

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 4.4.0.m1

Date: February 18, 2021

Batch file: CCMI-base-01-tag.bat

Integrator: rosenbrock_mz

Gas equation file: gas.eqn

Replacement file: mim1-CCMI-base-01

Selected reactions:

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

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 178

Aqueous phase: 0

All species: 178

Number of reactions in selected mechanism:

Gas phase (Gnn): 218

Aqueous phase (Annn): 0

Henry (Hnn): 0

Photolysis (Jnn): 68

Aqueous phase photolysis (PHnn): 0

Heterogeneous (HETnn): 12

Equilibria (EQnn): 0

Isotope exchange (IEXnn): 0

Tagging equations (TAGnn): 0

Dummy (Dnn): 0

All equations: 298

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$\text{O}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	$3.3\text{E}-11*\text{EXP}(55./\text{temp})$	Burkholder et al. (2015)
G1001	UpStTrG	$\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{O}_3$	$6.0\text{E}-34*((\text{temp}/300.)**(-2.4))$ $*\text{cair}$	Burkholder et al. (2015)
G1002a	UpStG	$\text{O}_3 + \text{O}(^1\text{D}) \rightarrow 2.0 \text{ o3lossxo} + 2.0 \text{ LossO3O} + 2.0 \text{ LossO3} + 2 \text{ O}_2$	$1.2\text{E}-10$	Burkholder et al. (2015)*
G1003	UpStG	$\text{O}_3 + \text{O}(^3\text{P}) \rightarrow 2.0 \text{ LossO3O} + 2.0 \text{ LossO3} + 2 \text{ O}_2$	$8.0\text{E}-12*\text{EXP}(-2060./\text{temp})$	Burkholder et al. (2015)
G2100	UpStTrG	$\text{H} + \text{O}_2 \rightarrow 1.0 \text{ LossG2100} + \text{HO}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 4.4\text{E}-32, 1.3, 7.5\text{E}-11, -0.2, 0.6)$	Burkholder et al. (2015)
G2101	UpStG	$\text{H} + \text{O}_3 \rightarrow 1.0 \text{ o3lossxo} + 1.0 \text{ LossO3H} + 1.0 \text{ LossO3} + \text{OH} + \text{O}_2$	$1.4\text{E}-10*\text{EXP}(-470./\text{temp})$	Burkholder et al. (2015)
G2102	UpStG	$\text{H}_2 + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 1.0 \text{ LossO3H} + 1.0 \text{ LossO3} + \text{H} + \text{OH}$	$1.2\text{E}-10$	Burkholder et al. (2015)
G2103	UpStG	$\text{OH} + \text{O}(^3\text{P}) \rightarrow 1.0 \text{ LossG2103} + 1.0 \text{ LossO3H} + 1.0 \text{ LossO3} + \text{H} + \text{O}_2$	$1.8\text{E}-11*\text{EXP}(180./\text{temp})$	Burkholder et al. (2015)
G2104	UpStTrG	$\text{OH} + \text{O}_3 \rightarrow 1.0 \text{ LossG2104} + 1.0 \text{ o3lossoh} + 1.0 \text{ LossO3H} + \text{LossOH} + 1.0 \text{ LossO3} + \text{HO}_2 + \text{O}_2$	$1.7\text{E}-12*\text{EXP}(-940./\text{temp})$	Burkholder et al. (2015)
G2105	UpStTrG	$\text{OH} + \text{H}_2 \rightarrow 1.0 \text{ LossG2105} + \text{H}_2\text{O} + \text{H}$	$2.8\text{E}-12*\text{EXP}(-1800./\text{temp})$	Burkholder et al. (2015)
G2106	UpStG	$\text{HO}_2 + \text{O}(^3\text{P}) \rightarrow 1. \text{ LossG2106} + 1.0 \text{ LossO3H} + 1.0 \text{ LossO3} + \text{OH} + \text{O}_2$	$3.\text{E}-11*\text{EXP}(200./\text{temp})$	Burkholder et al. (2015)
G2107	UpStTrG	$\text{HO}_2 + \text{O}_3 \rightarrow 1. \text{ LossG2107} + 1.0 \text{ o3lossho2} + 1.0 \text{ LossO3H} + \text{LossHO2} + 1.0 \text{ LossO3} + \text{OH} + 2 \text{ O}_2$	$1.\text{E}-14*\text{EXP}(-490./\text{temp})$	Burkholder et al. (2015)
G2108a	UpStG	$\text{HO}_2 + \text{H} \rightarrow 2 \text{ OH}$	$7.2\text{E}-11$	Burkholder et al. (2015)
G2108b	UpStG	$\text{HO}_2 + \text{H} \rightarrow \text{H}_2 + \text{O}_2$	$6.9\text{E}-12$	Burkholder et al. (2015)
G2108c	UpStG	$\text{HO}_2 + \text{H} \rightarrow 1.0 \text{ ProdO3} + \text{O}(^3\text{P}) + \text{H}_2\text{O}$	$1.6\text{E}-12$	Burkholder et al. (2015)
G2109	UpStTrG	$\text{HO}_2 + \text{OH} \rightarrow 1. \text{ LossG2109} + \text{lossho2oh} + \text{H}_2\text{O} + \text{O}_2$	$4.8\text{E}-11*\text{EXP}(250./\text{temp})$	Burkholder et al. (2015)
G2110	UpStTrG	$\text{HO}_2 + \text{HO}_2 \rightarrow 1. \text{ LossG2110} + \text{ho2lossHO2} + \text{H}_2\text{O}_2 + \text{O}_2$	k_H02_H02	Burkholder et al. (2015)*
G2111	UpStTrG	$\text{H}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 1. \text{ LossG2111} + 1.0 \text{ o3lossxo} + 1.0 \text{ LossO3O} + \text{LossO1D} + 1.0 \text{ LossO3} + 2 \text{ OH}$	$1.63\text{E}-10*\text{EXP}(60./\text{temp})$	Burkholder et al. (2015)
G2112	UpStTrG	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow 1. \text{ LossG2112} + \text{H}_2\text{O} + \text{HO}_2$	$1.8\text{E}-12$	Burkholder et al. (2015)
G3100	UpStGN	$\text{N} + \text{O}_2 \rightarrow 1.0 \text{ ProdO3} + \text{NO} + \text{O}(^3\text{P})$	$1.5\text{E}-11*\text{EXP}(-3600./\text{temp})$	Burkholder et al. (2015)
G3101	UpStTrGN	$\text{N}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{N}_2$	$2.15\text{E}-11*\text{EXP}(110./\text{temp})$	Burkholder et al. (2015)
G3102a	UpStGN	$\text{N}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + \text{noprodN2O} + 1.0 \text{ LossO3O} + 1.0 \text{ LossO3} + 2 \text{ NO}$	$7.259\text{E}-11*\text{EXP}(20./\text{temp})$	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G3102b	StGN	$\text{N}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 1.0 \text{ LossO3O} + 1.0 \text{ LossO3}$ $+ \text{N}_2 + \text{O}_2$	$4.641\text{E-}11 * \text{EXP}(20./\text{temp})$	Burkholder et al. (2015)
G3103	UpStTrGN	$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$	$3.0\text{E-}12 * \text{EXP}(-1500./\text{temp})$	Burkholder et al. (2015)
G3104	UpStGN	$\text{NO} + \text{N} \rightarrow 1.0 \text{ ProdO3} + \text{O}(^3\text{P}) + \text{N}_2$	$2.1\text{E-}11 * \text{EXP}(100./\text{temp})$	Burkholder et al. (2015)
G3105	UpStGN	$\text{NO}_2 + \text{O}(^3\text{P}) \rightarrow 2.0 \text{ LossO3N} + 2.0 \text{ LossO3} + \text{NO} + \text{O}_2$	$5.1\text{E-}12 * \text{EXP}(210./\text{temp})$	Burkholder et al. (2015)
G3106	StTrGN	$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$	$1.2\text{E-}13 * \text{EXP}(-2450./\text{temp})$	Burkholder et al. (2015)
G3107	UpStGN	$\text{NO}_2 + \text{N} \rightarrow \text{N}_2\text{O} + \text{O}(^3\text{P})$	$5.8\text{E-}12 * \text{EXP}(220./\text{temp})$	Burkholder et al. (2015)
G3108	StTrGN	$\text{NO}_3 + \text{NO} \rightarrow 2 \text{ NO}_2$	$1.5\text{E-}11 * \text{EXP}(170./\text{temp})$	Burkholder et al. (2015)
G3109	UpStTrGN	$\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	k_N03_N02	Burkholder et al. (2015)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$k_N03_N02 / (5.8\text{E-}27 * \text{EXP}(10840./\text{temp}))$	Burkholder et al. (2015)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow 1. \text{ LossG3200} + \text{HONO}$	$k_3\text{rd}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6, 3.6\text{E-}11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow 1. \text{ LossG3201} + 1.0 \text{ o3prodho2} + \text{ProdHO2}$ $+ 1.0 \text{ ProdO3} + \text{NO}_2 + \text{OH}$	$3.3\text{E-}12 * \text{EXP}(270./\text{temp})$	Burkholder et al. (2015)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow 1. \text{ LossG3202} + \text{ohlossNO2} + \text{HNO}_3$	$k_3\text{rd}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0, 2.8\text{E-}11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow 1. \text{ LossG3203} + \text{HNO}_4$	k_N02_H02	Burkholder et al. (2015)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow 1.0 \text{ o3lossno} + 1.0 \text{ LossO3N} + 1.0 \text{ LossO3}$ $+ \text{NO}_2 + \text{OH} + \text{O}_2$	3.5E-12	Burkholder et al. (2015)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow 1.0 \text{ o3prodho2} + \text{ohlossNO2} + 1.0 \text{ ProdO3}$ $+ \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11 * \text{EXP}(-390./\text{temp})$	Burkholder et al. (2015)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow 1.0 \text{ o3prodho2} + \text{ohlossNO2} + 1.0 \text{ ProdO3}$ $+ \text{H}_2\text{O} + \text{NO}_3$	k_HN03_OH	Dulitz et al. (2018)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow 1. \text{ LossG3207} + \text{NO}_2 + \text{HO}_2$	$k_N02_H02 / (2.1\text{E-}27 * \text{EXP}(10900./\text{temp}))$	Burkholder et al. (2015)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E-}12 * \text{EXP}(380./\text{temp})$	Burkholder et al. (2015)
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	$\text{NH}_2 + \text{O}_3 \rightarrow 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12 * \text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E-}07 * \text{EXP}(-628./\text{temp}) * (\text{temp})^{**(-1.32)}$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E-}09 * \text{EXP}(-356./\text{temp}) * (\text{temp})^{**(-1.12)}$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12 * ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11 * ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)

