

The Chemical Mechanism of MAFOR v2.2

KPP version: 2.2.3_rs3

MECCA version: 4.0

Date: November 30, 2024

Batch file: mafor.bat

Integrator: rosenbrock_posdef

Gas equation file: gas.eqn

Replacement file: maforchem

Selected reactions:

“Tr && (G | | Aa) && !Br && !Hg”

Number of aerosol phases: 3

Number of species in selected mechanism:

Gas phase: 782

Aqueous phase: 465

All species: 1247

Number of reactions in selected mechanism:

Gas phase (Gnn): 1873

Aqueous phase (Annn): 714

Henry (Hnn): 378

Photolysis (Jnn): 356

Aqueous phase photolysis (PHnn): 39

Heterogeneous (HETnn): 0

Equilibria (EQnn): 300

Isotope exchange (IEXnn): 0

Tagging equations (TAGnn): 0

Dummy (Dnn): 3

All equations: 3663

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.3E-11*EXP(55./temp)$	Burkholder et al. (2015)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.0E-34*((temp/300.)**(-2.4))$ $*c_{air}$	Burkholder et al. (2015)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	$k_3rd(temp, c_{air}, 4.4E-32, 1.3,$ $7.5E-11, -0.2, 0.6)$	Burkholder et al. (2015)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Burkholder et al. (2015)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Burkholder et al. (2015)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Burkholder et al. (2015)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Burkholder et al. (2015)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_H02_H02	Burkholder et al. (2015)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$1.63E-10*EXP(60./temp)$	Burkholder et al. (2015)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$1.8E-12$	Burkholder et al. (2015)
G2117	UpStTrG	$H_2O + H_2O \rightarrow (H_2O)_2$	$6.521E-26*temp*EXP(1851.09/temp)$ $*EXP(-5.10485E-3*temp)$	Scribano et al. (2006)*
G2118	UpStTrG	$(H_2O)_2 \rightarrow H_2O + H_2O$	$1.E0$	see note*
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.0E-12*EXP(-1500./temp)$	Burkholder et al. (2015)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Burkholder et al. (2015)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Burkholder et al. (2015)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_N03_N02	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_N03_N02/(5.8E-27*EXP(10840./$ $temp))$	Burkholder et al. (2015)*
G3200	TrGN	$NO + OH \rightarrow HONO$	$k_3rd(temp, c_{air}, 7.0E-31, 2.6,$ $3.6E-11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	$3.3E-12*EXP(270./temp)$	Burkholder et al. (2015)
G3202	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	$k_3rd(temp, c_{air}, 1.8E-30, 3.0,$ $2.8E-11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_N02_H02	Burkholder et al. (2015)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	$3.5E-12$	Burkholder et al. (2015)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	$1.8E-11*EXP(-390./temp)$	Burkholder et al. (2015)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Dulitz et al. (2018)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k_N02_H02/(2.1E-27*EXP(10900./$ $temp))$	Burkholder et al. (2015)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	$1.3E-12*EXP(380./temp)$	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	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$(k_{\text{CH302}} - 7.4\text{E}-13 * \text{EXP}(-520./\text{temp})) * R02 * 2.$	Atkinson et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{CH}_3\text{O}_2 + .4 \text{HCHO} + .4 \text{OH} + \text{H}_2\text{O}$	$k_{\text{CH300H_OH}}$	Wallington et al. (2018)
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	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	$k_{\text{N02_CH302}}$	Burkholder et al. (2015)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$k_{\text{N02_CH302}} / (9.5\text{E}-29 * \text{EXP}(11234./\text{temp}))$	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	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E}-14 * \text{exp}(-663./\text{temp}) * c(\text{ind_02})$	Chai et al. (2014)
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 8.1\text{E}-29, 4.5, 2.1\text{E}-11, 0., 0.44)$	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	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 2.6\text{E}-29, 2.8, 3.3\text{E}-11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/900.), \text{SP}))$	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	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(k_{\text{CH302}} * 5.5\text{E}-12) ** 0.5 * R02 * 2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(k_{\text{CH302}} * 5.7\text{E}-14 * \text{EXP}(750./\text{temp})) ** 0.5 * R02 * 2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_{roohro}	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{rohro}} + k_{\text{s*f_sooh*f_soh}}$	Taraborrelli (2010)*

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

#	labels	reaction	rate coefficient	reference
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$2 \cdot k_{\text{rohro}} + k_{\text{s}} \cdot f_{\text{soh}} \cdot f_{\text{soh}}$	Taraborrelli (2010)*
G4133	StTrG	$\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$	$1.4\text{E}-10$	Bossolasco et al. (2014)*
G4134	StTrG	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E}+14 \cdot \text{EXP}(-10000/\text{temp})$	see note*
G4135	StTrG	$\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$	$k_{\text{CH200_N02}} \cdot 3.6\text{E}-6$	Ouyang et al. (2013)*
G4136	StTrG	$\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$	$5.2\text{E}-12$	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$	$6\text{E}-14$	Welz et al. (2012)*
G4138	StTrGN	$\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$	$k_{\text{CH200_N02}}$	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$	$3.6\text{E}-14$	Vereecken et al. (2012)
G4141	StTrG	$\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$	$1\text{E}-10$	Welz et al. (2014)*
G4142	StTrG	$\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$	$1.7\text{E}-12$	Stone et al. (2014)*
G4143	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$	$5\text{E}-12$	Vereecken et al. (2012)*
G4144	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$	$5\text{E}-12$	Vereecken et al. (2012)*
G4145	StTrG	$\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$	$5\text{E}-12$	Vereecken et al. (2012)
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	$1\text{E}-12$	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	$6\text{E}-11$	Buras et al. (2014)
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	$k_{\text{N02_CH302}}$	see note*
G4149	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$	$k_{\text{N02_CH302}} / (9.5\text{E}-29 \cdot \text{EXP}(11234./\text{temp}))$	Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp}) \cdot f_{\text{soh}}$	see note*
G4151	StTrG	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 7.0\text{E}-31, 3., 1.8\text{E}-12, -1.1, 0.33)$	Atkinson et al. (2006)
G4152	StTrG	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{HCHO} + .956 \text{H} + .044 \text{CH}_3\text{O} + \text{O}_2$	$5.1\text{E}-12 \cdot \text{exp}(-210./\text{temp})$	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{HCHO} + .83 \text{H} + .17 \text{CO} + .17 \text{H}_2 + .17 \text{H}$	$1.3\text{E}-10$	Atkinson et al. (2006)
G4154	StTrG	$\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$	$2.53\text{E}-14$	Albaladejo et al. (2002)*
G4155	StTrG	$\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{CH}_3 + .75 \text{O}_2 + .25 \text{HCHO} + .25 \text{OH}$	$2.5\text{E}-11$	Baulch et al. (2005)
G4156	StTrG	$\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$	$4.3\text{E}-11$	Zellner et al. (1988)
G4157	StTrG	$\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{OH} + .7 \text{CO} + .3 \text{H} + .3 \text{CO}_2 + \text{HO}_2$	$3.4\text{E}-11 \cdot \text{EXP}(-1600./\text{temp})$	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	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	$\text{k_3rd}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$	Kleinböhle 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)*
G42000	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(-499./\text{temp})$	Atkinson et al. (2006)
G42001	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{OO}^*$	$9.1\text{E-}15 * \text{EXP}(-2580./\text{temp})$	Atkinson et al. (2006)*
G42002	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42003	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13 * \text{EXP}(700./\text{temp})$	Burkholder et al. (2015)
G42004a	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * (1. - \text{beta_C2H5NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * \text{beta_C2H5NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42005	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Wallington et al. (2018)
G42006	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .8 \text{CH}_3\text{CHO} + .6 \text{HO}_2 + .2 \text{C}_2\text{H}_5\text{OH}$	$2. * (7.6\text{E-}14 * \text{k_CH3O2}) * (.5) * \text{R02}$	Sander et al. (2018), Atkinson et al. (2006)
G42007a	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G42007b	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{OH}$	k_sf_sooh	Sander et al. (2018)
G42008a	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.95$	Atkinson et al. (2006)
G42008b	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.05$	Atkinson et al. (2006)
G42009	TrGCN	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42010	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$	k_CH3CO2H_OH	Atkinson et al. (2006)*
G42011a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.61$	Groß et al. (2014)
G42011b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.23$	Groß et al. (2014)
G42011c	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.16$	Groß et al. (2014)
G42012	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E-}12 * \text{EXP}(270./\text{temp})$	Tyndall et al. (2001a)

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

#	labels	reaction	rate coefficient	reference
G42013	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3C03_N02	Burkholder et al. (2015)*
G42014	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G42017a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3 + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2018)
G42017b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOH}$	k1_R02RC03*0.1	Sander et al. (2018)
G42018	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	k_roohro	Rickard and Pascoe (2009)*
G42020	TrGCN	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	3.00E-14	Rickard and Pascoe (2009)
G42021	TrGCN	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Burkholder et al. (2015)*
G42022a	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.71	Burkholder et al. (2015)*
G42022b	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$	k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.29	Burkholder et al. (2015)*
G42023a	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$	8.00E-12*0.80	Atkinson et al. (2006)
G42023b	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$	8.00E-12*0.20	Atkinson et al. (2006)
G42024a	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$	5.1E-12*(1.-1./(1+1.85E-18*cair))	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42024b	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	5.1E-12*1./(1+1.85E-18*cair)	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42025	TrGC	$\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Sander et al. (2018)
G42026	TrGCN	$\text{HOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42027a	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.9	Sander et al. (2018)
G42027b	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	k1_R02RC03*0.1	Sander et al. (2018)
G42028a	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	KAPH02*rco3_oh	Sander et al. (2018), Groß et al. (2014)
G42028b	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Sander et al. (2018), Groß et al. (2014)
G42028c	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rco3_o3	Sander et al. (2018), Groß et al. (2014)
G42029	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G42030	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G42031	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G42032	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{ HCHO} + .09 \text{ CO}_2 + .91 \text{ HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	k_co2h+k_sf_soh*f_co2h	Sander et al. (2018)
G42033a	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	k_sf_soh*f_co2h	Sander et al. (2018)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G42035	TrGCN	PHAN + OH \rightarrow HCHO + CO + NO ₂ + H ₂ O	k_s*f_soh*f_cpan+k_rohro	Sander et al. (2018)
G42036	TrGC	GLYOX + OH \rightarrow HCOCO + H ₂ O	3.1E-12*EXP(340./temp)	Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013)
G42037	TrGCN	GLYOX + NO ₃ \rightarrow HCOCO + HNO ₃	KN03AL	Rickard and Pascoe (2009)
G42038a	TrGC	HCOCO \rightarrow CO + CO + HO ₂	7.E11*EXP(-3160./temp) +5.E-12*c(ind_02)	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	HCOCO \rightarrow HCOCO ₃	5.E-12*c(ind_02)*3.2*exp(-550./temp)	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	HCOCO \rightarrow OH + CO + CO ₂	5.E-12*c(ind_02) *(1.-3.2*exp(-550./temp))	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	HCOCO ₃ \rightarrow CO + HO ₂ + CO ₂	k1_R02RC03*0.9	Sander et al. (2018)
G42039b	TrGC	HCOCO ₃ \rightarrow HCOCO ₂ H	k1_R02RC03*0.1	Sander et al. (2018)
G42040	TrGC	HCOCO ₃ + HO ₂ \rightarrow HO ₂ + CO + CO ₂ + OH	KAPH02	Feierabend et al. (2008), Sander et al. (2018)
G42041	TrGCN	HCOCO ₃ + NO \rightarrow HO ₂ + CO + NO ₂ + CO ₂	KAPN0	Rickard and Pascoe (2009)
G42042	TrGCN	HCOCO ₃ + NO ₃ \rightarrow HO ₂ + CO + NO ₂ + CO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G42043	TrGCN	HCOCO ₃ + NO ₂ \rightarrow HO ₂ + CO + NO ₃ + CO ₂	k_CH3CO3_N02	Orlando and Tyndall (2001), Sander et al. (2018)
G42044	TrGC	HCOCO ₂ H + OH \rightarrow CO + HO ₂ + CO ₂ + H ₂ O	k_co2h+k_t*f_o*f_co2h	Sander et al. (2018)
G42045a	TrGC	HCOCO ₃ H + OH \rightarrow HCOCO ₃ + H ₂ O	k_roohro	Sander et al. (2018)
G42045b	TrGC	HCOCO ₃ H + OH \rightarrow CO + CO ₂ + H ₂ O + OH	k_t*f_o*f_co2h	Sander et al. (2018)
G42046	TrGC	HOCH ₂ CH ₂ O ₂ \rightarrow .6 HOCH ₂ CH ₂ O + .2 HOCH ₂ CHO + .2 ETHGLY	2.*(7.8E-14*EXP(1000./temp) *k_CH302)**(.5)*R02	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	HOCH ₂ CH ₂ O ₂ + NO \rightarrow .25 HO ₂ + .5 HCHO + .75 HOCH ₂ CH ₂ O + NO ₂	KR02N0*(1.-alpha_AN(3,1,0,0,0, temp, cair))	Rickard and Pascoe (2009)*
G42048	TrGCN	HOCH ₂ CH ₂ O ₂ + NO \rightarrow ETHOHNO3	KR02N0*alpha_AN(3,1,0,0,0,temp, cair)	Sander et al. (2018)
G42049a	TrGC	HOCH ₂ CH ₂ O ₂ + HO ₂ \rightarrow HYETHO2H	1.53E-13*EXP(1300./temp) *(1.-rchohch2o2_oh)	Rickard and Pascoe (2009)
G42049b	TrGC	HOCH ₂ CH ₂ O ₂ + HO ₂ \rightarrow HOCH ₂ CH ₂ O + OH	1.53E-13*EXP(1300./temp) *rchohch2o2_oh	Rickard and Pascoe (2009)
G42050	TrGCN	ETHOHNO3 + OH \rightarrow .93 NO ₃ CH2CHO + .93 HO ₂ + .07 HOCH ₂ CHO + .07 NO ₂ + H ₂ O	k_s*(f_soh*f_ch2ono2+f_ono2*f_ pch2oh)+k_rohro	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G42051a	TrGC	HYETHO2H + OH \rightarrow HOCH ₂ CH ₂ O ₂ + H ₂ O	k_roohro	Rickard and Pascoe (2009)*
G42051b	TrGC	HYETHO2H + OH \rightarrow HOCH ₂ CHO + OH + H ₂ O	k_s*f_sooH*f_pch2oh	Sander et al. (2018)
G42051c	TrGC	HYETHO2H + OH \rightarrow HOOCH ₂ CHO + HO ₂ + H ₂ O	k_s*f_soh*f_pch2oh+k_rohro	Sander et al. (2018)
G42052a	TrGC	HOCH ₂ CH ₂ O \rightarrow HO ₂ + HOCH ₂ CHO	6.00E-14*EXP(-550./temp) *C(ind_02)	Rickard and Pascoe (2009)
G42052b	TrGC	HOCH ₂ CH ₂ O \rightarrow HO ₂ + HCHO + HCHO	9.50E13*EXP(-5988./temp)	Rickard and Pascoe (2009)
G42053	TrGC	ETHGLY + OH \rightarrow HOCH ₂ CHO + HO ₂ + H ₂ O	2*k_s*f_soh*f_pch2oh+2*k_rohro	Sander et al. (2018)
G42054	TrGC	HCOCH ₂ O ₂ \rightarrow .6 HCHO + .6 CO + .6 HO ₂ + .2 GLYOX + .2 HOCH ₂ CHO	k1_R02p0R02	Sander et al. (2018)
G42055a	TrGC	HCOCH ₂ O ₂ + HO ₂ \rightarrow HOOCH ₂ CHO	KR02H02(2)*rcoch2o2_ooh	Sander et al. (2018)
G42055b	TrGC	HCOCH ₂ O ₂ + HO ₂ \rightarrow HCHO + CO + HO ₂ + OH	KR02H02(2)*rcoch2o2_oh	Sander et al. (2018)
G42056a	TrGCN	HCOCH ₂ O ₂ + NO \rightarrow NO ₂ + HCHO + CO + HO ₂	KR02N0*(1.-alpha_AN(3,1,1,0,0, temp, cair))	Sander et al. (2018)
G42056b	TrGCN	HCOCH ₂ O ₂ + NO \rightarrow NO ₃ CH ₂ CHO	KR02N0*alpha_AN(3,1,1,0,0,temp, cair)	Sander et al. (2018)
G42057	TrGCN	HCOCH ₂ O ₂ + NO ₃ \rightarrow HCHO + CO + HO ₂ + NO ₂	KR02N03	Sander et al. (2018)
G42058a	TrGC	HOOCH ₂ CHO + OH \rightarrow HCOCH ₂ O ₂	k_roohro	Sander et al. (2018)
G42058b	TrGC	HOOCH ₂ CHO + OH \rightarrow HCHO + CO + OH	0.8*8.E-12	Sander et al. (2018)*
G42058c	TrGC	HOOCH ₂ CHO + OH \rightarrow GLYOX + OH	k_s*f_sooH*f_cho	Sander et al. (2018)
G42059	TrGCN	HOOCH ₂ CHO + NO ₃ \rightarrow OH + HCHO + CO + HNO ₃	KN03AL	Rickard and Pascoe (2009)
G42060	TrGCN	HOOCH ₂ CO ₃ + NO \rightarrow NO ₂ + OH + HCHO + CO ₂	KAPN0	Sander et al. (2018)
G42061	TrGCN	HOOCH ₂ CO ₃ + NO ₃ \rightarrow NO ₂ + OH + HCHO + CO ₂	KR02N03*1.74	Sander et al. (2018)
G42062a	TrGC	HOOCH ₂ CO ₃ + HO ₂ \rightarrow 2 OH + HCHO + CO ₂	KAPH02*rco3_oh	Sander et al. (2018)
G42062b	TrGC	HOOCH ₂ CO ₃ + HO ₂ \rightarrow HOOCH ₂ CO ₃ H	KAPH02*rco3_ooh	Sander et al. (2018)
G42062c	TrGC	HOOCH ₂ CO ₃ + HO ₂ \rightarrow HOOCH ₂ CO ₂ H + O ₃	KAPH02*rco3_o3	Sander et al. (2018)
G42063a	TrGC	HOOCH ₂ CO ₃ \rightarrow OH + HCHO + CO ₂	k1_R02RC03*0.9	Sander et al. (2018)
G42063b	TrGC	HOOCH ₂ CO ₃ \rightarrow HOOCH ₂ CO ₂ H	k1_R02RC03*0.1	Sander et al. (2018)
G42064a	TrGC	HOOCH ₂ CO ₃ H + OH \rightarrow HOOCH ₂ CO ₃ + H ₂ O	2.*k_roohro	Sander et al. (2018)
G42064b	TrGC	HOOCH ₂ CO ₃ H + OH \rightarrow HCOCO ₃ H + OH + H ₂ O	k_s*f_sooH*f_co2h	Sander et al. (2018)
G42065	TrGC	HOOCH ₂ CO ₂ H + OH \rightarrow HCOCO ₂ H + OH + H ₂ O	k_s*f_sooH*f_co2h+k_co2h	Sander et al. (2018)
G42066	TrGC	CH ₂ CO + OH \rightarrow .6 HCHO + .6 HO ₂ + .6 CO + .4 HOOCH ₂ CO ₂ H	2.8E-12*exp(510./temp)	Baulch et al. (2005), Sander et al. (2018)
G42067a	TrGC	CH ₃ CHOHOOH + OH \rightarrow CH ₃ COOH + OH	(k_t*f_tooh*f_toh + k_rohro)	Sander et al. (2018)
G42067b	TrGC	CH ₃ CHOHOOH + OH \rightarrow CH ₃ CHOHO ₂	k_roohro	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G42068	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$3.46\text{E}12 * \text{EXP}(-12500./(1.98 * \text{temp}))$	Hermans et al. (2005), Sander et al. (2018)
G42069	TrGC	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$	$3.46\text{E}12 * \text{EXP}(-12500./(1.98 * \text{temp})) / (6.34\text{E}26 * \text{EXP}(-14700./(1.98 * \text{temp})))$	Hermans et al. (2005), Sander et al. (2018)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{CH}_3\text{CHOHOOH} + .3 \text{CH}_3\text{COOH} + .2 \text{CH}_3 + .2 \text{HCOOH} + .2 \text{OH}$	$5.6\text{E}-15 * \text{EXP}(2300./\text{temp})$	Sander et al. (2018)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	k1_R02s0R02	Sander et al. (2018)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KR02N0	Sander et al. (2018)
G42073	TrGCN	$\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$	$6.7\text{E}-13 * \text{EXP}(-395./\text{temp})$	Atkinson et al. (2006)
G42074a	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{NO}_2 + \text{H}_2\text{O}$	k_s*f_ch2ono2*f_cho	Paulot et al. (2009a), Sander et al. (2018)*
G42074b	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{H}_2\text{O}$	k_t*f_o*f_ch2ono2*3.	Paulot et al. (2009a), Sander et al. (2018)*
G42075	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{OH}$	KAPH02	Rickard and Pascoe (2009)*
G42076	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G42077	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G42078	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G42079	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42080	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2\text{NO}_2$	k_3rd_iupac(temp, cair, 1.3E-29, 6.2, 8.8E-12, 0.0, 0.31)	Atkinson et al. (2006)
G42081	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$	k_3rd_iupac(temp, cair, REAL(4.8E-4*EXP(-9285./temp), SP), 0.0, REAL(8.8E15*EXP(-10440./temp), SP), 0.0, 0.31)	Atkinson et al. (2006)
G42082	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 * \text{EXP}(-650./\text{temp})$	Sander et al. (2018)*
G42083a	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$5.1\text{E}-12 * (1. - 1./(1. + 9.4\text{E}-18 * \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42083b	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$	$5.1\text{E}-12 * 1./(1. + 9.4\text{E}-18 * \text{cair})$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{C}_2\text{H}_5\text{O}_2 + .95 \text{HO}_2 + .05 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$3.0\text{E}-12 * \text{EXP}(20./\text{temp})$	Sander et al. (2018), Atkinson et al. (2006)
G42085a	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$	$8.1\text{E}-13 * \text{EXP}(-1080./\text{temp}) * 0.40$	Atkinson et al. (2006), Tyndall et al. (2001b)*

