

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 3.8m

Date: November 14, 2020.

Selected reactions:

“Tr && (G | | (Aa && Mb1)) && !C && !Hg”

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase: 325

Aqueous phase: 148

All species: 473

Number of reactions in selected mechanism:

Gas phase (Gnn): 185

Aqueous phase (Annn): 25

Henry (Hnnn): 47

Photolysis (Jnnn): 49

Aqueous phase photolysis (PHnnn): 0

Heterogeneous (HETnnn): 0

Equilibria (EQnn): 34

Isotope exchange (IEXnnn): 0

Tagging equations (TAGnnn): 0

Dummy (Dnn): 1

All equations: 341

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	$\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{O}_3$	$6.0\text{E-}34*((\text{temp}/300.)^{**}(-2.4))$ *cair	Burkholder et al. (2015)
G2100	UpStTrG	$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 4.4\text{E-}32, 1.3,$ $7.5\text{E-}11, -0.2, 0.6)$	Burkholder et al. (2015)
G2104	UpStTrG	$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$1.7\text{E-}12*\text{EXP}(-940./\text{temp})$	Burkholder et al. (2015)
G2105	UpStTrG	$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$2.8\text{E-}12*\text{EXP}(-1800./\text{temp})$	Burkholder et al. (2015)
G2107	UpStTrG	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2 \text{O}_2$	$1.\text{E-}14*\text{EXP}(-490./\text{temp})$	Burkholder et al. (2015)
G2109	UpStTrG	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	$4.8\text{E-}11*\text{EXP}(250./\text{temp})$	Burkholder et al. (2015)
G2110	UpStTrG	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	k_HO2_HO2	Burkholder et al. (2015)*
G2111	UpStTrG	$\text{H}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 2 \text{OH}$	$1.63\text{E-}10*\text{EXP}(60./\text{temp})$	Burkholder et al. (2015)
G2112	UpStTrG	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	$1.8\text{E-}12$	Burkholder et al. (2015)
G2117	UpStTrG	$\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow (\text{H}_2\text{O})_2$	$6.521\text{E-}26*\text{temp}*\text{EXP}(1851.09/\text{temp})$ * $\text{EXP}(-5.10485\text{E-}3*\text{temp})$	Scribano et al. (2006)*
G2118	UpStTrG	$(\text{H}_2\text{O})_2 \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	$1.\text{E0}$	see note*
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)
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)
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)
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_NO3_NO2	Burkholder et al. (2015)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$\text{k_NO3_NO2}/(5.8\text{E-}27*\text{EXP}(10840./$ $\text{temp}))$	Burkholder et al. (2015)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$\text{k_3rd}(\text{temp}, \text{cair}, 7.0\text{E-}31, 2.6,$ $3.6\text{E-}11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.3\text{E-}12*\text{EXP}(270./\text{temp})$	Burkholder et al. (2015)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$\text{k_3rd}(\text{temp}, \text{cair}, 1.8\text{E-}30, 3.0,$ $2.8\text{E-}11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	k_NO2_HO2	Burkholder et al. (2015)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E-}12$	Burkholder et al. (2015)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E-}11*\text{EXP}(-390./\text{temp})$	Burkholder et al. (2015)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	k_HNO3_OH	Burkholder et al. (2015)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$\text{k_NO2_HO2}/(2.1\text{E-}27*\text{EXP}(10900./$ $\text{temp}))$	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)