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

#	labels	reaction	rate coefficient	reference
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11 * ((\text{temp}/298.) ** (-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11 * ((\text{temp}/298.) ** (-2.0))$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{NH}_2 + \text{O}_2$	$1.2\text{E-}14$	Kohlmann and Poppe (1999)
G3218	TrGN	$\text{NH}_2\text{O} \rightarrow \text{NHOH}$	$1.3\text{E}3$	Kohlmann and Poppe (1999)
G3219	TrGN	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	$8.0\text{E-}11 * \text{EXP}(-500./\text{temp})$	Kohlmann and Poppe (1999)
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E-}12 * \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{HONO} + \text{NO}$	$1.0\text{E-}12 * \text{EXP}(-1000./\text{temp})$	Kohlmann and Poppe (1999)
G3222	TrGN	$\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$	$1.66\text{E-}12$	Kohlmann and Poppe (1999)
G3223	TrGN	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11 * \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14 * \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4100	UpStG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 1.0 \text{ LossO3O} + 1.0 \text{ LossO3} + .75 \text{ CH}_3\text{O}_2 + .75 \text{ OH} + .25 \text{ HCHO} + .4 \text{ H} + .05 \text{ H}_2$	$1.75\text{E-}10$	Sander et al. (2011)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow 1. \text{ LossG4101} + \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E-}20 * \text{EXP}(2.82 * \text{LOG}(\text{temp}) - 987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow 1. \text{ OHlossHO2prodNMHC} + \text{HCHO} + \text{HO}_2$	$2.9\text{E-}12 * \text{EXP}(-345./\text{temp})$	Sander et al. (2011)
G4103	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{ho2loss} + \text{CH}_3\text{OOH} + \text{O}_2$	$4.1\text{E-}13 * \text{EXP}(750./\text{temp})$	Sander et al. (2011)*
G4104	UpStTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow 1. \text{ HO2prodNMHCNOy} + 1.0 \text{ o3prodro2} + \text{noprodHO2} + \text{ProdMeO2} + 1.0 \text{ ProdO3} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E-}12 * \text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow 1. \text{ HO2prodNMHCNOy} + 1.0 \text{ o3lossno} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E-}12$	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{ HCHO} + 2 \text{ HO}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 1./26.2 * \text{EXP}(1130./\text{temp}))$	Sander et al. (2011)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E-}14 * \text{EXP}(390./\text{temp}) / (1. + 26.2 * \text{EXP}(-1130./\text{temp}))$	Sander et al. (2011)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow 0.7 \text{ OHlossNMHC} + .7 \text{ CH}_3\text{O}_2 + .3 \text{ HCHO} + .3 \text{ OH} + \text{H}_2\text{O}$	$k_ \text{CH300H_OH}$	Wallington et al. (2018)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow 1. \text{ OHlossHO2prodNMHC} + \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 * \text{EXP}(2.03 * \text{LOG}(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow 1. \text{ HO2prodNMHCNOy} + 1.0 \text{ o3lossno} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 * \text{EXP}(-1900./\text{temp})$	Sander et al. (2011)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow 1. \text{ LossG4110} + \text{H} + \text{CO}_2$	$(1.57\text{E-}13 + \text{cair} * 3.54\text{E-}33)$	McCabe et al. (2001)