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

#	labels	reaction	rate coefficient	reference
G42085b	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$	$8.1\text{E-}13*\text{EXP}(-1080./\text{temp})*(1.-0.40)$	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})$ $*0.0269*\text{EXP}(137./\text{temp})$	Strekowski et al. (2010)
G42086b	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{H} + \text{CO} + \text{HCN}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})*0.16$	Strekowski et al. (2010)*
G42086c	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{CH}_3 + .5 \text{NCO} + .5 \text{NCCH}_2\text{O}_2 + .5 \text{OH}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})*(1.- (0.16+ 0.0269*\text{EXP}(137./\text{temp})))$	Strekowski et al. (2010)*
G42087	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N0	see note*
G42088	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$	KR02H02(2)	see note*
G42089a	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{HCHO}$	k_CH2CHOH_OH_HCOOH	Sander et al. (2018), So et al. (2014)*
G42089b	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2$	k_CH2CHOH_OH_ALD	Sander et al. (2018), So et al. (2014)
G42090	TrGC	$\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G42091	TrGC	$\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G43000a	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_s	Sander et al. (2018)
G43000b	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	2.*k_p	Sander et al. (2018)
G43001a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{CHOHO}_2 + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.57$	Atkinson et al. (2006)*
G43001b	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{OO}^*$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.43$	Atkinson et al. (2006)*
G43002	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO}_2$	$k_{3\text{rd_iupac}}(\text{temp}, \text{cair}, 8.6\text{E-}27, 3.5, 3.\text{E-}11, 1., 0.5)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO}_3\text{BO}_2$	$4.6\text{E-}13*\text{EXP}(-1155./\text{temp})$	Wallington et al. (2018)
G43004	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$1.9\text{E-}13*\text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43005a	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Wallington et al. (2018)
G43005b	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{ONO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair})$	Wallington et al. (2018)
G43006	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{CH}_3\text{COCH}_3 + .2 \text{IPROPOL} + .6 \text{HO}_2$	$2.*(1.6\text{E-}12*\text{EXP}(-2200./\text{temp})*k_{\text{CH302}})**(.5)*R02$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G43007b	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{OH}$	k_t*f_tooh	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G43008	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	$1.9\text{E-}13*\text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43009a	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\text{alpha_AN}(3,1,0,0,0,\text{temp},\text{cair}))$	Wallington et al. (2018)
G43009b	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_3\text{H}_7\text{ONO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*\text{alpha_AN}(3,1,0,0,0,\text{temp},\text{cair})$	Wallington et al. (2018)
G43010	TrGC	$\text{C}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{ CH}_3\text{COCH}_3 + .2 \text{ NPROPOL} + .6 \text{ HO}_2$	$2.*(k_CH3O2*3.E-13)**(.5)*R02$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43011	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$(8.8\text{E-}12*\text{EXP}(-1320./\text{temp}) + 1.7\text{E-}14*\text{EXP}(423./\text{temp}))$	Atkinson et al. (2006)*
G43012a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E-}13*\text{EXP}(700./\text{temp})*\text{rcoch2o2_ooh}$	Tyndall et al. (2001a), Sander et al. (2018)
G43012b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{C(O)} + \text{HCHO}$	$8.6\text{E-}13*\text{EXP}(700./\text{temp})*\text{rcoch2o2_oh}$	Tyndall et al. (2001a), Sander et al. (2018)
G43013a	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{NO}_2$	$2.9\text{E-}12*\text{EXP}(300./\text{temp})*(1.-\text{alpha_AN}(4,1,1,0,0,\text{temp},\text{cair}))$	Burkholder et al. (2015)
G43013b	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NOA}$	$2.9\text{E-}12*\text{EXP}(300./\text{temp})*\text{alpha_AN}(4,1,1,0,0,\text{temp},\text{cair})$	Burkholder et al. (2015)
G43014	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .3 \text{ CH}_3\text{C(O)} + .3 \text{ HCHO} + .5 \text{ MGLYOX} + .2 \text{ CH}_3\text{COCH}_2\text{OH}$	$k1_R02p0R02$	Orlando and Tyndall (2012)
G43015a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_roohro	see note*
G43015b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	$k_s*f_sooh*f_co$	Sander et al. (2018)
G43016	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$1.6\text{E-}12*\text{EXP}(305./\text{temp})$	Atkinson et al. (2006)
G43017	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{ CH}_3 + .6 \text{ CH}_3\text{C(O)} + 1.4 \text{ CO} + \text{H}_2\text{O}$	$1.9\text{E-}12*\text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$i\text{C}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13*\text{EXP}(-230./\text{temp})$	Wallington et al. (2018)
G43021	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{NO}_2$	KRO2N03	Rickard and Pascoe (2009)
G43022	TrGC	$\text{HYPROPO2} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	$k1_R02s0R02$	Rickard and Pascoe (2009)
G43023a	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{HYPROPO2H}$	$\text{KRO2H02}(3)*(1.-\text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G43023b	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KRO2H02}(3)*\text{rchohch2o2_oh}$	Rickard and Pascoe (2009)
G43024a	TrGCN	$\text{HYPROPO2} + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KRO2N0}*(1.-\text{alpha_AN}(4,1,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009)
G43024b	TrGCN	$\text{HYPROPO2} + \text{NO} \rightarrow \text{PROPOLNO3}$	$\text{KRO2N0}*\text{alpha_AN}(4,1,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G43025	TrGCN	$\text{HYPROPO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KRO2N03	Rickard and Pascoe (2009)
G43026a	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{HYPROPO2}$	k_roohro	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43026b	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{s*f_soh*f_pch2oh} + k_{t*f_tooh*f_pch2oh})$	Sander et al. (2018)
G43027	TrGCN	$\text{PRONO3BO2} + \text{HO}_2 \rightarrow \text{PR2O2HNO3}$	KR02H02(3)	Rickard and Pascoe (2009)
G43028	TrGCN	$\text{PRONO3BO2} + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43029	TrGCN	$\text{PRONO3BO2} + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43030a	TrGCN	$\text{PR2O2HNO3} + \text{OH} \rightarrow \text{PRONO3BO2}$	k_roohro	Rickard and Pascoe (2009)
G43030b	TrGCN	$\text{PR2O2HNO3} + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{t*f_tooh*f_ch2ono2}$	Sander et al. (2018)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Rickard and Pascoe (2009)
G43032	TrGCN	$\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$	$(k_{s*f_co*f_ono2} + k_{p*f_co})$	Sander et al. (2018)
G43033	TrGC	$\text{HOCH2COCHO} + \text{OH} \rightarrow .8609 \text{HOCH2CO} + .8609 \text{CO} + .1391 \text{HCOCOCHO} + .1391 \text{HO}_2$	$(1.9\text{E}-12*\text{EXP}(575./\text{temp}) + k_{s*f_soh*f_co})$	Sander et al. (2018)
G43034	TrGCN	$\text{HOCH2COCHO} + \text{NO}_3 \rightarrow \text{HOCH2CO} + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Sander et al. (2018)
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E}-14*\text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Sander et al. (2018)
G43036	TrGC	$\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{HCOCO} + .6 \text{HCHO} + .2 \text{HCOCOCHO} + .2 \text{HOCH2COCHO}$	k1_R02p0R02	Sander et al. (2018)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$\text{KR02H02(3)*rcoch2o2_ooh}$	Sander et al. (2018)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{KR02H02(3)*rcoch2o2_oh}$	Sander et al. (2018)
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N03	Sander et al. (2018)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{t*f_co*f_o}$	Sander et al. (2018)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{s*f_sooh*f_co}$	Sander et al. (2018)*
G43040c	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G43041	TrGCN	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Sander et al. (2018)
G43042	TrGC	$\text{HOCH2COCH2O2} \rightarrow \text{HCHO} + \text{HOCH2CO}$	k1_R02p0R02	Sander et al. (2018)
G43043a	TrGC	$\text{HOCH2COCH2O2} + \text{HO}_2 \rightarrow \text{HOCH2COCH2OOH}$	$\text{KR02H02(3)*rcoch2o2_ooh}$	Sander et al. (2018)
G43043b	TrGC	$\text{HOCH2COCH2O2} + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH2CO} + \text{OH}$	$\text{KR02H02(3)*rcoch2o2_oh}$	Sander et al. (2018)
G43044	TrGCN	$\text{HOCH2COCH2O2} + \text{NO} \rightarrow \text{HCHO} + \text{HOCH2CO} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G43045a	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HOCH2COCHO} + \text{OH}$	$k_{s*f_sooh*f_co}$	Sander et al. (2018)
G43045b	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HOCH2COCH2O2}$	k_roohro	Sander et al. (2018)
G43045c	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E}-12*\text{EXP}(305./\text{temp})$	Sander et al. (2018)*
G43046	TrGC	$\text{CH}_3\text{CHCO} + \text{OH} \rightarrow .72 \text{CO} + .72 \text{CH}_3\text{CHO} + .72 \text{HO}_2 + .21 \text{CH}_3\text{COCO}_2\text{H} + .07 \text{CH}_3\text{CHO} + .07 \text{HO}_2 + .07 \text{CO}_2$	$7.6\text{E}-11$	Hatakeyama et al. (1985), Sander et al. (2018)
G43047	TrGCN	$\text{PROPOLNO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{t*f_ono2*f_pch2oh} + k_{s*f_soh*f_ch2ono2}$	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G43048	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$2.3\text{E-}12 \cdot \text{EXP}(300./\text{temp})$	Tyndall et al. (2001a)*
G43049	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2$	$1.9\text{E}16 \cdot \text{EXP}(-10830./\text{temp})$	Sehested et al. (1998)*
G43050	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E-}13 \cdot \text{EXP}(-650./\text{temp}) \cdot \text{f_co}$	Sander et al. (2018)*
G43051a	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G43051b	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	k_s*f_sooH	Sander et al. (2018)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	k_s*f_pch2oh	Sander et al. (2018)*
G43052	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$4.9\text{E-}12 \cdot \text{EXP}(405./\text{temp})$	Atkinson et al. (2006)*
G43053	TrGCN	$\text{C}_2\text{H}_5\text{CHO} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HNO}_3$	6.3E-15	Atkinson et al. (2006)
G43054a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2018)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	k1_R02RC03*0.1	Sander et al. (2018)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Sander et al. (2018), Groß et al. (2014)
G43055b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Sander et al. (2018), Groß et al. (2014)
G43055c	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rco3_o3	Sander et al. (2018), Groß et al. (2014)
G43056	TrGCN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G43057	TrGCN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G43058	TrGCN	$\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43059	TrGC	$\text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	k_co2h+k_p+k_s*f_co2h	Sander et al. (2018)*
G43060a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G43060b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	k_s*f_co2h+k_p	Sander et al. (2018)*
G43061	TrGCN	$\text{PPN} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	k_s*f_cpan+k_p	Sander et al. (2018)*
G43062	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_3 + \text{H}_2\text{O}$	k_roohro	Sander et al. (2018)
G43063a	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Sander et al. (2018)
G43063b	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	KAPH02*(rco3_ooh+rco3_o3)	Sander et al. (2018)
G43064	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_2$	KAPNO	Sander et al. (2018)
G43065	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_3$	k_CH3C03_N02	Sander et al. (2018)*
G43066	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Sander et al. (2018)
G43067	TrGC	$\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2$	k1_R02RC03	Sander et al. (2018)
G43068	TrGC	$\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{ CO} + \text{HO}_2$	2.*k_t*f_co*f_o	Sander et al. (2018)
G43069	TrGC	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$	$2.6\text{E-}12 \cdot \text{EXP}(200./\text{temp})$	Atkinson et al. (2006)
G43070a	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$4.6\text{E-}12 \cdot \text{EXP}(70./\text{temp}) \cdot (\text{k_s*f_soh}/(\text{k_p}+\text{k_s*f_pch2oh}+\text{k_s*f_soh}))$	Atkinson et al. (2006), Sander et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G43070b	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO2} + \text{H}_2\text{O}$	$4.6\text{E-}12 \cdot \text{EXP}(70./\text{temp}) \cdot ((k_{\text{p}} + k_{\text{s*f_pch2oh}}) / (k_{\text{p}} + k_{\text{s*f_pch2oh}} + k_{\text{s*f_soh}}))$	Atkinson et al. (2006), Sander et al. (2018)*
G43071a	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$	$k_{\text{CH2CHOH_OH_HCOOH}}$	Sander et al. (2018), So et al. (2014)*
G43072	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCOOH}$	$k_{\text{CH2CHOH_HCOOH}}$	Sander et al. (2018), da Silva (2010)*
G43073	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH}$	$k_{\text{ALD_HCOOH}}$	Sander et al. (2018), da Silva (2010)*
G43074	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{s*f_sooh*f_co}} + k_{\text{roohro}}$	Sander et al. (2018)*
G43202	TrGTerC	$\text{HCOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{CO}_3$	$4.29\text{E-}11$	Rickard and Pascoe (2009)
G43203	TrGTerCN	$\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$	$2 \cdot \text{KNO3AL} \cdot 2.4$	Rickard and Pascoe (2009)
G43204a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Sander et al. (2018)
G43204b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$k1_{\text{R02RC03}} \cdot 0.1$	Sander et al. (2018)
G43205	TrGTerCN	$\text{HCOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43206	TrGTerCN	$\text{HCOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN2}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G43207a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{rco3_ooh}$	Rickard and Pascoe (2009)
G43207b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{rco3_o3}$	Rickard and Pascoe (2009)
G43207c	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3_oh}$	Rickard and Pascoe (2009)
G43210	TrGTerCN	$\text{C}_3\text{PAN2} \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G43211	TrGTerCN	$\text{C}_3\text{PAN2} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	$2.10\text{E-}11$	Rickard and Pascoe (2009)
G43212	TrGTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$2.14\text{E-}11$	Rickard and Pascoe (2009)
G43213a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Sander et al. (2018)
G43213b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$k1_{\text{R02RC03}} \cdot 0.1$	Sander et al. (2018)
G43214	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{rco3_ooh}$	Rickard and Pascoe (2009)
G43215b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3_oh}$	Rickard and Pascoe (2009)
G43215c	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{rco3_o3}$	Rickard and Pascoe (2009)
G43218	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN1}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G43219	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$1.39\text{E-}11$	Rickard and Pascoe (2009)
G43220	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3$	$1.73\text{E-}11$	Rickard and Pascoe (2009)
G43221	TrGTerCN	$\text{C}_3\text{PAN1} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G43222	TrGTerCN	$\text{C}_3\text{PAN1} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{CO} + \text{NO}_2$	$4.51\text{E-}12$	Rickard and Pascoe (2009)
G43223	TrGTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$2.49\text{E-}11$	Rickard and Pascoe (2009)*
G43415	TrGAroC	$\text{C3DIALOOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{OH}$	$1.44\text{E-}10$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43418a	TrGAroC	$\text{C3DIALO2} + \text{HO}_2 \rightarrow \text{C3DIALOOH}$	$\text{KR02H02(3)} * (\text{rco3_ooh} + \text{rco3_o3})$	Rickard and Pascoe (2009)
G43418b	TrGAroC	$\text{C3DIALO2} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(3)} * \text{rco3_oh}$	Rickard and Pascoe (2009)
G43419	TrGAroCN	$\text{C3DIALO2} + \text{NO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43420	TrGAroCN	$\text{C3DIALO2} + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G43421	TrGAroC	$\text{C3DIALO2} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G43422a	TrGAroC	$\text{HCOCOHCO3} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$\text{KAPH02} * \text{rco3_oh}$	Rickard and Pascoe (2009)
G43422b	TrGAroC	$\text{HCOCOHCO3} + \text{HO}_2 \rightarrow \text{HCOCOHCO3H}$	$\text{KAPH02} * (\text{rco3_ooh} + \text{rco3_o3})$	Rickard and Pascoe (2009)
G43424	TrGAroCN	$\text{HCOCOHCO3} + \text{NO} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G43425	TrGAroCN	$\text{HCOCOHCO3} + \text{NO}_2 \rightarrow \text{HCOCOH PAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G43426	TrGAroCN	$\text{HCOCOHCO3} + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03} * 1.74$	Rickard and Pascoe (2009)
G43427	TrGAroC	$\text{HCOCOHCO3} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G43428	TrGAroC	$\text{METACETHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2$	$9.82\text{E-}11$	Rickard and Pascoe (2009)
G43442	TrGAroCN	$\text{HCOCOH PAN} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	$6.97\text{E-}11$	Rickard and Pascoe (2009)
G43443	TrGAroCN	$\text{HCOCOH PAN} \rightarrow \text{HCOCOHCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	$\text{C32OH13CO} + \text{OH} \rightarrow \text{HCOCOHCO3}$	$1.36\text{E-}10$	Rickard and Pascoe (2009)
G43446	TrGAroC	$\text{HCOCOHCO3H} + \text{OH} \rightarrow \text{HCOCOHCO3}$	$7.33\text{E-}11$	Rickard and Pascoe (2009)
G44000	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$2.03\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(78./\text{temp})$	Atkinson et al. (2006)*
G44001a	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$(\text{k1_R02pR02} * 0.1273 + \text{k1_R02sR02} * 0.8727) * 0.1273$	Rickard and Pascoe (2009), Sander et al. (2018)
G44001b	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$(\text{k1_R02pR02} * 0.1273 + \text{k1_R02sR02} * 0.8727) * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2018)*
G44002	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N0} * (1. - (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) * 0.1273$	Rickard and Pascoe (2009), Sander et al. (2018)
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N0} * (1. - (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2018)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC}_4\text{H}_9\text{NO3}$	$\text{KR02N0} * (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G44004a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N03} * 0.1273$	Rickard and Pascoe (2009), Sander et al. (2018)
G44004b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N03} * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44005a	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{roohro}	Sander et al. (2018)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}}*f_{\text{tooh}}*f_{\text{alk}}*(k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2018)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t}}*f_{\text{tooh}}*f_{\text{alk}}*(k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2018)
G44006a	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E-}17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp})$	Atkinson (2003)
G44006b	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$*k_{\text{t}}/(3.*k_{\text{p}}+k_{\text{t}})$ $1.17\text{E-}17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp})$ $*3.*k_{\text{p}}/(3.*k_{\text{p}}+k_{\text{t}})$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$k1_{\text{R02tR02}}$	Rickard and Pascoe (2009), Sander et al. (2018)
G44008	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{TC}_4\text{H}_9\text{OOH}$	$\text{KR02H02}(4)$	Rickard and Pascoe (2009)
G44009a	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(4,3,0,0,0,$ $\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2018)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*\alpha_{\text{AN}}(4,3,0,0,0,\text{temp},$ $\text{cair})$	Rickard and Pascoe (2009)
G44010a	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{roohro}	Sander et al. (2018)
G44010b	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$3.*k_{\text{p}}*f_{\text{tch2oh}}$	Sander et al. (2018)*
G44011	TrGCN	$\text{TC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$3.*k_{\text{p}}*f_{\text{ch2ono2}}$	Sander et al. (2018)*
G44012	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k1_{\text{R02sR02}}$	Rickard and Pascoe (2009), Sander et al. (2018)
G44013	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$	$\text{KR02H02}(4)$	Rickard and Pascoe (2009)
G44014a	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(4,2,0,0,0,$ $\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2018)
G44014b	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},$ $\text{cair})$	Rickard and Pascoe (2009)
G44015a	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{roohro}	Sander et al. (2018)
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{sooh}}+2.*k_{\text{s}}+k_{\text{t}}*f_{\text{pch2oh}}$	Sander et al. (2018)*
G44016	TrGCN	$\text{IC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{ono2}}+2.*k_{\text{p}}+k_{\text{t}}*f_{\text{ch2ono2}}$	Sander et al. (2018)*
G44017	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .87 \text{ MGLYOX} + .5481 \text{ CO} + .1392 \text{ HO}_2$ $+ .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .13 \text{ HCHO} + .04680 \text{ OH}$ $+ .04680 \text{ CO} + .07280 \text{ CH}_3\text{C}(\text{O}) + .026 \text{ CH}_3\text{CHO} + .026$ $\text{CO}_2 + .026 \text{ HCHO} + .026 \text{ HO}_2 + .02402 \text{ MGLYOX} +$ $.02402 \text{ H}_2\text{O}_2 + .00718 \text{ CH}_3\text{COCO}_2\text{H}$	$8.5\text{E-}16*\text{EXP}(-1520./\text{temp})$	Sander et al. (2018)
G44018	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{LHMKABO}_2$	$2.6\text{E-}12*\text{EXP}(610./\text{temp})$	Sander et al. (2018), Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G44019	TrGC	MEK + OH \rightarrow LMEKO2 + H ₂ O	1.5E-12*EXP(-90./temp)	Atkinson et al. (2006), Sander et al. (2018)*
G44020	TrGC	LMEKO2 + HO ₂ \rightarrow LMEKOOH	KR02H02(4)	Sander et al. (2018)
G44021a	TrGCN	LMEKO2 + NO \rightarrow .62 CH ₃ CHO + .62 CH ₃ C(O) + .38 HCHO + .38 CO ₂ + .38 HOCH ₂ CH ₂ O ₂ + NO ₂	KR02N0*(1.-(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair)))	Sander et al. (2018)*
G44021b	TrGCN	LMEKO2 + NO \rightarrow LMEKNO3	KR02N0*(.62*alpha_AN(4,2,1,0,0,temp,cair)+.38*alpha_AN(4,1,0,1,0,temp,cair))	Sander et al. (2018)
G44022a	TrGC	LMEKOOH + OH \rightarrow LMEKO2 + H ₂ O	k_roohro	Sander et al. (2018)
G44022b	TrGC	LMEKOOH + OH \rightarrow .62 BIACET + .38 HCHO + .38 CO ₂ + .38 HOCH ₂ CH ₂ O ₂ + H ₂ O + OH	(.62*k_t*f_tooh*f_co+.38*k_s*f_sooH)	Sander et al. (2018)
G44023a	TrGCN	LC4H9NO3 + OH \rightarrow MEK + NO ₂ + H ₂ O	(k_t*f_ono2*f_alk+k_p*f_alk+k_s*f_ch2ono2+k_p)*(k_s/(k_p+k_s))	Sander et al. (2018)*
G44023b	TrGCN	LC4H9NO3 + OH \rightarrow C ₃ H ₇ CHO + NO ₂ + H ₂ O	(k_p+k_s*(1+f_ch2ono2+f_ono2)*f_alk)*(k_p/(k_p+k_s))	Sander et al. (2018)*
G44024	TrGCN	MPAN + OH \rightarrow CH ₃ COCH ₂ OH + CO + NO ₂	3.2E-11	Orlando et al. (2002)
G44025	TrGCN	MPAN \rightarrow MACO3 + NO ₂	k_PAN_M	see note*
G44026	TrGC	LMEKO2 \rightarrow .538 HCHO + .538 CO ₂ + .459 HOCH ₂ CH ₂ O ₂ + .079 C ₂ H ₅ O ₂ + .462 CH ₃ C(O) + .462 CH ₃ CHO	(.62*k1_R02sOR02+.38*k1_R02pOR02)	Rickard and Pascoe (2009)*
G44027	TrGC	MACR + OH \rightarrow .45 MACO3 + .55 MACRO2	8.E-12*EXP(380./temp)	Orlando et al. (1999b), Sander et al. (2018)
G44028	TrGC	MACR + O ₃ \rightarrow .5481 CO + .1392 HO ₂ + .1392 OH + .3219 CH ₂ OO + .87 MGLYOX + .13 HCHO + .13 OH + .065 HCOCOCH ₂ O ₂ + .065 CO + .065 CH ₃ C(O)	1.36E-15*EXP(-2112./temp)	Sander et al. (2018)
G44029	TrGCN	MACR + NO ₃ \rightarrow MACO3 + HNO ₃	KN03AL*2.0	Rickard and Pascoe (2009)
G44030a	TrGC	MACO3 \rightarrow CH ₃ C(O) + HCHO + CO ₂	k1_R02RC03*0.9	Sander et al. (2018)
G44030b	TrGC	MACO3 \rightarrow MACO2H	k1_R02RC03*0.1	Sander et al. (2018)
G44031a	TrGC	MACO3 + HO ₂ \rightarrow MACO2 + OH	KAPH02*rco3_oh	Sander et al. (2018)
G44031b	TrGC	MACO3 + HO ₂ \rightarrow MACO3H	KAPH02*rco3_ooh	Sander et al. (2018)
G44031c	TrGC	MACO3 + HO ₂ \rightarrow MACO2H + O ₃	KAPH02*rco3_o3	Sander et al. (2018)
G44032	TrGCN	MACO3 + NO \rightarrow MACO2 + NO ₂	8.70E-12*EXP(290./temp)	Sander et al. (2018)
G44033	TrGCN	MACO3 + NO ₂ \rightarrow MPAN	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44034	TrGCN	MACO3 + NO ₃ \rightarrow MACO2 + NO ₂	KR02N03*1.74	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44035	TrGC	$\text{MACRO2} \rightarrow .7 \text{CH}_3\text{COCH}_2\text{OH} + .7 \text{HCHO} + .7 \text{HO}_2 + .3 \text{MACROH}$	$k_{1_R02t0R02}$	Rickard and Pascoe (2009)*
G44036a	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACRO} + \text{OH}$	$\text{KR02H02(4)*rcoch2o2_oh}$	Sander et al. (2018)
G44036b	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACROOH}$	$\text{KR02H02(4)*rcoch2o2_ooh}$	Sander et al. (2018)
G44037a	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRO} + \text{NO}_2$	$\text{KR02N0*(1.-alpha_AN(6,3,1,0,0, temp, cair))}$	Sander et al. (2018)
G44037b	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRNO3}$	$\text{KR02N0*alpha_AN(6,3,1,0,0,temp, cair)}$	Sander et al. (2018)
G44038	TrGCN	$\text{MACRO2} + \text{NO}_3 \rightarrow \text{MACRO} + \text{NO}_2$	KR02N03	Sander et al. (2018)
G44039a	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{MACRO2}$	k_roohro	Sander et al. (2018)
G44039b	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$k_t*f_o*f_tch2oh*f_alk$	Sander et al. (2018)
G44039c	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$(k_s*f_soh*f_pch2oh + k_rohro)$	Sander et al. (2018)
G44040	TrGC	$\text{MACROH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2$	$k_t*f_o*f_tch2oh*f_alk$	Sander et al. (2018)
G44041	TrGC	$\text{MACRO} \rightarrow .885 \text{CH}_3\text{COCH}_2\text{OH} + .885 \text{CO} + .115 \text{MGLYOX} + .115 \text{HCHO} + \text{HO}_2$	KDEC	Sander et al. (2018)
G44042	TrGC	$\text{MACO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2 + \text{CO}_2$	$((k_adt+k_adp)*a_co2h+k_co2h)$	Sander et al. (2018)
G44043a	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{OH}$	$(k_adt+k_adp)*a_co2h$	Sander et al. (2018)
G44043b	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{MACO3}$	k_roohro	Sander et al. (2018)
G44044	TrGC	$\text{LHMKABO2} \rightarrow .024 \text{CO2H3CHO} + .072 \text{MGLYOX} + .072 \text{HO}_2 + .072 \text{HCHO} + .5280 \text{CH}_3\text{C(O)} + .5280 \text{HOCH}_2\text{CHO} + .176 \text{BIACETOH} + .2 \text{HO12CO3C4}$	$(.12*k_{1_R02p0R02}+.88*k_{1_R02s0R02})$	Sander et al. (2018)
G44045a	TrGC	$\text{LHMKABO2} + \text{HO}_2 \rightarrow \text{OH} + \text{HOCH}_2\text{CHO} + \text{CH}_3\text{C(O)}$	$\text{KR02H02(4)*.88*rcoch2o2_oh}$	Sander et al. (2018)
G44045b	TrGC	$\text{LHMKABO2} + \text{HO}_2 \rightarrow \text{LHMKABOOH}$	$\text{KR02H02(4)*(.12+.88*rcoch2o2_ooh)}$	Sander et al. (2018)
G44046a	TrGCN	$\text{LHMKABO2} + \text{NO} \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{HOCH}_2\text{CHO} + .88 \text{CH}_3\text{C(O)} + .12 \text{HCHO} + \text{NO}_2$	$\text{KR02N0*(1.-(.12*alpha_AN(6,1,0,1,0,0,temp, cair)+.88*alpha_AN(6,2,1,0,0,temp, cair)))}$	Sander et al. (2018)
G44046b	TrGCN	$\text{LHMKABO2} + \text{NO} \rightarrow \text{MKNO3}$	$\text{KR02N0*(.12*alpha_AN(6,1,0,1,0,0,temp, cair)+.88*alpha_AN(6,2,1,0,0,temp, cair))}$	Sander et al. (2018)*
G44047	TrGCN	$\text{LHMKABO2} + \text{NO}_3 \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{HOCH}_2\text{CHO} + .88 \text{CH}_3\text{C(O)} + .12 \text{HCHO} + .12 \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2018)
G44048a	TrGC	$\text{LHMKABOOH} + \text{OH} \rightarrow \text{LHMKABO2}$	k_roohro	Sander et al. (2018)
G44048b	TrGC	$\text{LHMKABOOH} + \text{OH} \rightarrow .12 \text{CO2H3CHO} + .88 \text{BIACETOH} + \text{OH}$	$(.12*k_s*f_sooh*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co)$	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44049a	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	$k_{\text{t}*f_{\text{o}}*f_{\text{alk}}}$	Sander et al. (2018)
G44049b	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{t}*f_{\text{co}}*f_{\text{toh}}*f_{\text{cho}}}$	Sander et al. (2018)
G44050	TrGCN	$\text{CO}_2\text{H}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{HNO}_3$	KN03AL*4.0	Rickard and Pascoe (2009)
G44051	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	$k_{1_R02RC03}$	Sander et al. (2018)
G44052a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	KAPH02*rco3_oh	Sander et al. (2018)
G44052b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rco3_o3	Sander et al. (2018)
G44052c	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Sander et al. (2018)
G44053	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	KAPNO	Sander et al. (2018)
G44054	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	KR02N03*1.74	Sander et al. (2018)
G44055a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	k_{roohro}	Sander et al. (2018)
G44055b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{OH}$	$(k_{\text{t}*f_{\text{co2h}}*f_{\text{co}}*f_{\text{toh}}})$	Sander et al. (2018)
G44056	TrGC	$\text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCOCO}_2\text{H} + \text{HO}_2$	$k_{\text{t}*f_{\text{co2h}}*f_{\text{co}}*f_{\text{toh}}+k_{\text{co2h}}}$	Sander et al. (2018)
G44057a	TrGC	$\text{HO}_{12}\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{BIACETOH} + \text{HO}_2$	$k_{\text{t}*f_{\text{toh}}*f_{\text{alk}}*f_{\text{co}}}$	Sander et al. (2018)
G44057b	TrGC	$\text{HO}_{12}\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$	$k_{\text{s}*f_{\text{soh}}*f_{\text{alk}}}$	Sander et al. (2018)
G44058	TrGC	$\text{MACO}_2 \rightarrow .65 \text{CH}_3 + .65 \text{CO} + .65 \text{HCHO} + .35 \text{OH} + .35 \text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$	KDEC	Sander et al. (2018)
G44059	TrGC	$\text{LHMKABO}_2 \rightarrow .88 \text{MGLYOX} + .88 \text{HCHO} + .12 \text{HOOCH}_2\text{CHO} + .12 \text{CH}_3\text{C}(\text{O}) + \text{OH}$	KHSD	Sander et al. (2018)
G44060	TrGC	$\text{MACRO}_2 \rightarrow \text{MGLYOX} + \text{HCHO} + \text{OH}$	KHSB	Sander et al. (2018)
G44061a	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}*f_{\text{sooh}}*f_{\text{ch2ono2}}+k_{\text{rohro}}}$	Sander et al. (2018)*
G44061b	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{BIACETOH} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t}*f_{\text{ono2}}*f_{\text{co}}*f_{\text{pch2oh}}}$	Sander et al. (2018)*
G44062a	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t}*f_{\text{o}}*f_{\text{ch2ono2}}}$	Sander et al. (2018)*
G44062b	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{rohro}}+k_{\text{s}*f_{\text{sooh}}*f_{\text{ch2ono2}}}$	Sander et al. (2018)*
G44063	TrGC	$\text{MACRO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH} + \text{CO}$	K14HSAL	Sander et al. (2018)
G44064	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow .9 \text{CH}_3\text{COCHCO} + .1 \text{CH}_3\text{C}(\text{O}) + .01 \text{GLYOX} + .18 \text{CO} + .09 \text{HO}_2 + \text{OH}$	K15HS24VYNAL	Sander et al. (2018)
G44065	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOHCHCHO}$	KR02H02(4)	Sander et al. (2018)
G44066	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G44067	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	kR02N03	Sander et al. (2018)
G44068	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO}$	$k_{1_R02s0R02}$	Sander et al. (2018)
G44069	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCCH}_3\text{CO} + \text{OH}$	K15HS24VYNAL	Sander et al. (2018)
G44070	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G44071	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{HO}_2 \rightarrow \text{HCOCCH}_3\text{CHOOH}$	KR02H02(4)	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44072	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO}_3 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KR02N03	Sander et al. (2018)
G44073	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO}$	k1_R02p0R02	Sander et al. (2018)
G44074	TrGC	$\text{CH}_3\text{COOHCHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{OH}$	KHYDEC	Sander et al. (2018)
G44075	TrGC	$\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{OH}$	KHYDEC	Sander et al. (2018)
G44076	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G44077	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{NO}_2$	KR02N03	Sander et al. (2018)
G44078	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{OH}$	KR02H02(4)	Sander et al. (2018)*
G44079	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX}$	k1_R02s0R02	Sander et al. (2018)
G44080	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$	k1_R02t0R02	Sander et al. (2018)
G44081	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G44082	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	KR02H02(4)	Sander et al. (2018)*
G44083	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2018)
G44084	TrGC	$\text{HCOCCH}_3\text{CO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	1E-10*a_cho	Hatakeyama et al. (1985), Sander et al. (2018)
G44085	TrGC	$\text{CH}_3\text{COCHCO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	7.6E-11*a_coch3	Hatakeyama et al. (1985), Sander et al. (2018)*
G44086	TrGCN	$\text{LMEKNO}_3 + \text{OH} \rightarrow .62 \text{ MGLYOX} + .62 \text{ HCHO} + .62 \text{ HO}_2 + .62 \text{ NO}_2 + .38 \text{ CH}_3\text{C(O)} + .38 \text{ NO}_3\text{CH}_2\text{CHO}$	$.62*(k_p*(f_{\text{co}}+f_{\text{ch2ono2}})) + .38*(k_s*f_{\text{ch2ono2}}*f_{\text{co}})$	Sander et al. (2018)*
G44087	TrGC	$\text{MEPROPENE} + \text{OH} \rightarrow \text{IBUTOLBO}_2$	$9.4\text{E-}12*\text{EXP}(505./\text{temp})$	Atkinson et al. (2006)
G44088a	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_2\text{OO}^*$	$2.7\text{E-}15*\text{EXP}(-1630./\text{temp})*0.33$	Atkinson et al. (2006), Sander et al. (2018)
G44088b	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{OH} + \text{HCHO}$	$2.7\text{E-}15*\text{EXP}(-1630./\text{temp})*0.67$	Atkinson et al. (2006), Sander et al. (2018)
G44089	TrGCN	$\text{MEPROPENE} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2$	3.4E-13	Atkinson et al. (2006), Sander et al. (2018)*
G44090	TrGC	$\text{IBUTOLBO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$	k1_R02t0R02	Sander et al. (2018)
G44091a	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{IBUTOLBOOH}$	KR02H02(4)*rcoch2o2_ooh	Sander et al. (2018)
G44091b	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	KR02H02(4)*rcoch2o2_oh	Sander et al. (2018)
G44092a	TrGCN	$\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(5,3,0,0,0,\text{temp},\text{cair}))$	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44092b	TrGCN	IBUTOLBO2 + NO \rightarrow IBUTOLBNO3	KR02N0*alpha_AN(5,3,0,0,0,temp,cair)	Sander et al. (2018)
G44093	TrGCN	IBUTOLBO2 + NO ₃ \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02N03	Sander et al. (2018)
G44094a	TrGC	IBUTOLBOOH + OH \rightarrow IBUTOLBO2	k_roohro	Sander et al. (2018)
G44094b	TrGC	IBUTOLBOOH + OH \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂	k_s*f_sooh*f_pch2oh	Sander et al. (2018)
G44095	TrGCN	IBUTOLBNO3 + OH \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	3.*k_p	Sander et al. (2018)
G44096	TrGC	BUT1ENE + OH \rightarrow LBUT1ENO2	6.6E-12*EXP(465./temp)	Atkinson et al. (2006)*
G44097a	TrGC	BUT1ENE + O ₃ \rightarrow HCHO + .5 C ₂ H ₅ CHO + .5 H ₂ O ₂ + .5 CH ₃ CHO + .5 CO + .5 HO ₂	3.35E-15*EXP(-1745./temp)*.57	Atkinson et al. (2006), Sander et al. (2018)*
G44097b	TrGC	BUT1ENE + O ₃ \rightarrow C ₂ H ₅ CHO + CH ₂ OO*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Sander et al. (2018)*
G44098	TrGCN	BUT1ENE + NO ₃ \rightarrow C ₂ H ₅ CHO + HCHO + NO ₂	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Sander et al. (2018)*
G44099	TrGC	LBUT1ENO2 \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02s0R02	Sander et al. (2018)
G44100a	TrGC	LBUT1ENO2 + HO ₂ \rightarrow LBUT1ENOOH	KR02H02(4)*rcoch2o2_ooh	Sander et al. (2018)
G44100b	TrGC	LBUT1ENO2 + HO ₂ \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Sander et al. (2018)
G44101a	TrGCN	LBUT1ENO2 + NO \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(5,2,0,0,0,temp,cair))	Sander et al. (2018)
G44101b	TrGCN	LBUT1ENO2 + NO \rightarrow LBUT1ENNO3	KR02N0*alpha_AN(5,2,0,0,0,temp,cair)	Sander et al. (2018)
G44102	TrGCN	LBUT1ENO2 + NO ₃ \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂ + NO ₂	KR02N03	Sander et al. (2018)
G44103a	TrGC	LBUT1ENOOH + OH \rightarrow LBUT1ENO2	k_roohro	Sander et al. (2018)
G44103b	TrGC	LBUT1ENOOH + OH \rightarrow C ₂ H ₅ CO ₃ + HCHO + HO ₂	k_t*f_tooh*f_pch2oh	Sander et al. (2018)*
G44104	TrGCN	LBUT1ENNO3 + OH \rightarrow C ₂ H ₅ CHO + CO + HO ₂ + NO ₂	k_s*f_soh*f_ch2ono2	Sander et al. (2018)*
G44105	TrGC	CBUT2ENE + OH \rightarrow BUT2OLO2	1.1E-11*EXP(485./temp)	Atkinson et al. (2006)
G44106	TrGC	CBUT2ENE + O ₃ \rightarrow CH ₃ CHO + .16 CH ₃ CHOHOOH + .50 OH + .50 HCOCH ₂ O ₂ + .05 CH ₂ CO + .09 CH ₃ OH + .09 CO + .2 CH ₄ + .2 CO ₂	3.2E-15*EXP(-965./temp)	Atkinson et al. (2006), Sander et al. (2018)*
G44107	TrGCN	CBUT2ENE + NO ₃ \rightarrow 2 CH ₃ CHO + NO ₂	3.5E-13	Atkinson et al. (2006), Sander et al. (2018)*
G44108	TrGC	TBUT2ENE + OH \rightarrow BUT2OLO2	1.0E-11*EXP(553./temp)	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G44109	TrGC	TBUT2ENE + O ₃ → CH ₃ CHO + .16 CH ₃ CHOHOOH + .50 OH + .50 HCOCH ₂ O ₂ + .05 CH ₂ CO + .09 CH ₃ OH + .09 CO + .2 CH ₄ + .2 CO ₂	6.6E-15*EXP(-1060./temp)	Atkinson et al. (2006), Sander et al. (2018)
G44110	TrGCN	TBUT2ENE + NO ₃ → 2 CH ₃ CHO + NO ₂	1.78E-12*EXP(-530./temp) +1.28E-14*EXP(570./temp)	Atkinson et al. (2006), Sander et al. (2018)*
G44111	TrGC	BUT2OLO2 → C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02s0R02	Sander et al. (2018)
G44112a	TrGC	BUT2OLO2 + HO ₂ → BUT2OLOOH	KR02H02(4)*rcoch2o2_ooh	Sander et al. (2018)
G44112b	TrGC	BUT2OLO2 + HO ₂ → 2 CH ₃ CHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Sander et al. (2018)
G44113a	TrGCN	BUT2OLO2 + NO → 2 CH ₃ CHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(5,2,0,0,0, temp, cair))	Sander et al. (2018)
G44113b	TrGCN	BUT2OLO2 + NO → BUT2OLNO3	KR02N0*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2018)
G44114	TrGCN	BUT2OLO2 + NO ₃ → 2 CH ₃ CHO + HO ₂ + NO ₂	KR02N03	Sander et al. (2018)
G44115a	TrGC	BUT2OLOOH + OH → BUT2OLO2	k_roohro	Sander et al. (2018)
G44115b	TrGC	BUT2OLOOH + OH → LMEKOOH + HO ₂	k_t*f_toh*f_pch2oh	Sander et al. (2018)
G44115c	TrGC	BUT2OLOOH + OH → BUT2OLO + OH	k_t*f_tooh*f_pch2oh	Sander et al. (2018)
G44116	TrGCN	BUT2OLNO3 + OH → LMEKNO3 + HO ₂	k_t*f_toh*f_ch2ono2	Sander et al. (2018)
G44117	TrGC	BUT2OLO + OH → BIACET + HO ₂	k_t*f_toh*f_co	Sander et al. (2018)
G44118	TrGC	IPRCHO + OH → IPRCO3 + H ₂ O	6.8E-12*EXP(410./temp)	Atkinson et al. (2006)
G44119	TrGCN	IPRCHO + NO ₃ → IPRCO3 + HNO ₃	1.67E-12*EXP(-1460./temp)	Atkinson et al. (2006)
G44120	TrGC	IPRCO3 → iC ₃ H ₇ O ₂ + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G44121a	TrGC	IPRCO3 + HO ₂ → PERIBUACID	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G44121b	TrGC	IPRCO3 + HO ₂ → iC ₃ H ₇ O ₂ + CO ₂ + OH	KAPH02*(1-rco3_ooh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44122	TrGCN	IPRCO3 + NO ₂ → PIPN	k_CH3C03_N02	Rickard and Pascoe (2009)
G44123	TrGCN	IPRCO3 + NO → iC ₃ H ₇ O ₂ + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G44124a	TrGC	PERIBUACID + OH → IPRCO3 + H ₂ O	k_roohro	Rickard and Pascoe (2009)
G44124b	TrGC	PERIBUACID + OH → CH ₃ COCH ₃ + H ₂ O + CO ₂	k_s*f_co2h	Sander et al. (2018)*
G44125	TrGCN	PIPn → IPRCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	PIPn + OH → CH ₃ COCH ₃ + CO ₂ + NO ₂	k_s*f_cpan	Sander et al. (2018)*
G44127	TrGC	MPROPENOL + OH → HCOOH + OH + CH ₃ COCH ₃	k_CH2CHOH_OH_HCOOH	Sander et al. (2018), So et al. (2014)*
G44128	TrGC	MPROPENOL + HCOOH → IPRCHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*