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

#	labels	reaction	rate coefficient	reference
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)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	$1.85\text{E}-20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp})$ $-987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{HCHO} + .85 \text{HO}_2 + .15 \text{CH}_3\text{O} + \text{H}_2\text{O}$	$6.38\text{E}-18 \cdot (\text{temp}^{**}2) \cdot \text{EXP}(144./\text{temp})$	Atkinson et al. (2006)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$3.8\text{E}-13 \cdot \text{EXP}(780./\text{temp}) / (1.+1./$ $498. \cdot \text{EXP}(1160./\text{temp}))$	Atkinson et al. (2006)
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$3.8\text{E}-13 \cdot \text{EXP}(780./\text{temp}) / (1.+$ $498. \cdot \text{EXP}(-1160./\text{temp}))$	Atkinson et al. (2006)
G4104a	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot (1.-\text{beta}_$ $\text{CH3NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot \text{beta}_$ CH3NO3	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$	$1.2\text{E}-12$	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{O}_2$	$7.4\text{E}-13 \cdot \text{EXP}(-520./\text{temp}) \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$(\text{k_CH302}-7.4\text{E}-13*\text{EXP}(-520./\text{temp}))$ $*\text{R02}*2.$	Atkinson et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{CH}_3\text{O}_2 + .4 \text{HCHO} + .4 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Wallington et al. (2017)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18*\text{EXP}(2.03*\text{LOG}(\text{temp})$ $+636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13*\text{EXP}(-1900./\text{temp})$	Burkholder et al. (2015)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E}-13+\text{cair}*3.54\text{E}-33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$2.94\text{E}-14*\text{exp}(786./\text{temp})$ $+9.85\text{E}-13*\text{EXP}(-1036./\text{temp})$	Paulot et al. (2011)
G4114	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	k_NO2_CH302	Burkholder et al. (2015)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$\text{k_NO2_CH302}/(9.5\text{E}-29*\text{EXP}(11234./$ $\text{temp}))$	Burkholder et al. (2015)*
G4116	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$	$3.00\text{E}-14$	see note*
G4117	StTrGN	$\text{CH}_3\text{ONO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}_2$	$4.0\text{E}-13*\text{EXP}(-845./\text{temp})$	Atkinson et al. (2006)
G4118	StTrG	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E}-14*\text{exp}(-663./\text{temp})*\text{c}(\text{ind_02})$	Chai et al. (2014)
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.1\text{E}-29,$ $4.5, 2.1\text{E}-11, 0., 0.44)$	Atkinson et al. (2006)
G4119b	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$	$9.6\text{E}-12*\text{EXP}(-1150./\text{temp})$	Atkinson et al. (2006)
G4120a	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 2.6\text{E}-29,$ $2.8, 3.3\text{E}-11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/$ $900.), \text{SP}))$	Atkinson et al. (2006)
G4120b	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$	$2.3\text{E}-12*(\text{temp}/300.)*0.7$	Atkinson et al. (2006)
G4121	StTrG	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E}-16*\text{exp}(-1000./\text{temp})$	Burkholder et al. (2015)
G4122	StTrGN	$\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$	$1.\text{E}-10*\text{exp}(-1764./\text{temp})$	Nielsen et al. (1991)
G4123	StTrG	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$9.7\text{E}-15*\text{EXP}(625./\text{temp})$	Atkinson et al. (2006)
G4124	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.4\text{E}12*\text{EXP}(-7000./\text{temp})$	Atkinson et al. (2006)
G4125	StTrG	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2$ $\text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$	$5.6\text{E}-15*\text{EXP}(2300./\text{temp})$	Atkinson et al. (2006)
G4126	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$0.7275*2.3\text{E}-12*\text{EXP}(360./\text{temp})$	Atkinson et al. (2006)*
G4127	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$1.2\text{E}-12$	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(\text{k_CH302}*5.5\text{E}-12)**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(\text{k_CH302}*5.7\text{E}-14*\text{EXP}(750./\text{temp}))$ $**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*\text{k_CH300H_OH}$	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$\text{k_rohro} + \text{k_s*f_sooh}*f_soh$	Taraborrelli (2010)*