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

#	labels	reaction	rate coefficient	reference
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow 1. \text{ OHlossHO2prodNMHC} + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	4.0E-13	Sander et al. (2011)
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17*\text{temp}*\text{temp}*\text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow 1.0 \text{ o3lossro} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{HCHO} + .63 \text{ CO} + .13 \text{ HO}_2 + 0.23125 \text{ HCOOH} + 0.13875 \text{ HCHO} + 0.13875 \text{ H}_2\text{O}_2 + .13 \text{ OH}$	$1.2\text{E-}14*\text{EXP}(-2630./\text{temp})$	Sander et al. (2011)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	$k_3\text{rd}(\text{temp}, \text{cair}, 1.0\text{E-}28, 4.5, 7.5\text{E-}12, 0.85, 0.6)$	Sander et al. (2011)
G4203	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13*\text{EXP}(700./\text{temp})$	Sander et al. (2011)
G4204	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow 1. \text{ HO2prodNMHCNOy} + 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1.0 \text{ ProdO3} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E-}12*\text{EXP}(365./\text{temp})$	Sander et al. (2011)
G4205	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow 1. \text{ HO2prodNMHCNOy} + 1.0 \text{ o3lossno} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	2.3E-12	Wallington et al. (2018)
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	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow 0.3 \text{ OHlossNMHC} + .3 \text{ C}_2\text{H}_5\text{O}_2 + .7 \text{ CH}_3\text{CHO} + .7 \text{ OH}$	k_CH300H_OH	see note*
G4208	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$4.4\text{E-}12*\text{EXP}(365./\text{temp})$	Atkinson et al. (2006)
G4209	TrGCN	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow 1.0 \text{ o3lossno} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E-}12*\text{EXP}(-1900./\text{temp})$	Sander et al. (2011)
G4210	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$4.2\text{E-}14*\text{EXP}(855./\text{temp})$	Atkinson et al. (2006)
G4211a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{CH}_3\text{C}(\text{O})\text{OOH}$	$4.3\text{E-}13*\text{EXP}(1040./\text{temp})/(1.+1./37.*\text{EXP}(660./\text{temp}))$	Tyndall et al. (2001)
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + 1.0 \text{ o3prodro2} + 1.0 \text{ ProdO3} + \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E-}13*\text{EXP}(1040./\text{temp})/(1.+37.*\text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1.0 \text{ ProdO3} + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E-}12*\text{EXP}(270./\text{temp})$	Tyndall et al. (2001)
G4213	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{panprod} + \text{PAN}$	k_CH3C03_N02	Sander et al. (2011)*
G4214	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow 1.0 \text{ o3lossno} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	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)

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

#	labels	reaction	rate coefficient	reference
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. (2018), 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	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow 1. \text{OHlossNMHC} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G4219	TrGCN	$\text{NACA} + \text{OH} \rightarrow 1. \text{OHlossNMHC} + \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6\text{E}-12 * \text{EXP}(270./\text{temp})$	Pöschl et al. (2000)
G4220	TrGCN	$\text{PAN} + \text{OH} \rightarrow 1. \text{OHlossNMHC} + \text{panloss} + \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$9.50\text{E}-13 * \text{EXP}(-650./\text{temp})$	Rickard and Pascoe (2009)
G4221	TrGCN	$\text{PAN} \rightarrow \text{panloss} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	$k_{\text{PAN_M}}$	Sander et al. (2011)*
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow 1. \text{OHlossNMHC} + .82 \text{iC}_3\text{H}_7\text{O}_2 + .18 \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65\text{E}-17 * \text{temp} * \text{temp} * \text{EXP}(-87./\text{temp})$	Atkinson (2003)
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow 1.0 \text{LossO3R} + 1.0 \text{LossO3} + .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .04 \text{MGLYOX} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5\text{E}-15 * \text{EXP}(-1900./\text{temp})$	Sander et al. (2011)
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow 1. \text{OHlossNMHC} + \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 8.\text{E}-27, 3.5, 3.\text{E}-11, 0., 0.5)$	Wallington et al. (2018)
G4303	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow 1.0 \text{o3lossno} + 1.0 \text{LossO3R} + 1.0 \text{LossO3} + \text{LC4H9NO3}$	$4.6\text{E}-13 * \text{EXP}(-1155./\text{temp})$	Wallington et al. (2018)
G4304	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow 1. \text{HO2lossNMHC} + \text{iC}_3\text{H}_7\text{OOH}$	$k_{\text{Pr02_H02}}$	Atkinson (1997)
G4305	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow 0.96 \text{HO2prodNMHCNOy} + 1.0 \text{o3prodho2} + \text{ProdRO2} + 1.0 \text{ProdO3} + .96 \text{CH}_3\text{COCH}_3 + .96 \text{HO}_2 + .96 \text{NO}_2 + .04 \text{iC}_3\text{H}_7\text{ONO}_2$	$k_{\text{Pr02_N0}}$	Wallington et al. (2018)
G4306	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{HCHO} + .8 \text{HO}_2 + .2 \text{CH}_3\text{OH}$	$k_{\text{Pr02_CH302}}$	Kirchner and Stockwell (1996)
G4307	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow 0.3 \text{OHlossNMHC} + .3 \text{iC}_3\text{H}_7\text{O}_2 + .7 \text{CH}_3\text{COCH}_3 + .7 \text{OH}$	$k_{\text{CH300H_OH}}$	see note*
G4308	TrGC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HO}_2 \rightarrow 1. \text{HO2lossNMHC} + \text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH}$	$6.5\text{E}-13 * \text{EXP}(650./\text{temp})$	Müller and Brasseur (1995)
G4309	TrGCN	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow 0.98 \text{HO2prodNMHCNOy} + 1.0 \text{o3prodho2} + \text{ProdRO2} + 1.0 \text{ProdO3} + .98 \text{CH}_3\text{CHO} + .98 \text{HCHO} + .98 \text{HO}_2 + .98 \text{NO}_2 + .02 \text{LC4H9NO3}$	$4.2\text{E}-12 * \text{EXP}(180./\text{temp})$	Müller and Brasseur (1995)
G4310	TrGC	$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH} + \text{OH} \rightarrow 0.5 \text{OHlossNMHC} + .5 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{OH} + \text{H}_2\text{O}$	$3.8\text{E}-12 * \text{EXP}(200./\text{temp})$	Müller and Brasseur (1995)