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

#	labels	reaction	rate coefficient	reference
G44129	TrGC	IPRCHO + HCOOH \rightarrow MPROPENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G44130	TrGC	BUTENOL + OH \rightarrow HCOOH + OH + C ₂ H ₅ CHO	k_CH2CHOH_OH_HCOOH	Sander et al. (2018), So et al. (2014)*
G44131	TrGC	BUTENOL + HCOOH \rightarrow C ₃ H ₇ CHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G44132	TrGC	C ₃ H ₇ CHO + HCOOH \rightarrow BUTENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G44133	TrGC	HVMK + OH \rightarrow HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2018), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	HVMK + HCOOH \rightarrow CO ₂ C ₃ CHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G44135	TrGC	CO ₂ C ₃ CHO + HCOOH \rightarrow HVMK + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G44136	TrGC	HMAC + OH \rightarrow HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2018), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	HMAC + HCOOH \rightarrow IBUTDIAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G44138	TrGC	IBUTDIAL + HCOOH \rightarrow HMAC + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G44139	TrGC	CO ₂ C ₃ CHO + OH \rightarrow CH ₃ COCH ₂ O ₂ + CO ₂ + H ₂ O	k_t*f_o*f_alk+k_s*f_cho*f_co	Sander et al. (2018)*
G44140	TrGCN	CO ₂ C ₃ CHO + NO ₃ \rightarrow CH ₃ COCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*4.0	Sander et al. (2018)*
G44141	TrGC	IBUTDIAL + OH \rightarrow CH ₃ CHO + CO + HO ₂ + CO ₂ + H ₂ O	2.*k_t*f_o*f_alk+k_t*f_cho*f_cho	Sander et al. (2018)*
G44142	TrGCN	IBUTDIAL + NO ₃ \rightarrow CH ₃ CHO + CO + HO ₂ + CO ₂ + HNO ₃	2.*KN03AL*4.0	Sander et al. (2018)*
G44200	TrGTerC	CH ₃ COCOCH ₂ O ₂ \rightarrow CH ₃ C(O) + HCHO + CO	k1_R02p0R02	Rickard and Pascoe (2009)
G44201	TrGTerC	CH ₃ COCOCH ₂ O ₂ + HO ₂ \rightarrow CH ₃ COCOCH ₂ OOH	KR02H02(4)	Rickard and Pascoe (2009)
G44202	TrGTerCN	CH ₃ COCOCH ₂ O ₂ + NO \rightarrow CH ₃ C(O) + HCHO + CO + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44203a	TrGTerC	CH ₃ COCOCH ₂ OOH + OH \rightarrow CH ₃ COCOCHO + OH	k_s*f_co*f_sooH	Rickard and Pascoe (2009)*
G44203b	TrGTerC	CH ₃ COCOCH ₂ OOH + OH \rightarrow CH ₃ COCOCH ₂ O ₂	k_roohro	Rickard and Pascoe (2009)
G44204	TrGTerC	C44O ₂ + HO ₂ \rightarrow C44OOH	KR02H02(4)	Rickard and Pascoe (2009)
G44205	TrGTerCN	C44O ₂ + NO \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O ₂ \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44207	TrGTerC	$\text{C44OOH} + \text{OH} \rightarrow \text{C44O2}$	$7.46\text{E-}11$	Rickard and Pascoe (2009)
G44208	TrGTerC	$\text{CHOC3COO2} \rightarrow \text{HCOCH2CO3} + \text{HCHO}$	k1_R02p0R02	Rickard and Pascoe (2009)
G44209	TrGTerC	$\text{CHOC3COO2} + \text{HO}_2 \rightarrow \text{C413COOOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	$\text{CHOC3COO2} + \text{NO} \rightarrow \text{HCOCH2CO3} + \text{HCHO} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44211	TrGTerC	$\text{C413COOOH} + \text{OH} \rightarrow \text{CHOC3COO2}$	$8.33\text{E-}11$	Rickard and Pascoe (2009)
G44212	TrGTerC	$\text{C4CODIAL} + \text{OH} \rightarrow \text{C312COCO3}$	$3.39\text{E-}11$	Rickard and Pascoe (2009)
G44213	TrGTerCN	$\text{C4CODIAL} + \text{NO}_3 \rightarrow \text{C312COCO3} + \text{HNO}_3$	$2.\text{*KN03AL*4.0}$	Rickard and Pascoe (2009)
G44214	TrGTerC	$\text{C312COCO3} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G44215a	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{C312COCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44215b	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02*(1-rco3_ooh)}$	Rickard and Pascoe (2009)
G44216	TrGTerCN	$\text{C312COCO3} + \text{NO}_2 \rightarrow \text{C312COPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G44217	TrGTerCN	$\text{C312COCO3} + \text{NO} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G44218	TrGTerC	$\text{C312COCO3H} + \text{OH} \rightarrow \text{C312COCO3}$	$1.63\text{E-}11$	Rickard and Pascoe (2009)
G44219	TrGTerCN	$\text{C312COPAN} \rightarrow \text{C312COCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G44220	TrGTerCN	$\text{C312COPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO} + \text{NO}_2$	$1.27\text{E-}11$	Rickard and Pascoe (2009)
G44221	TrGTerC	$\text{CH}_3\text{COCOCHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + 2\text{ CO}$	$8.4\text{E-}13\text{*EXP(830./temp)}$	Sander et al. (2018)*
G44222	TrGTerCN	$\text{CH}_3\text{COCOCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + 2\text{ CO} + \text{HNO}_3$	KN03AL*4.0	Rickard and Pascoe (2009)
G44223	TrGTerC	$\text{IBUTALOH} + \text{OH} \rightarrow \text{IPRHOCO3}$	$1.4\text{E-}11$	Rickard and Pascoe (2009)
G44224a	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G44224b	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009), Sander et al. (2018)
G44224c	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G44225	TrGTerCN	$\text{IPRHOCO3} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G44226	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_2 \rightarrow \text{C4PAN5}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G44227	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G44228a	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.7	Rickard and Pascoe (2009)
G44228b	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{IPRHOCO2H}$	k1_R02RC03*0.3	Rickard and Pascoe (2009)
G44229	TrGTerC	$\text{IPRHOCO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$1.72\text{E-}12$	Rickard and Pascoe (2009)
G44230	TrGTerC	$\text{OH} + \text{IPRHOCO3H} \rightarrow \text{IPRHOCO3}$	$4.80\text{E-}12$	Rickard and Pascoe (2009)
G44231	TrGTerCN	$\text{C4PAN5} \rightarrow \text{IPRHOCO3} + \text{NO}_2$	K_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	$\text{C4PAN5} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO} + \text{NO}_2$	$4.75\text{E-}13$	Rickard and Pascoe (2009)
G44233a	TrGTerC	$\text{MBOOO} \rightarrow \text{IPRHOCO2H}$	$1.60\text{E-}17\text{*C(ind_H20)*(0.08+0.15)}$	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G44233b	TrGTerC	MBOOO \rightarrow IBUTALOH + H ₂ O ₂	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Sander et al. (2018)
G44234	TrGTerC	MBOOO + CO \rightarrow IBUTALOH + CO ₂	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	MBOOO + NO \rightarrow IBUTALOH + NO ₂	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	MBOOO + NO ₂ \rightarrow IBUTALOH + NO ₃	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	MALANHY + OH \rightarrow MALANHYO2	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	MALDIALOOH + OH \rightarrow HOCOC4DIAL + OH	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	MALDIALOOH + OH \rightarrow MALDIALO2	k_roohro	Rickard and Pascoe (2009)
G44402	TrGAroCN	NC4DCO2H + OH \rightarrow MALANHY + NO ₂	k_roohro	Rickard and Pascoe (2009)*
G44403	TrGAroC	CO14O3CO2H + OH \rightarrow HCOCH ₂ O ₂ + 2 CO ₂	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	BZFUOOH + OH \rightarrow BZFUO2	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	HOCOC4DIAL + OH \rightarrow CO2C4DIAL + HO ₂	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow MALDALCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44406b	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow MALDALCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44406c	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)*
G44407	TrGAroCN	MALDIALCO3 + NO \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)*
G44408	TrGAroCN	MALDIALCO3 + NO ₂ \rightarrow MALDIALPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO3 + NO ₃ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KR02NO3*1.74	Rickard and Pascoe (2009)*
G44410	TrGAroC	MALDIALCO3 \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	k1_R02RCO3	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO ₃ \rightarrow NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O ₃ \rightarrow .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H ₂ O ₂ + .5 CO + .5 CO ₂ + .5 HCOCH ₂ O ₂ + .5 OH	2.20E-19	see note*
G44413	TrGAroC	BZFUONE + OH \rightarrow BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH \rightarrow NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH \rightarrow MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH \rightarrow C3DIALO2 + CO ₂	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow C3DIALO2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO \rightarrow C3DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44419	TrGAroCN	EPXDLCO3 + NO ₂ → EPXDLPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44420	TrGAroCN	EPXDLCO3 + NO ₃ → C3DIALO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G44421	TrGAroC	EPXDLCO3 → C3DIALO2 + CO ₂	k1_R02RCO3	Rickard and Pascoe (2009)*
G44422	TrGAroC	MALNHYOHCO + OH → CO + CO + CO + CO ₂ + HO ₂	5.68E-12	Rickard and Pascoe (2009)
G44423	TrGAroCN	MALDIAL + NO ₃ → MALDIALCO3 + HNO ₃	2*KN03AL*2.0	Rickard and Pascoe (2009)
G44424	TrGAroC	MALDIAL + O ₃ → 1.0675 GLYOX + .125 HCHO + .1125 HCOCO ₂ H + .0675 H ₂ O ₂ + .82 HO ₂ + .57 OH + 1.265 CO + .25 CO ₂	2.00E-18	Rickard and Pascoe (2009)*
G44425	TrGAroC	MALDIAL + OH → .83 MALDIALCO3 + .17 MALDIALO2	5.20E-11	Rickard and Pascoe (2009)*
G44426	TrGAroC	MALANHYOOH + OH → MALNHYOHCO + OH	4.66E-11	Rickard and Pascoe (2009)
G44427	TrGAroCN	MALDIALPAN + OH → GLYOX + CO + CO + NO ₂	3.70E-11	Rickard and Pascoe (2009)
G44428	TrGAroCN	MALDIALPAN → MALDIALCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44429a	TrGAroC	MALANHYO2 + HO ₂ → MALANHYOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44429b	TrGAroC	MALANHYO2 + HO ₂ → HCOCOHCOC3 + CO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCOHCOC3 + CO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44431	TrGAroCN	MALANHYO2 + NO ₃ → HCOCOHCOC3 + CO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 → HCOCOHCOC3 + CO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44433	TrGAroC	EPXDLCO3H + OH → EPXDLCO3	2.62E-11	Rickard and Pascoe (2009)
G44434	TrGAroC	CO2C4DIAL + OH → CO + CO + CO + CO + HO ₂	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	NBZFUO2 + HO ₂ → NBZFUOOH	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44435b	TrGAroCN	NBZFUO2 + HO ₂ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G44436	TrGAroCN	NBZFUO2 + NO → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44437	TrGAroCN	NBZFUO2 + NO ₃ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44438	TrGAroCN	NBZFUO2 → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44439	TrGAroC	MALDALCO2H + OH → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	3.70E-11	Rickard and Pascoe (2009)*
G44440	TrGAroCN	EPXC4DIAL + NO ₃ → EPXDLCO3 + HNO ₃	2*KN03AL*4.0	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44441	TrGAroC	EPXC4DIAL + OH \rightarrow EPXDLCO3	4.32E-11	Rickard and Pascoe (2009)
G44442a	TrGAroC	MECOACETO2 + HO ₂ \rightarrow MECOACEOOH	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44442b	TrGAroC	MECOACETO2 + HO ₂ \rightarrow CH ₃ C(O)OO + HCHO + CO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G44443	TrGAroCN	MECOACETO2 + NO \rightarrow CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44444	TrGAroCN	MECOACETO2 + NO ₃ \rightarrow CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44445	TrGAroC	MECOACETO2 \rightarrow CH ₃ C(O)OO + HCHO + CO ₂	k1_R02p0R02	Rickard and Pascoe (2009)*
G44446	TrGAroCN	CO14O3CHO + NO ₃ \rightarrow CO + HCOCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	CO14O3CHO + OH \rightarrow CO + HCOCH ₂ O ₂ + CO ₂	3.44E-11	Rickard and Pascoe (2009)
G44448	TrGAroCN	NBZFUONE + OH \rightarrow BZFUCO + NO ₂	1.16E-12	Rickard and Pascoe (2009)
G44449a	TrGAroC	BZFUO2 + HO ₂ \rightarrow BZFUOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44449b	TrGAroC	BZFUO2 + HO ₂ \rightarrow CO14O3CHO + HO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G44450	TrGAroCN	BZFUO2 + NO \rightarrow CO14O3CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44451	TrGAroCN	BZFUO2 + NO ₃ \rightarrow CO14O3CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44452	TrGAroC	BZFUO2 \rightarrow CO14O3CHO + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44453	TrGAroC	BZFUCO + OH \rightarrow CO14O3CHO + HO ₂	1.78E-11	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO ₂ \rightarrow MALDIALOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO ₂ \rightarrow GLYOX + GLYOX + HO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)
G44457	TrGAroCN	MALDIALO2 + NO \rightarrow GLYOX + GLYOX + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44458	TrGAroCN	MALDIALO2 + NO ₃ \rightarrow GLYOX + GLYOX + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44459	TrGAroC	MALDIALO2 \rightarrow GLYOX + GLYOX + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH \rightarrow HCOCOCHO + CO + NO ₂	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN \rightarrow EPXDLCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH \rightarrow MECOACETO2	3.59E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45000	TrGC	$C_5H_8 + O_3 \rightarrow .3508 \text{ MACR} + .01518 \text{ MACO2H} + .2440 \text{ MVK} + .7085 \text{ HCHO} + .11 \text{ CH}_2\text{OO} + .1275 \text{ C}_3\text{H}_6 + .1575 \text{ CH}_3\text{C(O)} + .0510 \text{ CH}_3 + .2625 \text{ HO}_2 + .27 \text{ OH} + .09482 \text{ H}_2\text{O}_2 + .255 \text{ CO}_2 + .522 \text{ CO} + .07182 \text{ HCHO} + .03618 \text{ HCOCH}_2\text{O}_2 + .01782 \text{ CO} + 0.05408 \text{ LCARBON}$	$1.03E-14 * \exp(-1995./\text{temp})$	Atkinson et al. (2006), Sander et al. (2018)
G45001	TrGC	$C_5H_8 + OH \rightarrow .63 \text{ LISOPAB} + .30 \text{ LISOPCD} + .07 \text{ LISOPEFO2}$	$2.7E-11 * \exp(390./\text{temp})$	Atkinson et al. (2006), Sander et al. (2018)
G45002	TrGCN	$C_5H_8 + NO_3 \rightarrow \text{NISOP O2}$	$3.0E-12 * \exp(-450./\text{temp})$	Atkinson et al. (2006)
G45003a	TrGC	$\text{LISOPAB} + O_2 \rightarrow \text{LISOPACO2}$	$5.530E-13$	Sander et al. (2018)
G45003b	TrGC	$\text{LISOPAB} + O_2 \rightarrow \text{ISOPBO2}$	$3.E-12$	Sander et al. (2018)
G45004a	TrGC	$\text{LISOPCD} + O_2 \rightarrow \text{LDISOPACO2}$	$6.780E-13$	Sander et al. (2018)
G45004b	TrGC	$\text{LISOPCD} + O_2 \rightarrow \text{ISOPDO2}$	$3.E-12$	Sander et al. (2018)
G45005	TrGC	$\text{LISOPACO2} \rightarrow \text{LISOPAB} + O_2$	$3.1E12 * \exp(-7900./\text{temp}) * .6 + 7.8E13 * \exp(-8600./\text{temp}) * .4$	Sander et al. (2018)
G45006	TrGC	$\text{ISOPBO2} \rightarrow \text{LISOPAB} + O_2$	$3.7E14 * \exp(-9570./\text{temp}) + 4.2E14 * \exp(-9970./\text{temp})$	Sander et al. (2018)
G45007	TrGC	$\text{LDISOPACO2} \rightarrow \text{LISOPCD} + O_2$	$5.65E12 * \exp(-8410./\text{temp}) * .42 + 1.4E14 * \exp(-9110./\text{temp}) * .58$	Sander et al. (2018)
G45008	TrGC	$\text{ISOPDO2} \rightarrow \text{LISOPCD} + O_2$	$5.0E14 * \exp(-10120./\text{temp}) + 8.25E14 * \exp(-10220./\text{temp})$	Sander et al. (2018)
G45009a	TrGC	$\text{LISOPACO2} \rightarrow \text{C1ODC2O2C4OOH}$	$K16HSZ14 * 2./3. * (1 - fhpal)$	Sander et al. (2018)
G45009b	TrGC	$\text{LISOPACO2} \rightarrow \text{LZCODC23DBCOOH} + HO_2$	$K16HSZ14 * (2./3. * fhpal + 1./3.)$	Sander et al. (2018)
G45010a	TrGC	$\text{LDISOPACO2} \rightarrow \text{C1OOHC3O2C4OD}$	$k16HSZ41 * 2./3. * (1 - fhpal)$	Sander et al. (2018)
G45010b	TrGC	$\text{LDISOPACO2} \rightarrow \text{LZCODC23DBCOOH} + HO_2$	$k16HSZ41 * (2./3. * fhpal + 1./3.)$	Sander et al. (2018)
G45011	TrGC	$\text{LISOPACO2} \rightarrow .9 \text{ LISOPACO} + .1 \text{ ISOPAOH}$	$k1_R02LISOPACO2$	Rickard and Pascoe (2009), Sander et al. (2018)
G45012	TrGC	$\text{LISOPACO2} + HO_2 \rightarrow \text{LISOPACOOH} + 0.024 \text{ BLOV} + 0.119 \text{ BSOV}$	$KR02H02(5)$	Rickard and Pascoe (2009)
G45013a	TrGCN	$\text{LISOPACO2} + NO \rightarrow \text{LISOPACO} + NO_2 + 0.003 \text{ BLOV} + 0.101 \text{ BSOV}$	$KR02N0 * (1 - \alpha_AN(6, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2018)
G45013b	TrGCN	$\text{LISOPACO2} + NO \rightarrow \text{LISOPACNO3}$	$KR02N0 * \alpha_AN(6, 1, 0, 0, 0, \text{temp}, \text{cair})$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2018)
G45014	TrGCN	$\text{LISOPACO2} + NO_3 \rightarrow \text{LISOPACO} + NO_2$	$KR02N03$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45015	TrGC	LDISOPACO2 \rightarrow .9 LISOPACO + .1 ISOPAOH	k1_R02LISOPACO2	Rickard and Pascoe (2009), Sander et al. (2018)
G45016	TrGC	LDISOPACO2 + HO ₂ \rightarrow LISOPACOOH + 0.024 BLOV + 0.119 BSOV	KR02H02(5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO \rightarrow LISOPACO + NO ₂ + 0.003 BLOV + 0.101 BSOV	KR02N0*(1.-alpha_AN(6,1,0,0,0,temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2018)
G45017b	TrGCN	LDISOPACO2 + NO \rightarrow LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0,temp,cair)	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2018)
G45018	TrGCN	LDISOPACO2 + NO ₃ \rightarrow LISOPACO + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH \rightarrow LISOPACO2	k_roohro	Sander et al. (2018)
G45019b	TrGC	LISOPACOOH + OH \rightarrow LZCODC23DBCOOH + HO ₂	k_s*f_allyl*f_soh	Sander et al. (2018)
G45019c	TrGC	LISOPACOOH + OH \rightarrow LHC4ACCHO + OH	(k_s*f_soh*f_allyl+ k_rohro)	Sander et al. (2018)
G45019d	TrGC	LISOPACOOH + OH \rightarrow LIEPOX + OH	(k_adt+k_ads)*a_ch2oh*a_ch2ooh	Sander et al. (2018)*
G45020	TrGC	ISOPAOH + OH \rightarrow LHC4ACCHO + HO ₂	(k_adt+k_ads)*a_ch2oh*a_ch2oh+k_s*f_soh*f_allyl+k_rohro	Sander et al. (2018)
G45021	TrGCN	LISOPACNO3 + OH \rightarrow LISOPACNO3O2	(k_adt+k_ads)*a_ch2ono2*a_ch2oh	Sander et al. (2018)*
G45022	TrGC	ISOPBO2 \rightarrow .8 MVK + .8 HCHO + .8 HO ₂ + .2 ISOPBOH	k1_R02ISOPBO2	Rickard and Pascoe (2009)
G45023a	TrGC	ISOPBO2 + HO ₂ \rightarrow ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2018)
G45023b	TrGC	ISOPBO2 + HO ₂ \rightarrow MVK + HCHO + HO ₂ + OH + 0.024 BLOV + 0.119 BSOV	KR02H02(5)*rchohch2o2_oh	Sander et al. (2018)
G45024a	TrGCN	ISOPBO2 + NO \rightarrow MVK + HCHO + HO ₂ + NO ₂ + 0.003 BLOV + 0.101 BSOV	KR02N0*(1.-alpha_AN(6,3,0,0,0,temp,cair))	Lockwood et al. (2010), Sander et al. (2018)
G45024b	TrGCN	ISOPBO2 + NO \rightarrow ISOPBNO3	KR02N0*alpha_AN(6,3,0,0,0,temp,cair)	Lockwood et al. (2010), Sander et al. (2018)
G45025	TrGCN	ISOPBO2 + NO ₃ \rightarrow MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45026a	TrGC	ISOPBOOH + OH \rightarrow LIEPOX + OH	(k_ads+k_adp)*a_ch2ooh	Paulot et al. (2009b), Sander et al. (2018)
G45026b	TrGC	ISOPBOOH + OH \rightarrow ISOPBO2	k_roohro	Sander et al. (2018)
G45026c	TrGC	ISOPBOOH + OH \rightarrow MGLYOX + HOCH ₂ CHO	k_rohro+k_s*f_alk*f_soh	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45027	TrGC	ISOPBOOH + O ₃ → .1368 MACROOH + .1368 H ₂ O ₂ + .2280 HO ₂ + .4332 CH ₃ COCH ₂ OH + .2280 CO ₂ + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO ₂ + .06880 OH + .2709 CO + .1591 CH ₂ OO	1.E-17	Sander et al. (2018)
G45028	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃	k _s *f _{alk} *f _{soh} +(k _{adp} +k _{ads})*a _{ch2oh}	Sander et al. (2018)
G45029	TrGCN	ISOPBNO ₃ + OH → ISOPBDNO ₃ O ₂	(k _{adt} +k _{adp})*f _{ch2ono2}	Sander et al. (2018)
G45030	TrGC	ISOPDO ₂ → .8 MACR + .8 HCHO + .8 HO ₂ + .1 HCOC ₅ + .1 ISOPDOH	k1_R02ISOPD02	Rickard and Pascoe (2009)
G45031a	TrGC	ISOPDO ₂ + HO ₂ → ISOPDOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2018)
G45031b	TrGC	ISOPDO ₂ + HO ₂ → MACR + HCHO + HO ₂ + OH + 0.024 BLOV + 0.119 BLOV	KR02H02(5)*rchohch2o2_oh	Sander et al. (2018)
G45032a	TrGCN	ISOPDO ₂ + NO → MACR + HCHO + HO ₂ + NO ₂ + 0.003 BLOV + 0.101 BSOV	KR02N0*(1.-alpha_AN(6,2,0,0,0,temp,cair))	Lockwood et al. (2010), Sander et al. (2018)
G45032b	TrGCN	ISOPDO ₂ + NO → ISOPDNO ₃	KR02N0*alpha_AN(6,2,0,0,0,temp,cair)	Lockwood et al. (2010), Sander et al. (2018)
G45033	TrGCN	ISOPDO ₂ + NO ₃ → MACR + HCHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45034a	TrGC	ISOPDOOH + OH → LIEPOX + OH	(k _{adt} +k _{adp})*a _{ch2ooh}	Paulot et al. (2009b), Sander et al. (2018)
G45034b	TrGC	ISOPDOOH + OH → ISOPDO ₂	k _{roohro}	Sander et al. (2018)
G45034c	TrGC	ISOPDOOH + OH → HCOC ₅ + OH	k _t *f _{tooh} *f _{allyl} *f _{pch2oh}	Sander et al. (2018)
G45034d	TrGC	ISOPDOOH + OH → CH ₃ COCH ₂ OH + GLYOX + OH	k _s *f _{pch2oh} *f _{soh}	Sander et al. (2018)
G45035	TrGC	ISOPDOOH + O ₃ → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO ₂ + .2079 CO + .1221 CH ₂ OO	1.E-17	Sander et al. (2018)
G45036	TrGC	ISOPDOH + OH → HCOC ₅ + HO ₂	2.*k _{rohro} +(k _t *f _{toh} *f _{allyl} +k _s *f _{soh})*f _{pch2oh} +(k _{adt} +k _{adp})*a _{ch2oh}	Sander et al. (2018)
G45037	TrGCN	ISOPDNO ₃ + OH → ISOPBDNO ₃ O ₂	(k _{adp} +k _{ads})*a _{ch2ono2}	Sander et al. (2018)*
G45038	TrGCN	NISOP ₂ → .8 NC ₄ CHO + .6 HO ₂ + .2 LISOPACNO ₃	k1_R02LISOPAC02	Rickard and Pascoe (2009)
G45039	TrGCN	NISOP ₂ + HO ₂ → NISOP ₂ OOH	KR02H02(5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOP ₂ + NO → NC ₄ CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOP ₂ + NO ₃ → NC ₄ CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45042	TrGCN	NISOP ₂ OOH + OH → NC ₄ CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC ₄ CHO + OH → LNISO ₃	(k _{adt} +k _{ads})*a _{cho} *a _{ch2ono2}	Sander et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G45044	TrGCN	$\text{NC4CHO} + \text{O}_3 \rightarrow .27 \text{ NOA} + .027 \text{ HCOCO}_2\text{H} + .0162 \text{ GLYOX} + .0162 \text{ H}_2\text{O}_2 + .1458 \text{ HCOCO} + .0405 \text{ HCOOH} + .0405 \text{ CO} + .8758 \text{ OH} + .365 \text{ MGLYOX} + .73 \text{ NO}_2 + 0.7705 \text{ HCHO} + .4055 \text{ CO}_2 + .73 \text{ GLYOX}$	2.40E-17	Sander et al. (2018)
G45045	TrGCN	$\text{NC4CHO} + \text{NO}_3 \rightarrow \text{LNISO3} + \text{HNO}_3$	KN03AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	$\text{LNISO3} + \text{HO}_2 \rightarrow \text{LNISOOH}$	0.5*KR02H02(5)+0.5*KAPH02	Rickard and Pascoe (2009)
G45047	TrGCN	$\text{LNISO3} + \text{NO} \rightarrow \text{NOA} + .5 \text{ HOCHCHO} + .5 \text{ CO} + .5 \text{ HO}_2 + \text{NO}_2 + .5 \text{ CO}_2$	0.5*KAPN0+0.5*KR02N0	Rickard and Pascoe (2009)*
G45048	TrGCN	$\text{LNISO3} + \text{NO}_3 \rightarrow \text{NOA} + .5 \text{ HOCHCHO} + .5 \text{ CO} + .5 \text{ HO}_2 + \text{NO}_2 + .5 \text{ CO}_2$	KR02N03*1.37	Rickard and Pascoe (2009)
G45049	TrGCN	$\text{LNISOOH} + \text{OH} \rightarrow \text{LNISO3}$	2.65E-11	Rickard and Pascoe (2009)
G45050a	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LC578O2}$	(k_adtertprim+k_ads)*a_cho*a_ch2oh	Sander et al. (2018)
G45050b	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LHC4ACCO3}$	k_t*f_o	Sander et al. (2018)
G45050c	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{C4MDIAL} + \text{HO}_2$	k_s*f_soh*f_allyl	Sander et al. (2018)
G45051	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow .2225 \text{ CH}_3\text{C(O)} + .89 \text{ CO} + .0171875 \text{ HOCH}_2\text{CO}_2\text{H} + .075625 \text{ H}_2\text{O}_2 + .0171875 \text{ HCOCO}_2\text{H} + .2775 \text{ CH}_3\text{COCH}_2\text{OH} + .6675 \text{ HO}_2 + .2603125 \text{ GLYOX} + .2225 \text{ HCHO} + .89 \text{ OH} + .2603125 \text{ HOCH}_2\text{CHO} + .5 \text{ MGLYOX}$	2.40E-17	Rickard and Pascoe (2009)
G45052	TrGCN	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO3} + \text{HNO}_3$	KN03AL*4.25	Rickard and Pascoe (2009)
G45053	TrGC	$\text{LC578O2} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2$	k1_R02t0R02	Rickard and Pascoe (2009)
G45054a	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO} + \text{OH}$	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45054b	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{LC578OOH}$	KR02H02(5)*rcoch2o2_ooh	Rickard and Pascoe (2009)
G45055	TrGCN	$\text{LC578O2} + \text{NO} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45056	TrGCN	$\text{LC578O2} + \text{NO}_3 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45057	TrGC	$\text{LC578O2} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCH}_2\text{CHO} + .75 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	KHSB	Sander et al. (2018)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	k_roohro	Sander et al. (2018)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C1ODC2OOHC4OD} + \text{HO}_2$	k_t*f_o*f_tch2oh*f_alk+k_t*f_toh*f_pch2oh*f_pch2oh+k_s*f_soh*f_pch2oh	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45059a	TrGC	$\text{LHC4ACCO3} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	$k1_R02RC03*0.9$	Sander et al. (2018)
G45059b	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LHC4ACCO2H}$	$k1_R02RC03*0.1$	Sander et al. (2018)
G45060a	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 2 \text{ OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	KAPH02*rc03_oh	Sander et al. (2018)
G45060b	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO3H}$	KAPH02*rc03_ooh	Sander et al. (2018)
G45060c	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$	KAPH02*rc03_o3	Sander et al. (2018)
G45061	TrGCN	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KAPN0	Sander et al. (2018)
G45062	TrGCN	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45063	TrGCN	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KR02N03*1.74	Sander et al. (2018)
G45064a	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	$2.52\text{E-}11$	Sander et al. (2018)
G45064b	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$2.88\text{E-}11$	Rickard and Pascoe (2009)
G45065	TrGCN	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45066	TrGCN	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)
G45067	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	$3.81\text{E-}11$	Rickard and Pascoe (2009)
G45068	TrGC	$\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{ H}_2\text{O}_2 + .67 \text{ HCHO} + .2079 \text{ CO} + .1221 \text{ CH}_2\text{OO} + .05280 \text{ OH}$	$7.51\text{E-}16*\text{EXP}(-1521./\text{temp})$	Sander et al. (2018)
G45069	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$k1_R02t0R02$	Sander et al. (2018)
G45070a	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$\text{KR02H02(5)*rcoch2o2_oh}$	Sander et al. (2018)
G45070b	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	$\text{KR02H02(5)*rcoch2o2_ooh}$	Sander et al. (2018)
G45071	TrGCN	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G45072	TrGCN	$\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N03	Sander et al. (2018)
G45073	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	$9.7\text{E-}12$	Rickard and Pascoe (2009)
G45074	TrGC	$\text{LIEPOX} + \text{OH} \rightarrow \text{DB1O2} + \text{H}_2\text{O}$	$5.78\text{E-}11*\text{EXP}(-400./\text{temp}) * (1.52/3.+0.98*2./3.)/1.51$	Paulot et al. (2009b), Bates et al. (2014), Sander et al. (2018)*
G45075	TrGC	$\text{ISOPBO2} \rightarrow \text{MVK} + \text{HCHO} + \text{OH}$	KH5B	Sander et al. (2018)
G45076	TrGC	$\text{ISOPDO2} \rightarrow \text{MACR} + \text{HCHO} + \text{OH}$	KH5D	Sander et al. (2018)
G45077a	TrGC	$\text{LZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC2O2C4OOH} + .4 \text{ C1OOHC2O2C4OD}$	$k_adt*a_cho*a_ch2ooh$	Sander et al. (2018)
G45077b	TrGC	$\text{LZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC3O2C4OOH} + .4 \text{ C1OOHC3O2C4OD}$	$k_ads*a_cho*a_ch2ooh$	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45077c	TrGC	LZCODC23DBCOOH + OH → LZCO3HC23DBCOD	k_t*f_o*f_alk+k_roohro	Sander et al. (2018)
G45077d	TrGC	LZCODC23DBCOOH + OH → C4MDIAL + OH	k_s*f_sooh*f_allyl	Sander et al. (2018)
G45078	TrGC	LZCODC23DBCOOH + O ₃ → .4672 OH + .2336 HCOCOCH ₂ O ₂ + .2336 CO + .2336 CH ₃ C(O) + .4672 HOOCH ₂ CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH ₂ CHO + .02765 H ₂ O ₂ + .02592 CH ₃ OOH + .02592 CO ₂ + .01037 HCOCO + .01555 CH ₂ OO + .01555 CO + .006908 HOOCH ₂ CO ₃ + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH ₂ OOH + .2628 GLYOX + .0972 CH ₃ COCH ₂ O ₂ H + .00972 HCOCO ₂ H + .005832 GLYOX + .005832 H ₂ O ₂ + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO ₂ + .01458 HCOOH + .01458 CO	2.4E-17	Sander et al. (2018)
G45079	TrGC	C1OOHC2O2C4OD → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH	k1_R02t0R02	Sander et al. (2018)
G45080	TrGCN	C1OOHC2O2C4OD + NO → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH + NO ₂	KR02N0	Sander et al. (2018)*
G45081a	TrGC	C1OOHC2O2C4OD + HO ₂ → C1OOHC2OOHC4OD	KR02H02(5)*rcoch2o2_ooh	Sander et al. (2018)
G45081b	TrGC	C1OOHC2O2C4OD + HO ₂ → .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + 1.22 OH	KR02H02(5)*rcoch2o2_oh	Sander et al. (2018)
G45082	TrGC	C1OOHC2O2C4OD → CH ₃ COCH ₂ O ₂ H + GLYOX + OH	KHSB	Sander et al. (2018)
G45083	TrGC	C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD	K15HSDHB	Sander et al. (2018)
G45084a	TrGC	C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH	2.*k_s*f_sooh*f_tch2oh	Sander et al. (2018)
G45084b	TrGC	C1OOHC2OOHC4OD + OH → CH ₃ COCH ₂ O ₂ H + 2 CO + 2 HO ₂ + OH	k_t*f_toh*f_pch2oh*f_pch2oh	Sander et al. (2018)
G45084c	TrGC	C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD	k_roohro	Sander et al. (2018)
G45085	TrGC	C1ODC2OOHC4OD + OH → CO ₂ H ₃ CHO + CO + H ₂ O + OH	k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho	Sander et al. (2018)
G45086	TrGC	C1ODC3O2C4OOH → MGLYOX + HOOCH ₂ CHO + HO ₂	k1_R02s0R02	Sander et al. (2018)
G45087	TrGCN	C1ODC3O2C4OOH + NO → MGLYOX + HOOCH ₂ CHO + HO ₂ + NO ₂	KR02N0	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45088	TrGC	$\text{C1ODC3O2C4OOH} + \text{HO}_2 \rightarrow .5 \text{ CH}_3\text{C(O)} + .5 \text{ CO} + .5 \text{ MGLYOX} + .5 \text{ HO}_2 + \text{HOOCH}_2\text{CO}_3$	KR02H02(5)	Sander et al. (2018)
G45089	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{OH} + \text{HOOCH}_2\text{CHO}$	KHSD	Sander et al. (2018)
G45090	TrGC	$\text{C1OOHC3O2C4OD} \rightarrow .625 \text{ MGLYOX} + 2 \text{ CO} + 1.625 \text{ HO}_2 + .375 \text{ CH}_3\text{C(O)} + .375 \text{ CO}_2 + \text{OH}$	K15HSDHB	Sander et al. (2018)
G45091	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LZCO3HC23DBCOD} + \text{HO}_2$	K16HS	Sander et al. (2018)
G45092a	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{C1ODC2O2C4OD}$	$(k_{\text{adt}}+k_{\text{ads}})*a_{\text{cho}}*a_{\text{cho}}$	Sander et al. (2018)*
G45092b	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{LZCO3C23DBCOD}$	$2*k_{\text{t}}*f_{\text{o}}*f_{\text{alk}}$	Sander et al. (2018)*
G45093	TrGCN	$\text{C4MDIAL} + \text{NO}_3 \rightarrow \text{LZCO3C23DBCOD} + \text{HNO}_3$	$\text{KN03AL}*4.25*2.$	Sander et al. (2018)*
G45094a	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$	$\text{KR02H02(5)}*r_{\text{coch2o2_oh}}$	Sander et al. (2018)
G45094b	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1ODC2OOHC4OD}$	$\text{KR02H02(5)}*r_{\text{coch2o2_ooh}}$	Sander et al. (2018)
G45095	TrGCN	$\text{C1ODC2O2C4OD} + \text{NO} \rightarrow \text{NO}_2 + \text{MGLYOX} + \text{HOCHCHO}$	KR02N0	Sander et al. (2018)*
G45096	TrGC	$\text{C1ODC2O2C4OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$	$k1_R02t0R02$	Sander et al. (2018)
G45097a	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO}$	$(2*k_{\text{t}}*f_{\text{o}}*f_{\text{tch2oh}}*f_{\text{alk}}+k_{\text{t}}*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$	Sander et al. (2018)
G45097b	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + \text{OH}$	$(2*k_{\text{t}}*f_{\text{o}}*f_{\text{tch2oh}}*f_{\text{alk}}+k_{\text{t}}*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$	Sander et al. (2018)
G45098	TrGCN	$\text{LISOPACNO3O2} + \text{NO} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2 + \text{NO}_2$	KR02N0	Sander et al. (2018)*
G45099	TrGCN	$\text{LISOPACNO3O2} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2$	$k1_R02t0R02+\text{KR02H02(5)}*c(\text{ind_H02})$	Sander et al. (2018)
G45100	TrGCN	$\text{ISOPBDNO3O2} + \text{NO} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRNO3} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + 1.6 \text{ NO}_2$	KR02N0	Sander et al. (2018)*
G45101	TrGCN	$\text{ISOPBDNO3O2} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRNO3} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + .6 \text{ NO}_2$	$k1_R02s0R02+\text{KR02H02(5)}*c(\text{ind_H02})$	Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45102	TrGCN	LISOPACNO3 + O ₃ → .8704 OH + .365 HO ₂ + .73 MGLYOX + .4325 NO ₃ CH ₂ CHO + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .4325 NO ₂ + .0891 H ₂ O ₂ + .135 NOA + .0675 HOCHCHO + .3866 HOCH ₂ CHO + .0405 CH ₃ OH + .0405 CO + .0054 HOCH ₂ CO	2.8E-17	Feierabend et al. (2008), Sander et al. (2018)
G45103	TrGC	DB1O2 → DB1O2	k1_R02s0R02	Sander et al. (2018)
G45104a	TrGC	DB1O2 + HO ₂ → DB1OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2018)*
G45104b	TrGC	DB1O2 + HO ₂ → DB1O2 + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2018)
G45105a	TrGCN	DB1O2 + NO → DB1O2 + NO ₂	KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair))	Sander et al. (2018)
G45105b	TrGCN	DB1O2 + NO → DB1NO3	KR02N0*alpha_AN(7,2,0,0,0,temp, cair)	Sander et al. (2018)
G45106	TrGCN	DB1O2 + NO ₃ → DB1O2 + NO ₂	KR02N03	Sander et al. (2018)
G45107	TrGC	DB1O2 → DB1O2 + OH	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 → DB1O2	KDEC*0.72	see note*
G45108b	TrGC	DB1O2 → .5 HVMK + .5 HMAc + HCHO + HO ₂	KDEC*0.28	see note*
G45109	TrGC	DB1O2 → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂	k1_R02s0R02	Sander et al. (2018)
G45110a	TrGC	DB1O2 + HO ₂ → DB2OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2018)
G45110b	TrGC	DB1O2 + HO ₂ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2018)
G45111	TrGCN	DB1O2 + NO → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02N0	see note*
G45112	TrGCN	DB1O2 + NO ₃ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02N03	Sander et al. (2018)
G45113	TrGC	DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH	K14HSAL	Sander et al. (2018)
G45114a	TrGC	DB1OOH + OH → DB1O2	k_roohro	Sander et al. (2018)
G45114b	TrGC	DB1OOH + OH → HCOOH + HO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2018)*
G45115	TrGC	DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH	4.67E-26*temp**3.286*EXP(4509./(1.987*temp))	Sander et al. (2018), da Silva (2010)*
G45116	TrGCN	DB1NO3 + OH → HCOOH + NO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2018)*
G45117	TrGC	DB2OOH + OH → DB1O2	k_roohro	Sander et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G45118	TrGC	LISOPACOOH + O ₃ → 1.3272 OH + .36986 HO ₂ + .0432 H ₂ O ₂ + .08422 CO + .2025 CH ₃ OOH + .01215 CH ₂ OO + .3704 HCHO + .00405 CH ₃ OH + .0405 CO ₂ + .1825 HOCH ₂ COCH ₂ O ₂ + .365 MGLYOX + .3866 HOOCH ₂ CHO + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .00324 HCOCO + .3866 HOCH ₂ CHO + .135 CH ₃ COCH ₂ O ₂ H + .0675 HOCHCHO + .0054 HOCH ₂ CO	4.829E-16	Sander et al. (2018)
G45119a	TrGC	LZCO3HC23DBCOD + OH → .62 CO ₂ H ₃ CHO + .62 OH + .62 CO ₂ + .38 MGLYOX + .38 HCOCO ₃ H + .38 HO ₂	k _{adt} *a _{cho} *a _{co2h}	Sander et al. (2018)
G45119b	TrGC	LZCO3HC23DBCOD + OH → .62 CH ₃ COCO ₃ H + 1.24 CO + 1.24 HO ₂ + .38 MGLYOX + .38 HO ₂ + .38 CO + .38 HO ₂ + .38 OH + .38 CO ₂	k _{ads} *a _{cho} *a _{co2h}	Sander et al. (2018)
G45120	TrGC	LISOPEFO ₂ → LISOPEFO	k1_R02p0R02	Sander et al. (2018)
G45121a	TrGCN	LISOPEFO ₂ + NO → LISOPEFO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0,temp,cair))	Sander et al. (2018)
G45121b	TrGCN	LISOPEFO ₂ + NO → ISOPDNO ₃	KR02N0*alpha_AN(6,1,0,0,0,temp,cair)	Sander et al. (2018)*
G45122a	TrGC	LISOPEFO ₂ + HO ₂ → .7143 ISOPDOOH + .2857 ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Sander et al. (2018)
G45122b	TrGC	LISOPEFO ₂ + HO ₂ → LISOPEFO + OH	KR02H02(5)*rchohch2o2_oh	Sander et al. (2018)
G45123	TrGCN	LISOPEFO ₂ + NO ₃ → LISOPEFO + NO ₂	KR02N03	Sander et al. (2018)
G45124	TrGC	LISOPEFO ₂ → .7143 MACR + .2857 MVK + HCHO + OH	0.7143*KHSD+.2857*KHSB	Sander et al. (2018)
G45125	TrGC	LISOPEFO → .7143 MACR + .2857 MVK + HCHO + HO ₂	KDEC	Sander et al. (2018)
G45126a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2018), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2018), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2018), Paulot et al. (2009a), Francisco-Marquez et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G45127b	TrGC	LISOPACO \rightarrow .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2018), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	3METHYLFURAN + OH \rightarrow L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Sander et al. (2018)*
G45129	TrGCN	3METHYLFURAN + NO ₃ \rightarrow L3METHYLFURANO2 + NO ₂	1.9E-11	Sander et al. (2018), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 \rightarrow C4MDIAL + HO ₂	k1_R02s0R02	Sander et al. (2018)
G45131	TrGCN	L3METHYLFURANO2 + NO \rightarrow C4MDIAL + HO ₂ + NO ₂	KR02N0	Sander et al. (2018)*
G45132	TrGC	L3METHYLFURANO2 + HO ₂ \rightarrow C4MDIAL + HO ₂	KR02H02(5)	Sander et al. (2018)*
G45133	TrGC	LZCO3C23DBCOD \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂	k1_R02RC03	Sander et al. (2018)
G45134a	TrGC	LZCO3C23DBCOD + HO ₂ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH	KAPH02*rco3_oh	Sander et al. (2018)
G45134b	TrGC	LZCO3C23DBCOD + HO ₂ \rightarrow LZCO3HC23DBCOD	KAPH02*(rco3_ooh+rco3_o3)	Sander et al. (2018)*
G45135	TrGCN	LZCO3C23DBCOD + NO \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KAPN0	Sander et al. (2018)
G45136	TrGCN	LZCO3C23DBCOD + NO ₂ \rightarrow LZCPANC23DBCOD	k_CH3C03_N02	Rickard and Pascoe (2009)
G45137	TrGCN	LZCO3C23DBCOD + NO ₃ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KR02N03*1.74	Sander et al. (2018)
G45138	TrGCN	LZCPANC23DBCOD \rightarrow LZCO3C23DBCOD + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	LZCPANC23DBCOD + OH \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	2.52E-11	Sander et al. (2018)*
G45200	TrGTerC	C511O2 \rightarrow CH ₃ C(O) + HCOCH2CHO	k1_R02s0R02	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO \rightarrow CH ₃ C(O) + HCOCH2CHO + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45202a	TrGTerC	C511O2 + HO ₂ \rightarrow C511OOH	KR02H02(5)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G45202b	TrGTerC	C511O2 + HO ₂ \rightarrow CH ₃ C(O) + HCOCH2CHO + OH	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G45203	TrGTerC	C511OOH + OH \rightarrow C511O2	7.49E-11	Rickard and Pascoe (2009)
G45204	TrGTerC	CO23C4CHO + OH \rightarrow CO23C4CO3	6.65E-11	Rickard and Pascoe (2009)
G45205	TrGTerCN	CO23C4CHO + NO ₃ \rightarrow CO23C4CO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G45206	TrGTerC	CO23C4CO3 \rightarrow CH ₃ COCOCH ₂ O ₂ + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G45207	TrGTerCN	CO23C4CO3 + NO \rightarrow CH ₃ COCOCH ₂ O ₂ + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)*
G45208	TrGTerCN	CO23C4CO3 + NO ₂ \rightarrow C5PAN9	k_CH3C03_N02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45209a	TrGTerC	$\text{CO}_2\text{C}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{C}_4\text{CO}_3\text{H}$	$\text{KAPH02}*(\text{rco3_ooh}+\text{rco3_o3})$	Rickard and Pascoe (2009)
G45209b	TrGTerC	$\text{CO}_2\text{C}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*\text{rco3_oh}$	Rickard and Pascoe (2009)
G45210	TrGTerCN	$\text{C}_5\text{PAN}_9 \rightarrow \text{CO}_2\text{C}_4\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45211	TrGTerCN	$\text{C}_5\text{PAN}_9 + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{CO} + \text{NO}_2$	$3.12\text{E}-13$	Rickard and Pascoe (2009)
G45212	TrGTerC	$\text{C}_5\text{I}_2\text{O}_2 \rightarrow \text{C}_5\text{I}_3\text{O}_2$	k1_R02pR02	Rickard and Pascoe (2009)
G45213	TrGTerC	$\text{C}_5\text{I}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_5\text{I}_2\text{OOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009)
G45214	TrGTerCN	$\text{C}_5\text{I}_2\text{O}_2 + \text{NO} \rightarrow \text{C}_5\text{I}_3\text{O}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45215	TrGTerC	$\text{C}_5\text{I}_2\text{OOH} + \text{OH} \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{OH}$	$1.01\text{E}-10$	Rickard and Pascoe (2009)