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

#	labels	reaction	rate coefficient	reference
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$\text{k_rohro} + 2.*\text{k_s*f_soh*f_soh}$	Taraborrelli (2010)*
G4133	StTrG	$\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$	1.4E-10	Bossolasco et al. (2014)*
G4134	StTrG	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E}+14*\text{EXP}(-10000/\text{temp})$	see note*
G4135	StTrG	$\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$	$\text{k_CH200_N02}*3.6\text{E}-6$	Ouyang et al. (2013)*
G4136	StTrG	$\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$	5.2E-12	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$	6.E-14	Welz et al. (2012)*
G4138	StTrGN	$\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$	k_CH200_N02	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$	3.6E-14	Vereecken et al. (2012)
G4141	StTrG	$\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$	1.E-10	Welz et al. (2014)*
G4142	StTrG	$\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$	1.7E-12	Stone et al. (2014)*
G4143	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4144	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4145	StTrG	$\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$	5.E-12	Vereecken et al. (2012)
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	1.E-12	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	6.E-11	Buras et al. (2014)
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	k_NO2_CH302	see note*
G4149	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$	$\text{k_NO2_CH302}/(9.5\text{E}-29*\text{EXP}(11234./\text{temp}))$	Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13*\text{EXP}(-650./\text{temp})*\text{f_soh}$	see note*
G4151	StTrG	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 7.0\text{E}-31, 3., 1.8\text{E}-12, -1.1, 0.33)$	Atkinson et al. (2006)
G4152	StTrG	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{HCHO} + .956 \text{H} + .044 \text{CH}_3\text{O} + \text{O}_2$	$5.1\text{E}-12*\text{exp}(-210./\text{temp})$	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{HCHO} + .83 \text{H} + .17 \text{CO} + .17 \text{H}_2 + .17 \text{H}$	1.3E-10	Atkinson et al. (2006)
G4154	StTrG	$\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$	2.53E-14	Albaladejo et al. (2002)*
G4155	StTrG	$\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{CH}_3 + .75 \text{O}_2 + .25 \text{HCHO} + .25 \text{OH}$	2.5E-11	Baulch et al. (2005)
G4156	StTrG	$\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$	4.3E-11	Zellner et al. (1988)
G4157	StTrG	$\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{OH} + .7 \text{CO} + .3 \text{H} + .3 \text{CO}_2 + \text{HO}_2$	$3.4\text{E}-11*\text{EXP}(-1600./\text{temp})$	Burkholder et al. (2015)
G4158	TrG	$\text{CH}_2\text{OO}^* \rightarrow .37 \text{CH}_2\text{OO} + .47 \text{CO} + .47 \text{H}_2\text{O} + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH}$	KDEC	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4159	TrGN	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$	Kleinböhl et al. (2006)
G4160a	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{HCN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.15 * \text{EXP}(200/\text{temp})$	Strekowski et al. (2010)
G4160b	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{NCO}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.68/2.$	Strekowski et al. (2010)*
G4160c	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{CN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * (1. - (0.68/2. + 0.15 * \text{EXP}(200/\text{temp})))$	Strekowski et al. (2010)*
G4161	TrGN	$\text{HCN} + \text{O}(^3\text{P}) \rightarrow \text{H} + \text{NCO}$	$1.0\text{E-}11 * \text{EXP}(-4000./\text{temp})$	Burkholder et al. (2015)*
G4162	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}(^3\text{P})$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.75$	Baulch et al. (2005)
G4163	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{CO} + \text{NO}$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.25$	Baulch et al. (2005)
G4164	TrGN	$\text{NCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{NO}$	$7.\text{E-}15$	Becker et al. (2000)*
G6100	UpStTrGCl	$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	$2.8\text{E-}11 * \text{EXP}(-250./\text{temp})$	Atkinson et al. (2007)
G6102a	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$	$1.0\text{E-}12 * \text{EXP}(-1590./\text{temp})$	Atkinson et al. (2007)
G6102b	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow 2 \text{Cl} + \text{O}_2$	$3.0\text{E-}11 * \text{EXP}(-2450./\text{temp})$	Atkinson et al. (2007)
G6102c	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl} + \text{OClO}$	$3.5\text{E-}13 * \text{EXP}(-1370./\text{temp})$	Atkinson et al. (2007)
G6102d	StTrGCl	$\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2\text{O}_2$	$k_{\text{ClO-ClO}}$	Burkholder et al. (2015)
G6103	StTrGCl	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	$k_{\text{ClO-ClO}} / (2.16\text{E-}27 * \text{EXP}(8537./\text{temp}))$	Burkholder et al. (2015)*
G6202	StTrGCl	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	$1.1\text{E-}11 * \text{EXP}(-980./\text{temp})$	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	$2.2\text{E-}12 * \text{EXP}(340./\text{temp})$	Atkinson et al. (2007)*
G6205	StTrGCl	$\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$	$1.7\text{E-}12 * \text{EXP}(-230./\text{temp})$	Atkinson et al. (2007)
G6300	UpStTrGCIN	$\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$	$6.2\text{E-}12 * \text{EXP}(295./\text{temp})$	Atkinson et al. (2007)
G6301	StTrGCIN	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$k_{\text{3rd-iupac}}(\text{temp}, \text{cair}, 1.6\text{E-}31, 3.4, 7.\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G6302	TrGCIN	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	$6.918\text{E-}7 * \text{EXP}(-10909./\text{temp}) * \text{cair}$	Anderson and Fahey (1990)
G6304	StTrGCIN	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	$6.2\text{E-}12 * \text{EXP}(145./\text{temp})$	Atkinson et al. (2007)
G6400	StTrGCl	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$	$6.6\text{E-}12 * \text{EXP}(-1240./\text{temp})$	Atkinson et al. (2006)
G6401	StTrGCl	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$	$8.1\text{E-}11 * \text{EXP}(-34./\text{temp})$	Atkinson et al. (2006)
G6402	StTrGCl	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{HCl} + \text{OH}$	$5.9\text{E-}11$	Atkinson et al. (2006)*
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$1.8\text{E-}12 * \text{EXP}(-600./\text{temp})$	Burkholder et al. (2015)
G6413	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{HCl} + \text{HCHO} + \text{NO}_2$	$1.3\text{E-}11 * \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6414	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO} \rightarrow \text{HCl} + \text{HCHO} + \text{NO}$	$2.1\text{E-}12$	Sokolov et al. (1999)
G6415	StTrGCl	$\text{Cl} + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ClO} + .5 \text{CH}_3\text{O} + .5 \text{HCl} + .5 \text{CH}_2\text{OO}$	$1.6\text{E-}10$	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)