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

#	labels	reaction	rate coefficient	reference
G4311	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$1.33\text{E-}13 + 3.82\text{E-}11 * \text{EXP}(-2000./\text{temp})$	Sander et al. (2011)
G4312	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E-}13 * \text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1.0 \text{ ProdO3} + \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{NO}_2$	$2.9\text{E-}12 * \text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ MGLYOX} + .5 \text{ CH}_3\text{OH} + .3 \text{ CH}_3\text{C(O)OO} + .8 \text{ HCHO} + .3 \text{ HO}_2 + .2 \text{ CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E-}13 * \text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4315	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow 0.3 \text{ OHlossNMHC} + .3 \text{ CH}_3\text{COCH}_2\text{O}_2 + .7 \text{ MGLYOX} + .7 \text{ OH}$	$k_{\text{CH300H_OH}}$	see note*
G4316	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow 1. \text{ OHlossHO2prodNMHC} + \text{MGLYOX} + \text{HO}_2$	$2.15\text{E-}12 * \text{EXP}(305./\text{temp})$	Dillon et al. (2006)
G4317	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{CH}_3\text{C(O)OO} + \text{CO}$	$8.4\text{E-}13 * \text{EXP}(830./\text{temp})$	Tyndall et al. (1995)
G4320	TrGCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13 * \text{EXP}(-230./\text{temp})$	Wallington et al. (2018)
G4400	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.81\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(114./\text{temp})$	Atkinson (2003)
G4401	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .88 \text{ MEK} + .68 \text{ HCHO} + 1.23 \text{ HO}_2 + .12 \text{ CH}_3\text{CHO} + .12 \text{ C}_2\text{H}_5\text{O}_2 + .18 \text{ CH}_3\text{OH}$	$k_{\text{PrO2_CH302}}$	see note*
G4402	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{LC}_4\text{H}_9\text{OOH}$	$k_{\text{PrO2_H02}}$	see note*
G4403	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow 0.56 \text{ HO2prodNMHCNOy} + 1.0 \text{ o3prodro2} + \text{ProdRO2} + 1.0 \text{ ProdO3} + .84 \text{ NO}_2 + .56 \text{ MEK} + .56 \text{ HO}_2 + .28 \text{ C}_2\text{H}_5\text{O}_2 + .28 \text{ CH}_3\text{CHO} + .16 \text{ LC}_4\text{H}_9\text{NO}_3$	$k_{\text{PrO2_N0}}$	see note*
G4404	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow 0.14999998 \text{ OHlossNMHC} + .15 \text{ LC}_4\text{H}_9\text{O}_2 + .85 \text{ MEK} + .85 \text{ OH} + .85 \text{ H}_2\text{O}$	$k_{\text{CH300H_OH}}$	see note*
G4405	TrGC	$\text{MVK} + \text{O}_3 \rightarrow 1.0 \text{ o3lossro} + 1.0 \text{ LossO3R} + 1.0 \text{ LossO3} + .45 \text{ HCOOH} + .9 \text{ MGLYOX} + .1 \text{ CH}_3\text{C(O)OO} + .19 \text{ OH} + .22 \text{ CO} + .32 \text{ HO}_2$	$.5 * (1.36\text{E-}15 * \text{EXP}(-2112./\text{temp}) + 7.51\text{E-}16 * \text{EXP}(-1521./\text{temp}))$	Pöschl et al. (2000)
G4406	TrGC	$\text{MVK} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + \text{MVKO2}$	$.5 * (4.1\text{E-}12 * \text{EXP}(452./\text{temp}) + 1.9\text{E-}11 * \text{EXP}(175./\text{temp}))$	Pöschl et al. (2000)
G4407	TrGC	$\text{MVKO2} + \text{HO}_2 \rightarrow 1. \text{ HO2lossNMHC} + \text{MVKOOH}$	$1.82\text{E-}13 * \text{EXP}(1300./\text{temp})$	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
G4408	TrGCN	MVKO2 + NO \rightarrow 0.75 HO2prodNMHCNOy + 1.0 o3prodro2 + ProdRO2 + 1.0 ProdO3 + NO ₂ + .25 CH ₃ C(O)OO + .25 CH ₃ COCH ₂ OH + .75 HCHO + .25 CO + .75 HO ₂ + .5 MGLYOX	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGCN	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 MGLYOX + .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 + MGLYOX + .5 CO + .5 HCHO + HO ₂	2.E-12	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH \rightarrow 1. OHlossNMHC + MVKO2	3.E-11	Pöschl et al. (2000)
G4413	TrGC	MEK + OH \rightarrow 1. OHlossNMHC + LMEKO2	1.3E-12*EXP(-25./temp)	Wallington et al. (2018)
G4414	TrGC	LMEKO2 + HO ₂ \rightarrow 1. HO2lossNMHC + LMEKOOH	k_PrO2_HO2	see note*
G4415	TrGCN	LMEKO2 + NO \rightarrow 1.0 o3prodro2 + ProdRO2 + 1.0 ProdO3 + .985 CH ₃ CHO + .985 CH ₃ C(O)OO + .985 NO ₂ + .015 LC4H9NO3	k_PrO2_NO	see note*
G4416	TrGC	LMEKOOH + OH \rightarrow 0.19999999 OHlossNMHC + .8 BIACET + .8 OH + .2 LMEKO2	k_CH300H_OH	see note*
G4417	TrGCN	LC4H9NO3 + OH \rightarrow 1. OHlossNMHC + MEK + NO ₂ + H ₂ O	1.7E-12	Wallington et al. (2018)
G4418	TrGCN	MPAN + OH \rightarrow 1. OHlossNMHC + CH ₃ COCH ₂ OH + NO ₂	3.2E-11	Orlando et al. (2002)
G4419	TrGCN	MPAN \rightarrow MVKO2 + NO ₂	k_PAN_M	see note*
G4500	TrGC	C ₅ H ₈ + O ₃ \rightarrow 1.0 LossO3R + 1.0 LossO3 + .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)
G4501	TrGC	C ₅ H ₈ + OH \rightarrow 1. OHlossNMHC + ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGCN	C ₅ H ₈ + NO ₃ \rightarrow 1.0 o3lossno + 1.0 LossO3R + 1.0 LossO3 + ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO ₂ \rightarrow 1. HO2lossNMHC + ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)
G4504	TrGCN	ISO2 + NO \rightarrow 0.956 HO2prodNMHCNOy + 1.0 o3prodro2 + ProdRO2 + 1.0 ProdO3 + .956 NO ₂ + .956 MVK + .956 HCHO + .956 HO ₂ + .044 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
G4505	TrGC	ISO2 + CH ₃ O ₂ → .5 MVK + 1.25 HCHO + HO ₂ + .25 MGLYOX + .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	TrGCN	ISON + OH → 1. OHlossNMHC + CH ₃ COCH ₂ OH + NACA	1.3E-11	Pöschl et al. (2000)
G6100	UpStTrGCl	Cl + O ₃ → ClO + O ₂	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + O(³ P) → 2.0 LossO3Cl + 2.0 LossO3 + Cl + O ₂	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → 2.0 LossO3Cl + 2.0 LossO3 + Cl ₂ + O ₂	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2.0 LossO3Cl + 2.0 LossO3 + 2 Cl + O ₂	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → 1.0 LossO3Cl + 1.0 LossO3 + Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl ₂ O ₂	k_ClO_ClO	Burkholder et al. (2015)
G6103	StTrGCl	Cl ₂ O ₂ → ClO + ClO	k_ClO_ClO/(2.16E-27*EXP(8537./ temp))	Burkholder et al. (2015)*
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 → 1.0 ProdO3 + 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 → 1. LossG6203 + 1.0 LossO3Cl + 1.0 LossO3 + .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 → 1. LossG6204 + HOCl + O ₂	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)	Burkholder et al. (2015)
G6300	UpStTrGCIN	ClO + NO → NO ₂ + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGCIN	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	TrGCIN	ClNO ₃ → ClO + NO ₂	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGCIN	ClNO ₃ + O(³ P) → ClO + NO ₃	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGCIN	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)*
G6403	StTrGCl	ClO + CH ₃ O ₂ → 1.0 o3lossro + 1.0 LossO3Cl + 1.0 LossO3 + HO ₂ + Cl + HCHO	1.8E-12*EXP(-600./temp)	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow 4.0 \text{ ProdLCl} + \text{LCARBON} + \text{ClO} + 3 \text{ Cl}$	3.3E-10	Burkholder et al. (2015)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 1.0 \text{ ProdLCl} + 1.0 \text{ LossO3Cl} + 1.0 \text{ LossO3} + \text{OH} + \text{Cl}$	1.65E-10	see note*
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow 1.0 \text{ ProdLCl} + \text{LCARBON} + \text{H}_2\text{O} + \text{Cl}$	$1.96\text{E-}12*\text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 1.0 \text{ o3lossxo} + 3.0 \text{ ProdLCl} + 1.0 \text{ LossO3Cl} + 1.0 \text{ LossO3} + 2 \text{ LCARBON} + \text{OH} + 3 \text{ Cl}$	3.25E-10	Burkholder et al. (2015)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 3.0 \text{ ProdLCl} + 2 \text{ LCARBON} + \text{H}_2\text{O} + 3 \text{ Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Burkholder et al. (2015)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})\text{OO}$	8.0e-11	Atkinson et al. (2006)
G6500	StGCIF	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow 2.0 \text{ ProdLCl} + \text{LCARBON} + 2 \text{ LFLUORINE} + \text{ClO} + \text{Cl}$	1.4E-10	Burkholder et al. (2015)
G6501	StGCIF	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow 3.0 \text{ ProdLCl} + \text{LCARBON} + 2 \text{ LFLUORINE} + \text{ClO} + 2 \text{ Cl}$	2.3E-10	Burkholder et al. (2015)
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	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow 2.0 \text{ LossO3Br} + 2.0 \text{ LossO3} + \text{Br} + \text{O}_2$	$1.9\text{E-}11*\text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2.0 \text{ LossO3Br} + 2.0 \text{ LossO3} + 2 \text{ Br} + \text{O}_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2.0 \text{ LossO3Br} + 2.0 \text{ LossO3} + \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14*\text{EXP}(840./\text{temp})$	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	$\text{BrO} + \text{HO}_2 \rightarrow 1. \text{ LossG7201} + \text{HOBr} + \text{O}_2$	$4.5\text{E-}12*\text{EXP}(500./\text{temp})$	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	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3} + \text{OH} + \text{BrO}$	$1.2\text{E-}10*\text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow 1.0 \text{ ProdO3} + \text{HOBr} + \text{Br}$	$2.0\text{E-}11*\text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGBrN	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.7\text{E-}12*\text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGBrN	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$\text{k_BrO_NO2}/(5.44\text{E-}9*\text{EXP}(14192./\text{temp})*1.\text{E6}*R_gas*\text{temp}/(\text{atm2Pa}*N_A))$	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	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{HCHO}$	f_BrO_CH3O2*5.7E-12	Aranda et al. (1997)