G45216	TrGTerC	$\text{C}_5\text{I}_3\text{O}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3$	k1_R02s0R02	Rickard and Pascoe (2009)
G45217	TrGTerCN	$\text{C}_5\text{I}_3\text{O}_2 + \text{NO} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45218a	TrGTerC	$\text{C}_5\text{I}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_5\text{I}_3\text{OOH}$	$\text{KR02H02}(5)*\text{rcoch2o2_ooh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G45218b	TrGTerC	$\text{C}_5\text{I}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$\text{KR02H02}(5)*\text{rcoch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G45219	TrGTerC	$\text{CO}_2\text{C}_4\text{CHO} + \text{OH} \rightarrow \text{CHOC}_3\text{COCO}_3$	$1.33\text{E}-10$	Rickard and Pascoe (2009)
G45220	TrGTerCN	$\text{CO}_2\text{C}_4\text{CHO} + \text{NO}_3 \rightarrow \text{CHOC}_3\text{COCO}_3 + \text{HNO}_3$	$2.*\text{KN03AL}*5.5$	Rickard and Pascoe (2009)
G45221	TrGTerC	$\text{C}_5\text{I}_3\text{OOH} + \text{OH} \rightarrow \text{C}_5\text{I}_3\text{CO} + \text{OH}$	$9.23\text{E}-11$	Rickard and Pascoe (2009)
G45222	TrGTerC	$\text{CHOC}_3\text{COCO}_3 \rightarrow \text{CHOC}_3\text{COO}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45223	TrGTerC	$\text{CHOC}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CHOC}_3\text{COOOH}$	KAPH02	Rickard and Pascoe (2009)
G45224	TrGTerCN	$\text{CHOC}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CHOC}_3\text{COPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45225	TrGTerCN	$\text{CHOC}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CHOC}_3\text{COO}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)*
G45226	TrGTerC	$\text{C}_5\text{I}_3\text{CO} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{CO} + \text{CO}$	$2.64\text{E}-11$	Rickard and Pascoe (2009)
G45227	TrGTerC	$\text{C}_5\text{I}_4\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_5\text{I}_4\text{OOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009)
G45228a	TrGTerCN	$\text{C}_5\text{I}_4\text{O}_2 + \text{NO} \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\text{alpha_AN}(7,2,0,1,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2018)
G45228b	TrGTerCN	$\text{C}_5\text{I}_4\text{O}_2 + \text{NO} \rightarrow \text{C}_5\text{I}_4\text{NO}_3$	$\text{KR02N0}*\text{alpha_AN}(7,2,0,1,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009), Sander et al. (2018)
G45229	TrGTerCN	$\text{C}_5\text{I}_4\text{O}_2 + \text{NO}_3 \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45230	TrGTerC	$\text{C}_5\text{I}_4\text{O}_2 \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{HO}_2$	k1_R02sR02	Rickard and Pascoe (2009)
G45231	TrGTerC	$\text{C}_5\text{I}_4\text{OOH} + \text{OH} \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{OH}$	$1.10\text{E}-10$	Rickard and Pascoe (2009)
G45232	TrGTerCN	$\text{C}_5\text{I}_4\text{NO}_3 + \text{OH} \rightarrow \text{CO}_2\text{C}_4\text{CHO} + \text{NO}_2$	$4.33\text{E}-11$	Rickard and Pascoe (2009)
G45233	TrGTerC	$\text{CHOC}_3\text{COOOH} + \text{OH} \rightarrow \text{CHOC}_3\text{COCO}_3$	$7.55\text{E}-11$	Rickard and Pascoe (2009)
G45234	TrGTerCN	$\text{CHOC}_3\text{COPAN} \rightarrow \text{CHOC}_3\text{COCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45235	TrGTerCN	$\text{CHOC}_3\text{COPAN} + \text{OH} \rightarrow \text{C}_4\text{CODIAL} + \text{CO} + \text{NO}_2$	$7.19\text{E}-11$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45236	TrGTerC	$\text{MBO} + \text{OH} \rightarrow \text{LMBOABO2}$	$8.1\text{E-}12 * \text{EXP}(610./\text{TEMP})$	Rickard and Pascoe (2009), Sander et al. (2018)*
G45237a	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{COCH}_3 + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH} + .84 \text{MBOOO}$	$1.0\text{E-}17 * 0.57$	Rickard and Pascoe (2009), Sander et al. (2018)
G45237b	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{IBUTALOH} + .63 \text{CO} + .37 \text{HOCH}_2\text{OOH} + .16 \text{OH} + .16 \text{HO}_2$	$1.0\text{E-}17 * 0.43$	Rickard and Pascoe (2009), Sander et al. (2018)
G45238	TrGTerCN	$\text{MBO} + \text{NO}_3 \rightarrow \text{LNMBOABO2}$	$4.6\text{E-}14 * \text{EXP}(-400./\text{TEMP})$	Rickard and Pascoe (2009), Sander et al. (2018)
G45239	TrGTerC	$\text{LMBOABO2} + \text{HO}_2 \rightarrow \text{LMBOABOOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009), Sander et al. (2018)
G45240a	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{LMBOABNO3}$	$\text{KR02N0} * (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2018)
G45240b	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .67$	Rickard and Pascoe (2009), Sander et al. (2018)
G45240c	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .33$	Rickard and Pascoe (2009), Sander et al. (2018)
G45241a	TrGTerC	$\text{LMBOABO2} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2$	$k1_R02s0R02 * .67$	Rickard and Pascoe (2009), Sander et al. (2018)
G45241b	TrGTerC	$\text{LMBOABO2} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2$	$k1_R02p0R02 * .33$	Rickard and Pascoe (2009), Sander et al. (2018)
G45242a	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{MBOACO}$	$0.67 * 2.93\text{E-}11 + .33 * 2.05\text{E-}12$	Rickard and Pascoe (2009), Sander et al. (2018)
G45242b	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{LMBOABO2}$	k_roohro	Rickard and Pascoe (2009), Sander et al. (2018)
G45243	TrGTerCN	$\text{LMBOABNO3} + \text{OH} \rightarrow \text{MBOACO} + \text{NO}_2$	$0.67 * 1.75\text{E-}12 + .33 * 2.69\text{E-}12$	Rickard and Pascoe (2009), Sander et al. (2018)
G45244	TrGTerC	$\text{MBOACO} + \text{OH} \rightarrow \text{MBOCOCO} + \text{HO}_2$	$3.79\text{E-}12$	Rickard and Pascoe (2009)
G45245	TrGTerC	$\text{MBOCOCO} + \text{OH} \rightarrow \text{CO} + \text{IPRHOCO3}$	$1.38\text{E-}11$	Rickard and Pascoe (2009)
G45246	TrGTerCN	$\text{LNMBOABO2} + \text{HO}_2 \rightarrow \text{LNMBOABOOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G45247	TrGTerCN	$\text{LNMBOABO2} + \text{NO} \rightarrow .65 \text{ NO}_3\text{CH2CHO} + .65 \text{ CH}_3\text{COCH}_3 + .65 \text{ HO}_2 + .35 \text{ IBUTALOH} + .35 \text{ HCHO} + .35 \text{ NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009), Sander et al. (2018)*
G45248	TrGTerCN	$\text{LNMBOABO2} + \text{NO}_3 \rightarrow .65 \text{ NO}_3\text{CH2CHO} + .65 \text{ CH}_3\text{COCH}_3 + .65 \text{ HO}_2 + .35 \text{ IBUTALOH} + .35 \text{ HCHO} + .35 \text{ NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009), Sander et al. (2018)
G45249	TrGTerCN	$\text{LNMBOABO2} \rightarrow .65 \text{ NO}_3\text{CH2CHO} + .65 \text{ CH}_3\text{COCH}_3 + .65 \text{ HO}_2 + .35 \text{ IBUTALOH} + .35 \text{ HCHO} + .35 \text{ NO}_2$	k1_R02s0R02	Rickard and Pascoe (2009), Sander et al. (2018)
G45250a	TrGTerCN	$\text{LNMBOABOOH} + \text{OH} \rightarrow .65 \text{ C4MCONO3OH} + .35 \text{ NMBOBCO}$	$0.65*4.89\text{E-}12 + .35*2.52\text{E-}12$	Rickard and Pascoe (2009), Sander et al. (2018)
G45250b	TrGTerCN	$\text{LNMBOABOOH} + \text{OH} \rightarrow \text{LNMBOABO2}$	k_roohro	Rickard and Pascoe (2009), Sander et al. (2018)
G45251	TrGTerCN	$\text{NMBOBCO} + \text{OH} \rightarrow \text{NC4OHCO3}$	$4.26\text{E-}12$	Rickard and Pascoe (2009)
G45252a	TrGTerCN	$\text{NC4OHCO3} + \text{HO}_2 \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G45252b	TrGTerCN	$\text{NC4OHCO3} + \text{HO}_2 \rightarrow \text{NC4OHCO3H}$	KAPH02*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Sander et al. (2018)
G45253	TrGTerCN	$\text{NC4OHCO3} + \text{NO} \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G45254	TrGTerCN	$\text{NC4OHCO3} + \text{NO}_2 \rightarrow \text{NC4OHCPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45255	TrGTerCN	$\text{NC4OHCO3} + \text{NO}_3 \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45256	TrGTerCN	$\text{NC4OHCO3} \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45257	TrGTerCN	$\text{NC4OHCO3H} + \text{OH} \rightarrow \text{NC4OHCO3}$	$4.50\text{E-}12$	Rickard and Pascoe (2009)
G45258	TrGTerCN	$\text{NC4OHCPAN} + \text{OH} \rightarrow \text{IBUTALOH} + \text{CO} + \text{NO}_2 + \text{NO}_2$	$1.27\text{E-}12$	Rickard and Pascoe (2009)
G45259	TrGTerCN	$\text{NC4OHCPAN} \rightarrow \text{NC4OHCO3} + \text{NO}_2$	K_PAN_M	Rickard and Pascoe (2009)
G45260	TrGTerCN	$\text{C4MCONO3OH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	$1.23\text{E-}12$	Rickard and Pascoe (2009), Sander et al. (2018)
G45400	TrGAroCN	$\text{NC4MDCO2HN} + \text{OH} \rightarrow \text{MMALANHY} + \text{NO}_2$	k_roohro	Rickard and Pascoe (2009)*
G45401	TrGAroCN	$\text{C54CO} + \text{NO}_3 \rightarrow 3 \text{ CO} + \text{CH}_3\text{C(O)OO} + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	$\text{C54CO} + \text{OH} \rightarrow 3 \text{ CO} + \text{CH}_3\text{C(O)OO}$	$1.72\text{E-}11$	Rickard and Pascoe (2009)
G45403a	TrGAroCN	$\text{NTLFUO2} + \text{HO}_2 \rightarrow \text{NTLFUOOH}$	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	$\text{NTLFUO2} + \text{HO}_2 \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{OH}$	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45404	TrGAroCN	$\text{NTLFUO2} + \text{NO} \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45405	TrGAroCN	$\text{NTLFUO2} + \text{NO}_3 \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45406	TrGAroCN	$\text{NTLFUO2} \rightarrow \text{ACCOMMECHO} + \text{NO}_2$	k1_R02t0R02	Rickard and Pascoe (2009)*
G45407	TrGAroC	$\text{C5134CO2OH} + \text{OH} \rightarrow \text{C54CO} + \text{HO}_2$	$7.48\text{E-}11$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45408	TrGAroCN	$C5COO2NO2 + OH \rightarrow MGLYOX + CO + CO + NO_2$	5.43E-11	Rickard and Pascoe (2009)
G45409	TrGAroCN	$C5COO2NO2 \rightarrow C5CO14O2 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45410	TrGAroC	$C5DIALOOH + OH \rightarrow C5DIALCO + OH$	7.52E-11	Rickard and Pascoe (2009)
G45411a	TrGAroC	$C4CO2DBC03 + HO_2 \rightarrow C4CO2DCO3H$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45411b	TrGAroC	$C4CO2DBC03 + HO_2 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G45412	TrGAroCN	$C4CO2DBC03 + NO \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G45413	TrGAroCN	$C4CO2DBC03 + NO_2 \rightarrow C4CO2DBPAN$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$C4CO2DBC03 + NO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45415	TrGAroC	$C4CO2DBC03 \rightarrow HO_2 + CO + HCOCOCHO + CO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45416	TrGAroC	$MMALANHY + OH \rightarrow MMALANHYO2$	1.50E-12	Rickard and Pascoe (2009)
G45421a	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow MMALNHYOOH$	KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G45421b	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow CO2H3CO3 + CO_2 + OH$	KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G45422	TrGAroCN	$MMALANHYO2 + NO \rightarrow CO2H3CO3 + CO_2 + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$MMALANHYO2 + NO_3 \rightarrow CO2H3CO3 + CO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)*
G45424	TrGAroC	$MMALANHYO2 \rightarrow CO2H3CO3 + CO_2$	k1_R02t0R02	Rickard and Pascoe (2009)*
G45428	TrGAroCN	$C4CO2DBPAN + OH \rightarrow HCOCOCHO + CO_2 + CO + NO_2$	2.74E-11	Rickard and Pascoe (2009)
G45429	TrGAroCN	$C4CO2DBPAN \rightarrow C4CO2DBC03 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	$C5CO14O2 + HO_2 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)*
G45430b	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OH + O_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G45430c	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OOH$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G45431	TrGAroCN	$C5CO14O2 + NO \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)*
G45432	TrGAroCN	$C5CO14O2 + NO_2 \rightarrow C5COO2NO2$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45433	TrGAroCN	$C5CO14O2 + NO_3 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	$C5CO14O2 \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2$	k1_R02RC03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45436	TrGAroC	C5CO14OH + OH \rightarrow .83 MALANHY + .83 CH ₃ + .17 MGLYOX + .17 HO ₂ + .17 CO + .17 CO ₂	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	C5DICARB + NO ₃ \rightarrow C5CO14O2 + HNO ₃	KN03AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	C5DICARB + O ₃ \rightarrow .5338 GLYOX + .063 CH ₃ CHO + .348 CH ₃ C(O)OO + .918 CO + .57 OH + .473 HO ₂ + .0563 CH ₃ COCO ₂ H + .5338 MGLYOX + .676 H ₂ O ₂ + .063 HCHO + .0563 HCOCO ₂ H + .2465 CO ₂	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	C5DICARB + OH \rightarrow .48 C5CO14O2 + .52 C5DICARBO2	6.2E-11	Rickard and Pascoe (2009)
G45444	TrGAroC	MC3ODBCO2H + OH \rightarrow .35 GLYOX + .35 CH ₃ + .35 CO + .35 CO ₂ + .65 MMALANHY + .65 HO ₂	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	TLFUONE + NO ₃ \rightarrow NTLFUO2	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	TLFUONE + O ₃ \rightarrow .5 CO + .5 OH + .5 MECOACETO2 + .3125 C24O3CCO2H + .1875 ACCOMECHO + .1875 H ₂ O ₂	8.00E-19	see note*
G45453	TrGAroC	TLFUONE + OH \rightarrow TLFUO2	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	ACCOMECO3 + HO ₂ \rightarrow ACCOMECHO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	ACCOMECO3 + HO ₂ \rightarrow MECOACETO2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45455	TrGAroCN	ACCOMECO3 + NO \rightarrow MECOACETO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	ACCOMECO3 + NO ₂ \rightarrow ACCOMECHAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45457	TrGAroCN	ACCOMECO3 + NO ₃ \rightarrow MECOACETO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	ACCOMECO3 \rightarrow MECOACETO2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G45459	TrGAroC	C4CO2DCO3H + OH \rightarrow C4CO2DBCO3	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	ACCOMETCHO + NO ₃ \rightarrow ACCOMECHO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	ACCOMETCHO + OH \rightarrow ACCOMECHO3	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	MMALNHYOOH + OH \rightarrow MMALANHYO2	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	C5DICAROOH + OH \rightarrow C5134CO2OH + OH	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	C5DICAROOH + OH \rightarrow C5DICARBO2	k_roohro	Rickard and Pascoe (2009)
G45468	TrGAroC	C24O3CCO2H + OH \rightarrow MECOACETO2 + CO ₂	8.76E-13	Rickard and Pascoe (2009)
G45469	TrGAroCN	NTLFUOOH + OH \rightarrow NTLFUO2	4.44E-12	Rickard and Pascoe (2009)
G45470	TrGAroCN	ACCOMEPAN + OH \rightarrow METACETHO + CO + CO + NO ₂	1.00E-14	Rickard and Pascoe (2009)
G45471	TrGAroCN	ACCOMEPAN \rightarrow ACCOMECHO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G45476a	TrGAroC	TLFUO2 + HO ₂ \rightarrow TLFUOOH	KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45476b	TrGAroC	$\text{TLFUO2} + \text{HO}_2 \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(5)} * (\text{rcoch2o2_oh} + \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)*
G45477	TrGAroCN	$\text{TLFUO2} + \text{NO} \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45478	TrGAroCN	$\text{TLFUO2} + \text{NO}_3 \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45479	TrGAroC	$\text{TLFUO2} \rightarrow \text{ACCOMMECHO} + \text{HO}_2$	k1_R02t0R02	Rickard and Pascoe (2009)*
G45480	TrGAroC	$\text{C5CO14OOH} + \text{OH} \rightarrow \text{C5CO14O2}$	3.59E-12	Rickard and Pascoe (2009)
G45483	TrGAroC	$\text{TLFUOOH} + \text{OH} \rightarrow \text{TLFUO2}$	2.53E-11	Rickard and Pascoe (2009)
G45485	TrGAroC	$\text{ACCOMECO3H} + \text{OH} \rightarrow \text{ACCOMECO3}$	3.59E-12	Rickard and Pascoe (2009)
G45486a	TrGAroC	$\text{C5DIALO2} + \text{HO}_2 \rightarrow \text{C5DIALOOH}$	$\text{KR02H02(5)} * (1 - \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)
G45486b	TrGAroC	$\text{C5DIALO2} + \text{HO}_2 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(5)} * \text{rcoch2o2_oh}$	Rickard and Pascoe (2009)*
G45487	TrGAroCN	$\text{C5DIALO2} + \text{NO} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45488	TrGAroCN	$\text{C5DIALO2} + \text{NO}_3 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45489	TrGAroC	$\text{C5DIALO2} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G45490a	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{C5DICAROOH}$	$\text{KR02H02(5)} * (\text{rco3_ooh} + \text{rco3_o3})$	Rickard and Pascoe (2009)
G45491b	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(5)} * \text{rco3_oh}$	Rickard and Pascoe (2009)*
G45492	TrGAroCN	$\text{C5DICARBO2} + \text{NO} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45493	TrGAroCN	$\text{C5DICARBO2} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45494	TrGAroC	$\text{C5DICARBO2} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46200a	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO235C6OOH}$	$\text{KR02H02(6)} * \text{rcoch2o2_ooh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G46200b	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$	$\text{KR02H02(6)} * \text{rcoch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G46201	TrGTerCN	$\text{CO235C6O2} + \text{NO} \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46202	TrGTerC	$\text{CO235C6O2} \rightarrow \text{CO23C4CO3} + \text{HCHO}$	k1_R02p0R02	Rickard and Pascoe (2009)
G46203	TrGTerC	$\text{CO235C6OOH} + \text{OH} \rightarrow \text{CO235C6O2}$	1.01E-11	Rickard and Pascoe (2009)
G46204	TrGTerC	$\text{C614O2} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)
G46205a	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G46205b	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{C614NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G46206a	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{C614OOH}$	$\text{KR02H02(6)} * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G46206b	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G46207	TrGTerCN	$\text{C614NO3} + \text{OH} \rightarrow \text{C614CO} + \text{NO}_2$	7.11E-12	Rickard and Pascoe (2009)
G46208	TrGTerC	$\text{C614OOH} + \text{OH} \rightarrow \text{C614CO} + \text{OH}$	8.69E-11	Rickard and Pascoe (2009)
G46209	TrGTerC	$\text{C614CO} + \text{OH} \rightarrow \text{CO235C5CHO} + \text{HO}_2$	3.22E-12	Rickard and Pascoe (2009)
G46210	TrGTerC	$\text{CO235C5CHO} + \text{OH} \rightarrow \text{CO23C4CO3} + \text{CO}$	1.33E-11	Rickard and Pascoe (2009)
G46211	TrGTerCN	$\text{CO235C5CHO} + \text{NO}_3 \rightarrow \text{CO23C4CO3} + \text{CO} + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G46400	TrGAroC	$\text{PHENOOH} + \text{OH} \rightarrow \text{PHENO2}$	1.16E-10	Rickard and Pascoe (2009)
G46401	TrGAroC	$\text{C6CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{CO} + \text{HCOCOCHO}$	7.70E-11	Rickard and Pascoe (2009)
G46402	TrGAroC	$\text{C5CO2DCO3H} + \text{OH} \rightarrow \text{C5CO2DBCO3}$	3.60E-11	Rickard and Pascoe (2009)
G46403	TrGAroCN	$\text{NDNPHENOOH} + \text{OH} \rightarrow \text{NDNPHENO2}$	k_roohro	Rickard and Pascoe (2009)
G46404a	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C615CO2OOH}$	$\text{KR02H02(6)*(1.-rcoch2o2_oh)}$	Rickard and Pascoe (2009)
G46404b	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(6)*rcoch2o2_oh}$	Rickard and Pascoe (2009)*
G46405	TrGAroCN	$\text{C615CO2O2} + \text{NO} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46406	TrGAroCN	$\text{C615CO2O2} + \text{NO}_3 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46407	TrGAroC	$\text{C615CO2O2} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46408	TrGAroCN	$\text{BZEMUCPAN} + \text{OH} \rightarrow \text{MALDIAL} + \text{CO} + \text{CO}_2 + \text{NO}_2$	4.05E-11	Rickard and Pascoe (2009)
G46409	TrGAroCN	$\text{BZEMUCPAN} \rightarrow \text{BZEMUCCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46410	TrGAroCN	$\text{BZBIPERNO3} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{NO}_2$	7.30E-11	Rickard and Pascoe (2009)
G46411	TrGAroCN	$\text{HOC6H4NO2} + \text{NO}_3 \rightarrow \text{NPHEN1O} + \text{HNO}_3$	9.00E-14	Rickard and Pascoe (2009)
G46412	TrGAroCN	$\text{HOC6H4NO2} + \text{OH} \rightarrow \text{NPHEN1O}$	9.00E-13	Rickard and Pascoe (2009)
G46413a	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NDNPHENOOH}$	$\text{KR02H02(6)*(1.-rchohch2o2_oh)}$	Rickard and Pascoe (2009)
G46413b	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G46414	TrGAroCN	$\text{NDNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46415	TrGAroCN	$\text{NDNPHENO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46416	TrGAroCN	$\text{NDNPHENO2} \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46417	TrGAroC	$\text{PBZQCO} + \text{OH} \rightarrow \text{C5CO2OHCO3}$	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	$\text{CATECHOL} + \text{NO}_3 \rightarrow \text{CATEC1O} + \text{HNO}_3$	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	$\text{CATECHOL} + \text{O}_3 \rightarrow \text{MALDALCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	9.2E-18	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46420	TrGAroC	CATECHOL + OH \rightarrow CATEC1O	1.0E-10	Rickard and Pascoe (2009)
G46421	TrGAroC	C5COOHCO3H + OH \rightarrow C5CO2OHCO3	8.01E-11	Rickard and Pascoe (2009)
G46422	TrGAroCN	NCATECHOL + NO ₃ \rightarrow NNCATECO2	2.60E-12	Rickard and Pascoe (2009)
G46423	TrGAroCN	NCATECHOL + OH \rightarrow NCATECO2	3.47E-12	Rickard and Pascoe (2009)
G46424a	TrGAroC	C5CO2OHCO3 + HO ₂ \rightarrow C5COOHCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46424b	TrGAroC	C5CO2OHCO3 + HO ₂ \rightarrow HOCOC4DIAL + HO ₂ + CO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46425	TrGAroCN	C5CO2OHCO3 + NO \rightarrow HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46426	TrGAroCN	C5CO2OHCO3 + NO ₂ \rightarrow C5CO2OHPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46427	TrGAroCN	C5CO2OHCO3 + NO ₃ \rightarrow HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46428	TrGAroC	C5CO2OHCO3 \rightarrow HOCOC4DIAL + HO ₂ + CO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46429	TrGAroCN	BZEPOXMUC + NO ₃ \rightarrow BZEMUCCO3 + HNO ₃	2*KN03AL*2.75	Rickard and Pascoe (2009)
G46430	TrGAroC	BZEPOXMUC + O ₃ \rightarrow EPXC4DIAL + .125 HCHO + .1125 HCOCO ₂ H + .0675 GLYOX + .0675 H ₂ O ₂ + .82 HO ₂ + .57 OH + 1.265 CO + .25 CO ₂	2.00E-18	Rickard and Pascoe (2009)*
G46431	TrGAroC	BZEPOXMUC + OH \rightarrow .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard and Pascoe (2009)
G46432a	TrGAroCN	NCATECO2 + HO ₂ \rightarrow NCATECOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	NCATECO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46433	TrGAroCN	NCATECO2 + NO \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46434	TrGAroCN	NCATECO2 + NO ₃ \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46435	TrGAroCN	NCATECO2 \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46436	TrGAroCN	NPHEN1OOH + OH \rightarrow NPHEN1O2	9.00E-13	Rickard and Pascoe (2009)
G46437a	TrGAroCN	NPHENO2 + HO ₂ \rightarrow NPHENOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46437b	TrGAroCN	NPHENO2 + HO ₂ \rightarrow MALDALCO2H + GLYOX + NO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46438	TrGAroCN	NPHENO2 + NO \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46439	TrGAroCN	NPHENO2 + NO ₃ \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46440	TrGAroCN	NPHENO2 \rightarrow MALDALCO2H + GLYOX + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46441	TrGAroC	BENZENE + OH \rightarrow .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO ₂ + .53 PHENOL + .53 HO ₂	2.3E-12*EXP(-190/TEMP)	Rickard and Pascoe (2009)*
G46442	TrGAroCN	C5CO2OHPAN + OH \rightarrow HOCOC4DIAL + CO + CO + NO ₂	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	C5CO2OHPAN \rightarrow C5CO2OHCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G46444	TrGAroCN	CATEC1O + NO ₂ \rightarrow NCATECHOL	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46445	TrGAroC	CATEC1O + O ₃ \rightarrow CATEC1O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G46446	TrGAroC	BZEMUCCO + OH \rightarrow EPXDLCO3 + GLYOX	9.20E-11	Rickard and Pascoe (2009)
G46447a	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NNCATECOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46447b	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46448	TrGAroCN	NNCATECO2 + NO \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46449	TrGAroCN	NNCATECO2 + NO ₃ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46450	TrGAroCN	NNCATECO2 \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46451	TrGAroC	BZEMUCCO2H + OH \rightarrow C5DIALO2 + CO ₂	4.06E-11	Rickard and Pascoe (2009)
G46452	TrGAroCN	NNCATECOOH + OH \rightarrow NNCATECO2	k_roohro	Rickard and Pascoe (2009)
G46453	TrGAroCN	NPHEN1O + NO ₂ \rightarrow DNPHEN	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46454	TrGAroCN	NPHEN1O + O ₃ \rightarrow NPHEN1O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G46455	TrGAroCN	DNPHEN + NO ₃ \rightarrow NDNPHENO2	2.25E-15	Rickard and Pascoe (2009)
G46456	TrGAroCN	DNPHEN + OH \rightarrow DNPHEO2	3.00E-14	Rickard and Pascoe (2009)
G46457	TrGAroCN	PHENOL + NO ₃ \rightarrow .742 C6H5O + .742 HNO ₃ + .258 NPHENO2	3.8E-12	Rickard and Pascoe (2009)*
G46458	TrGAroC	PHENOL + OH \rightarrow .06 C6H5O + .8 CATECHOL + .8 HO ₂ + .14 PHENO2	4.7E-13*EXP(1220/TEMP)	Rickard and Pascoe (2009)*
G46459	TrGAroCN	PBZQONE + NO ₃ \rightarrow NBZQO2	3.00E-13	Rickard and Pascoe (2009)
G46460	TrGAroC	PBZQONE + OH \rightarrow PBZQO2	4.6E-12	Rickard and Pascoe (2009)
G46461a	TrGAroC	PHENO2 + HO ₂ \rightarrow PHENO2OH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46461b	TrGAroC	PHENO2 + HO ₂ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46462	TrGAroCN	PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46463	TrGAroCN	PHENO2 + NO ₃ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46464	TrGAroC	PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46465	TrGAroC	C615CO2OOH + OH → C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
G46466a	TrGAroC	C5CO2DBCO3 + HO ₂ → C5CO2DCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBCO3 + HO ₂ → CH ₃ C(O) + HCOCOCHO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBCO3 + NO → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBCO3 + NO ₂ → C5CO2DBPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBCO3 + NO ₃ → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBCO3 → CH ₃ C(O) + HCOCOCHO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46471	TrGAroCN	NPHEN1O2 + HO ₂ → NPHEN1OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46472a	TrGAroCN	NPHEN1O2 + NO → NPHEN1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46472b	TrGAroCN	NPHEN1O2 + NO ₂ → NPHEN1O + NO ₃	k_C6H502_N02	Jagiella and Zabel (2007)*
G46473	TrGAroCN	NPHEN1O2 + NO ₃ → NPHEN1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46474	TrGAroCN	NPHEN1O2 → NPHEN1O	k1_R02sR02	Rickard and Pascoe (2009)
G46475	TrGAroCN	NPHENOOH + OH → NPHENO2	1.07E-10	Rickard and Pascoe (2009)
G46476	TrGAroCN	C6H5O + NO ₂ → HOC6H4NO2	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O ₃ → C6H5O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G46478	TrGAroCN	NCATECOOH + OH → NCATECO2	k_roohro	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH → PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)
G46480a	TrGAroC	PBZQO2 + HO ₂ → PBZQOOH	KR02H02(6)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46480b	TrGAroC	PBZQO2 + HO ₂ → C5CO2OHCO3 + OH	KR02H02(6)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G46481	TrGAroCN	PBZQO2 + NO → C5CO2OHCO3 + NO ₂	KR02N0	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46482	TrGAroCN	PBZQO2 + NO ₃ → C5CO2OHCO3 + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46483	TrGAroC	PBZQO2 → C5CO2OHCO3	k1_R02s0R02	Rickard and Pascoe (2009)*
G46484	TrGAroC	BZOBIPEROH + OH → MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	DNPHEO2 + HO ₂ → DNPHEOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46485b	TrGAroCN	DNPHEO2 + HO ₂ → NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46486	TrGAroCN	DNPHEO2 + NO → NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46487	TrGAroCN	DNPHEO2 + NO ₃ → NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46488	TrGAroCN	DNPHEO2 → NC4DCO2H + HCOCO ₂ H + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46489	TrGAroC	BZBIPEROOH + OH → BZOBIPEROH + OH	9.77E-11	Rickard and Pascoe (2009)
G46490a	TrGAroC	BZEMUCO2 + HO ₂ → BZEMUCOOH	KR02H02(6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	BZEMUCO2 + HO ₂ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + OH	KR02H02(6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	BZEMUCO2 + NO → BZEMUCNO3	KR02N0*alpha_AN(10,2,0,1,0, temp, cair)	Rickard and Pascoe (2009)
G46491b	TrGAroCN	BZEMUCO2 + NO → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + NO ₂	KR02N0*(1.-alpha_AN(10,2,0,1,0, temp, cair))	Rickard and Pascoe (2009)*
G46492	TrGAroCN	BZEMUCO2 + NO ₃ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46493	TrGAroC	BZEMUCO2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO	k1_R02s0R02	Rickard and Pascoe (2009)*
G46494	TrGAroCN	C5CO2DBPAN + OH → HCOCOCHO + CH ₃ CHO + CO ₂ + NO ₂	3.28E-11	Rickard and Pascoe (2009)
G46495	TrGAroCN	C5CO2DBPAN → C5CO2DBCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	NBZQOOH + OH → NBZQO2	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	CATEC1OOH + OH → CATEC1O2	k_roohro	Rickard and Pascoe (2009)
G46498	TrGAroC	C6125CO + OH → C5CO14O2 + CO	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	NBZQO2 + HO ₂ → NBZQOOH	KR02H02(6)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46499b	TrGAroCN	NBZQO2 + HO ₂ → C6CO4DB + NO ₂ + OH	KR02H02(6)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G46500	TrGAroCN	NBZQO2 + NO → C6CO4DB + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46501	TrGAroCN	NBZQO2 + NO ₃ → C6CO4DB + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46502	TrGAroCN	NBZQO2 → C6CO4DB + NO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G46503	TrGAroCN	DNPHEOOH + OH → DNPHEO2	k_roohro	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46504	TrGAroC	CATEC1O2 + HO ₂ → CATEC1OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46505a	TrGAroCN	CATEC1O2 + NO → CATEC1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46505b	TrGAroCN	CATEC1O2 + NO ₂ → CATEC1O + NO ₃	K_C6H502_N02	Jagiella and Zabel (2007)*
G46506	TrGAroCN	CATEC1O2 + NO ₃ → CATEC1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46507	TrGAroC	CATEC1O2 → CATEC1O	k1_R02s0R02	Rickard and Pascoe (2009)
G46508	TrGAroC	BZEMUCCO3H + OH → BZEMUCCO3	4.37E-11	Rickard and Pascoe (2009)
G46509	TrGAroC	C6H5OOH + OH → C6H5O2	3.60E-12	Rickard and Pascoe (2009)
G46510	TrGAroC	BZEMUCOOH + OH → BZEMUCCO + OH	1.31E-10	Rickard and Pascoe (2009)
G46511a	TrGAroC	BZEMUCCO3 + HO ₂ → BZEMUCCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G46511b	TrGAroC	BZEMUCCO3 + HO ₂ → BZEMUCCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G46511c	TrGAroC	BZEMUCCO3 + HO ₂ → C5DIALO2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46512	TrGAroCN	BZEMUCCO3 + NO → C5DIALO2 + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46513	TrGAroCN	BZEMUCCO3 + NO ₂ → BZEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G46514	TrGAroCN	BZEMUCCO3 + NO ₃ → C5DIALO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46515	TrGAroC	BZEMUCCO3 → C5DIALO2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G46516	TrGAroC	C6H5O2 + HO ₂ → C6H5OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46517a	TrGAroCN	C6H5O2 + NO → C6H5O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46517b	TrGAroCN	C6H5O2 + NO ₂ → C6H5O + NO ₃	K_C6H502_N02	Jagiella and Zabel (2007)*
G46518	TrGAroCN	C6H5O2 + NO ₃ → C6H5O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46519	TrGAroC	C6H5O2 → C6H5O	k1_R02sR02	Rickard and Pascoe (2009)
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO ₂	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	BZBIPERO2 + HO ₂ → BZBIPEROOH	KR02H02(6)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G46522b	TrGAroC	BZBIPERO2 + HO ₂ → OH + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02H02(6)*rbipero2_oh	Rickard and Pascoe (2009), Bird- sall et al. (2010)*
G46523a	TrGAroCN	BZBIPERO2 + NO → BZBIPERNO3	KR02N0*alpha_AN(9,2,0,0,1,temp, cair)	Rickard and Pascoe (2009)
G46523b	TrGAroCN	BZBIPERO2 + NO → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N0*(1.-alpha_AN(9,2,0,0,1, temp,cair))	Rickard and Pascoe (2009)*
G46524	TrGAroCN	BZBIPERO2 + NO ₃ → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N03	Rickard and Pascoe (2009)*
G46525	TrGAroC	BZBIPERO2 → GLYOX + HO ₂ + BZFUONE	k1_R02s0R02	Rickard and Pascoe (2009)*
G47200	TrGTerCN	CO235C6CHO + NO ₃ → CO235C6CO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	CO235C6CO3 + HO ₂ → C235C6CO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO ₂ → CO235C6O2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47203	TrGTerCN	$\text{CO235C6CO3} + \text{NO} \rightarrow \text{CO235C6O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G47204	TrGTerCN	$\text{CO235C6CO3} + \text{NO}_2 \rightarrow \text{C7PAN3}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G47205	TrGTerC	$\text{CO235C6CO3} \rightarrow \text{CO235C6O2} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G47206	TrGTerC	$\text{C235C6CO3H} + \text{OH} \rightarrow \text{CO235C6CO3}$	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	$\text{C7PAN3} + \text{OH} \rightarrow \text{CO235C5CHO} + \text{CO} + \text{NO}_2$	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	$\text{C7PAN3} \rightarrow \text{CO235C6CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G47209a	TrGTerC	$\text{C716O2} + \text{HO}_2 \rightarrow \text{C716OOH}$	KR02H02(7)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G47209b	TrGTerC	$\text{C716O2} + \text{HO}_2 \rightarrow \text{CO13C4CHO} + \text{CH}_3\text{C(O)} + \text{OH}$	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G47210	TrGTerCN	$\text{C716O2} + \text{NO} \rightarrow \text{CO13C4CHO} + \text{CH}_3\text{C(O)} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47211	TrGTerC	$\text{C716O2} \rightarrow \text{CO13C4CHO} + \text{CH}_3\text{C(O)}$	k1_R02s0R02	Rickard and Pascoe (2009)
G47212	TrGTerC	$\text{C716OOH} + \text{OH} \rightarrow \text{CO235C6CHO} + \text{OH}$	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	$\text{C721O2} + \text{HO}_2 \rightarrow \text{C721OOH}$	KR02H02(7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	$\text{C721O2} + \text{NO} \rightarrow \text{C722O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47215	TrGTerC	$\text{C721O2} \rightarrow \text{C722O2}$	k1_R02pR02	Rickard and Pascoe (2009)
G47216	TrGTerC	$\text{C721OOH} + \text{OH} \rightarrow \text{C721O2}$	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	$\text{C722O2} + \text{HO}_2 \rightarrow \text{C722OOH}$	KR02H02(7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	$\text{C722O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C44O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47219	TrGTerC	$\text{C722O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C44O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G47220	TrGTerC	$\text{C722OOH} + \text{OH} \rightarrow \text{C722O2}$	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	$\text{ROO6R3O2} \rightarrow \text{ROO6R5O2}$	5.68E10*EXP(-8745./TEMP)	Vereecken and Peeters (2012)
G47222	TrGTerCN	$\text{ROO6R3O2} + \text{NO} \rightarrow \text{ROO6R3O} + \text{NO}_2$	KR02N0	Vereecken and Peeters (2012)*
G47223	TrGTerC	$\text{ROO6R3O2} + \text{HO}_2 \rightarrow 7 \text{ L CARBON}$	KR02H02(7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	$\text{ROO6R3O2} \rightarrow \text{ROO6R3O}$	k1_R02sR02	Vereecken and Peeters (2012)
G47225	TrGTerC	$\text{ROO6R3O} \rightarrow 7 \text{ L CARBON} + \text{HO}_2$	5.7E10*EXP(-2949./TEMP)	Vereecken and Peeters (2012)*
G47226	TrGTerC	$\text{ROO6R5O2} \rightarrow 7 \text{ L CARBON} + \text{OH}$	9.17E10*EXP(-8706./TEMP)	Vereecken and Peeters (2012)*
G47400	TrGAroC	$\text{TOLUENE} + \text{OH} \rightarrow .07 \text{ C6H5CH2O2} + .18 \text{ CRESOL} + .18 \text{ HO}_2 + .65 \text{ TLBIPERO2} + .10 \text{ TLEPOXMUC} + .10 \text{ HO}_2 + .04 \text{ AELV}$	1.8E-12*EXP(340/TEMP)	Rickard and Pascoe (2009)*
G47401	TrGAroC	$\text{C6H5CH2O2} + \text{HO}_2 \rightarrow \text{C6H5CH2OOH}$	1.5E-13*EXP(1310/TEMP)	Rickard and Pascoe (2009)
G47402a	TrGAroCN	$\text{C6H5CH2O2} + \text{NO} \rightarrow \text{C6H5CH2NO3}$	KR02N0*alpha_AN(7,1,0,0,0,temp,cair)	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	$\text{C6H5CH2O2} + \text{NO} \rightarrow \text{BENZAL} + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-alpha_AN(7,1,0,0,0,temp,cair))	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47403	TrGAroCN	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{BENZAL} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47404	TrGAroC	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 \rightarrow \text{BENZAL} + \text{HO}_2$	$2 \cdot (\text{k_CH302} \cdot 2.4\text{E-}14 \cdot \text{EXP}(1620./\text{TEMP})) \cdot 0.5 \cdot \text{R02}$	Rickard and Pascoe (2009)*
G47405	TrGAroCN	$\text{CRESOL} + \text{NO}_3 \rightarrow .103 \text{ CRESO}_2 + .103 \text{ HNO}_3 + .506 \text{ NCRESO}_2 + .391 \text{ TOLIO} + .391 \text{ HNO}_3$	$1.4\text{E-}11$	Rickard and Pascoe (2009)*
G47406	TrGAroC	$\text{CRESOL} + \text{OH} \rightarrow .2 \text{ CRESO}_2 + .727 \text{ MCATECHOL} + .727 \text{ HO}_2 + .073 \text{ TOLIO}$	$4.65\text{E-}11$	Rickard and Pascoe (2009)*
G47407a	TrGAroC	$\text{TLBIPERO}_2 + \text{HO}_2 \rightarrow \text{TLBIPEROOH}$	$\text{KR02H02}(7) \cdot (1 - \text{rbipero2_oh})$	Rickard and Pascoe (2009)
G47407b	TrGAroC	$\text{TLBIPERO}_2 + \text{HO}_2 \rightarrow \text{OH} + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL} + 0.780 \text{ ALOV}$	$\text{KR02H02}(7) \cdot \text{rbipero2_oh}$	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G47408a	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO} \rightarrow \text{NO}_2 + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL} + 0.097 \text{ ALOV} + 0.748 \text{ ASOV}$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(11, 2, 0, 0, 1, \text{temp, cair}))$	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO} \rightarrow \text{TLBIPERNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(11, 2, 0, 0, 1, \text{temp, cair})$	Rickard and Pascoe (2009)*
G47409	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	KR02N03	Rickard and Pascoe (2009)*
G47410	TrGAroC	$\text{TLBIPERO}_2 \rightarrow .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	k1_R02s0R02	Rickard and Pascoe (2009)*
G47411	TrGAroCN	$\text{TLEPOXMUC} + \text{NO}_3 \rightarrow \text{TLEMUCCO}_3 + \text{HNO}_3$	$\text{KN03AL} \cdot 2.75$	Rickard and Pascoe (2009)
G47412	TrGAroC	$\text{TLEPOXMUC} + \text{O}_3 \rightarrow \text{EPXC4DIAL} + .125 \text{ CH}_3\text{CHO} + .695 \text{ CH}_3\text{C(O)} + .57 \text{ CO} + .57 \text{ OH} + .125 \text{ HO}_2 + .1125 \text{ CH}_3\text{COCO}_2\text{H} + .0675 \text{ MGLYOX} + .0675 \text{ H}_2\text{O}_2 + .25 \text{ CO}_2$	$5.00\text{E-}18$	Rickard and Pascoe (2009)*
G47413	TrGAroC	$\text{TLEPOXMUC} + \text{OH} \rightarrow .31 \text{ TLEMUCCO}_3 + .69 \text{ TLEMUCO}_2$	$7.99\text{E-}11$	Rickard and Pascoe (2009)*
G47414	TrGAroC	$\text{C}_6\text{H}_5\text{CH}_2\text{OOH} + \text{OH} \rightarrow \text{BENZAL} + \text{OH}$	$2.05\text{E-}11$	Rickard and Pascoe (2009)
G47415	TrGAroCN	$\text{C}_6\text{H}_5\text{CH}_2\text{NO}_3 + \text{OH} \rightarrow \text{BENZAL} + \text{NO}_2$	$6.03\text{E-}12$	Rickard and Pascoe (2009)
G47416	TrGAroCN	$\text{BENZAL} + \text{NO}_3 \rightarrow \text{C}_6\text{H}_5\text{CO}_3 + \text{HNO}_3$	$2.40\text{E-}15$	Rickard and Pascoe (2009)