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

#	labels	reaction	rate coefficient	reference
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14*\text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E-}12*\text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E-}12*\text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E-}12*\text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E-}11*\text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
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	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$\text{k_BrO_NO2}/(5.44\text{E-}9*\text{EXP}(14192./\text{temp})*1.\text{E6}*\text{R_gas}*\text{temp}/(\text{atm2Pa}*\text{N_A}))$	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)
G7402	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{CH}_2\text{OO}$	$2.42\text{E-}14*\text{EXP}(1617./\text{temp})$	Shallcross et al. (2015)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + \text{Br}$	$1.42\text{E-}12*\text{EXP}(-1150./\text{temp})$	Burkholder et al. (2015)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Br}$	$9.0\text{E-}13*\text{EXP}(-360./\text{temp})$	Burkholder et al. (2015)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	Burkholder et al. (2015)*
G7600	TrGBrCl	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	3.32E-15	Manion et al. (2015)
G7601	TrGBrCl	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	1.10E-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	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$1.6\text{E-}12*\text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E-}12*\text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	$5.8\text{E-}13*\text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGBrCl	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	1.45E-11	Clyne and Cruse (1972)
G7605	TrGBrCl	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{LCARBON} + 2 \text{LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	see note*
G7606	TrGBrCl	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + 2 \text{Br}$	$2.0\text{E-}12*\text{EXP}(-840./\text{temp})$	see note*
G7607	TrGBrCl	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.1\text{E-}12*\text{EXP}(-880./\text{temp})$	Burkholder et al. (2015)*
G8100	TrGI	$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	$2.1\text{E-}11*\text{EXP}(-830./\text{temp})$	Atkinson et al. (2007)
G8102	TrGI	$\text{OIO} + \text{OIO} \rightarrow \text{I}(\text{part})$	5.E-11	von Glasow et al. (2002)*
G8103	TrGI	$\text{IO} + \text{IO} \rightarrow .38 \text{OIO} + 1.62 \text{I} + .62 \text{O}_2$	$5.4\text{E-}11*\text{EXP}(180./\text{temp})$	Atkinson et al. (2007)*
G8200	TrGI	$\text{I} + \text{HO}_2 \rightarrow \text{HI} + \text{O}_2$	$1.5\text{E-}11*\text{EXP}(-1090./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G8201	TrGI	$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	$1.4\text{E-}11 \cdot \text{EXP}(540./\text{temp})$	Atkinson et al. (2007)
G8202	TrGI	$\text{HI} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O}$	$1.6\text{E-}11 \cdot \text{EXP}(440./\text{temp})$	Atkinson et al. (2007)
G8203	TrGI	$\text{OIO} + \text{OH} \rightarrow \text{HIO}_3$	$2.2\text{E-}10 \cdot \text{EXP}(243./\text{temp})$	Plane et al. (2006)
G8204	TrGI	$\text{I}_2 + \text{OH} \rightarrow \text{HOI} + \text{I}$	$2.1\text{E-}10$	Atkinson et al. (2007)
G8300	TrGIN	$\text{I} + \text{NO}_2 \rightarrow \text{INO}_2$	k_I_NO2	Atkinson et al. (2007)*
G8301	TrGIN	$\text{I} + \text{NO}_3 \rightarrow \text{IO} + \text{NO}_2$	$1.\text{E-}10$	Dillon et al. (2008)
G8302	TrGIN	$\text{IO} + \text{NO} \rightarrow \text{I} + \text{NO}_2$	$7.15\text{E-}12 \cdot \text{EXP}(300./\text{temp})$	Atkinson et al. (2007)
G8303	TrGIN	$\text{IO} + \text{NO}_2 \rightarrow \text{INO}_3$	k_3rd_iupac(temp, cair, $7.7\text{E-}31$, 5., $1.6\text{E-}11$, 0., 0.4)	Atkinson et al. (2007)
G8304	TrGIN	$\text{OIO} + \text{NO} \rightarrow \text{NO}_2 + \text{IO}$	$1.1\text{E-}12 \cdot \text{EXP}(542./\text{temp})$	Atkinson et al. (2007)
G8305	TrGIN	$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	k_I_NO2/($3.7\text{E-}7 \cdot \text{EXP}(9568./\text{temp})$ $\cdot 1.\text{E6} \cdot \text{R_gas} \cdot \text{temp}/(\text{atm2Pa} \cdot \text{N_A})$)	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGIN	$\text{INO}_3 \rightarrow \text{IO} + \text{NO}_2$	0.	see note*
G8307	TrGIN	$\text{I}_2 + \text{NO}_3 \rightarrow \text{I} + \text{INO}_3$	$1.5\text{E-}12$	Atkinson et al. (2007)
G8308	TrGIN	$\text{IO} + \text{NO}_3 \rightarrow \text{OIO} + \text{NO}_2$	$9.\text{E-}12$	Dillon et al. (2008)
G8401	TrGI	$\text{CH}_3\text{O}_2 + \text{IO} \rightarrow .4 \text{ I} + .6 \text{ OIO} + \text{HCHO} + \text{HO}_2$	$2.\text{E-}12$	Dillon et al. (2006), Bale et al. (2005)*
G8402	TrGIN	$\text{CH}_3\text{I} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{HCHO} + \text{IO}$	$3.4\text{E-}17$	Wayne et al. (1991)*
G8600	TrGCH	$\text{IO} + \text{ClO} \rightarrow .2 \text{ ICl} + .25 \text{ Cl} + .55 \text{ OClO} + .8 \text{ I} + .45 \text{ O}_2$	$4.7\text{E-}12 \cdot \text{EXP}(280./\text{temp})$	Atkinson et al. (2007)
G8700	TrGBrI	$\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br}$	$1.2\text{E-}11$	Burkholder et al. (2015)
G8701	TrGBrI	$\text{IO} + \text{BrO} \rightarrow \text{Br} + .8 \text{ OIO} + .2 \text{ I} + .2 \text{ O}_2$	$1.5\text{E-}11 \cdot \text{EXP}(510./\text{temp})$	Atkinson et al. (2007)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	k_3rd(temp, cair, $3.3\text{E-}31$, 4.3, $1.6\text{E-}12$, 0., 0.6)	Burkholder et al. (2015)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3$	$1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	$3.\text{E-}13$	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5.\text{E-}11$	Barone et al. (1995)
G9408	StTrGS	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	k_CH200_S02	Welz et al. (2012), Stone et al. (2014)*

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_{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. (2017) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

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 $k^{1\text{st}} = 2 \times \sqrt{k_{\text{self}} \times k_{\text{CH3O2}}} \times [\text{RO}_2]$ 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

G2110: The rate coefficient is: `k_HO2_HO2` = $(3.0\text{E-}13 \times \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 \times \text{EXP}(920./\text{temp}) \times \text{cair}) \times (1. + 1.4\text{E-}21 \times \text{EXP}(2200./\text{temp}) \times \text{C}(\text{ind_H2O}))$.