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

#	labels	reaction	rate coefficient	reference
G7402b	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow 1.0 \text{ o3lossro} + 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3} + \text{Br} + \text{HCHO} + \text{HO}_2$	$(1.-\text{f_BrO_CH3O2})*5.7\text{E-}12$	Aranda et al. (1997)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow 1.0 \text{ ProdLBr} + \text{LCARBON} + \text{H}_2\text{O} + \text{Br}$	$1.42\text{E-}12*\text{EXP}(-1150./\text{temp})$	Burkholder et al. (2015)
G7404	TrGBrC	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow .6666667 \text{ CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HBr}$	$2.8\text{E-}13*\text{EXP}(224./\text{temp})/(1.+1.13\text{E}24*\text{EXP}(-3200./\text{temp})/\text{C}(\text{ind_O2}))$	Atkinson et al. (2006)
G7405	TrGBrC	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})\text{OO}$	$1.8\text{e-}11*\text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow 3.0 \text{ ProdSBr} + \text{LCARBON} + \text{H}_2\text{O} + 3 \text{ Br}$	$9.0\text{E-}13*\text{EXP}(-360./\text{temp})$	Burkholder et al. (2015)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow 2.0 \text{ ProdSBr} + \text{LCARBON} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	Burkholder et al. (2015)*
G7600	TrGBrCl	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	$3.32\text{E-}15$	Manion et al. (2015)
G7601	TrGBrCl	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	$1.10\text{E-}15$	Dolson and Leone (1987)
G7602	TrGBrCl	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E-}10*\text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow 0.5 \text{ LossO3Br} + 0.5 \text{ LossO3Cl} + 1.0 \text{ LossO3} + \text{Br} + \text{OClO}$	$1.6\text{E-}12*\text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3Cl} + 2.0 \text{ LossO3} + \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E-}12*\text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3Cl} + 2.0 \text{ LossO3} + \text{BrCl} + \text{O}_2$	$5.8\text{E-}13*\text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGBrCl	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	$1.45\text{E-}11$	Clyne and Cruse (1972)
G7605	TrGBrCl	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow 1.0 \text{ ProdSBr} + 2.0 \text{ ProdSCl} + \text{LCARBON} + 2 \text{ Cl} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	see note*
G7606	TrGBrCl	$\text{CHClBr}_2 + \text{OH} \rightarrow 2.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + \text{LCARBON} + \text{Cl} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	see note*
G7607	TrGBrCl	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow 1.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + \text{LCARBON} + \text{Cl} + \text{H}_2\text{O} + \text{Br}$	$2.1\text{E-}12*\text{EXP}(-880./\text{temp})$	Burkholder et al. (2015)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 3.3\text{E-}31, 4.3, 1.6\text{E-}12, 0., 0.6)$	Burkholder et al. (2015)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + 1.0 \text{ ProdO3} + \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E-}11*\text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow 1. \text{ OHlossNMHC} + 1.0 \text{ ProdO3} + \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow 1.0 \text{ o3lossro} + \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-}13*\text{EXP}(520./\text{temp})$	Atkinson et al. (2004)