G47417	TrGAroC	$\text{BENZAL} + \text{OH} \rightarrow \text{C}_6\text{H}_5\text{CO}_3$	$5.9\text{E-}12 \cdot \text{EXP}(225/\text{TEMP})$	Rickard and Pascoe (2009)
G47418a	TrGAroC	$\text{CRESO}_2 + \text{HO}_2 \rightarrow \text{CRESOOH}$	$\text{KR02H02}(7) \cdot (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47418b	TrGAroC	CRESO2 + HO ₂ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO2 + NO ₃ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47421	TrGAroC	CRESO2 → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO2 + HO ₂ → NCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO2 + HO ₂ → C5CO14OH + GLYOX + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO2 + NO → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO2 + NO ₃ → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO2 → C5CO14OH + GLYOX + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47426	TrGAroCN	TOL1O + NO ₂ → TOL1OHNO2	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O ₃ → OXYL1O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47428	TrGAroCN	MCATECHOL + NO ₃ → MCATEC1O + HNO ₃	1.7E-10*1.0	Rickard and Pascoe (2009)
G47429	TrGAroC	MCATECHOL + O ₃ → MC3ODBCO2H + HCOCO ₂ H + HO ₂ + OH	2.8E-17	Rickard and Pascoe (2009)*
G47430	TrGAroC	MCATECHOL + OH → MCATEC1O	2.0E-10*1.0	Rickard and Pascoe (2009)
G47431	TrGAroC	TLBIPEROOH + OH → TLOBIPEROH + OH	9.64E-11	Rickard and Pascoe (2009)
G47432	TrGAroCN	TLBIPERNO3 + OH → TLOBIPEROH + NO ₂	7.16E-11	Rickard and Pascoe (2009)
G47433	TrGAroC	TLOBIPEROH + OH → C5CO14O2 + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO3 + HO ₂ → C615CO2O2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO3 + HO ₂ → TLEMUCCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO3 + HO ₂ → TLEMUCCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO3 + NO → C615CO2O2 + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO3 + NO ₂ → TLEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO3 + NO ₃ → C615CO2O2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G47438	TrGAroC	TLEMUCCO3 → C615CO2O2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G47439a	TrGAroC	TLEMUCO2 + HO ₂ → TLEMUCOOH	KR02H02(7)*(1-rchohch2o2_ oh-rcoch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47439b	TrGAroC	$\text{TLEMUCO}_2 + \text{HO}_2 \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{OH}$	$\text{KR02H02}(7) * (\text{rchohch2o2_oh} + \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)*
G47440a	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO} \rightarrow \text{TLEMUCNO}_3$	$\text{KR02N0} * \alpha_{\text{AN}}(11, 2, 1, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G47440b	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO} \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(11, 2, 1, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G47441	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO}_3 \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{NO}_2$	KR02N0_3	Rickard and Pascoe (2009)*
G47442	TrGAroC	$\text{TLEMUCO}_2 \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G47443a	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{CO}_3\text{H}$	$1.1\text{E-}11 * \text{EXP}(364./\text{temp}) * 0.65$	Roth et al. (2010)
G47443b	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$1.1\text{E-}11 * \text{EXP}(364./\text{temp}) * 0.20$	Roth et al. (2010)
G47443c	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{PHCOOH} + \text{O}_3$	$1.1\text{E-}11 * \text{EXP}(364./\text{temp}) * 0.15$	Roth et al. (2010)
G47444	TrGAroCN	$\text{C}_6\text{H}_5\text{CO}_3 + \text{NO} \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G47445	TrGAroCN	$\text{C}_6\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PBZN}$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47446	TrGAroCN	$\text{C}_6\text{H}_5\text{CO}_3 + \text{NO}_3 \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2 + \text{NO}_2$	$\text{KR02N0}_3 * 1.74$	Rickard and Pascoe (2009)
G47447	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G47448	TrGAroC	$\text{CRESOOH} + \text{OH} \rightarrow \text{CRESO}_2$	$1.15\text{E-}10$	Rickard and Pascoe (2009)
G47449	TrGAroCN	$\text{NCRESOOH} + \text{OH} \rightarrow \text{NCRESO}_2$	$1.07\text{E-}10$	Rickard and Pascoe (2009)
G47450	TrGAroCN	$\text{TOL1OHNO}_2 + \text{NO}_3 \rightarrow \text{NCRES1O} + \text{HNO}_3$	$3.13\text{E-}13 * 1.0$	Rickard and Pascoe (2009)
G47451	TrGAroCN	$\text{TOL1OHNO}_2 + \text{OH} \rightarrow \text{NCRES1O}$	$2.8\text{E-}12$	Rickard and Pascoe (2009)
G47452	TrGAroC	$\text{OXYL1O}_2 + \text{HO}_2 \rightarrow \text{OXYL1OOH}$	$\text{KR02H02}(7)$	Rickard and Pascoe (2009)
G47453	TrGAroCN	$\text{OXYL1O}_2 + \text{NO} \rightarrow \text{TOL1O} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G47454	TrGAroCN	$\text{OXYL1O}_2 + \text{NO}_2 \rightarrow \text{TOL1O} + \text{NO}_3$	K_C6H502_N02	Jagiella and Zabel (2007)*
G47455	TrGAroCN	$\text{OXYL1O}_2 + \text{NO}_3 \rightarrow \text{TOL1O} + \text{NO}_2$	KR02N0_3	Rickard and Pascoe (2009)
G47456	TrGAroC	$\text{OXYL1O}_2 \rightarrow \text{TOL1O}$	k1_R02sR02	Rickard and Pascoe (2009)
G47457	TrGAroCN	$\text{MCATEC1O} + \text{NO}_2 \rightarrow \text{MNCATECH}$	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47458	TrGAroC	$\text{MCATEC1O} + \text{O}_3 \rightarrow \text{MCATEC1O}_2$	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47459	TrGAroC	$\text{TLEMUCCO}_2\text{H} + \text{OH} \rightarrow \text{C}_6\text{H}_5\text{CO}_2\text{O}_2 + \text{CO}_2$	$5.98\text{E-}11$	Rickard and Pascoe (2009)
G47460	TrGAroC	$\text{TLEMUCCO}_3\text{H} + \text{OH} \rightarrow \text{TLEMUCCO}_3$	$6.29\text{E-}11$	Rickard and Pascoe (2009)
G47461	TrGAroCN	$\text{TLEMUCPAN} + \text{OH} \rightarrow \text{C}_5\text{DICARB} + \text{CO} + \text{CO}_2 + \text{NO}_2$	$5.96\text{E-}11$	Rickard and Pascoe (2009)
G47462	TrGAroCN	$\text{TLEMUCPAN} \rightarrow \text{TLEMUCCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G47463	TrGAroC	$\text{TLEMUCOOH} + \text{OH} \rightarrow \text{TLEMUCCO} + \text{OH}$	$7.04\text{E-}11$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47464	TrGAroCN	TLEMUCNO3 + OH → TLEMUCCO + NO ₂	3.06E-11	Rickard and Pascoe (2009)
G47465	TrGAroC	TLEMUCCO + OH → CH ₃ C(O) + EPXC4DIAL + CO	4.06E-11	Rickard and Pascoe (2009)
G47466	TrGAroC	C6H5CO3H + OH → C6H5CO3	4.66E-12	Rickard and Pascoe (2009)
G47467	TrGAroC	PHCOOH + OH → C6H5O2 + CO ₂	1.10E-12	Rickard and Pascoe (2009)
G47468	TrGAroCN	PBZN + OH → C6H5OOH + CO + NO ₂	1.06E-12	Rickard and Pascoe (2009)
G47469	TrGAroCN	PBZN → C6H5CO3 + NO ₂	k_PAN_M*0.67	Rickard and Pascoe (2009)
G47470	TrGAroCN	PTLQONE + NO ₃ → NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
G47471	TrGAroC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard and Pascoe (2009)
G47472	TrGAroCN	NCRES1O + NO ₂ → DNCRES	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O ₃ → NCRES1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47474	TrGAroC	OXYL1OOH + OH → OXYL1O2	4.65E-11	Rickard and Pascoe (2009)
G47475	TrGAroCN	MNCATECH + NO ₃ → MNNCATECO2	5.03E-12	Rickard and Pascoe (2009)
G47476	TrGAroCN	MNCATECH + OH → MNCATECO2	6.83E-12	Rickard and Pascoe (2009)
G47477	TrGAroC	MCATEC1O2 + HO ₂ → MCATEC1OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47478	TrGAroCN	MCATEC1O2 + NO → MCATEC1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G47479	TrGAroCN	MCATEC1O2 + NO ₂ → MCATEC1O + NO ₃	K_C6H5O2_NO2	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO ₃ → MCATEC1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G47481	TrGAroC	MCATEC1O2 → MCATEC1O	k1_R02s0R02	Rickard and Pascoe (2009)
G47482a	TrGAroCN	NPTLQO2 + HO ₂ → NPTLQOOH	KR02H02(7)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO ₂ → C7CO4DB + NO ₂ + OH	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G47483	TrGAroCN	NPTLQO2 + NO → C7CO4DB + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47484	TrGAroCN	NPTLQO2 + NO ₃ → C7CO4DB + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47485	TrGAroCN	NPTLQO2 → C7CO4DB + NO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G47486a	TrGAroC	PTLQO2 + HO ₂ → PTLQOOH	KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO ₂ → C6CO2OHCO3 + OH	KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G47487	TrGAroCN	PTLQO2 + NO → C6CO2OHCO3 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47488	TrGAroCN	PTLQO2 + NO ₃ → C6CO2OHCO3 + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47489	TrGAroC	PTLQO2 → C6CO2OHCO3	k1_R02s0R02	Rickard and Pascoe (2009)*
G47490	TrGAroCN	DNCRES + NO ₃ → NDNCRESO2	7.83E-15	Rickard and Pascoe (2009)
G47491	TrGAroCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard and Pascoe (2009)
G47492	TrGAroCN	NCRES1O2 + HO ₂ → NCRES1OOH	KR02H02(7)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47493	TrGAroCN	$\text{NCRES1O2} + \text{NO} \rightarrow \text{NCRES1O} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G47494	TrGAroCN	$\text{NCRES1O2} + \text{NO}_2 \rightarrow \text{NCRES1O} + \text{NO}_3$	K_C6H502_N02	Jagiella and Zabel (2007)*
G47495	TrGAroCN	$\text{NCRES1O2} + \text{NO}_3 \rightarrow \text{NCRES1O} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G47496	TrGAroCN	$\text{NCRES1O2} \rightarrow \text{NCRES1O}$	k1_R02sR02	Rickard and Pascoe (2009)
G47497a	TrGAroCN	$\text{MNNCATECO2} + \text{HO}_2 \rightarrow \text{MNNCATCOOH}$	$\text{KR02H02(7)} * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G47497b	TrGAroCN	$\text{MNNCATECO2} + \text{HO}_2 \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H}$ $+ \text{NO}_2 + \text{OH}$	$\text{KR02H02(7)} * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G47498	TrGAroCN	$\text{MNNCATECO2} + \text{NO} \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H}$ $+ \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47499	TrGAroCN	$\text{MNNCATECO2} + \text{NO}_3 \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H}$ $+ \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47500	TrGAroCN	$\text{MNNCATECO2} \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)
G47501a	TrGAroCN	$\text{MNCATECO2} + \text{HO}_2 \rightarrow \text{MNCATECOOH}$	$\text{KR02H02(7)} * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G47501b	TrGAroCN	$\text{MNCATECO2} + \text{HO}_2 \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H}$ $+ \text{HO}_2 + \text{OH}$	$\text{KR02H02(7)} * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G47502	TrGAroCN	$\text{MNCATECO2} + \text{NO} \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} +$ $\text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47503	TrGAroCN	$\text{MNCATECO2} + \text{NO}_3 \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H}$ $+ \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47504	TrGAroCN	$\text{MNCATECO2} \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{HO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47505	TrGAroC	$\text{MCATEC1OOH} + \text{OH} \rightarrow \text{MCATEC1O2}$	2.05E-10	Rickard and Pascoe (2009)
G47506	TrGAroCN	$\text{NPTLQOOH} + \text{OH} \rightarrow \text{NPTLQO2}$	8.56E-11	Rickard and Pascoe (2009)
G47507	TrGAroC	$\text{PTLQOOH} + \text{OH} \rightarrow \text{PTLQCO} + \text{OH}$	1.42E-10	Rickard and Pascoe (2009)
G47508	TrGAroC	$\text{PTLQCO} + \text{OH} \rightarrow \text{C6CO2OHCO3}$	7.95E-11	Rickard and Pascoe (2009)
G47509a	TrGAroCN	$\text{NDNCRESO2} + \text{HO}_2 \rightarrow \text{NDNCRESOOH}$	$\text{KR02H02(7)} * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G47509b	TrGAroCN	$\text{NDNCRESO2} + \text{HO}_2 \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + 2$ $\text{CO} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(7)} * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G47510	TrGAroCN	$\text{NDNCRESO2} + \text{NO} \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + 2 \text{ CO}$ $+ \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47511	TrGAroCN	$\text{NDNCRESO2} + \text{NO}_3 \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + 2$ $\text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47512	TrGAroCN	$\text{NDNCRESO2} \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + 2 \text{ CO} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47513a	TrGAroCN	$\text{DNCRESO2} + \text{HO}_2 \rightarrow \text{DNCRESOOH}$	$\text{KR02H02(7)} * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G47513b	TrGAroCN	$\text{DNCRESO2} + \text{HO}_2 \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} +$ $\text{NO}_2 + \text{OH}$	$\text{KR02H02(7)} * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47514	TrGAroCN	DNCRESO2 + NO → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47515	TrGAroCN	DNCRESO2 + NO ₃ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47516	TrGAroCN	DNCRESO2 → NC4MDCO2HN + HCOCO ₂ H + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47517	TrGAroCN	NCRES1OOH + OH → NCRES1O2	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	MNNCATCOOH + OH → MNNCATECO2	k_roohro	Rickard and Pascoe (2009)
G47519	TrGAroCN	MNCATECOOH + OH → MNCATECO2	k_roohro	Rickard and Pascoe (2009)
G47520	TrGAroC	C7CO4DB + OH → CO + CO + CH ₃ C(O) + HCOCOCHO	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	C6CO2OHCO3 + HO ₂ → C5134CO2OH + HO ₂ + CO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47521b	TrGAroC	C6CO2OHCO3 + HO ₂ → C6COOHCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47522	TrGAroCN	C6CO2OHCO3 + NO → C5134CO2OH + HO ₂ + CO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G47523	TrGAroCN	C6CO2OHCO3 + NO ₂ → C6CO2OHPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G47524	TrGAroCN	C6CO2OHCO3 + NO ₃ → C5134CO2OH + HO ₂ + CO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	C6CO2OHCO3 → C5134CO2OH + HO ₂ + CO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G47526	TrGAroCN	NDNCRESOOH + OH → NDNCRESO2	k_roohro	Rickard and Pascoe (2009)
G47527	TrGAroCN	DNCRESOOH + OH → DNCRESO2	k_roohro	Rickard and Pascoe (2009)
G47528	TrGAroC	C6COOHCO3H + OH → C6CO2OHCO3	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	C6CO2OHPAN + OH → C5134CO2OH + CO + CO + NO ₂	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	C6CO2OHPAN → C6CO2OHCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	C85O2 → C86O2	k1_R02tr02	Rickard and Pascoe (2009)
G48201	TrGTerC	C85O2 + HO ₂ → C85OOH	KR02H02(8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	C85O2 + NO → C86O2 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G48203	TrGTerC	C85OOH + OH → C85O2	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	C86O2 → C511O2 + CH ₃ COCH ₃	k1_R02tr02	Rickard and Pascoe (2009)
G48205	TrGTerCN	C86O2 + NO → C511O2 + CH ₃ COCH ₃ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G48206	TrGTerC	C86O2 + HO ₂ → C86OOH	KR02H02(8)	Rickard and Pascoe (2009)
G48207	TrGTerC	C86OOH + OH → C86O2	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	C811O2 → C812O2	k1_R02pr02	Rickard and Pascoe (2009)
G48209	TrGTerC	C811O2 + HO ₂ → 8 LCARBON	KR02H02(8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48210	TrGTerCN	$\text{C811O2} + \text{NO} \rightarrow \text{C812O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48211	TrGTerC	$\text{C812O2} \rightarrow \text{C813O2}$	k1_R02t0R02	Rickard and Pascoe (2009)
G48212	TrGTerCN	$\text{C812O2} + \text{NO} \rightarrow \text{C813O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48213	TrGTerC	$\text{C812O2} + \text{HO}_2 \rightarrow \text{C812OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48214	TrGTerC	$\text{C812OOH} + \text{OH} \rightarrow \text{C812O2}$	1.09E-11	Rickard and Pascoe (2009)
G48215	TrGTerC	$\text{C813O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G48216	TrGTerCN	$\text{C813O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48217	TrGTerC	$\text{C813O2} + \text{HO}_2 \rightarrow \text{C813OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48218	TrGTerC	$\text{C813OOH} + \text{OH} \rightarrow \text{C813O2}$	1.86E-11	Rickard and Pascoe (2009)
G48219	TrGTerCN	$\text{C721CHO} + \text{NO}_3 \rightarrow \text{C721CO3} + \text{HNO}_3$	KN03AL*8.5	Rickard and Pascoe (2009)
G48220	TrGTerC	$\text{C721CHO} + \text{OH} \rightarrow \text{C721CO3}$	2.63E-11	Rickard and Pascoe (2009)
G48221a	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721CO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G48221b	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G48221c	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{NORPINIC} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G48222	TrGTerCN	$\text{C721CO3} + \text{NO} \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)*
G48223	TrGTerCN	$\text{C721CO3} + \text{NO}_2 \rightarrow \text{C721PAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G48224	TrGTerCN	$\text{C721CO3} + \text{NO}_3 \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	$\text{C721CO3} \rightarrow \text{C721O2} + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2018)
G48226	TrGTerC	$\text{C721CO3} \rightarrow \text{NORPINIC}$	k1_R02RC03*0.1	Sander et al. (2018)
G48227	TrGTerC	$\text{C721CO3H} + \text{OH} \rightarrow \text{C721CO3}$	9.65E-12	Rickard and Pascoe (2009)
G48228	TrGTerC	$\text{NORPINIC} + \text{OH} \rightarrow \text{C721O2} + \text{CO}_2$	6.57E-12	Rickard and Pascoe (2009)
G48229	TrGTerCN	$\text{C721PAN} + \text{OH} \rightarrow \text{C721OOH} + \text{CO} + \text{NO}_2$	2.96E-12	Rickard and Pascoe (2009)
G48230	TrGTerCN	$\text{C721PAN} \rightarrow \text{C721CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G48231	TrGTerC	$\text{C8BC} + \text{OH} \rightarrow \text{C8BCO2}$	3.04E-12	Rickard and Pascoe (2009)
G48232	TrGTerC	$\text{C8BCO2} + \text{HO}_2 \rightarrow \text{C8BCOOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48233a	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C89O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C8BCNO3}$	KR02N0*alpha_AN(8,2,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G48234	TrGTerC	$\text{C8BCO2} \rightarrow \text{C89O2}$	k1_R02sR02	Rickard and Pascoe (2009)
G48235	TrGTerC	$\text{C8BCOOH} + \text{OH} \rightarrow \text{C8BCCO} + \text{OH}$	1.62E-11	Rickard and Pascoe (2009)
G48236	TrGTerCN	$\text{C8BCNO3} + \text{OH} \rightarrow \text{C8BCCO} + \text{NO}_2$	1.84E-12	Rickard and Pascoe (2009)
G48237	TrGTerC	$\text{C8BCCO} + \text{OH} \rightarrow \text{C89O2}$	3.94E-12	Rickard and Pascoe (2009)
G48238	TrGTerC	$\text{C89O2} + \text{HO}_2 \rightarrow \text{C89OOH}$	KR02H02(8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48239a	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C810O2} + \text{NO}_2$	$\text{KRO2N0} * (1 - \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G48239b	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C89NO3}$	$\text{KRO2N0} * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G48240	TrGTerCN	$\text{C89O2} + \text{NO}_3 \rightarrow \text{C810O2} + \text{NO}_2$	KRO2N03	Rickard and Pascoe (2009)
G48241	TrGTerC	$\text{C89O2} \rightarrow \text{C810O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G48242	TrGTerC	$\text{C89OOH} + \text{OH} \rightarrow \text{C89O2}$	3.61E-11	Rickard and Pascoe (2009)
G48243	TrGTerCN	$\text{C89NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	2.56E-11	Rickard and Pascoe (2009)
G48244	TrGTerC	$\text{C810O2} + \text{HO}_2 \rightarrow \text{C810OOH}$	KRO2H02(8)	Rickard and Pascoe (2009)
G48245a	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	$\text{KRO2N0} * (1 - \alpha_{\text{AN}}(10, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G48245b	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{C810NO3}$	$\text{KRO2N0} * \alpha_{\text{AN}}(10, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G48246	TrGTerCN	$\text{C810O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KRO2N03	Rickard and Pascoe (2009)
G48247	TrGTerC	$\text{C810O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G48248	TrGTerC	$\text{C810OOH} + \text{OH} \rightarrow \text{C810O2}$	8.35E-11	Rickard and Pascoe (2009)
G48249	TrGTerCN	$\text{C810NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	4.96E-11	Rickard and Pascoe (2009)
G48400a	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + \text{LCARBON} + 0.063 \text{ ALOV} + 0.424 \text{ ASOV}$	0.401E-11	Rickard and Pascoe (2009)*
G48400b	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{C6H5CH2O2} + \text{LCARBON}$	0.101E-11	Rickard and Pascoe (2009)*
G48400c	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{CRESOL} + \text{LCARBON}$	0.261E-11	Rickard and Pascoe (2009)*
G48400d	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLBIPERO2} + \text{HO}_2 + \text{LCARBON}$	0.932E-11	Rickard and Pascoe (2009)*
G48401	TrGAroCN	$\text{LXYL} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	3.9E-16	Rickard and Pascoe (2009)*
G48402	TrGAroC	$\text{EBENZ} + \text{OH} \rightarrow .10 \text{ TLEPOXMUC} + .07 \text{ C6H5CH2O2} + .18 \text{ CRESOL} + .65 \text{ TLBIPERO2} + .28 \text{ HO}_2 + \text{LCARBON}$	7.00E-12	Rickard and Pascoe (2009)*
G48403	TrGAroCN	$\text{EBENZ} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	1.20E-16	Rickard and Pascoe (2009)*
G48404	TrGAroCN	$\text{STYRENE} + \text{NO}_3 \rightarrow \text{NSTYRENO2}$	1.50E-12	Rickard and Pascoe (2009)
G48405	TrGAroC	$\text{STYRENE} + \text{O}_3 \rightarrow .545 \text{ HCHO} + .1 \text{ BENZENE} + .28 \text{ C6H5O2} + .56 \text{ CO} + .36 \text{ OH} + .28 \text{ HO}_2 + .075 \text{ PHCOOH} + .545 \text{ BENZAL} + .09 \text{ H}_2\text{O}_2 + .075 \text{ HCOOH} + .2 \text{ CO}_2$	1.70E-17	Rickard and Pascoe (2009)*
G48406	TrGAroC	$\text{STYRENE} + \text{OH} \rightarrow \text{STYRENO2}$	5.80E-11	Rickard and Pascoe (2009)
G48407	TrGAroCN	$\text{NSTYRENO2} + \text{HO}_2 \rightarrow \text{NSTYRENOOH}$	KRO2H02(8)	Rickard and Pascoe (2009)
G48408	TrGAroCN	$\text{NSTYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KRO2N0	Rickard and Pascoe (2009)*
G48409	TrGAroCN	$\text{NSTYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KRO2N03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G48410	TrGAroCN	NSTYRENO2 \rightarrow NO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
G48411	TrGAroCN	NSTYRENOOH + OH \rightarrow NSTYRENO2	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	STYRENO2 + HO ₂ \rightarrow STYRENOOH	KR02H02(8)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G48412b	TrGAroC	STYRENO2 + HO ₂ \rightarrow HO ₂ + OH + HCHO + BENZAL	KR02H02(8)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G48413	TrGAroCN	STYRENO2 + NO \rightarrow NO ₂ + HO ₂ + HCHO + BENZAL	KR02N0	Rickard and Pascoe (2009)*
G48414	TrGAroCN	STYRENO2 + NO ₃ \rightarrow NO ₂ + HO ₂ + HCHO + BENZAL	KR02N03	Rickard and Pascoe (2009)*
G48415	TrGAroC	STYRENO2 \rightarrow HO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
G48416	TrGAroC	STYRENOOH + OH \rightarrow STYRENO2	6.16E-11	Rickard and Pascoe (2009)
G49200	TrGTerC	C96O2 \rightarrow C97O2	k1_R02pR02	Rickard and Pascoe (2009)
G49201	TrGTerC	C96O2 + HO ₂ \rightarrow C96OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49202a	TrGTerCN	C96O2 + NO \rightarrow C97O2 + NO ₂	KR02N0*(1.-alpha_AN(10,1,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49202b	TrGTerCN	C96O2 + NO \rightarrow C96NO3	KR02N0*alpha_AN(10,1,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49203	TrGTerCN	C96NO3 + OH \rightarrow NORPINAL + NO ₂	2.88E-12	Rickard and Pascoe (2009)
G49204a	TrGTerC	C96OOH + OH \rightarrow C96O2	k_roohro	Rickard and Pascoe (2009)
G49205b	TrGTerC	C96OOH + OH \rightarrow NORPINAL + OH	1.30E-11	Rickard and Pascoe (2009)
G49206	TrGTerC	C97O2 \rightarrow C98O2	k1_R02tR02	Rickard and Pascoe (2009)
G49207	TrGTerCN	C97O2 + NO \rightarrow C98O2 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G49208a	TrGTerC	C97O2 + HO ₂ \rightarrow C97OOH	KR02H02(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G49208b	TrGTerC	C97O2 + HO ₂ \rightarrow C98O2 + OH	KR02H02(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G49209	TrGTerC	C97OOH + OH \rightarrow C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 \rightarrow C614O2 + CH ₃ COCH ₃	k1_R02tR02	Rickard and Pascoe (2009)
G49211a	TrGTerCN	C98O2 + NO \rightarrow C614O2 + CH ₃ COCH ₃ + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49211b	TrGTerCN	C98O2 + NO \rightarrow 9 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49212	TrGTerC	C98O2 + HO ₂ \rightarrow C98OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49213	TrGTerC	C98OOH + OH \rightarrow C98O2	2.05E-11	Rickard and Pascoe (2009)
G49214	TrGTerC	NORPINAL + OH \rightarrow C85CO3	2.64E-11	Rickard and Pascoe (2009)
G49215	TrGTerCN	NORPINAL + NO ₃ \rightarrow C85CO3 + HNO ₃	KN03AL*8.5	Rickard and Pascoe (2009)
G49216	TrGTerC	C85CO3 \rightarrow C85O2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G49217	TrGTerCN	C85CO3 + NO \rightarrow C85O2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49218	TrGTerCN	$\text{C85CO3} + \text{NO}_2 \rightarrow \text{C9PAN2}$	$k_{\text{CH3CO3_NO2}}$	Rickard and Pascoe (2009)
G49219a	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85CO3H}$	$\text{KAPH02}*(\text{rco3_ooh}+\text{rco3_o3})$	Rickard and Pascoe (2009)
G49219b	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*\text{rco3_oh}$	Rickard and Pascoe (2009)
G49220	TrGTerCN	$\text{C9PAN2} \rightarrow \text{C85CO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G49221	TrGTerCN	$\text{C9PAN2} + \text{OH} \rightarrow \text{C85OOH} + \text{CO} + \text{NO}_2$	6.60E-12	Rickard and Pascoe (2009)
G49222	TrGTerC	$\text{C85CO3H} + \text{OH} \rightarrow \text{C85CO3}$	1.02E-11	Rickard and Pascoe (2009)
G49223a	TrGTerC	$\text{C89CO3} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	$k1_{\text{R02RC03}*0.9}$	Sander et al. (2018)
G49223b	TrGTerC	$\text{C89CO3} \rightarrow \text{C89CO2H}$	$k1_{\text{R02RC03}*0.1}$	Sander et al. (2018)
G49224a	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO3H}$	$\text{KAPH02}*\text{rco3_ooh}$	Rickard and Pascoe (2009)
G49224b	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO2H} + \text{O}_3$	$\text{KAPH02}*\text{rco3_o3}$	Rickard and Pascoe (2009)
G49224c	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow .80 \text{ C811CO3} + .20 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	$\text{KAPH02}*\text{rco3_oh}$	Rickard and Pascoe (2009)
G49225	TrGTerCN	$\text{C89CO3} + \text{NO}_2 \rightarrow \text{C89PAN}$	$k_{\text{CH3CO3_NO2}}$	Rickard and Pascoe (2009)
G49226	TrGTerCN	$\text{C89CO3} + \text{NO} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G49227	TrGTerC	$\text{C89CO2H} + \text{OH} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	2.69E-11	Rickard and Pascoe (2009)
G49228	TrGTerC	$\text{C89CO3H} + \text{OH} \rightarrow \text{C89CO3}$	3.00E-11	Rickard and Pascoe (2009)
G49229	TrGTerCN	$\text{C89PAN} \rightarrow \text{C89CO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G49230	TrGTerCN	$\text{C89PAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{CO} + \text{NO}_2$	2.52E-11	Rickard and Pascoe (2009)
G49231a	TrGTerC	$\text{C811CO3} \rightarrow \text{C811O2} + \text{CO}_2$	$k1_{\text{R02RC03}*0.9}$	Sander et al. (2018)
G49231b	TrGTerC	$\text{C811CO3} \rightarrow \text{PINIC}$	$k1_{\text{R02RC03}*0.1}$	Sander et al. (2018)
G49232a	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811CO3H}$	$\text{KAPH02}*\text{rco3_ooh}$	Rickard and Pascoe (2009)
G49232b	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{PINIC} + \text{O}_3$	$\text{KAPH02}*\text{rco3_o3}$	Rickard and Pascoe (2009)
G49232c	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*\text{rco3_oh}$	Rickard and Pascoe (2009)
G49233	TrGTerCN	$\text{C811CO3} + \text{NO} \rightarrow \text{C811O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G49234	TrGTerCN	$\text{C811CO3} + \text{NO}_2 \rightarrow \text{C811PAN}$	$k_{\text{CH3CO3_NO2}}$	Rickard and Pascoe (2009)
G49235	TrGTerC	$\text{PINIC} + \text{OH} \rightarrow \text{C811O2} + \text{CO}_2$	7.29E-12	Rickard and Pascoe (2009)
G49236	TrGTerC	$\text{NOPINONE} + \text{OH} \rightarrow \text{NOPINDO2}$	1.55E-11	Capouet et al. (2008), Rickard and Pascoe (2009)
G49237a	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{NOPINDOOH}$	$\text{KR02H02(9)}*\text{rcoch2o2_ooh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	$\text{KR02H02(9)}*\text{rcoch2o2_oh}$	Rickard and Pascoe (2009), Sander et al. (2018)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G49239	TrGTerC	NOPINDO2 \rightarrow C89CO3	k1_R02p0R02	Rickard and Pascoe (2009)
G49240	TrGTerC	NOPINDOOH \rightarrow NOPINDCO	2.63E-11	Rickard and Pascoe (2009)
G49241	TrGTerC	NOPINDCO + OH \rightarrow C89CO3	3.07E-12	Rickard and Pascoe (2009)
G49242	TrGTerC	NOPINOO \rightarrow NOPINONE + H ₂ O ₂	6.00E-18*c(ind_H2O)	Rickard and Pascoe (2009)
G49243	TrGTerC	NOPINOO + CO \rightarrow NOPINONE + CO ₂	1.2E-15	Rickard and Pascoe (2009)
G49244	TrGTerCN	NOPINOO + NO \rightarrow NOPINONE + NO ₂	1.E-14	Rickard and Pascoe (2009)
G49245	TrGTerCN	NOPINOO + NO ₂ \rightarrow NOPINONE + NO ₃	1.E-15	Rickard and Pascoe (2009)
G49246	TrGTerC	NORPINENOL + OH \rightarrow HCOOH + OH + C86O2	k_CH2CHOH_OH_HCOOH	Sander et al. (2018), So et al. (2014)*
G49247	TrGTerC	NORPINENOL + HCOOH \rightarrow NORPINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G49248	TrGTerC	NORPINAL + HCOOH \rightarrow NORPINENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G49249	TrGTerC	C811CO3H + OH \rightarrow C811CO3	1.04E-11	Rickard and Pascoe (2009)
G49250	TrGTerCN	C811PAN \rightarrow C811CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	C811PAN + OH \rightarrow C721CHO + CO + NO ₂	6.77E-12	Rickard and Pascoe (2009)
G49400a	TrGAroC	LTMB + OH \rightarrow TLBIPERO2 + HO ₂ + 2 LCARBON + .04 ALOV	2.917E-11	Rickard and Pascoe (2009)*
G49400b	TrGAroC	LTMB + OH \rightarrow C6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard and Pascoe (2009)*
G49400c	TrGAroC	LTMB + OH \rightarrow CRESOL + 2 LCARBON	0.141E-11	Rickard and Pascoe (2009)*
G49400d	TrGAroC	LTMB + OH \rightarrow TLBIPERO2 + HO ₂ + 2 LCARBON	2.917E-11	Rickard and Pascoe (2009)*
G49401	TrGAroCN	LTMB + NO ₃ \rightarrow C6H5CH2O2 + HNO ₃ + 2 LCARBON	1.52E-15	Rickard and Pascoe (2009)*
G40200	TrGTerC	APINENE + OH \rightarrow .75 LAPINABO2 + .15 MENTHEN6ONE + .15 HO ₂ + .10 ROO6R1O2	1.2E-11*EXP(440./TEMP)	Atkinson et al. (2006)*
G40201a	TrGTerCN	LAPINABO2 + NO \rightarrow PINAL + HO ₂ + NO ₂ + 0.052 BLOV + 0.184 BSOV	KR02N0*(1-(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)))	Rickard and Pascoe (2009), Sander et al. (2018)
G40201b	TrGTerCN	LAPINABO2 + NO \rightarrow LAPINABNO3	KR02N0*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2018)
G40202a	TrGTerC	LAPINABO2 + HO ₂ \rightarrow LAPINABOOH	KR02H02(10)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009), Sander et al. (2018)
G40202b	TrGTerC	LAPINABO2 + HO ₂ \rightarrow PINAL + HO ₂ + OH	(1-ya_soan1-ya_soan2)*KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G40203	TrGTerC	LAPINABO2 \rightarrow PINAL + HO ₂	R02*(0.65*k1_R02t0R02+.35*k1_R02s0R02)	Rickard and Pascoe (2009)*
G40204	TrGTerC	LAPINABOOH + OH \rightarrow .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard and Pascoe (2009)*
G40205	TrGTerCN	LAPINABNO3 + OH \rightarrow .35 PINAL + .65 C96CO3 + NO ₂	4.29E-12	Rickard and Pascoe (2009)*
G40206	TrGTerC	MENTHEN6ONE + OH \rightarrow OHMENTHEN6ONEO2	6.46E-11	Vereecken et al. (2007)*
G40207	TrGTerCN	OHMENTHEN6ONEO2 + NO \rightarrow 2OHMENTHEN6ONE + HO ₂ + NO ₂	KR02N0	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO ₂ \rightarrow 2OHMENTHEN6ONE	KR02H02(10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 \rightarrow 2OHMENTHEN6ONE + HO ₂	k1_R02t0R02	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH \rightarrow 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH \rightarrow .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./TEMP)	Wallington et al. (2018)*
G40212	TrGTerCN	PINAL + NO ₃ \rightarrow C96CO3 + HNO ₃	2.0E-14	Wallington et al. (2018)*
G40213a	TrGTerC	C96CO3 \rightarrow C96O2 + CO ₂	k1_R02RC03*0.9	Rickard and Pascoe (2009)
G40213b	TrGTerC	C96CO3 \rightarrow PINONIC	k1_R02RC03*0.1	Rickard and Pascoe (2009)
G40214a	TrGTerC	C96CO3 + HO ₂ \rightarrow PERPINONIC	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO ₂ \rightarrow PINONIC + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO ₂ \rightarrow C96O2 + OH + CO ₂	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G40215	TrGTerCN	C96CO3 + NO ₂ \rightarrow C10PAN2	k_CH3C03_N02	Rickard and Pascoe (2009)
G40216	TrGTerCN	C96CO3 + NO \rightarrow C96O2 + NO ₂ + CO ₂	KAPN0	Rickard and Pascoe (2009)
G40217	TrGTerCN	C96CO3 + NO ₃ \rightarrow C96O2 + NO ₂ + CO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G40218	TrGTerCN	C10PAN2 \rightarrow C96CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G40219	TrGTerCN	C10PAN2 + OH \rightarrow NORPINAL + CO + NO ₂	3.66E-12	Rickard and Pascoe (2009)
G40220	TrGTerC	PINONIC + OH \rightarrow C96O2 + CO ₂	6.65E-12	Rickard and Pascoe (2009)
G40221	TrGTerC	PERPINONIC + OH \rightarrow C96CO3	9.73E-12	Rickard and Pascoe (2009)
G40222	TrGTerC	PINALO2 + HO ₂ \rightarrow PINALOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40223a	TrGTerCN	PINALO2 + NO \rightarrow C106O2 + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2018)
G40223b	TrGTerCN	PINALO2 + NO \rightarrow PINALNO3	KR02N0*alpha_AN(12,3,0,1,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2018)
G40224	TrGTerC	PINALO2 \rightarrow C106O2	k1_R02tR02	Rickard and Pascoe (2009)
G40225	TrGTerC	PINALOOH + OH \rightarrow PINALO2	2.75E-11	Rickard and Pascoe (2009)
G40226	TrGTerCN	PINALNO3 + OH \rightarrow CO235C6CHO + CH ₃ COCH ₃ + NO ₂	2.25E-11	Rickard and Pascoe (2009)
G40227	TrGTerC	C106O2 + HO ₂ \rightarrow C106OOH	KR02H02(10)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40228a	TrGTerCN	$\text{C106O2} + \text{NO} \rightarrow \text{C716O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$\text{KR02N0} * 0.875 * (1 - \alpha_{\text{AN}}(13, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2018)
G40228b	TrGTerCN	$\text{C106O2} + \text{NO} \rightarrow \text{C106NO3}$	$\text{KR02N0} * 0.875 * \alpha_{\text{AN}}(13, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009), Sander et al. (2018)
G40229	TrGTerC	$\text{C106O2} \rightarrow \text{C716O2} + \text{CH}_3\text{COCH}_3$	$k1_R02tR02$	Rickard and Pascoe (2009)
G40230	TrGTerC	$\text{C106OOH} + \text{OH} \rightarrow \text{C106O2}$	$8.01\text{E-}11$	Rickard and Pascoe (2009)
G40231	TrGTerCN	$\text{C106NO3} + \text{OH} \rightarrow \text{CO235C6CHO} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$7.03\text{E-}11$	Rickard and Pascoe (2009)
G40232	TrGTerC	$\text{APINENE} + \text{O}_3 \rightarrow .09 \text{ APINBOO} + .08 \text{ PINONIC} + .77 \text{ OH} + .33 \text{ NORPINAL} + .33 \text{ CO} + .33 \text{ HO}_2 + .06 \text{ APINAOO} + .44 \text{ C109O2} + 0.07 \text{ BELV} + 0.13 \text{ BLOV}$	$8.05\text{E-}16 * \text{EXP}(-640./\text{TEMP})$	Wallington et al. (2018), Ehn et al. (2014)*
G40233	TrGTerC	$\text{APINAOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * c(\text{ind_H2O})$	Rickard and Pascoe (2009)
G40234	TrGTerC	$\text{APINAOO} + \text{CO} \rightarrow \text{PINAL} + \text{CO}_2$	$1.20\text{E-}15$	Rickard and Pascoe (2009)
G40235	TrGTerCN	$\text{APINAOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2 + 0.052 \text{ BLOV} + 0.184 \text{ BSOV}$	$1.00\text{E-}14$	Rickard and Pascoe (2009)
G40236	TrGTerCN	$\text{APINAOO} + \text{NO}_2 \rightarrow \text{PINAL} + \text{NO}_3$	$1.00\text{E-}15$	Rickard and Pascoe (2009)
G40237a	TrGTerC	$\text{APINBOO} \rightarrow \text{PINONIC}$	$1.00\text{E-}17 * c(\text{ind_H2O}) * (0.08 + 0.15)$	Rickard and Pascoe (2009)
G40237b	TrGTerC	$\text{APINBOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * c(\text{ind_H2O}) * 0.77$	Rickard and Pascoe (2009)
G40238	TrGTerC	$\text{APINBOO} + \text{CO} \rightarrow \text{PINAL} + \text{CO}_2$	$1.20\text{E-}15$	Rickard and Pascoe (2009)
G40239	TrGTerCN	$\text{APINBOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2 + 0.052 \text{ BLOV} + 0.184 \text{ BSOV}$	$1.00\text{E-}14$	Rickard and Pascoe (2009)
G40240	TrGTerCN	$\text{APINBOO} + \text{NO}_2 \rightarrow \text{PINAL} + \text{NO}_3$	$1.00\text{E-}15$	Rickard and Pascoe (2009)
G40241	TrGTerC	$\text{C109O2} \rightarrow \text{C89CO3} + \text{HCHO}$	$k1_R02p0R02$	Rickard and Pascoe (2009)
G40242	TrGTerCN	$\text{C109O2} + \text{NO} \rightarrow \text{C89CO3} + \text{HCHO} + \text{NO}_2 + 0.052 \text{ BLOV} + 0.184 \text{ BSOV}$	KR02N0	Rickard and Pascoe (2009)*
G40243a	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C109OOH}$	$\text{KR02H02}(10) * r_{\text{coch2o2_ooh}}$	Rickard and Pascoe (2009), Sander et al. (2018)
G40243b	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{HCHO} + \text{OH}$	$(1 - y_{\text{a_soan1}} - y_{\text{a_soan2}}) * \text{KR02H02}(10) * r_{\text{coch2o2_oh}}$	Rickard and Pascoe (2009), Sander et al. (2018)
G40244	TrGTerC	$\text{C109OOH} + \text{OH} \rightarrow \text{C109CO} + \text{OH}$	$5.47\text{E-}11$	Rickard and Pascoe (2009)
G40245	TrGTerC	$\text{C109CO} + \text{OH} \rightarrow \text{C89CO3} + \text{CO}$	$5.47\text{E-}11$	Rickard and Pascoe (2009)
G40246	TrGTerCN	$\text{APINENE} + \text{NO}_3 \rightarrow \text{LNAPINABO2}$	$1.2\text{E-}12 * \text{EXP}(490./\text{temp})$	Wallington et al. (2018)*
G40247	TrGTerCN	$\text{LNAPINABO2} \rightarrow \text{PINAL} + \text{NO}_2$	$(0.65 * k1_R02tR02 + 0.35 * k1_R02sR02)$	Rickard and Pascoe (2009)
G40248	TrGTerCN	$\text{LNAPINABO2} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G40249	TrGTerCN	$\text{LNAPINABO2} + \text{HO}_2 \rightarrow \text{LNAPINABOOH}$	$\text{KR02H02}(10)$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40250	TrGTerCN	LNAPINABO2 + NO ₃ → PINAL + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G40251	TrGTerCN	LNAPINABOOH + OH → LNAPINABO2	(.65*6.87E-12+.35*1.23E-11)	Rickard and Pascoe (2009)
G40252a	TrGTerC	BPINENE + OH → BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40252b	TrGTerC	BPINENE + OH → ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO ₂ → BPINAOOH	KR02H02(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Sander et al. (2018)
G40253b	TrGTerC	BPINAO2 + HO ₂ → NOPINONE + HCHO + HO ₂ + OH	(1-ya_soan1-ya_soan2) *KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40254a	TrGTerCN	BPINAO2 + NO → NOPINONE + HCHO + HO ₂ + NO ₂ + 0.052 BLOV + 0.184 BSOV	KR02N0*(1.-alpha_AN(11,3,0,0,0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2018)
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KR02N0*alpha_AN(11,3,0,0,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2018)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO ₂	k1_R02t0R02	Rickard and Pascoe (2009)
G40256	TrGTerC	BPINAOOH + OH → BPINAO2	1.33E-11	Rickard and Pascoe (2009)
G40257	TrGTerCN	BPINANO3 + OH → NOPINONE + HCHO + NO ₂	4.70E-12	Rickard and Pascoe (2009)
G40258a	TrGTerCN	ROO6R1O2 + NO → ROO6R3O2 + CH ₃ COCH ₃ + NO ₂ + 0.052 BLOV + 0.184 BSOV	KR02N0*(1.-alpha_AN(13,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO → ROO6R1NO3	KR02N0*alpha_AN(13,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40260	TrGTerC	ROO6R1O2 → ROO6R3O2 + CH ₃ COCH ₃	k1_R02t0R02	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO → RO6R3O2 + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO → RO6R1NO3	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO ₂ → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 → RO6R3O2	k1_R02s0R02	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO → 9 LCARBON + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40264b	TrGTerCN	RO6R3O2 + NO → 10 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO ₂ → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)
G40266	TrGTerC	RO6R3O2 → 9 LCARBON + HCHO + HO ₂	k1_R02sR02	Vereecken and Peeters (2012)*