G2117: Converted to Kc [molec-1 cm3] = $\text{Kp} \times \text{R} \times \text{T} / \text{NA}$, where R is 82.05736 [cm3atmK1mol1].

G2118: Assuming fast equilibrium.

G3109: The rate coefficient is: `k_NO3_NO2` = `k_3rd(temp, cair, 2.4E-30, 3.0, 1.6E-12, -0.1, 0.6)`.

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

G3203: The rate coefficient is: `k_NO2_HO2` = `k_3rd(temp, cair, 1.9E-31, 3.4, 4.0E-12, 0.3, 0.6)`.

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

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

G4104b: Methyl nitrate yield according to Banic et al. (2003) but reduced by a factor of 10 according to the upper limit derived from measurements by Munger et al. (1999).

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

G4115: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4116: Same value as for PAN + OH.

G4126: Same as for G4104 but scaled to match the recommended value at 298K.

G4127: Same as for $\text{CH}_3\text{O}_2 + \text{NO}_3$ in G4105.

G4130a: SAR for H-abstraction by OH.

G4130b: SAR for H-abstraction by OH.

G4132: SAR for H-abstraction by OH.

G4133: Lower limit of the rate constant. Products uncertain but CH_3OH can be excluded because of a likely high energy barrier (L. Vereecken, pers. comm.). CH_2OO production cannot be excluded.

G4134: Estimate based on the decomposition lifetime of 3 s (Olzmann et al., 1997) and a 20 kcal/mol energy barrier (Vereecken and Francisco, 2012).

G4135: Rate constant for $\text{CH}_2\text{OO} + \text{NO}_2$ (G4138) multiplied by the factor from Ouyang et al. (2013).

G4136: Average of two measurements.

G4137: Upper limit.

G4138: Average of 7.E-12 and 1.5E-12.

G4141: $\text{HOOCH}_2\text{OCHO}$ forms and then decomposes to formic anhydride (Gruzdev et al., 1993) which hydrolyses in the humid atmosphere (Conn et al., 1942).

G4142: High-pressure limit.

G4143: Generic estimate for reaction with alcohols.

G4144: Generic estimate for reaction with RO_2 .

G4148: Same value as for $\text{NO}_2 + \text{CH}_3\text{O}_2$.

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of $\text{CH}_3\text{O}_2\text{NO}_2$.

G4150: Value for $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH}$, H-abstraction enhanced by the HO-group by f_{soh} .

G4154: Products assumed to be $\text{CH}_3\text{O}_2 + \text{O}_2$ (could also be $\text{HCHO} + \text{O}_2 + \text{OH}$).

G4160b: Half of the H-yield is attributed to fast secondary chemistry.

G4160c: The $\text{NH} + \text{CO}$ channel is also significant but neglected here.

G4161: No studies below 450 K and only the major channel is considered.

G4164: Upper limit. Dominant pathway under atmospheric conditions.

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 .

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

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 atoms but not Cl. The fate of the carbon atom is currently not considered.

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

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

G8102: It is assumed that the reaction produces new particles

G8103: The yield of 38 % OIO is from Atkinson et al. (2007). It is assumed here that the remaining 62 % produce $2 \text{I} + \text{O}_2$.

G8300: The rate coefficient is: $k_{\text{I}_2\text{NO}_2} = k_{3\text{rd_iupac}}(\text{temp}, \text{cair}, 3\text{E-}31, 1., 6.6\text{E-}11, 0., 0.63)$.

G8305: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (van den Bergh and Troe, 1976).

G8306: According to John Plane and John Crowley (pers. comm. 2007), the rate coefficient of $1.1\text{E}15 * \text{EXP}(-12060./\text{temp})$ suggested by Atkinson et al. (2007) is wrong.

G8401: The rate coefficient is from Dillon et al. (2006), the yield of I atoms is a lower limit given on page 2170 of Bale et al. (2005).

G8402: The products are from Nakano et al. (2005).

G8701: 80% Br + OIO production is from Atkinson et al. (2007). The remaining channels are assumed to produce $\text{Br} + \text{I} + \text{O}_2$.