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

#	labels	reaction	rate coefficient	reference
G9402	TrGCS	DMSO + OH \rightarrow 1. OHlossNMHC + 0.40 ProdO3 + .6 SO ₂ + HCHO + .6 CH ₃ O ₂ + .4 HO ₂ + .4 CH ₃ SO ₃ H	1.E-10	Hynes and Wine (1996)
G9403	TrGS	CH ₃ SO ₂ \rightarrow SO ₂ + CH ₃ O ₂	1.8E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	CH ₃ SO ₂ + O ₃ \rightarrow 1.0 o3lossxo + CH ₃ SO ₃	3.E-13	Barone et al. (1995)
G9405	TrGS	CH ₃ SO ₃ + HO ₂ \rightarrow CH ₃ SO ₃ H	5.E-11	Barone et al. (1995)
G9600	TrGCClS	DMS + Cl \rightarrow 1.0 ProdO3 + CH ₃ SO ₂ + HCl + HCHO	3.3E-10	Atkinson et al. (2004)
G9700	TrGBrCS	DMS + Br \rightarrow 1.0 ProdO3 + CH ₃ SO ₂ + HBr + HCHO	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGBrCS	DMS + BrO \rightarrow DMSO + Br	4.4E-13	Ingham et al. (1999)
G01Diag	StTrG	O ₃ (s) \rightarrow LO ₃ (s)	k_03s	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_{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 Wallington et al. (2018) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

Structure-Activity Relationships (SAR)

Some unmeasured rate coefficients are estimated with structure-activity relationships, using the following parameters and substituent factors:

k for H-abstraction by OH in $\text{cm}^{-3}\text{s}^{-1}$	
<code>k_p</code>	$4.49 \times 10^{-18} \times (T/\text{K})^2 \exp(-320 \text{ K}/T)$
<code>k_s</code>	$4.50 \times 10^{-18} \times (T/\text{K})^2 \exp(253 \text{ K}/T)$
<code>k_t</code>	$2.12 \times 10^{-18} \times (T/\text{K})^2 \exp(696 \text{ K}/T)$
<code>k_ROHRO</code>	$2.1 \times 10^{-18} \times (T/\text{K})^2 \exp(-85 \text{ K}/T)$
<code>k_CO2H</code>	$0.7 \times k_{\text{CH}_3\text{CO}_2\text{H}+\text{OH}}$
<code>k_ROOHRO</code>	$0.6 \times k_{\text{CH}_3\text{OOH}+\text{OH}}$
<code>f_alk</code>	1.23
<code>f_sOH</code>	3.44
<code>f_tOH</code>	2.68
<code>f_sOOH</code>	8.
<code>f_tOOH</code>	8.
<code>f_ONO2</code>	0.04
<code>f_CH2ONO2</code>	0.20
<code>f_cpan</code>	0.25
<code>f_allyl</code>	3.6
<code>f_CHO</code>	0.55
<code>f_CO2H</code>	1.67
<code>f_CO</code>	0.73
<code>f_O</code>	8.15
<code>f_pCH2OH</code>	1.29
<code>f_tCH2OH</code>	0.53

k for OH-addition to double bonds in $\text{cm}^{-3}\text{s}^{-1}$	
<code>k_adp</code>	$4.5 \times 10^{-12} \times (T/300 \text{ K})^{-0.85}$
<code>k_ads</code>	$1/4 \times (1.1 \times 10^{-11} \times \exp(485 \text{ K}/T) + 1.0 \times 10^{-11} \times \exp(553 \text{ K}/T))$
<code>k_adt</code>	$1.922 \times 10^{-11} \times \exp(450 \text{ K}/T) - k_{\text{ads}}$
<code>k_adsecprim</code>	3.0×10^{-11}
<code>k_adtertprim</code>	5.7×10^{-11}
<code>a_PAN</code>	0.56
<code>a_CHO</code>	0.31
<code>a_COCH3</code>	0.76
<code>a_CH2OH</code>	1.7
<code>a_CH2OOH</code>	1.7
<code>a_COH</code>	2.2
<code>a_COOH</code>	2.2
<code>a_CO2H</code>	0.25
<code>a_CH2ONO2</code>	0.64

RO₂ 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), as described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \text{k_CH3O2}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH3O2 = second-order rate coefficient of the self reaction of CH_3O_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: $k_{\text{H02_H02}} = (3.0\text{E-}13 * \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 * \text{EXP}(920./\text{temp}) * \text{cair}) * (1 + 1.4\text{E-}21 * \text{EXP}(2200./\text{temp}) * \text{C}(\text{ind_H20}))$.

G3109: The rate coefficient is: $k_{\text{N03_N02}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 2.4\text{E-}30, 3.0, 1.6\text{E-}12, -0.1, 0.6)$.

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

G3203: The rate coefficient is: $k_{\text{N02_H02}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 1.9\text{E-}31, 3.4, 4.0\text{E-}12, 0.3, 0.6)$.

G3206: The rate coefficient is: $k_{\text{HN03_OH}} = 1.32\text{E-}14 * \text{EXP}(527/\text{temp}) + 1 / (1 / (7.39\text{E-}32 * \text{EXP}(453/\text{temp}) * \text{cair}) + 1 / (9.73\text{E-}17 * \text{EXP}(1910/\text{temp})))$

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.

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: $k_{\text{CH3CO3_N02}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

G4221: The rate coefficient $\text{isk_PAN_M} = k_{\text{CH3CO3_N02}}/9.5\text{E-}29 * \text{EXP}(-14000./\text{temp})$, 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_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

G6405: Sander et al. (2006), but simplified shortcut to release all Cl

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

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.

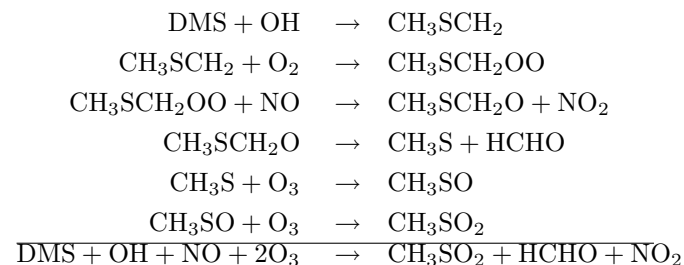
G7408: It is assumed that the reaction liberates all Br atoms. The fate of the carbon atom is currently not considered.

G7605: Same value as for G7408: $\text{CH}_2\text{Br}_2 + \text{OH}$ assumed. It is assumed that the reaction liberates all Br and all Cl. The fate of the carbon atom is currently not considered.

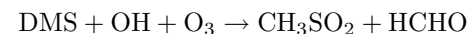
G7606: Same value as for G7408: $\text{CH}_2\text{Br}_2 + \text{OH}$ assumed. It is assumed that the reaction liberates all Br atoms and also Cl. The fate of the carbon atom is currently not considered.

