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see note
HET420	StHetNCl	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see note
HET421	StHetNCl	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H2O)</code>	see note
HET422	StHetNCl	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N2O5_HCl)</code>	see note
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see note
HET520	StHetNBr	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H2O)</code>	see note
HET540	StHetNClBr	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see note
HET541	StHetNClBr	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see note
HET542	StHetClBr	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see note
HET543	StHetClBr	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HCl)</code>	see note
HET1001	StTrHetHg	$\text{Hg} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_Hg) + khet_St(ihs_Hg)</code>	see note
HET1002	StTrHetHg	$\text{HgO} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1003	StTrHetHg	$\text{HgCl} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1004	StTrHetHg	$\text{HgCl}_2 \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1005	StTrHetHg	$\text{HgBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1006	StTrHetHg	$\text{HgBr}_2 \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1007	StTrHetHg	$\text{ClHgBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1008	StTrHetHg	$\text{BrHgOBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note
HET1009	StTrHetHg	$\text{ClHgOBr} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see note

*Notes:

Heterogeneous reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see www.messy-interface.org 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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