G9408: Average of $3.9\text{E-}11$ and $3.42\text{E-}11$.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	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)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_N02)	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	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	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HN03)	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HN04)	Sander et al. (2014)
J41000	StTrGJ	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	jx(ip_CH300H)	Sander et al. (2014)
J41001a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	Sander et al. (2014)
J41001b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	Sander et al. (2014)
J41004	StTrGJN	$CH_3ONO + h\nu \rightarrow CH_3O + NO$	jx(ip_CH30N0)	Sander et al. (2014)
J41005	StTrGJN	$CH_3ONO_2 + h\nu \rightarrow CH_3O + NO_2$	jx(ip_CH3N03)	Sander et al. (2014)
J41006	StTrGJN	$CH_3O_2NO_2 + h\nu \rightarrow .667 NO_2 + .667 CH_3O_2 + .333 NO_3 + .333 CH_3O$	jx(ip_CH302N02)	Sander et al. (2014)*
J41007	StTrGJ	$HOCH_2OOH + h\nu \rightarrow HCOOH + OH + HO_2$	jx(ip_CH300H)	Sander et al. (2014)
J41008	StTrGJ	$CH_3O_2 + h\nu \rightarrow HCHO + OH$	jx(ip_CH302)	Sander et al. (2014)
J41009	StTrGJ	$HCOOH + h\nu \rightarrow CO + HO_2 + OH$	jx(ip_HCOOH)	Sander et al. (2014)
J41010	StTrGJN	$HOCH_2O_2NO_2 + h\nu \rightarrow .667 NO_2 + .667 HOCH_2O_2 + .333 NO_3 + .333 HCOOH + .333 HO_2$	jx(ip_CH302N02)	Sander et al. (2014)
J6000	StTrGJCl	$Cl_2 + h\nu \rightarrow Cl + Cl$	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	$Cl_2O_2 + h\nu \rightarrow 2 Cl$	jx(ip_Cl202)	Sander et al. (2014)
J6101	StTrGJCl	$OClo + h\nu \rightarrow ClO + O(^3P)$	jx(ip_OC10)	Sander et al. (2014)
J6201	StTrGJCl	$HOCl + h\nu \rightarrow OH + Cl$	jx(ip_HOC1)	Sander et al. (2014)
J6300	TrGJClN	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	jx(ip_ClN02)	Sander et al. (2014)
J6301a	StTrGJClN	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	jx(ip_ClN03)	Sander et al. (2014)
J6301b	StTrGJClN	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	jx(ip_ClON02)	Sander et al. (2014)
J7000	StTrGJBr	$Br_2 + h\nu \rightarrow Br + Br$	jx(ip_Br2)	Sander et al. (2014)
J7100	StTrGJBr	$BrO + h\nu \rightarrow Br + O(^3P)$	jx(ip_Br0)	Sander et al. (2014)
J7200	StTrGJBr	$HOBr + h\nu \rightarrow Br + OH$	jx(ip_HOBr)	Sander et al. (2014)
J7300	TrGJBrN	$BrNO_2 + h\nu \rightarrow Br + NO_2$	jx(ip_BrN02)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7301	StTrGJBrN	$\text{BrNO}_3 + h\nu \rightarrow .85 \text{ Br} + .85 \text{ NO}_3 + .15 \text{ BrO} + .15 \text{ NO}_2$	jx(ip_BrNO3)	Sander et al. (2014)*
J7401	TrGJBr	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br}$	jx(ip_CH2Br2)	Sander et al. (2014)
J7402	TrGJBr	$\text{CHBr}_3 + h\nu \rightarrow \text{LCARBON} + 3 \text{ Br}$	jx(ip_CHBr3)	Sander et al. (2014)
J7600	StTrGJBrCl	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_BrCl)	Sander et al. (2014)
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + \text{Br} + \text{Cl}$	jx(ip_CH2ClBr)	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{LCARBON} + \text{Br} + 2 \text{ Cl}$	jx(ip_CHCl2Br)	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br} + \text{Cl}$	jx(ip_CHClBr2)	Sander et al. (2014)
J8000	TrGJI	$\text{I}_2 + h\nu \rightarrow \text{I} + \text{I}$	jx(ip_I2)	Sander et al. (2014)
J8100	TrGJI	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}(^3\text{P})$	jx(ip_IO)	Sander et al. (2014)
J8200	TrGJI	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	jx(ip_HOI)	Sander et al. (2014)
J8300	TrGJIN	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$	jx(ip_INO2)	Sander et al. (2014)
J8301	TrGJIN	$\text{INO}_3 + h\nu \rightarrow \text{I} + \text{NO}_3$	jx(ip_INO3)	Sander et al. (2014)
J8400	TrGJI	$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2 \text{ I} + 2 \text{ HO}_2 + \text{CO}$	jx(ip_CH2I2)	Sander et al. (2014)
J8401	TrGJI	$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3$	jx(ip_CH3I)	Sander et al. (2014)
J8403	TrGJClI	$\text{CH}_2\text{ClI} + h\nu \rightarrow \text{I} + \text{Cl} + 2 \text{ HO}_2 + \text{CO}$	jx(ip_CH2ClI)	Sander et al. (2014)
J8600	TrGJClI	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	jx(ip_ICl)	Sander et al. (2014)
J8700	TrGJBrI	$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$	jx(ip_IBr)	Sander et al. (2014)

General notes

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

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

J(11) \rightarrow jx(ip_COH2)

J(12) \rightarrow jx(ip_CHOH)

J(15) \rightarrow jx(ip_HOCH2CHO)

J(18) \rightarrow jx(ip_MACR)

J(22) \rightarrow jx(ip_ACETOL)

J(23)+J(24) \rightarrow jx(ip_MVK)

J(31)+J(32)+J(33) \rightarrow jx(ip_GLYOX)