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

#	labels	reaction	rate coefficient	reference
G40267a	TrGTerC	BPINENE + O ₃ → NOPINONE + .63 CO + .37 CH ₂ OO + .16 OH + .16 HO ₂ + 0.07 BELV + 0.13 BLOV	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	Wallington et al. (2018)*
G40267b	TrGTerC	BPINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267c	TrGTerC	BPINENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267d	TrGTerC	BPINENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) * (.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40268	TrGTerCN	BPINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40269	TrGTerCN	LNBPINABO2 + HO ₂ → LNBPINABOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40270	TrGTerCN	LNBPINABO2 + NO → NOPINONE + HCHO + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G40271	TrGTerCN	LNBPINABO2 + NO ₃ → NOPINONE + HCHO + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G40272a	TrGTerCN	LNBPINABO2 → NOPINONE + HCHO + NO ₂	k1_R02tR02*0.7	Rickard and Pascoe (2009)
G40272b	TrGTerCN	LNBPINABO2 → BPINAN03	k1_R02tR02*0.3	Rickard and Pascoe (2009)
G40273	TrGTerCN	LNBPINABOOH + OH → LNBPINABO2	9.58E-12	Rickard and Pascoe (2009)
G40274	TrGTerCN	ROO6R1NO3 + OH → ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40275	TrGTerCN	RO6R1NO3 + OH → 9 LCARBON + HCHO + HO ₂ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)
G40276	TrGTerC	PINEOL + OH → HCOOH + OH + NORPINAL	k_CH2CHOH_OH_HCOOH	Sander et al. (2018), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH → PINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2018), da Silva (2010)*
G40278	TrGTerC	PINAL + HCOOH → PINEOL + HCOOH	k_ALD_HCOOH	Sander et al. (2018), da Silva (2010)*
G40279a	TrGC	CARENE + OH → LAPINABO2	8.8E-11*(.50+.25)	Atkinson and Arey (2003)
G40279b	TrGC	CARENE + OH → MENTHEN6ONE + HO ₂	8.8E-11*.25*.60	Atkinson and Arey (2003)
G40279c	TrGC	CARENE + OH → ROO6R1O2	8.8E-11*.25*.40	Atkinson and Arey (2003)
G40280a	TrGC	CARENE + O ₃ → APINBOO	3.7E-17*.50*.18	Atkinson and Arey (2003)
G40280b	TrGC	CARENE + O ₃ → PINONIC	3.7E-17*.50*.16	Atkinson and Arey (2003)
G40280c	TrGC	CARENE + O ₃ → OH + NORPINAL + CO + HO ₂	3.7E-17*.50*.66	Atkinson and Arey (2003)
G40280d	TrGC	CARENE + O ₃ → APINAOO	3.7E-17*.50*.12	Atkinson and Arey (2003)
G40280e	TrGC	CARENE + O ₃ → OH + C109O2	3.7E-17*.50*(.22+.66)	Atkinson and Arey (2003)