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

G9400a: For the abstraction path, the assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:



Neglecting the effect on O_3 and NO_x , the remaining reaction is:



G9400b: For the addition path, the rate coefficient is: $k_{\text{DMS_OH}} = 1.0\text{E-}39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{ind_02}) / (1 + 5.0\text{E-}30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{ind_02}))$.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow o3prodo2 + 2.0 \text{ ProdO3} + O(^3P) + O(^3P)$	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	UpStGJN	$N_2O + h\nu \rightarrow 1.0 \text{ o3prodho2} + 1.0 \text{ ProdO3} + O(^1D) + N_2$	jx(ip_N20)	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_N02)	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow 1.0 \text{ ProdO3} + N + O(^3P)$	jx(ip_NO)	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow 2.0 \text{ LossO3N} + 2.0 \text{ LossO3} + NO + O_2$	jx(ip_N002)	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow 1. \text{ LossJ3200} + NO + OH$	jx(ip_H0N0)	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow 1. \text{ LossJ3201} + NO_2 + OH$	jx(ip_HN03)	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow 0.333 \text{ o3prodho2} + 0.333 \text{ ProdO3} + .667 \text{ NO}_2 + .667 \text{ HO}_2 + .333 \text{ NO}_3 + .333 \text{ OH}$	jx(ip_HN04)	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	$HCHO + h\nu \rightarrow 1. \text{ HO2prodNMHCphoto} + 1. \text{ LossJ4101b} + H + CO + HO_2$	jx(ip_CH0H)	Sander et al. (2014)
J4102	StGJ	$CO_2 + h\nu \rightarrow 1.0 \text{ ProdO3} + CO + O(^3P)$	jx(ip_C02)	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	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J4201	TrGJC	$CH_3CHO + h\nu \rightarrow 1. \text{ HO2prodNMHCphoto} + CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	Sander et al. (2014)
J4202	TrGJC	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3C03H)	Sander et al. (2014)
J4203	TrGJCN	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CH0H)	von Kuhlmann (2001)
J4204	TrGJCN	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	Sander et al. (2014)
J4300	TrGJC	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J4301	TrGJC	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3C0CH3)	Sander et al. (2014)
J4302	TrGJC	$CH_3COCH_2OH + h\nu \rightarrow 1. \text{ HO2prodNMHCphoto} + CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CH0H)	see note*
J4303	TrGJC	$MGLYOX + h\nu \rightarrow 1. \text{ HO2prodNMHCphoto} + CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4304	TrGJC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	see note*
J4306	TrGJCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow 1. \text{HO2prodNMHCphoto} + \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	$3.7*\text{jx}(\text{ip_PAN})$	von Kuhlmann et al. (2003)*
J4400	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .67 \text{MEK} + .67 \text{HO}_2 + .33 \text{C}_2\text{H}_5\text{O}_2 + .33 \text{CH}_3\text{CHO}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J4401	TrGJC	$\text{MVK} + h\nu \rightarrow 1. \text{HO2prodNMHCphoto} + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO} + \text{HO}_2$	$0.019*\text{jx}(\text{ip_COH2}) + .015*\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2014)
J4402	TrGJC	$\text{MVKOOH} + h\nu \rightarrow \text{OH} + .5 \text{MGLYOX} + .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{HCHO} + .75 \text{HO}_2 + .25 \text{CH}_3\text{C}(\text{O})\text{OO} + .25 \text{CO}$	$\text{jx}(\text{ip_CH300H})$	see note*
J4403	TrGJC	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2$	$0.42*\text{jx}(\text{ip_CHOH})$	von Kuhlmann et al. (2003)
J4404	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J4405	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C}(\text{O})\text{OO}$	$2.15*\text{jx}(\text{ip_MGLYOX})$	see note*
J4406	TrGJCN	$\text{LC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow 0.67 \text{HO2prodNMHCphoto} + \text{NO}_2 + .67 \text{MEK} + .67 \text{HO}_2 + .33 \text{C}_2\text{H}_5\text{O}_2 + .33 \text{CH}_3\text{CHO}$	$3.7*\text{jx}(\text{ip_PAN})$	von Kuhlmann (2001)
J4407	TrGJCN	$\text{MPAN} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$\text{jx}(\text{ip_PAN})$	see note*
J4500	TrGJC	$\text{ISOOH} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	see note*
J4501	TrGJCN	$\text{ISON} + h\nu \rightarrow 1. \text{HO2prodNMHCphoto} + \text{MVK} + \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$3.7*\text{jx}(\text{ip_PAN})$	von Kuhlmann (2001)
J6000	StTrGJCl	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$\text{jx}(\text{ip_Cl2})$	Sander et al. (2014)
J6100	StTrGJCl	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2.0 \text{LossO3Cl} + 2.0 \text{LossO3} + 2 \text{Cl}$	$\text{jx}(\text{ip_Cl2O2})$	Sander et al. (2014)
J6101	StTrGJCl	$\text{OCIO} + h\nu \rightarrow 1.0 \text{ProdO3} + \text{ClO} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip_OC10})$	Sander et al. (2014)
J6200	StGJCl	$\text{HCl} + h\nu \rightarrow \text{Cl} + \text{H}$	$\text{jx}(\text{ip_HCl})$	Sander et al. (2014)
J6201	StTrGJCl	$\text{HOCl} + h\nu \rightarrow 1.0 \text{LossO3Cl} + 1.0 \text{LossO3} + \text{OH} + \text{Cl}$	$\text{jx}(\text{ip_HOC1})$	Sander et al. (2014)
J6300	TrGJCIN	$\text{ClNO}_2 + h\nu \rightarrow 1.0 \text{ProdO3} + \text{Cl} + \text{NO}_2$	$\text{jx}(\text{ip_ClNO2})$	Sander et al. (2014)
J6301a	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	$\text{jx}(\text{ip_ClNO3})$	Sander et al. (2014)
J6301b	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$\text{jx}(\text{ip_ClON02})$	Sander et al. (2014)
J6400	StGJCl	$\text{CH}_3\text{Cl} + h\nu \rightarrow 1.0 \text{ProdLCl} + \text{Cl} + \text{CH}_3\text{O}_2$	$\text{jx}(\text{ip_CH3Cl})$	Sander et al. (2014)
J6401	StGJCl	$\text{CCl}_4 + h\nu \rightarrow 4.0 \text{ProdLCl} + \text{LCARBON} + 4 \text{Cl}$	$\text{jx}(\text{ip_CC14})$	Sander et al. (2014)
J6402	StGJCCl	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3.0 \text{ProdLCl} + 2 \text{LCARBON} + 3 \text{Cl}$	$\text{jx}(\text{ip_CH3CC13})$	Sander et al. (2014)
J6500	StGJCIF	$\text{CFCl}_3 + h\nu \rightarrow 3.0 \text{ProdLCl} + 3 \text{Cl} + \text{LCARBON} + \text{LFLUORINE}$	$\text{jx}(\text{ip_CFC13})$	Sander et al. (2014)
J6501	StGJCIF	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2.0 \text{ProdLCl} + 2 \text{Cl} + \text{LCARBON} + 2 \text{LFLUORINE}$	$\text{jx}(\text{ip_CF2Cl2})$	Sander et al. (2014)
J7000	StTrGJBr	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	$\text{jx}(\text{ip_Br2})$	Sander et al. (2014)
J7100	StTrGJBr	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip_BrO})$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7200	StTrGJBr	$\text{HOBr} + h\nu \rightarrow 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3} + \text{Br} + \text{OH}$	<code>jx(ip_HOBr)</code>	Sander et al. (2014)
J7300	TrGJBrN	$\text{BrNO}_2 + h\nu \rightarrow 1.0 \text{ ProdO3} + \text{Br} + \text{NO}_2$	<code>jx(ip_BrNO2)</code>	Sander et al. (2014)
J7301	StTrGJBrN	$\text{BrNO}_3 + h\nu \rightarrow .85 \text{ Br} + .85 \text{ NO}_3 + .15 \text{ BrO} + .15 \text{ NO}_2$	<code>jx(ip_BrNO3)</code>	Sander et al. (2014)*
J7400	StGJBr	$\text{CH}_3\text{Br} + h\nu \rightarrow 1.0 \text{ ProdLBr} + \text{Br} + \text{CH}_3\text{O}_2$	<code>jx(ip_CH3Br)</code>	Sander et al. (2014)
J7401	TrGJBr	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow 2.0 \text{ ProdSBr} + \text{LCARBON} + 2 \text{ Br}$	<code>jx(ip_CH2Br2)</code>	Sander et al. (2014)
J7402	TrGJBr	$\text{CHBr}_3 + h\nu \rightarrow 3.0 \text{ ProdSBr} + \text{LCARBON} + 3 \text{ Br}$	<code>jx(ip_CHBr3)</code>	Sander et al. (2014)
J7500	StGJBrF	$\text{CF}_3\text{Br} + h\nu \rightarrow 1.0 \text{ ProdLBr} + \text{LCARBON} + 3 \text{ LFLUORINE} + \text{Br}$	<code>jx(ip_CF3Br)</code>	Sander et al. (2014)
J7600	StTrGJBrCl	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	<code>jx(ip_BrCl)</code>	Sander et al. (2014)
J7601	StGJBrClF	$\text{CF}_2\text{ClBr} + h\nu \rightarrow 1.0 \text{ ProdLBr} + 1.0 \text{ ProdLCl} + \text{LCARBON} + 2 \text{ LFLUORINE} + \text{Br} + \text{Cl}$	<code>jx(ip_CF2ClBr)</code>	Sander et al. (2014)
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow 1.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + \text{LCARBON} + \text{Br} + \text{Cl}$	<code>jx(ip_CH2ClBr)</code>	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow 1.0 \text{ ProdSBr} + 2.0 \text{ ProdSCl} + \text{LCARBON} + \text{Br} + 2 \text{ Cl}$	<code>jx(ip_CHCl2Br)</code>	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow 2.0 \text{ ProdSBr} + 1.0 \text{ ProdSCl} + \text{LCARBON} + 2 \text{ Br} + \text{Cl}$	<code>jx(ip_CHClBr2)</code>	Sander et al. (2014)
J8401a	StTrGJI	$\text{CH}_3\text{I} + h\nu \rightarrow \text{CH}_3\text{O}_2$	<code>JX(ip_CH3I)</code>	Sander et al. (2014)
PH (aqueous)				