J(34) \rightarrow jx(ip_MGLYOX)

J(41) \rightarrow jx(ip_CH3OOH)

J(53) \rightarrow J(isopropyl nitrate)

J(54) \rightarrow J(isopropyl nitrate)

J(55) \rightarrow J(isopropyl nitrate)

J(56)+J(57) \rightarrow jx(ip_NOA)

Specific notes

J41006: product distribution as for HNO4

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
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{O3})$	see general notes*
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(01, \text{ind}_{O3})$	see general notes*
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{H2O2})$	see general notes*
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(01, \text{ind}_{H2O2})$	see general notes*
H3200f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{NH3})$	see general notes*
H3200b_a01	TrAa01MblScScmN	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(01, \text{ind}_{NH3})$	see general notes*
H3201_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf_N205}}(01) * C(\text{ind}_{H2O_a01})$	Behnke et al. (1994), Behnke et al. (1997)
H3203f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{HNO3})$	see general notes*
H3203b_a01	TrAa01MblScScmN	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(01, \text{ind}_{HNO3})$	see general notes*
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{CO2})$	see general notes*
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(01, \text{ind}_{CO2})$	see general notes*
H6000f_a01	TrAa01MblScCl	$Cl_2 \rightarrow Cl_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{Cl2})$	see general notes*
H6000b_a01	TrAa01MblScCl	$Cl_2(aq) \rightarrow Cl_2$	$k_{\text{exb}}(01, \text{ind}_{Cl2})$	see general notes*
H6200f_a01	TrAa01MblScScmCl	$HCl \rightarrow HCl(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCl})$	see general notes*
H6200b_a01	TrAa01MblScScmCl	$HCl(aq) \rightarrow HCl$	$k_{\text{exb}}(01, \text{ind}_{HCl})$	see general notes*
H6201f_a01	TrAa01MblScCl	$HOCl \rightarrow HOCl(aq)$	$k_{\text{exf}}(01, \text{ind}_{HOCl})$	see general notes*
H6201b_a01	TrAa01MblScCl	$HOCl(aq) \rightarrow HOCl$	$k_{\text{exb}}(01, \text{ind}_{HOCl})$	see general notes*
H6300_a01	TrAa01MblClN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	$k_{\text{exf_N205}}(01) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)
H6301_a01	TrAa01MblClN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	$k_{\text{exf_ClN03}}(01) * C(\text{ind}_{H2O_a01})$	see general notes*
H6302_a01	TrAa01MblClN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	$k_{\text{exf_ClN03}}(01) * 5.E2$	see general notes*
H7000f_a01	TrAa01MblScBr	$Br_2 \rightarrow Br_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{Br2})$	see general notes*
H7000b_a01	TrAa01MblScBr	$Br_2(aq) \rightarrow Br_2$	$k_{\text{exb}}(01, \text{ind}_{Br2})$	see general notes*
H7200f_a01	TrAa01MblScScmBr	$HBr \rightarrow HBr(aq)$	$k_{\text{exf}}(01, \text{ind}_{HBr})$	see general notes*
H7200b_a01	TrAa01MblScScmBr	$HBr(aq) \rightarrow HBr$	$k_{\text{exb}}(01, \text{ind}_{HBr})$	see general notes*
H7201f_a01	TrAa01MblScBr	$HOBr \rightarrow HOBr(aq)$	$k_{\text{exf}}(01, \text{ind}_{HOBr})$	see general notes*
H7201b_a01	TrAa01MblScBr	$HOBr(aq) \rightarrow HOBr$	$k_{\text{exb}}(01, \text{ind}_{HOBr})$	see general notes*
H7300_a01	TrAa01MblBrN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	$k_{\text{exf_N205}}(01) * 3.E5$	Behnke et al. (1994), Behnke et al. (1997)
H7301_a01	TrAa01MblBrN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	$k_{\text{exf_BrN03}}(01) * C(\text{ind}_{H2O_a01})$	see general notes*
H7302_a01	TrAa01MblBrN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	$k_{\text{exf_BrN03}}(01) * 3.E5$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H7600f_a01	TrAa01MblScBrCl	$\text{BrCl} \rightarrow \text{BrCl(aq)}$	$k_{\text{exf}}(01, \text{ind_BrCl})$	see general notes*
H7600b_a01	TrAa01MblScBrCl	$\text{BrCl(aq)} \rightarrow \text{BrCl}$	$k_{\text{exb}}(01, \text{ind_BrCl})$	see general notes*
H7601_a01	TrAa01MblBrClN	$\text{ClNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(01) * 3.E5$	see general notes*
H7602_a01	TrAa01MblBrClN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl(aq)} + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * 5.E2$	see general notes*
H8100f_a01	TrAa01MblScI	$\text{IO} \rightarrow \text{IO(aq)}$	$k_{\text{exf}}(01, \text{ind_IO})$	see general notes*
H8100b_a01	TrAa01MblScI	$\text{IO(aq)} \rightarrow \text{IO}$	$k_{\text{exb}}(01, \text{ind_IO})$	see general notes*
H8200f_a01	TrAa01MblScI	$\text{HOI} \rightarrow \text{HOI(aq)}$	$k_{\text{exf}}(01, \text{ind_HOI})$	see general notes*
H8200b_a01	TrAa01MblScI	$\text{HOI(aq)} \rightarrow \text{HOI}$	$k_{\text{exb}}(01, \text{ind_HOI})$	see general notes*
H8201_a01	TrAa01MblScI	$\text{HI} \rightarrow \text{H}^+(\text{aq}) + \text{I}^-(\text{aq})$	$k_{\text{mt}}(\text{HI}) \cdot \text{lwc}$	see general notes*
H8301_a01	TrAa01MblIN	$\text{INO}_3 \rightarrow \text{HOI(aq)} + \text{HNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_INO3})$	see general notes*
H8600f_a01	TrAa01MblScClI	$\text{ICl} \rightarrow \text{ICl(aq)}$	$k_{\text{exf}}(01, \text{ind_ICl})$	see general notes*
H8600b_a01	TrAa01MblScClI	$\text{ICl(aq)} \rightarrow \text{ICl}$	$k_{\text{exb}}(01, \text{ind_ICl})$	see general notes*
H8700f_a01	TrAa01MblScBrI	$\text{IBr} \rightarrow \text{IBr(aq)}$	$k_{\text{exf}}(01, \text{ind_IBr})$	see general notes*
H8700b_a01	TrAa01MblScBrI	$\text{IBr(aq)} \rightarrow \text{IBr}$	$k_{\text{exb}}(01, \text{ind_IBr})$	see general notes*
H9100f_a01	TrAa01MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_SO2})$	see general notes*
H9100b_a01	TrAa01MblScScmS	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(01, \text{ind_SO2})$	see general notes*
H9200_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$\text{xnom7sulf} * k_{\text{exf}}(01, \text{ind_H2SO4})$	see general notes*
H9401_a01	TrAa01MblS	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3SO3H})$	see general notes*