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

#	labels	reaction	rate coefficient	reference
G40281	TrGCN	CARENE + NO ₃ → LNAPINABO2	9.1E-12	Atkinson and Arey (2003)
G40282a	TrGTerC	SABINENE + OH → BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40282b	TrGTerC	SABINENE + OH → ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40283a	TrGTerC	SABINENE + O ₃ → NOPINONE + .63 CO + .37 HOCH ₂ OOH + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	Wallington et al. (2018)*
G40283b	TrGTerC	SABINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283c	TrGTerC	SABINENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283d	TrGTerC	SABINENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40284	TrGTerCN	SABINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40285a	TrGTerC	CAMPHENE + OH → BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40285b	TrGTerC	CAMPHENE + OH → ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40286a	TrGTerC	CAMPHENE + O ₃ → NOPINONE + .63 CO + .37 HOCH ₂ OOH + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	Wallington et al. (2018)*
G40286b	TrGTerC	CAMPHENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286c	TrGTerC	CAMPHENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286d	TrGTerC	CAMPHENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40287	TrGTerCN	CAMPHENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40400	TrGAroC	LHAROM + OH → .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + .18 HO ₂ + 4 LCARBON	5.67E-11	Rickard and Pascoe (2009)*
G40401	TrGAroCN	LHAROM + NO ₃ → C6H5CH2O2 + HNO ₃ + 4 LCARBON	2.60E-15	Rickard and Pascoe (2009)*
G6100	UpStTrGCl	Cl + O ₃ → ClO + O ₂	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl ₂ + O ₂	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O ₂	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 2 \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Burkholder et al. (2015)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C(O)}$	$8.0\text{e-}11$	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{LCARBON} + \text{CH}_3 + \text{HCl}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 6.1\text{e-}30, 3.0, 2.0\text{e-}10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$8.3\text{E-}11*\text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
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)
G6416	TrGCCIN	$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{NCCH}_2\text{O}_2 + \text{HCl}$	$1.6\text{E-}11*\text{EXP}(-2104./\text{temp})$	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2018)
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	$\text{OIO} + \text{OIO} \rightarrow \text{I}(\text{part})$	$5.\text{E-}11$	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)
G8201	TrGI	$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	$1.4\text{E-}11*\text{EXP}(540./\text{temp})$	Atkinson et al. (2007)
G8202	TrGI	$\text{HI} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O}$	$1.6\text{E-}11*\text{EXP}(440./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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)
G8205	TrGI	$\text{HOI} + \text{OH} \rightarrow \text{IO} + \text{H}_2\text{O}$	$5.0\text{E-}12$	Riffault et al. (2005)
G8300	TrGIN	$\text{I} + \text{NO}_2 \rightarrow \text{INO}_2$	$k_{\text{I_NO2}}$	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	$\text{IO} + \text{NO}_2 \rightarrow \text{INO}_3$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 7.7\text{E-}31, 5., 1.6\text{E-}11, 0., 0.4)$	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	$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	$k_{\text{I_NO2}} / (3.7\text{E-}7 \cdot \text{EXP}(9568./\text{temp}) \cdot 1.\text{E6} \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm2Pa} \cdot N_{\text{A}}))$	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGIN	$\text{INO}_3 \rightarrow \text{IO} + \text{NO}_2$	$2.1\text{e}15 \cdot \text{EXP}(-13670./\text{temp})$	Kaltsayannis and Plane (2008)
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)
G8309	TrGIN	$\text{I} + \text{INO}_3 \rightarrow \text{I}_2 + \text{NO}_3$	$9.1\text{E-}11 \cdot \text{EXP}(-146./\text{temp})$	Kaltsayannis and Plane (2008)
G8400	TrGCI	$\text{CH}_3\text{CHICH}_3 + \text{OH} \rightarrow 2 \text{LCARBON} + \text{CH}_3\text{O}_2 + \text{I}$	$1.22\text{E-}12$	Carl and Crowley (2001)
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. (2006b), 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	TrGCI	$\text{IO} + \text{ClO} \rightarrow .2 \text{ICl} + .25 \text{Cl} + .55 \text{OCIO} + .8 \text{I} + .45 \text{O}_2$	$4.7\text{E-}12 \cdot \text{EXP}(280./\text{temp})$	Atkinson et al. (2007)
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{HSO}_3$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.\text{E-}31, -3.3, 1.5\text{E-}12, 0., 0.6)$	Burkholder et al. (2015)
G9201	StTrGS	$\text{HSO}_3 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_3$	$1.3\text{E-}12 \cdot \exp(-330/\text{temp})$	Burkholder et al. (2015)
G9202	StTrGS	$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$	$2.4\text{E-}15$	Reiner and Arnold (1993)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SCH}_2 + \text{H}_2\text{O}$	$1.13\text{E-}11 \cdot \text{EXP}(-253./\text{temp})$	Hynes and Wine (1996)
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{DMSOH} + \text{HO}_2$	$k_{\text{DMS_OH}}$	Hynes and Wine (1996)
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SCH}_2 + \text{HNO}_3$	$1.9\text{E-}13 \cdot \text{EXP}(520./\text{temp})$	Karl et al. (2007)
G9402a	TrGCS	$\text{DMSO} + \text{OH} \rightarrow \text{DMSOHO}$	$k_{\text{DMSO_OH_B1}}$	Karl et al. (2007)
G9402b	TrGCS	$\text{DMSO} + \text{OH} \rightarrow \text{CH}_3\text{SOCH}_2 + \text{H}_2\text{O}$	$k_{\text{DMSO_OH_B2}}$	Karl et al. (2007)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.0\text{E}13 \cdot \text{EXP}((-16500. \cdot f_{\text{ch3so2}} / 1.98635) / \text{temp})$	Karl et al. (2007)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3 + \text{O}_2$	$k_{\text{CH3SO2_O3}}$	Karl et al. (2007)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H} + \text{O}_2$	$k_{\text{CH3SO3_HO2}}$	Karl et al. (2007)
G9408	StTrGS	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	$k_{\text{CH200_SO2}}$	Welz et al. (2012), Stone et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
G9409	TrGTerCS	$\text{NOPINOO} + \text{SO}_2 \rightarrow \text{NOPINONE} + \text{H}_2\text{SO}_4$	7.E-14	Rickard and Pascoe (2009)
G9410	TrGTerCS	$\text{APINAOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G9411	TrGTerCS	$\text{APINBOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G9412	TrGTerCS	$\text{MBOOO} + \text{SO}_2 \rightarrow \text{IBUTALOH} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G9420aMK	TrGCS	$\text{DMSOH} + \text{O}_2 \rightarrow \text{DMSO} + \text{HO}_2$	5.0E-13	Karl et al. (2007)
G9420bMK	TrGCS	$\text{DMSOH} + \text{O}_2 \rightarrow \text{DMSOHOO}$	3.0E-14	Karl et al. (2007)
G9421MK	TrGCS	$\text{DMSOH} \rightarrow \text{CH}_3\text{SOH} + \text{CH}_3\text{O}_2$	5.0E+5	Karl et al. (2007)
G9422MK	TrGCNS	$\text{DMSOHOO} + \text{NO} \rightarrow \text{DMSOHO} + \text{NO}_2$	5.0E-12	Karl et al. (2007)
G9423MK	TrGCS	$\text{DMSOHO} + \text{O}_2 \rightarrow \text{DMSO}_2 + \text{HO}_2$	1.0E-13	Karl et al. (2007)
G9424MK	TrGCS	$\text{DMSOHO} \rightarrow \text{CH}_3\text{SOOH} + \text{CH}_3\text{O}_2$	6.0E+5	Karl et al. (2007)
G9425MK	TrGCS	$\text{CH}_3\text{SOCH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{SOCH}_2\text{O}_2$	0.5E-13	Karl et al. (2007)
G9426MK	TrGCNS	$\text{CH}_3\text{SOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{SO} + \text{HCHO} + \text{NO}_2$	1.0E-11	Karl et al. (2007)
G9427MK	TrGCS	$\text{CH}_3\text{SCH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{SCH}_2\text{OO}$	5.7E-12	Karl et al. (2007)
G9428MK	TrGCNS	$\text{CH}_3\text{SCH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{CH}_3\text{S} + \text{NO}_2$	1.9E-11	Karl et al. (2007)
G9429MK	TrGCS	$\text{CH}_3\text{SCH}_2\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{SCH}_2\text{OOH} + \text{O}_2$	1.5E-12	Karl et al. (2007)
G9430MK	TrGCS	$\text{CH}_3\text{SCH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{S} + 2 \text{HCHO} + \text{HO}_2$	1.8E-13	Karl et al. (2007)
G9431MK	TrGS	$\text{CH}_3\text{S} + \text{O}_3 \rightarrow \text{CH}_3\text{SO} + \text{O}_2$	$1.36\text{E-12} \cdot \text{EXP}(374./\text{temp})$	Karl et al. (2007)
G9432MK	TrGNS	$\text{CH}_3\text{S} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO} + \text{NO}$	$2.8\text{E-11} \cdot \text{EXP}(240./\text{temp})$	Karl et al. (2007)
G9433aMK	TrGS	$\text{CH}_3\text{S} + \text{O}_2 \rightarrow \text{CH}_3\text{SOO}$	1.5E-14	Karl et al. (2007)
G9433bMK	TrGS	$\text{CH}_3\text{S} + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2$	3.0E-18	Karl et al. (2007)
G9434MK	TrGS	$\text{CH}_3\text{S} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO} + \text{HCHO} + \text{HO}_2$	6.1E-11	Karl et al. (2007)
G9435MK	TrGS	$\text{CH}_3\text{SO} + \text{O}_3 \rightarrow 0.5 \text{CH}_3\text{SO}_2 + 0.5 \text{O}_2 + 0.5 \text{CH}_3\text{O}_2 + 0.5 \text{SO}_2$	3.2E-13	Karl et al. (2007)
G9436aMK	TrGNS	$\text{CH}_3\text{SO} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{NO}$	$1.2\text{E-11} \cdot 0.75$	Cala et al. (2023)
G9436bMK	TrGNS	$\text{CH}_3\text{SO} + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2 + \text{NO}$	$1.2\text{E-11} \cdot 0.25$	Cala et al. (2023)
G9437MK	TrGS	$\text{CH}_3\text{SO} + \text{O}_2 \rightarrow \text{CH}_3\text{SOO}_2$	7.7E-18	Karl et al. (2007)
G9438MK	TrGS	$\text{CH}_3\text{SO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO} + \text{HO}_2$	3.0E-12	Karl et al. (2007)
G9439MK	TrGS	$\text{CH}_3\text{SOH} + \text{OH} \rightarrow \text{CH}_3\text{SO} + \text{H}_2\text{O}$	1.10E-10	Karl et al. (2007)
G9440MK	TrGNS	$\text{CH}_3\text{SOH} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO} + \text{HNO}_3$	3.4E-12	Karl et al. (2007)
G9441MK	TrGS	$\text{CH}_3\text{SOH} + \text{HO}_2 \rightarrow \text{CH}_3\text{SO} + \text{H}_2\text{O}_2$	8.5E-13	Karl et al. (2007)
G9442MK	TrGS	$\text{CH}_3\text{SOH} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO} + \text{CH}_3\text{OOH}$	8.5E-13	Karl et al. (2007)
G9443MK	TrGS	$\text{CH}_3\text{SOO} + \text{O}_3 \rightarrow \text{CH}_3\text{SO} + 2\text{O}_2$	8.0E-13	Karl et al. (2007)
G9444MK	TrGNS	$\text{CH}_3\text{SOO} + \text{NO} \rightarrow \text{CH}_3\text{SO} + \text{NO}_2$	1.1E-11	Karl et al. (2007)
G9445MK	TrGS	$\text{CH}_3\text{SOO} + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2$	2.0E-17	Karl et al. (2007)
G9446aMK	TrGS	$\text{CH}_3\text{SOO} \rightarrow \text{CH}_3\text{S} + \text{O}_2$	$3.50\text{E+10} \cdot \text{EXP}(-3560./\text{temp})$	Cala et al. (2023)

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

#	labels	reaction	rate coefficient	reference
G9446bMK	TrGS	$\text{CH}_3\text{SOO} \rightarrow \text{CH}_3\text{O}_2 + \text{SO}_2$	$5.60\text{E}+16*\text{EXP}(-10870./\text{temp})$	Cala et al. (2023)
G9447MK	TrGS	$\text{CH}_3\text{SOO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO} + \text{HCHO} + \text{HO}_2$	$5.5\text{E}-12$	Karl et al. (2007)
G9448MK	TrGS	$\text{CH}_3\text{SOOH} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{H}_2\text{O}$	$k_{\text{MSIA_OH}}$	Karl et al. (2007)
G9449MK	TrGNS	$\text{CH}_3\text{SOOH} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3$	$1.0\text{E}-13$	Karl et al. (2007)
G9450MK	TrGS	$\text{CH}_3\text{SOOH} + \text{HO}_2 \rightarrow \text{CH}_3\text{SOO} + \text{H}_2\text{O}_2$	$1.0\text{E}-15$	Karl et al. (2007)
G9451MK	TrGS	$\text{CH}_3\text{SOOH} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{CH}_3\text{OOH}$	$1.0\text{E}-15$	Karl et al. (2007)
G9452MK	TrGS	$\text{CH}_3\text{SO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{OH}$	$2.5\text{E}-13$	Karl et al. (2007)
G9453MK	TrGNS	$\text{CH}_3\text{SO}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{NO}$	$2.2\text{E}-11$	Karl et al. (2007)
G9454MK	TrGS	$\text{CH}_3\text{SO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{HCHO} + \text{HO}_2$	$2.5\text{E}-13$	Karl et al. (2007)
G9455MK	TrGNS	$\text{CH}_3\text{SO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{SOO}_2\text{NO}_2$	$3.0\text{E}-15$	Karl et al. (2007)
G9456MK	TrGS	$\text{CH}_3\text{SO}_3 \rightarrow \text{SO}_3 + \text{CH}_3\text{O}_2$	$k_{\text{CH3S03_dec}}$	Cala et al. (2023)
G9457MK	TrGNS	$\text{CH}_3\text{SOO}_2 + \text{NO} \rightarrow \text{CH}_3\text{SO}_2 + \text{NO}_2$	$1.0\text{E}-11$	Karl et al. (2007)
G9458MK	TrGS	$\text{CH}_3\text{SOO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{SOO}_2\text{H} + \text{O}_2$	$3.0\text{E}-12$	Karl et al. (2007)
G9459MK	TrGS	$\text{CH}_3\text{SOO}_2 \rightarrow \text{CH}_3\text{SO} + \text{O}_2$	$170.$	Karl et al. (2007)
G9460MK	TrGS	$\text{CH}_3\text{SOO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO} + \text{HO}_2$	$5.5\text{E}-12$	Karl et al. (2007)
G9461MK	TrGNS	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{SO}_3 + \text{NO}_2$	$1.0\text{E}-11$	Karl et al. (2007)
G9462MK	TrGS	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_4\text{H}$	$2.0\text{E}-12$	Karl et al. (2007)
G9463MK	TrGS	$\text{CH}_3\text{SO}_2\text{O}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{O}_2$	$170.$	Karl et al. (2007)
G9464MK	TrGS	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{HCHO} + \text{HO}_2$	$5.5\text{E}-12$	Karl et al. (2007)
G9465MK	TrGNS	$\text{CH}_3\text{SO}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_2\text{O}_2\text{NO}_2$	$5.89\text{E}-12$	Karl et al. (2007)
G9466MK	TrGNS	$\text{CH}_3\text{SOO}_2\text{NO}_2 \rightarrow \text{CH}_3\text{SO}_3 + \text{NO}_2$	$1.15\text{E}-2$	Karl et al. (2007)
G9467MK	TrGNS	$\text{CH}_3\text{SO}_2\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{SO}_2\text{O}_2 + \text{NO}_2$	$1.15\text{E}-2$	Karl et al. (2007)
G9468MK	TrGCS	$\text{DMSO}_2 + \text{OH} \rightarrow \text{DMSO}_2\text{OO}$	$k_{\text{DMS02_OH}}$	Karl et al. (2007)
G9469MK	TrGCNS	$\text{DMSO}_2\text{OO} + \text{NO} \rightarrow \text{DMSO}_2\text{O} + \text{NO}_2$	$5.0\text{E}-12$	Karl et al. (2007)
G9470MK	TrGCS	$\text{DMSO}_2\text{OO} + \text{HO}_2 \rightarrow \text{DMSO}_2\text{OOH} + \text{O}_2$	$1.5\text{E}-12$	Karl et al. (2007)
G9471MK	TrGCS	$\text{DMSO}_2\text{O} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.0\text{E}+1$	Karl et al. (2007)
G9474MK	TrGS	$\text{CH}_3\text{SO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{SO}_3$	$2.24\text{E}-14$	Cala et al. (2023)
G9475MK	TrGCS	$\text{CH}_3\text{SCH}_2\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{SCHO}$	$7.03\text{E}-11$	Cala et al. (2023)
G9476MK	TrGCS	$\text{CH}_3\text{SCHO} + \text{OH} \rightarrow \text{CH}_3\text{S} + \text{CO}$	$1.11\text{E}-11$	Cala et al. (2023)
G9477MK	TrGCS	$\text{CH}_3\text{SCH}_2\text{OO} \rightarrow \text{HPMTF} + \text{OH}$	$k_{\text{MTMP_isom}}$	Veres et al. (2020)
G9478MK	TrGCS	$\text{HPMTF} + \text{OH} \rightarrow \text{HOOCH}_2\text{SCO}$	$1.4\text{E}-12$	Wollesen de Jonge et al. (2021)
G9479MK	TrGCS	$\text{HOOCH}_2\text{SCO} \rightarrow \text{HOOCH}_2\text{S} + \text{H}_2\text{O} + \text{CO}$	$9.2\text{E}9*\text{EXP}(-505.4/\text{temp})$	Wollesen de Jonge et al. (2021)
G9480MK	TrGCS	$\text{HOOCH}_2\text{SCO} \rightarrow \text{OCS} + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$1.6\text{E}7*\text{EXP}(-1468.6/\text{temp})$	Wollesen de Jonge et al. (2021)
G9481MK	TrGS	$\text{HOOCH}_2\text{S} + \text{O}_3 \rightarrow \text{HOOCH}_2\text{SO}$	$1.15\text{E}-12*\text{EXP}(430./\text{temp})$	Wu et al. (2015)
G9482MK	TrGNS	$\text{HOOCH}_2\text{S} + \text{NO}_2 \rightarrow \text{HOOCH}_2\text{SO} + \text{NO}$	$6.00\text{E}-11*\text{EXP}(240./\text{temp})$	Wu et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G9483MK	TrGS	$\text{HOOCH}_2\text{S} + \text{O}_2 \rightarrow \text{HOOCH}_2\text{SOO}$	$1.20\text{E}-16 \cdot \text{EXP}(1580./\text{temp})$	Cala et al. (2023)
G9484aMK	TrGS	$\text{HOOCH}_2\text{SOO} \rightarrow \text{HOOCH}_2\text{S} + \text{O}_2$	$3.50\text{E}+10 \cdot \text{EXP}(-3560./\text{temp})$	Cala et al. (2023)
G9484bMK	TrGS	$\text{HOOCH}_2\text{SOO} \rightarrow \text{HCHO} + \text{OH} + \text{SO}_2$	$5.60\text{E}-16 \cdot \text{EXP}(-10870./\text{temp})$	Cala et al. (2023)
G9485MK	TrGS	$\text{HOOCH}_2\text{SO} + \text{O}_3 \rightarrow \text{HCHO} + \text{OH} + \text{SO}_2$	$4.0\text{E}-13$	Wu et al. (2015)
G9486MK	TrGNS	$\text{HOOCH}_2\text{SO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{OH} + \text{NO} + \text{SO}_2$	$1.2\text{E}-11$	Wu et al. (2015)
G9600	TrGCCIS	$\text{DMS} + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCl} + \text{HCHO}$	$3.3\text{E}-10$	Atkinson et al. (2004)
G9800	TrGCIS	$\text{DMS} + \text{IO} \rightarrow \text{DMSO} + \text{I}$	$3.2\text{E}-13 \cdot \text{EXP}(-925./\text{temp})$	Dillon et al. (2006a)
G3126MK	StTrGN	$\text{NO} + \text{NO}_2 \rightarrow \text{N}_2\text{O}_3$	$7.9\text{E}-12$	Atkinson et al. (2004)
G3127MK	StTrGN	$\text{NO}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_4$	$1.0\text{E}-12$	Atkinson et al. (2004)
G3128MK	StTrGN	$\text{N}_2\text{O}_3 \rightarrow \text{NO} + \text{NO}_2$	$3.6\text{E}8$	Atkinson et al. (2004)
G3129MK	StTrGN	$\text{N}_2\text{O}_4 \rightarrow \text{NO}_2 + \text{NO}_2$	$4.4\text{E}6$	Atkinson et al. (2004)
G4170aMK	TrGAmin	$\text{MMA} + \text{OH} \rightarrow .3 \text{CH}_2\text{NH} + .3 \text{HO}_2 + .1 \text{MMAO}_2 + .6 \text{CH}_3\text{NH}$	$(1-\text{ya_soan1}-\text{ya_soan2}-\text{ya_soan5})$ $\cdot \text{k_MMA_OH} \cdot \text{xgcamin}$	Karl (2012)
G4170bMK	TrGAmin	$\text{MMA} + \text{OH} \rightarrow \text{BSOV} + \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan1} \cdot \text{k_MMA_OH}$	Karl (2012)
G4170cMK	TrGAmin	$\text{MMA} + \text{OH} \rightarrow \text{BLOV} + \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan2} \cdot \text{k_MMA_OH}$	Karl (2012)
G4170dMK	TrGAmin	$\text{MMA} + \text{OH} \rightarrow \text{BELV} + \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan5} \cdot \text{k_MMA_OH}$	Karl (2012)
G4171MK	TrGAmin	$\text{CH}_3\text{NH} + \text{NO}_2 \rightarrow .5 \text{MMNNO}_2 + .5 \text{CH}_2\text{NH} + .5 \text{HONO}$	$10 \cdot 1.1\text{E}-12 \cdot \text{xgcanno}$	Karl (2012)
G4172MK	TrGAmin	$\text{CH}_3\text{NH} + \text{O}_2 \rightarrow \text{CH}_2\text{NH} + \text{HO}_2$	$2.4\text{E}-17$	Nielsen et al. (2011)
G4173MK	TrGAmin	$\text{MMAO}_2 + \text{NO} \rightarrow \text{H}_2\text{NCHO} + \text{HO}_2 + \text{NO}_2$	$0.5 \cdot 7.7\text{E}-12$	Nielsen et al. (2011)
G4174MK	TrGAmin	$\text{H}_2\text{NCHO} + \text{OH} \rightarrow \text{HNCO} + \text{H}_2\text{O}$	$\text{k_H}_2\text{NCHO_OH}$	Karl (2012)
G4175MK	TrGAmin	$\text{MMA} + \text{CH}_2\text{NH} \rightarrow \text{CH}_2\text{NCH}_3 + \text{NH}_3$	$4.0\text{E}-17 \cdot \text{wall}$	Karl (2012)
G4200aMK	TrGAminCN	$\text{MEA} + \text{OH} \rightarrow 0.05 \text{H}_2\text{NCH}_2\text{CHO} + 0.8 \text{MEABO}_2 + 0.15 \text{MEAN} + 0.05 \text{HO}_2$	$(1-\text{ya_soan1}-\text{ya_soan2}-\text{ya_soan5})$ $\cdot \text{k_MEA_OH} \cdot \text{fkoh_mea} \cdot \text{xgcamin}$	Karl et al. (2012a)
G4200bMK	TrGAminCN	$\text{MEA} + \text{OH} \rightarrow \text{BSOV} + 2 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan1} \cdot \text{k_MEA_OH} \cdot \text{fkoh_mea}$	Karl et al. (2012a)
G4200cMK	TrGAminCN	$\text{MEA} + \text{OH} \rightarrow \text{BLOV} + 2 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan2} \cdot \text{k_MEA_OH} \cdot \text{fkoh_mea}$	Karl et al. (2012a)
G4200dMK	TrGAminCN	$\text{MEA} + \text{OH} \rightarrow \text{BELV} + 2 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan5} \cdot \text{k_MEA_OH} \cdot \text{fkoh_mea}$	Karl et al. (2012a)
G4201MK	TrGAminCN	$\text{H}_2\text{NCH}_2\text{CHO} + \text{OH} \rightarrow 0.8 \text{H}_2\text{NCH}_2\text{CO}_3 + 0.2 \text{H}_2\text{NCHO}_2\text{CHO} + \text{H}_2\text{O}$	k_AAC_OH	Karl et al. (2012a)
G4202MK	TrGAminCN	$\text{H}_2\text{NCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{MMAO}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Karl et al. (2012a)
G4203MK	TrGAminCN	$\text{H}_2\text{NCHO}_2\text{CHO} + \text{NO} \rightarrow \text{H}_2\text{NCOCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KRO}_2\text{NO} \cdot 2$	Karl et al. (2012a)
G4204MK	TrGAminCN	$\text{H}_2\text{NCOCHO} + \text{OH} \rightarrow \text{H}_2\text{NCOCO}_3 + \text{H}_2\text{O}$	k_OXA_OH	Karl et al. (2012a)
G4205MK	TrGAminCN	$\text{H}_2\text{NCOCO}_3 + \text{NO} \rightarrow \text{H}_2\text{NCHO} + \text{CO}_2 + \text{NO}_2$	KAPNO	Karl et al. (2012a)
G4206MK	TrGAminCN	$\text{MEABO}_2 + \text{NO} \rightarrow \text{MEABO} + \text{NO}_2$	KRO_2NO	Karl et al. (2012a)
G4207MK	TrGAminCN	$\text{MEABO} + \text{O}_2 \rightarrow \text{H}_2\text{NCOCH}_2\text{OH} + \text{HO}_2$	$\text{k_RO_O}_2 \cdot 0.25$	Karl et al. (2012a)
G4208MK	TrGAminCN	$\text{MEABO} \rightarrow \text{H}_2\text{NCHO} + \text{HCHO}$	$\text{k_DEC} \cdot 0.2$	Karl et al. (2012a)

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

#	labels	reaction	rate coefficient	reference
G4209MK	TrGAmiCN	$\text{H2NCOCH2OH} + \text{OH} \rightarrow \text{H2NCOCHO} + \text{HO}_2$	$k_{\text{HAC_OH}}$	Karl et al. (2012a)
G4210MK	TrGAmiCN	$\text{MEAN} + \text{NO}_2 \rightarrow 0.5 \text{ MEANNO}_2 + 0.5 \text{ HNCHCH2OH} + 0.5 \text{ HONO}$	$1.4\text{E-}13 \text{ *xgcnnno}$	Karl et al. (2012a)
G4211MK	TrGAmiCN	$\text{MEAN} + \text{O}_2 \rightarrow \text{HNCHCH2OH} + \text{HO}_2$	$1.2\text{E-}19$	Karl et al. (2012a)
G4212MK	TrGAmiCN	$\text{MEAN} + \text{NO} \rightarrow \text{MEANNO}$	$8.5\text{E-}14 \text{ *xgcnnno}$	Karl et al. (2012a)
G4213MK	TrGAmiCN	$\text{MEANNO}_2 + \text{OH} \rightarrow \text{MEANHA} + \text{HO}_2$	$k_{\text{NITRAMA_OH}}$	Karl et al. (2012a)
G4214MK	TrGAmiCN	$\text{HNCHCH2OH} + \text{OH} \rightarrow \text{H2NCOCH2OH} + \text{HO}_2$	$3.00\text{E-}13$	Karl et al. (2012a)
G4220aMK	TrGAmiCN	$\text{DMA} + \text{OH} \rightarrow .4 \text{ CH3NCH3} + .5 \text{ DMAO2} + .1 \text{ CH2NCH3} + .1 \text{ HO}_2$	$(1\text{-ya_soan1-ya_soan2-ya_soan5})$ $*k_{\text{DMA_OH*xgcamin}}$	Karl (2012)
G4220bMK	TrGAmiCN	$\text{DMA} + \text{OH} \rightarrow \text{BSOV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan1*k_DMA_OH	Karl (2012)
G4220cMK	TrGAmiCN	$\text{DMA} + \text{OH} \rightarrow \text{BLOV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan2*k_DMA_OH	Karl (2012)
G4220dMK	TrGAmiCN	$\text{DMA} + \text{OH} \rightarrow \text{BELV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan5*k_DMA_OH	Karl (2012)
G4221MK	TrGAmiCN	$\text{CH3NCH3} + \text{NO} \rightarrow \text{NDMA}$	$2.39\text{E-}13 \text{ *xgcnnno}$	Nielsen et al. (2011)
G4222MK	TrGAmiCN	$\text{CH3NCH3} + \text{O}_2 \rightarrow \text{CH2NCH3} + \text{HO}_2$	$9.54\text{E-}20$	Nielsen et al. (2011)
G4223MK	TrGAmiCN	$\text{CH3NCH3} + \text{NO}_2 \rightarrow .6 \text{ CH2NCH3} + .7 \text{ HONO} + .3 \text{ DMNNO}_2 + .1 \text{ CH3NO} + .1 \text{ CH}_3\text{O}_2$	$3.18\text{E-}13 \text{ *xgcnnno}$	Lazarou et al. (1994)
G4224MK	TrGAmiCN	$\text{DMNNO}_2 + \text{OH} \rightarrow \text{CH2NCH3} + \text{NO}_2 + \text{H}_2\text{O}$	$4.5\text{E-}12$	Karl (2012)
G4225MK	TrGAmiCN	$\text{DMAO2} + \text{NO} \rightarrow \text{CH3NHCHO} + 0.5 \text{ NO}_2 + 0.5 \text{ HO}_2 + 0.5 \text{ HONO}$	$8.5\text{E-}12$	Karl (2012)
G4226MK	TrGAmiCN	$\text{NDMA} + \text{OH} \rightarrow \text{CH2NCH3} + \text{NO} + \text{H}_2\text{O}$	$3.0\text{E-}12$	Karl (2012)
G4230aMK	TrGAmiCN	$\text{CH2NCH3} + \text{OH} \rightarrow \text{CH3NHCHO} + \text{HO}_2$	$(1\text{-ya_soan1-ya_soan2-ya_soan5})$ $*k_{\text{MMI_OH}}$	Karl (2012)
G4230bMK	TrGAmiCN	$\text{CH2NCH3} + \text{OH} \rightarrow \text{BSOV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan1*k_MMI_OH	Karl (2012)
G4230cMK	TrGAmiCN	$\text{CH2NCH3} + \text{OH} \rightarrow \text{BLOV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan2*k_MMI_OH	Karl (2012)
G4230dMK	TrGAmiCN	$\text{CH2NCH3} + \text{OH} \rightarrow \text{BELV} + 2 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan5*k_MMI_OH	Karl (2012)
G4300aMK	TrGAmiCN	$\text{TMA} + \text{OH} \rightarrow \text{TMAO2} + \text{H}_2\text{O}$	$(1\text{-ya_soan1-ya_soan2-ya_soan5})$ $*k_{\text{TMA_OH*xgcamin}}$	Karl (2012)
G4300bMK	TrGAmiCN	$\text{TMA} + \text{OH} \rightarrow \text{BSOV} + 3 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan1*k_TMA_OH	Karl (2012)
G4300cMK	TrGAmiCN	$\text{TMA} + \text{OH} \rightarrow \text{BLOV} + 3 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan2*k_TMA_OH	Karl (2012)
G4300dMK	TrGAmiCN	$\text{TMA} + \text{OH} \rightarrow \text{BELV} + 3 \text{ LCARBON} + \text{LNITROGEN}$	ya_soan5*k_TMA_OH	Karl (2012)
G4301MK	TrGAmiCN	$\text{TMAO2} + \text{NO} \rightarrow .3 \text{ DMNCHO} + .3 \text{ HONO} + .7 \text{ TMAO} + .7 \text{ NO}_2 + .7 \text{ HO}_2$	$8.5\text{E-}12$	Karl (2012)

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

#	labels	reaction	rate coefficient	reference
G4302MK	TrGAmiCN	$\text{TMAO} + \text{O}_2 \rightarrow \text{DMNCHO} + \text{HO}_2$	$2.4\text{E-}15*5$	Karl (2012)
G4303MK	TrGAmiCN	$\text{TMAO} \rightarrow \text{CH}_3\text{NCH}_3 + \text{HCHO}$	$4.0\text{E}+05$	Karl (2012)
G4304MK	TrGAmiCN	$\text{DMNCHO} + \text{OH} \rightarrow \text{DMNCHOO}_2$	$1.4\text{E-}11*0.25$	Karl (2012)
G4305MK	TrGAmiCN	$\text{DMNCHOO}_2 + \text{NO} \rightarrow \text{TMADF} + \text{NO}_2 + \text{HO}_2$	$8.5\text{E-}12$	Karl (2012)
G4306MK	TrGAmiCN	$\text{HOETNHCHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CONHCHO} + \text{HO}_2$	$k_{\text{HAC_OH}}$	Karl (2012)
G4310MK	TrGAmiCN	$\text{DMCNH}_2 + \text{O}_2 \rightarrow 0.8 \text{DMCOONH}_2 + 0.1 \text{CH}_2\text{CNH}_2\text{CH}_3 + 0.1 \text{DMCNH} + \text{HO}_2$	$k_{\text{R0_02}}*0.25$	Nielsen and Schade (2012)
G4311MK	TrGAmiCN	$\text{DMCOONH}_2 + \text{NO} \rightarrow \text{H}_2\text{NCOCH}_3 + \text{HCHO} + \text{NO}_2$	KAPNO	Nielsen and Schade (2012)
G4312MK	TrGAmiCN	$\text{CH}_3\text{CNH}_2\text{MOH} + \text{NO} \rightarrow 0.5 \text{H}_2\text{NCOCH}_3 + 0.5 \text{H}_2\text{NCOCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2$	KAPNO	Nielsen and Schade (2012)
G4313MK	TrGAmiCN	$\text{CH}_3\text{CNH}_2\text{MOH} + \text{O}_2 \rightarrow 0.8 \text{HNCCH}_3\text{MOH} + 0.1 \text{H}_2\text{NCCHOHCH}_3 + 0.1 \text{H}_2\text{NCCH}_2\text{MOH} + \text{HO}_2$	$k_{\text{R0_02}}*0.25$	Nielsen and Schade (2012)
G4320MK	TrGC	$\text{CH}_3\text{CHOCH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2$	$k_{\text{R0_02}}$	Rickard and Pascoe (2009)
G4400MK	TrGAmiCN	$\text{DEA} + \text{OH} \rightarrow .4 \text{HOETNETOH} + .5 \text{DEAO}_2 + .1 \text{HOETNHCH}_2\text{CHO} + .1 \text{HO}_2$	$k_{\text{DEA_OH}}*xgcamin$	Karl (2012)
G4401MK	TrGAmiCN	$\text{HOETNETOH} + \text{NO} \rightarrow \text{NDELA}$	$2.39\text{E-}13 *xgcnno$	Nielsen et al. (2011)
G4402MK	TrGAmiCN	$\text{HOETNETOH} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CHNETOH} + \text{HO}_2$	$9.54\text{E-}20$	Nielsen et al. (2011)
G4403MK	TrGAmiCN	$\text{HOETNETOH} + \text{NO}_2 \rightarrow .6 \text{HOCH}_2\text{CHNETOH} + .7 \text{HONO} + .3 \text{DEANNO}_2 + .1 \text{HOCH}_2\text{CH}_2\text{NO} + .1 \text{HOCH}_2\text{CH}_2\text{O}_2$	$3.18\text{E-}13 *xgcnno$	Lazarou et al. (1994)
G4404MK	TrGAmiCN	$\text{DEANNO}_2 + \text{OH} \rightarrow \text{HOCH}_2\text{CHNETOH} + \text{NO}_2 + \text{H}_2\text{O}$	$1.74\text{E-}11$	Karl (2012)
G4405MK	TrGAmiCN	$\text{DEAO}_2 + \text{NO} \rightarrow \text{HOETNHCHO} + \text{HCHO} + 0.5 \text{NO}_2 + 0.5 \text{HO}_2 + 0.5 \text{HONO}$	$8.5\text{E-}12$	Karl (2012)
G4406MK	TrGAmiCN	$\text{NDELA} + \text{OH} \rightarrow \text{HOCH}_2\text{CHNETOH} + \text{NO} + \text{H}_2\text{O}$	$1.61\text{E-}11$	Karl (2012)
G4407MK	TrGAmiCN	$\text{HOCH}_2\text{CHNETOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CONETOH} + \text{HO}_2$	$k_{\text{MMI_OH}}$	Karl (2012)
G4410aMK	TrGAmiCN	$\text{AMP} + \text{OH} \rightarrow 0.30 \text{AMPN} + 0.65 \text{DMCNH}_2\text{CHO} + 0.5 \text{HO}_2 + 0.05 \text{NH}_3 + 0.05 \text{MACR}$	$(1-\text{ya_soan1}-\text{ya_soan2}-\text{ya_soan5}) *k_{\text{AMP_OH}}*fkoh_mea$	Harris and J. N. Pitts (1983)
G4410bMK	TrGAmiCN	$\text{AMP} + \text{OH} \rightarrow \text{BSOV} + 4 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan1}*k_{\text{AMP_OH}}*fkoh_mea$	Harris and J. N. Pitts (1983)
G4410cMK	TrGAmiCN	$\text{AMP} + \text{OH} \rightarrow \text{BLOV} + 4 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan2}*k_{\text{AMP_OH}}*fkoh_mea$	Harris and J. N. Pitts (1983)
G4410dMK	TrGAmiCN	$\text{AMP} + \text{OH} \rightarrow \text{BELV} + 4 \text{LCARBON} + \text{LNITROGEN}$	$\text{ya_soan5}*k_{\text{AMP_OH}}*fkoh_mea$	Harris and J. N. Pitts (1983)
G4411MK	TrGAmiCN	$\text{AMPN} + \text{NO} \rightarrow \text{NAMP}$	$0.26*3.18\text{E-}13$	Nielsen and Schade (2012)
G4412MK	TrGAmiCN	$\text{AMPN} + \text{NO}_2 \rightarrow \text{AMPNNO}_2$	$3.18\text{E-}13$	Lazarou et al. (1994)
G4413MK	TrGAmiCN	$\text{AMPN} + \text{O}_3 \rightarrow \text{AMPOX}$	$1.7\text{E-}13$	Nielsen and Schade (2012)
G4414MK	TrGAmiCN	$\text{DMCNH}_2\text{CHO} + \text{OH} \rightarrow \text{DMCNH}_2\text{CO}_3 + \text{H}_2\text{O}$	$k_{\text{AAC_OH}}$	Nielsen and Schade (2012)
G4415MK	TrGAmiCN	$\text{DMCNH}_2\text{CO}_3 + \text{NO} \rightarrow \text{DMCNH}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Nielsen and Schade (2012)