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:

`j(11) → jx(ip_COH2)`
`j(12) → jx(ip_CHOH)`
`j(15) → jx(ip_HOCH2CHO)`
`j(18) → jx(ip_MACR)`
`j(22) → jx(ip_ACETOL)`
`j(23)+j(24) → jx(ip_MVK)`
`j(31)+j(32)+j(33) → jx(ip_GLYOX)`
`j(34) → jx(ip_MGLYOX)`

`j(41) → jx(ip_CH3OOH)`
`j(53) → j(isopropyl nitrate)`
`j(54) → j(isopropyl nitrate)`
`j(55) → j(isopropyl nitrate)`
`j(56)+j(57) → jx(ip_NOA)`

Specific notes

J4302: It is assumed that $J(\text{CH}_3\text{COCH}_2\text{OH})$ is 0.074 times that of J4101b.
J4304: It is assumed that $J(\text{CH}_3\text{COCH}_2\text{O}_2\text{H})$ is the same as $J(\text{CH}_3\text{OOH})$.
J4306: Following von Kuhlmann et al. (2003), we use $J(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7 * jx(ip_PAN)$.

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

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

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

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

J7301: The quantum yields are recommended by Burkholder et al. (2015) for $\lambda > 300\text{nm}$ and used here for the entire spectrum.

Table 3: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
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General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry’s law constants from chemprop (see `chemprop.pdf`).

For uptake of X (X = N₂O₅, ClNO₃, or BrNO₃) and

subsequent reaction with H₂O, Cl[−], and Br[−] 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_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt} . The factors only affect

the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[\text{Cl}^-] > 0.1 \text{ M}$ (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\text{H}_2\text{O}]/[\text{Cl}^-]$ is less than 5×10^2 . The ratio $5 \times 10^2 / 3 \times 10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N₂O₅. Here, they are also used for ClNO₃ and BrNO₃.

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 1.0 \text{ o3lossno} + 1.0 \text{ LossO3N} + 1.0 \text{ LossO3} + 2 \text{ HNO}_3$	<code>khet_St(ihs_N205_H20)</code>	see general notes*
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 3.0 \text{ LossO3N} + 3.0 \text{ LossO3} + 2 \text{ NO}_3^-(\text{cs}) + 2 \text{ H}^+(\text{cs})$	<code>khet_Tr(iht_N205)</code>	see general notes*
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow 1.0 \text{ LossO3Cl} + 1.0 \text{ LossO3} + \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see general notes*
HET420	StHetClN	$\text{ClNO}_3 + \text{HCl} \rightarrow 1.0 \text{ o3lossno} + 0.5 \text{ LossO3Cl} + 0.5 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see general notes*
HET421	StHetClN	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H20)</code>	see general notes*
HET422	StHetClN	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow 1.0 \text{ LossO3Cl} + 1.0 \text{ LossO3N} + 2.0 \text{ LossO3} + \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N205_HCl)</code>	see general notes*
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow 1.0 \text{ LossO3Br} + 1.0 \text{ LossO3} + \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see general notes*
HET520	StHetBrN	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H20)</code>	see general notes*
HET540	StHetBrClN	$\text{ClNO}_3 + \text{HBr} \rightarrow 1.0 \text{ o3lossno} + 0.333333 \text{ LossO3Br} + 0.333333 \text{ LossO3Cl} + 0.333333 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see general notes*
HET541	StHetBrClN	$\text{BrNO}_3 + \text{HCl} \rightarrow 1.0 \text{ o3lossno} + 0.333333 \text{ LossO3Br} + 0.333333 \text{ LossO3Cl} + 0.333333 \text{ LossO3N} + 1.0 \text{ LossO3} + \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see general notes*
HET542	StHetBrCl	$\text{HOCl} + \text{HBr} \rightarrow 0.5 \text{ LossO3Br} + 0.5 \text{ LossO3Cl} + 1.0 \text{ LossO3} + \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see general notes*
HET543	StHetBrCl	$\text{HOBr} + \text{HCl} \rightarrow 0.5 \text{ LossO3Br} + 0.5 \text{ LossO3Cl} + 1.0 \text{ LossO3} + \text{BrCl} + \text{H}_2\text{O}$	<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 for details)

Table 5: Acid-base and other equilibria

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

Table 6: 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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