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 ($X = \text{N}_2\text{O}_5$, ClNO_3 , or BrNO_3) and

subsequent reaction with H_2O , 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 N_2O_5 . Here, they are also used for ClNO_3 and BrNO_3 .

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
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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)

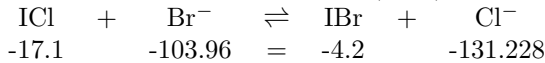
Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ21_a01	TrAa01MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a01	TrAa01MblScScmN	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ32_a01	TrAa01MblScScmN	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ40_a01	TrAa01MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ61_a01	TrAa01MblScScmCl	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ71_a01	TrAa01MblScScmBr	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ73_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01MblBrCl	$\text{Br}_2 + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01MblBrCl	$\text{Br}^- + \text{Cl}_2 \rightleftharpoons \text{BrCl}_2^-$	4.2E6	14072	Wang et al. (1994)
EQ80_a01	TrAa01MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ81_a01	TrAa01MblScBrI	$\text{IBr} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2.9E2		Troy and Margerum (1991)
EQ82_a01	TrAa01MblScBrClI	$\text{ICl} + \text{Br}^- \rightleftharpoons \text{IBr} + \text{Cl}^-$	3.3E2		see note*
EQ90_a01	TrAa01MblScScmS	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01MblScScmS	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01MblScScmS	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)

Specific notes

EQ40_a01: For $pK_a(\text{CO}_2)$, see also Dickson and Millero (1987).

EQ82_a01: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):



$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[\text{Cl}^-]/[\text{Br}^-]$ ratio equals 330.

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A6204_a01	TrAa01MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6208_a01	TrAa01MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A7202_a01	TrAa01MblBr	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7208_a01	TrAa01MblBr	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7602_a01	TrAa01MblBrCl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a01	TrAa01MblBrCl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		Liu and Margerum (2001)*
A7604_a01	TrAa01MblBrCl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A8100_a01	TrAa01MblI	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a01	TrAa01MblI	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A8200_a01	TrAa01MblI	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A8202_a01	TrAa01MblI	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A8203_a01	TrAa01MblI	$IO_2^- + I^- + H^+ \rightarrow 2 HOI + OH^-$	2.0E10		Edblom et al. (1987)
A8600_a01	TrAa01MblClI	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601_a01	TrAa01MblClI	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8603_a01	TrAa01MblClI	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8700_a01	TrAa01MblBrI	$IBr \rightarrow HOI + H^+ + Br^-$	8.0E5		Troy et al. (1991)
A8701_a01	TrAa01MblBrI	$I^- + HOBr \rightarrow IBr + OH^-$	5.0E9		Troy and Margerum (1991)
A8703_a01	TrAa01MblBrI	$HOI + Br^- + H^+ \rightarrow IBr$	3.3E12		Troy et al. (1991)
A9101_a01	TrAa01MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206_a01	TrAa01MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9209_a01	TrAa01MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9601_a01	TrAa01MblClS	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9605_a01	TrAa01MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A9702_a01	TrAa01MblBrS	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9705_a01	TrAa01MblBrS	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note*

Specific notes

A9605_a01: Assumed to be the same as for $SO_3^{2-} + HOCl$.
A9705_a01: Assumed to be the same as for $SO_3^{2-} + HOBr$.

A7603_a01: The rate coefficient is defined as backward reaction divided by equilibrium constant.

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