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

#	labels	reaction	rate coefficient	reference
G4416MK	TrGAmiCN	DMCNH2CO3 + NO ₂ → AMPAN	k_CH3C03_N02	Sander et al. (2006)
G4417MK	TrGAmiCN	AMPAN → DMCNH2CO3 + NO ₂	k_PAN_M	Sander et al. (2006)
G4418MK	TrGAmiCN	AMPO + O ₂ → DMOCNH2MOH + HO ₂	k_R0_02*0.25	Nielsen and Schade (2012)
G4419MK	TrGAmiCN	AMPO → CH3CNH2MOH + HCHO	k_DEC*0.2	Nielsen and Schade (2012)
G4420MK	TrGAmiCN	AMPNNO2 + OH → AMPNA + HO ₂	k_NITRAMA_OH	Nielsen and Schade (2012)
G4421MK	TrGAmiCN	AMP + NO ₃ → 0.5 AMPN + 0.4 DMCNH2CHO + 0.1 AMPO + 0.5 HO ₂ + HNO ₃	k_AMP_N03	Carter (2008)
G4500MK	TrGAmiCN	DEANCH2O2 + NO → DEANCHO + NO ₂ + HO ₂	8.5E-12	Karl (2012)
G4600MK	TrGAmiCN	TEA + OH → TEAO2 + H ₂ O	k_TEA_OH*xgcamin	Karl (2012)
G4601MK	TrGAmiCN	TEAO2 + NO → .3 DEANCH2CHO + .3 HONO + .7 TEAO + .7 NO ₂ + .7 HO ₂	8.5E-12	Karl (2012)
G4602MK	TrGAmiCN	TEAO + O ₂ → DEANCOCH2OH + HO ₂	2.4E-15*5	Karl (2012)
G4603MK	TrGAmiCN	TEAO → HOETNETOH + CH ₃ CHO	4.0E+05	Karl (2012)
G4604MK	TrGAmiCN	TEAO + O ₂ → DEANCH2O2 + HCHO	2.4E-15	Karl (2012)
G4605MK	TrGAmiCN	DEANCH2CHO + OH → DEANCH2COO2	1.4E-11	Karl (2012)
G4606MK	TrGAmiCN	DEANCH2COO2 + NO → DEANCHO + HCHO + NO ₂ + HO ₂	8.5E-12	Karl (2012)
G4610MK	TrGC	TME + O ₃ → CH ₃ COCH ₃ + CH ₃ COCH ₂ O ₂ + OH	3.03E-15*EXP(-294./temp)	Rickard and Pascoe (2009)
G4611MK	TrGC	TME + OH → TMEO2	1.1E-10	Rickard and Pascoe (2009)
G4612MK	TrGCN	TMEO2 + NO → 2.0 CH ₃ COCH ₃ + NO ₂ + HO ₂	KR02N0	Rickard and Pascoe (2009)
G4620MK	TrGC	CHEX + OH → CHEXO2	2.88E-17*temp*temp*exp(309./temp)	Rickard and Pascoe (2009)
G4621MK	TrGC	CHEXO2 → 0.6 CHEXO + 0.2 CHEXOL + 0.2 CHEXONE	9.20E-14*R02	Rickard and Pascoe (2009)
G4622MK	TrGC	CHEXO2 + HO ₂ → CHEXOOH	0.770*KR02H02(6)	Rickard and Pascoe (2009)
G4623MK	TrGCN	CHEXO2 + NO → CHEXO + NO ₂	KR02N0	Rickard and Pascoe (2009)
G4624MK	TrGC	CHEXO + O ₂ → CHEXONE + HO ₂	k_R0_02	Rickard and Pascoe (2009)
G40202c	TrGTerC	LAPINABO2 + HO ₂ → BSOV + 10 LCARBON	ya_soan1*KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40202d	TrGTerC	LAPINABO2 + HO ₂ → BLOV + 10 LCARBON	ya_soan2*KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40243c	TrGTerC	C109O2 + HO ₂ → BSOV + 10 LCARBON	ya_soan1*KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40243d	TrGTerC	C109O2 + HO ₂ → BLOV + 10 LCARBON	ya_soan2*KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40253c	TrGTerC	BPINAO2 + HO ₂ → BSOV + 10 LCARBON	ya_soan1*KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G40253d	TrGTerC	BPINAO2 + HO ₂ → BLOV + 10 LCARBON	ya_soan2*KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Sander et al. (2018)
G40259a	TrGTerC	ROO6R1O2 + HO ₂ → 10 LCARBON	(1-ya_soan1-ya_soan2) *KR02H02(10)	Vereecken and Peeters (2012)*
G40259b	TrGTerC	ROO6R1O2 + HO ₂ → BSOV + 10 LCARBON	ya_soan1*KR02H02(10)	Rickard and Pascoe (2009), Sander et al. (2018)
G40259ac	TrGTerC	ROO6R1O2 + HO ₂ → BLOV + 10 LCARBON	ya_soan2*KR02H02(10)	Rickard and Pascoe (2009), Sander et al. (2018)
G40600	TrGTer	BSOV + OH → BLOV	4.0E-11	Tsimpidi et al. (2010)
G40601	TrGTer	BLOV + OH → BELV	4.0E-11	Tsimpidi et al. (2010)
G40602	TrGTer	BSOV → BELV	9.6E-06	Carlton et al. (2010)
G40603	TrGTer	BLOV → BELV	9.6E-06	Carlton et al. (2010)
G40700	TrGTer	ASOV + OH → ALOV	4.0E-11	Tsimpidi et al. (2010)
G40701	TrGTer	ALOV + OH → AELV	4.0E-11	Tsimpidi et al. (2010)
G40702	TrGTer	ASOV → AELV	9.6E-06	Carlton et al. (2010)
G40703	TrGTer	ALOV → AELV	9.6E-06	Carlton et al. (2010)
G40704	TrGTer	PIOV + OH → PSOV	2.0E-11	Lambe et al. (2009)
G40705	TrGTer	PSOV + OH → PELV	2.0E-11	Lambe et al. (2009)
G40706	TrGTer	PELV → PSOV	5.0E-04	Lim and Ziemann (2009)

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 $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \text{k_CH302}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH302 = second-order rate coefficient of the self reaction of CH_3O_2 , and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

G2110: The rate coefficient is: $k_{\text{H02_H02}} = (3.0\text{E-}13 * \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 * \text{EXP}(920./\text{temp}) * \text{cair}) * (1 + 1.4\text{E-}21 * \text{EXP}(2200./\text{temp}) * \text{C}(\text{ind_H20}))$.

G2117: Converted to $K_c [\text{molec-1 cm}^3] = K_p * R * T / N_A$, where R is 82.05736 [$\text{cm}^3 \text{ atm K-1 mol-1}$].

G2118: Assuming fast equilibrium.

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.

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 $\text{PAN} + \text{OH}$.

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 $7\text{E-}12$ and $1.5\text{E-}12$.

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.

G42001: The product distribution is from Rickard and Pascoe (2009), after substitution of the energized Criegee intermediate, CH_2OO , by its decomposition products and reaction of the stabilized CI with the water dimer.

G42010: Only major channel considered as the end products are essentially the same.

G42013: The rate coefficient is: $k_{\text{CH3CO3_N02}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

G42018: The rate coefficient is the same as for the CH_3 channel in G4107 ($\text{CH}_3\text{OOH} + \text{OH}$).

G42021: The rate coefficient is $k_{\text{PAN_M}} = k_{\text{CH3CO3_N02}}/9.0\text{E-}29 * \text{EXP}(-14000./\text{temp})$, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G42022a: Quantum yields and products are from Glowacki et al. (2012).

G42022b: Quantum yields and products are from Glowacki et al. (2012).

G42024a: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42024b: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42047: Orlando et al. (1998) estimated that about 25% of the $\text{HOCH}_2\text{CH}_2\text{O}$ in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 $\text{HCHO} + \text{HO}_2$.

G42051a: Same as for the CH_3O_2 channel in G4107: $\text{CH}_3\text{OOH} + \text{OH}$.

G42058b: The aldehydic H is assumed to be like the analogous H of HOCH₂CHO.

G42074a: Factor of 3 to match the estimate of $k = 1.E-11$ molec/cm³/s by Paulot et al. (2009a).

G42074b: Factor of 3 to match the estimate of $k = 1.E-11$ molec/cm³/s by Paulot et al. (2009a).

G42075: NO₃CH₂CO₂H and NO₃CH₂CO₃H neglected.

G42078: NO₃CH₂CO₂H neglected.

G42082: Same rate constant as for PAN + OH.

G42083a: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42083b: Rate constant is the high-pressure limit as recommended by Atkinson et al. (2006).

G42085a: Uncertainties on the kinetics at pressures < 0.1 bar.

G42085b: Channel proposed by Hynes and Wine 1991, OH + HCHO + HOCN, could not be confirmed by Tyndall et al. (2001b). There is no alternative mechanism at the moment. Products assumed to be OH + CH₃CO₃ + NO

G42086b: Assuming HCN is from channel 2h, HCO + H + HCN. HCO is replaced by H + CO.

G42086c: Assuming exothermic channels 2b and 2d are equally important.

G42087: HCOCN is produced but replaced here by its likely oxidation products (HCN + CO₂) as studied by Tyndall et al. (2001b). The rate constant for a typical RO₂ + NO reaction is used.

G42088: NCCH₂OOH is produced but replaced here by its likely oxidation products (HCN + CO₂) as studied by Tyndall et al. (2001b). The rate constant for a typical RO₂ + HO₂ reaction is used.

G42089a: The minor channel with $k=5.2E-12$ is combined with the major one producing HCOOH.

G42090: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G42091: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G43001a: Branching ratios according to Rickard et al. (1999).

G43001b: Branching ratios according to Rickard et al. (1999).

G43004: The value for the generic RO₂ + HO₂ reaction from Atkinson (1997) is used here.

G43008: The value for the generic RO₂ + HO₂ reaction from Atkinson (1997) is used here.

G43011: Strong positive deviation of k below 240 K compared to the expression recommended by JPL (Burkholder et al., 2015).

G43015a: The same value as for G4107 (CH₃OOH + OH) is used, multiplied by the branching ratio of the CH₃O₂ channel.

G43028: Alkyl nitrate formation neglected. (also not considered in MCM).

G43037: Alkyl nitrate formation neglected. (also not considered in MCM).

G43040a: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43040b: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43044: Alkyl nitrate formation neglected.

G43045c: Rate coefficient assumed to equal to the one of hydroxyacetone (ACETOL) for this channel.

G43048: Using the high-pressure limit.

G43049: The pressure fall-off between 1000 and 100 mbar is only 3% (Kirchner et al., 1999).

G43050: Value for CH₃O₂NO₂ + OH, H-abstraction enhanced by the CH₃CO-group by f_{co}.

G43051c: Products approximated with C₂H₅CHO + HO₂.

G43052: Only major H-abstraction channel considered.

G43059: Products approximated with the major end-product CH₃CHO.

G43060b: Products approximated with the major end-product CH₃CHO.

G43061: Products approximated with the likely end-product CH₃CHO.

G43065: As for HCOCO₃.

G43070a: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43070b: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43071a: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

G43072: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G43073: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G43074: HCOCOCHO would be produced but undergoes fast photolysis (faster than MGLYOX) and is substituted with its products.

G43223: Products simplified

G43419: KDEC C3DIALO → GLYOX + CO + HO₂

G43420: KDEC C3DIALO → GLYOX + CO + HO₂

G43421: Permutation reaction (minor channels removed).

G44000: The LC₄H₉O₂ composition (nC₄H₉O₂:sC₄H₉O₂ ratio) is assumed to be equal to the ratio of the production rates at 298K: $k_p/(k_p+k_s) = 0.1273$ and $k_s/(k_p+k_s) = 0.8727$.

G44001b: $\text{sC}_4\text{H}_9\text{O}_2$ products are substituted with 0.636 $\text{MEK} + \text{HO}_2$ and 0.364 $\text{CH}_3\text{CHO} + \text{C}_2\text{H}_5\text{O}_2$ at 1 bar and 298 K.

G44003c: The alkyl nitrate yield is the weighted average yield for the two isomers forming from $\text{nC}_4\text{H}_9\text{O}_2$ and $\text{sC}_4\text{H}_9\text{O}_2$.

G44010b: H-abstraction from primary C and substitution of the resulting peroxy radical with its products from the reaction with NO.

G44011: H-abstraction from primary C and substitution of the resulting peroxy radical with its products from the reaction with NO.

G44015b: Products assumed to be only from H-abstraction from a secondary C bearing the -OOH group.

G44016: Products assumed to be only from H-abstraction from a secondary C bearing the -ONO₂ group.

G44018: LHMVKABO_2 is $0.12 \text{ HMVKAO}_2 + 0.88 \text{ HMVKBO}_2$.

G44019: LMEKO_2 represents $0.62 \text{ MEKBO}_2 + 0.38 \text{ MEKAO}_2$.

G44021a: The products of MEKAO are substituted with $\text{HCHO} + \text{CO}_2 + \text{HOCH}_2\text{CH}_2\text{O}_2$.

G44023a: Products from H-abstraction from the tertiary carbon bearing the ONO₂ group.

G44023b: Products from H-abstraction from the secondary carbon bearing the ONO₂ group.

G44025: Same value as for PAN.

G44026: Products as in G4415. Only the main channels for each isomer are considered. Weighted average for the isomers.

G44035: Rate constant replaced with the one of beta hydroxy RO₂.

G44046b: Using value for secondary nitrate (88% of total).

G44061a: Using value for secondary nitrate (88% of total).

G44061b: Using value for secondary nitrate (88% of total).

G44062a: Simplified products.

G44062b: Simplified products.

G44066: Alkyl nitrate formation neglected.

G44070: Alkyl nitrate formation neglected.

G44076: Alkyl nitrate formation neglected.

G44078: Other channel neglected.

G44081: Alkyl nitrate formation neglected.

G44082: Other channel neglected.

G44085: k for CH_3CHCO from Hatakeyama et al. (1985) adjusted.

G44086: Simplified product distribution.

G44089: The nitrated RO₂ is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO₂ isomers mostly $\text{C}_2\text{H}_5\text{CHO}$.

G44097a: Branching ratios according to Rickard et al. (1999). $\text{CH}_3\text{CHO}_2\text{CHO}$ is replaced with its major products $\text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2$.

G44097b: Branching ratios according to Rickard et al. (1999).

G44098: The nitrated RO₂ is replaced by its products upon reaction with NO.

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH_3CHOOA products as from $\text{C}_3\text{H}_6 + \text{O}_3$ reaction.

G44107: The nitrated RO₂ is replaced by its products upon reaction with NO.

G44110: The nitrated RO₂ is replaced by its products upon reaction with NO.

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

G44127: Only this channel considered as the intermediate radical is likely more stable than $\text{CHCH}(\text{OH})_2$.

G44128: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44129: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44130: Only this channel considered as the intermediate radical is likely more stable than $\text{CHCH}(\text{OH})_2$.

G44131: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44132: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44133: Only this channel considered as the intermediate radical is likely more stable than $\text{CHCH}(\text{OH})_2$.

G44134: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44135: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44136: Only this channel considered as the intermediate radical is likely more stable than $\text{CHCH}(\text{OH})_2$.

G44137: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44138: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G44139: Simplified oxidation.

G44140: Simplified oxidation.	G44432: Only major channel. KDEC MALANHYO \rightarrow HCOCOHCO ₃	G45037: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 4.2E-11.
G44141: Simplified oxidation.	G44436: KDEC NBZFUO \rightarrow 0.5 CO ₁₄ O ₃ CHO + 0.5 NO ₂ + 0.5 NBZFUONE + 0.5 HO ₂	G45040: Alkyl nitrate formation neglected.
G44142: Simplified oxidation.	G44437: KDEC NBZFUO \rightarrow 0.5 CO ₁₄ O ₃ CHO + 0.5 NO ₂ + 0.5 NBZFUONE + 0.5 HO ₂	G45043: Old MCM rate constant 4.16E-11.
G44202: Alkyl nitrate formation neglected.	G44438: KDEC NBZFUO \rightarrow 0.5 CO ₁₄ O ₃ CHO + 0.5 NO ₂ + 0.5 NBZFUONE + 0.5 HO ₂ and RO ₂ Only major channel.	G45047: Alkyl nitrate formation neglected.
G44203a: Rate coefficient estimated with SAR (Taraborrelli, 2010).	G44439: KDEC MALDIALCO ₂ \rightarrow 0.6 MALANHY + HO ₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO ₂	G45055: Alkyl nitrate formation neglected.
G44205: Alkyl nitrate formation neglected.	G44443: KDEC MECOACETO \rightarrow CH ₃ CO ₃ + HCHO	G45071: Alkyl nitrate formation neglected.
G44210: Alkyl nitrate formation neglected.	G44444: KDEC MECOACETO \rightarrow CH ₃ CO ₃ + HCHO	G45074: Formic acid production consistent with results of Bates et al. (2014). Here, the high yields of formic acid and hydroxycarbonyls at low NO from oxidation of cis-beta-LIEPOX (the most abundant isomer) are approximated with the production of DB1O which undergo both the Dibble double H-transfer to DB2O ₂ and HOCH ₂ elimination yielding HVMK and HMAc (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting from the ring opening after H-abstraction). The rate constant is from Paulot et al. (2009b) and adjusted based on Bates et al. (2014) that determined the single rate constants for the cis- and trans- beta isomer.
G44221: Same k as for MGLYOX + OH (Tyndall et al., 1995).	G44445: KDEC MECOACETO \rightarrow CH ₃ CO ₃ + HCHO	
G44402: KDEC NC ₄ DCO ₂ \rightarrow MALANHY + NO ₂	G44450: KDEC BZFUO \rightarrow CO ₁₄ O ₃ CHO + HO ₂	
G44406c: KDEC MALDIALCO ₂ \rightarrow 0.6 MALANHY + HO ₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO ₂	G44451: KDEC BZFUO \rightarrow CO ₁₄ O ₃ CHO + HO ₂	
G44407: KDEC MALDIALCO ₂ \rightarrow 0.6 MALANHY + HO ₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO ₂	G44452: KDEC BZFUO \rightarrow CO ₁₄ O ₃ CHO + HO ₂ . Only major channel.	
G44409: KDEC MALDIALCO ₂ \rightarrow 0.6 MALANHY + HO ₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO ₂	G44457: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO ₂	G45080: Alkyl nitrate formation neglected.
G44410: KDEC MALDIALCO ₂ \rightarrow 0.6 MALANHY + HO ₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO ₂	G44458: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO ₂	G45092a: C ₄ MDIAL = C ₄ DIAL in MCM only from aromatics.
G44412: KDEC BZFUONOOA \rightarrow 0.5 BZFUONOO + 0.5 CO + 0.5 CO ₂ + 0.5 HCOCH ₂ O ₂ + 0.5 OH and BZFUONOO \rightarrow 0.625 CO ₁₄ O ₃ CO ₂ H + 0.375 CO ₁₄ O ₃ CHO + 0.375 H ₂ O ₂	G44459: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO ₂ . Only major channel.	G45092b: Only one acyl peroxy radical considered.
G44421: Only major channel.	G44461: KBPAN \rightarrow k_PAN_M	G45093: Two aldehydic sites reacting with NO ₃ but only one isomer product considered.
G44424: KDEC: GLYOOA \rightarrow 0.125 HCHO + 0.18 GLYOO + 0.82 HO ₂ + 0.57 OH + 1.265 CO + 0.25 CO ₂ and H ₂ O substitution GLYOO \rightarrow 0.625 HCOCO ₂ H + 0.375 GLYOX + 0.375 H ₂ O ₂	G45019d: Delta-1 and delta-2 LIEPOX are not considered and replaced by beta-LIEPOX formed by ISOP-BOOH and ISOPDOOH.	G45095: Alkyl nitrate formation neglected.
G44425: Merged equations.	G45021: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 1.1E-11.	G45098: Alkyl nitrate formation neglected.
G44430: KDEC MALANHYO \rightarrow HCOCOHCO ₃		G45100: Alkyl nitrate formation neglected.
G44431: KDEC MALANHYO \rightarrow HCOCOHCO ₃		G45104a: DB1OOH is a hydroperoxide bearing a vinyl alcohol moiety that upon reaction with OH yields HCOOH (Davis et al., 1998).

G45107: OH production here is to take into account the hydroperoxidic function formed by the shift of the enolic hydrogen and not present in DB2O2. This approximation leads to spurious HO₂ production.

G45108a: Consistent with the results of Bates et al. (2014).

G45108b: Consistent with the results of Bates et al. (2014). Assuming that the enol alkoxy radical partly decomposes yielding a substitute vinyl alcohol.

G45111: Alkyl nitrate formation neglected.

G45114b: Here, formic acid is mechanistically produced by the OH-addition to the vinyl alcohol which, upon RO₂-to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with O₂ forming HCOOH + HO₂. Along CH₃COCHOHCHO should be produced but not in the mechanism. Only CH₃COCHO₂CHO. The rate constant is consistent with predictions by Ganzeveld et al. (2006) for ENOL. OH-addition to the OH-bearing carbon is considered the dominant channel as it is already for the ENOL (Ganzeveld et al., 2006).

G45115: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006). The product should be C1ODC3OOHC4OD but it is neglected in the mechanism.

G45116: As for DB1OOH + OH.

G45117: Additional sinks for DB2OOH are neglected.

G45121b: Nitrate assumed to be major isomer that is mostly similar to products of ISOPDO₂-chemistry.

G45128: Rate constant by Liljegren and Stevens (2013). A lumped RO₂ that upon conversion to RO yields 100% 2-methyl-butenedial (C4MDIAL) although Aschmann et al. (2014) quantified a 38% yield of the Z/E mixture.

G45129: As for 3METHYLFURAN + OH but with additional NO₂ production for mass conservation.

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

G45134b: ZCO₂HC₂3DBCOD formation is neglected. However, it is produced in MCM and in aromatic-related reactions under the name of MC3ODBCO₂H.

G45139: LZCPANC₂3DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO₂ = 0.67 MBOAO₂ + 0.33 MBOBO₂

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC₄MDCO₂ → MMALANHY + NO₂

G45404: KDEC NTLFUO → ACCOMECHO + NO₂

G45405: KDEC NTLFUO → ACCOMECHO + NO₂

G45406: KDEC NTLFUO → ACCOMECHO

G45409: KBPAN → k_PAN_M (renaming)

G45413: KFPAN → k_CH₃CO₃_NO₂ (renaming)

G45422: KDEC MMALANHYO → CO₂H₃CO₃

G45423: KDEC MMALANHYO → CO₂H₃CO₃

G45424: KDEC MMALANHYO → CO₂H₃CO₃ and Only major channel.

G45429: KBPAN → k_PAN_M (renamed)

G45430a: KDEC C₅CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + 0.17 MGLYOX + 0.17 HO₂ + 0.17 CO + 0.17 CO₂

G45431: KDEC C₅CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + 0.17 MGLYOX + 0.17 HO₂ + 0.17 CO + 0.17 CO₂

G45432: KFPAN → k_CH₃CO₃_NO₂ (renaming)

G45433: KDEC C₅CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + 0.17 MGLYOX + 0.17 HO₂ + 0.17 CO + 0.17 CO₂

G45434: KDEC C₅CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + 0.17 MGLYOX + 0.17 HO₂ + 0.17 CO + 0.17 CO₂ and only major channel.

G45436: KDEC C₅CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + 0.17 MGLYOX + 0.17 HO₂ + 0.17 CO + 0.17 CO₂

G45444: KDEC MC₃CODBCO₂ → 0.35 GLYOX + 0.35 CH₃ + 0.35 CO + 0.35 CO₂ + 0.65 MMALANHY + 0.65 HO₂

G45452: KDEC TLFUONOOA → 0.5 CO + 0.5 OH + 0.5 MECOACETO₂ + 0.5 TLFUONOO and H₂O subs TLFUONOO → 0.625 C₂₄O₃CCO₂H + 0.375 ACCOMECHO + 0.375 H₂O₂

G45456: KFPAN → k_CH₃CO₃_NO₂ (renaming)

G45476b: KDEC NTLFUO → ACCOMECHO + NO₂ and reactions with KRO₂HO₂.

G45477: KDEC NTLFUO → ACCOMECHO + NO₂

G45478: KDEC NTLFUO → ACCOMECHO + NO₂

G45479: KDEC NTLFUO → ACCOMECHO + NO₂

G45486b: KDEC C₅DIALO → MALDIAL + CO + HO₂ and reactions with KRO₂HO₂.

G45487: KDEC C₅DIALO → MALDIAL

G45488: KDEC C₅DIALO → MALDIAL

G45489: KDEC C₅DIALO → MALDIAL

G45491b: Reactions with KRO₂HO₂.

G45492: MGLYOX + GLYOX + HO2 from KDEC substitution

G45493: MGLYOX + GLYOX + HO2 from KDEC substitution

G45494: Permutation reaction (minor channels removed).

G46201: Alkyl nitrate formation neglected.

G46404b: Reactions with KRO2HO2 and KDEC C615CO2O \rightarrow C5DICARB + CO + HO2.

G46405: KDEC C615CO2O \rightarrow C5DICARB + CO + HO2

G46406: KDEC C615CO2O \rightarrow C5DICARB + CO + HO2

G46407: Only major channel.

G46413b: Reactions with KRO2HO2 and KDEC DNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2.

G46414: KDEC DNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2

G46415: KDEC DNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2

G46416: KDEC DNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2

G46418: KDEC CATECOOA \rightarrow MALDALCO2H + HCOCO2H + HO2 + OH

G46426: KFPAN \rightarrow k_CH3CO3_NO2

G46430: KDEC GLYOOA \rightarrow .125 HCHO + .18 GLYOO + .82 HO2 + .57 OH + 1.265 CO

G46432b: Reactions with KRO2HO2 and KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46433: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46434: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46435: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46437b: Reactions with KRO2HO2 and KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46438: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46439: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46440: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46441: Merged equations.

G46447b: reactions with KRO2HO2 and KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46448: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46449: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46450: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46457: Merged equations.

G46458: Merged equations.

G46461b: Reactions with KRO2HO2 and KDEC PHENO \rightarrow 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46462: KDEC PHENO \rightarrow 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46463: KDEC PHENO \rightarrow 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46464: KDEC PHENO \rightarrow 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2 and Only major channel.

G46468: KFPAN \rightarrow k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO \rightarrow C5CO2OHCO3

G46481: KDEC PBZQO \rightarrow C5CO2OHCO3

G46482: KDEC PBZQO \rightarrow C5CO2OHCO3

G46483: KDEC PBZQO \rightarrow C5CO2OHCO3 and Only major channel.

G46485b: Reactions with KRO2HO2 and KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46486: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46490b: Reactions with KRO2HO2 and KDEC BZEMUCO \rightarrow 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO.

G46491b: KDEC BZEMUCO \rightarrow 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO.

G46492: KDEC BZEMUCO \rightarrow 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO

G46493: KDEC BZEMUCO \rightarrow 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO and Only major channel.

G46499b: Reactions with KRO2HO2 and KDEC NBZQO \rightarrow C6CO4DB + NO2.

G46500: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46501: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46502: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

G46517b: New channel.

G46522b: In analogy to TLBIPERO2 from toluene (Birdsall et al., 2010).

G46523b: KDEC BZBIPERO \rightarrow GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46524: KDEC BZBIPERO \rightarrow GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46525: KDEC BZBIPERO \rightarrow GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE and Only major channel.

G47210: Alkyl nitrate formation neglected.

G47214: Alkyl nitrate formation neglected.

G47218: Alkyl nitrate formation neglected.

G47222: Alkyl nitrate formation neglected.

G47223: ROO6R3OOH produced but no sink for it.

G47225: ROO6R4P produced but no sink for it.

G47226: ROO6R5P produced but no sink for it

G47400: Merged.

G47402a: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47402b: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47403: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2.

G47404: KROPRIM*O2 fast reaction C6H5CH2O = BENZAL + HO2. C6H5CH2OH replaced by its oxidation product BENZAL.

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero2.oh is set to 0.4 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

G47408a: KDEC TLBIPERO \rightarrow 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 C4MDIAL + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47408b: KDEC TLBIPERO \rightarrow 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47409: KDEC TLBIPERO \rightarrow 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47410: Only major channel and KDEC TLBIPERO \rightarrow 0.6 GLYOX + 0.4 MGLYOX + HO2 + 0.2 ZCODC23DB COD + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

G47412: KDEC MGLOOB \rightarrow 0.125 CH3CHO + 0.695 CH3CO + 0.57 CO + 0.57 OH + 0.125 HO2 + 0.18 MGLOO + 0.25 CO2

G47413: Merged.

G47418b: Reactions with KRO2HO2 and KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE.

G47419: KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

G47420: KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

G47421: KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE and Only major channel.

G47422b: Reactions with KRO2HO2 and KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47423: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47425: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2 and Only major channel.

G47426: TOL1OHNO2 is a nitro-phenol

G47429: KDEC MCATECOOA \rightarrow MC3ODBCO2H + HCOCO2H + HO2 + OH

G47436: KFPAN \rightarrow k_CH3CO3_NO2

G47438: Only major channel.

G47439b: Reactions with KRO2HO2 and KDEC TLEMUCO \rightarrow 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47440b: KDEC TLEMUCO \rightarrow 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47441: KDEC TLEMUCO \rightarrow 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47442: KDEC TLEMUCO \rightarrow 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2 and Only major channel.

G47445: KFPAN \rightarrow k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

G47482b: Reactions with KRO2HO2 and KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47483: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47484: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47485: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO \rightarrow C6CO2OHCO3

G47487: KDEC PTLQO \rightarrow C6CO2OHCO3

G47488: KDEC PTLQO \rightarrow C6CO2OHCO3

G47489: Only major channel. KDEC PTLQO \rightarrow C6CO2OHCO3.

G47494: New channel.

G47497b: Reactions with KRO2HO2 and KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47498: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47501b: Reactions with KRO2HO2 and KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47502: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47509b: Reactions with KRO2HO2 and KDEC DNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47510: KDEC DNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47511: KDEC DNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47512: KDEC DNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

G47513b: Reactions with KRO2HO2 and KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47514: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G48202: Alkyl nitrate formation neglected.

G48205: Alkyl nitrate formation neglected.

G48210: Alkyl nitrate formation neglected.

G48212: Alkyl nitrate formation neglected.

G48216: Alkyl nitrate formation neglected.

G48222: Alkyl nitrate formation neglected.

G48400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(1.36\text{E-}11 \cdot 0.24 + 2.31\text{E-}11 \cdot 0.29 + 1.43\text{E-}11 \cdot 0.155)/3$, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400b: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(1.36\text{E-}11 \cdot 0.05 + 2.31\text{E-}11 \cdot 0.04 + 1.43\text{E-}11 \cdot 0.10)/3$, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(1.36\text{E-}11 \cdot 0.16 + 2.31\text{E-}11 \cdot 0.17 + 1.43\text{E-}11 \cdot 0.12)/3$, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48400d: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(1.36\text{E-}11 \cdot 0.55 + 2.31\text{E-}11 \cdot 0.50 + 1.43\text{E-}11 \cdot 0.625)/3$, where k and coefficients are for the single isomers ortho, meta and para from MCM.

G48401: Same products as for toluene. The rate constant is the average of m, p, o $k = (4.10\text{E-}16 + 2.60\text{E-}16 + 5.00\text{E-}16)/3 = 3.9\text{E-}16$.

G48402: merged under same rate constant

G48403: Same products as for toluene

G48405: KDEC CH2OOB \rightarrow 0.24 CH2OO + 0.40 CO + 0.36 HO2 + 0.36 CO + 0.36 OH and H2O + PHCHOO \rightarrow 0.625 PHCOOH + 0.375 BENZAL + 0.375 H2O2 + 0.2 CO2

G48408: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48409: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48410: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48412b: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL and reactions with KRO2HO2.

G48413: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

G48414: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

G48415: KDEC STYRENO \rightarrow HO2 + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

G49246: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)2. Instead of the (lacking) carbonyl a product of further degradation is assumed.

G49247: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G49248: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11 \cdot 0.70 + 3.25\text{E-}11 \cdot 0.61 + 5.67\text{E-}11 \cdot 0.79)/3$, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400b: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11 \cdot 0.06 + 3.25\text{E-}11 \cdot 0.06 + 5.67\text{E-}11 \cdot 0.03)/3$, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11 \cdot 0.03 + 3.25\text{E-}11 \cdot 0.03 + 5.67\text{E-}11 \cdot 0.04)/3$, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400d: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11 \cdot 0.70 + 3.25\text{E-}11 \cdot 0.61 + 5.67\text{E-}11 \cdot 0.79)/3$, where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49401: Same products as for toluene. The rate constant is the average of m, p, o $k = (1.90 + 1.80 + 0.88)\text{E-}15/3 = 1.52\text{E-}15$.

G40200: Products from Vereecken et al. (2007). $\text{LAP-INABO2} = 0.65 \text{ APINAO2} + 0.35 \text{ APINBO2}$

G40203: Weighted average for isomers A and B, $k = 0.33 \cdot 9.20\text{E-}14 + 0.67 \cdot 8.80\text{E-}13$.

G40204: Weighted average for isomers A and B, $k = 0.35 \cdot 1.83\text{E-}11 + 0.65 \cdot 3.28\text{E-}11$.

G40205: Weighted average for isomers A and B, $k = 0.35 \cdot 5.50\text{E-}12 + 0.65 \cdot 3.64\text{E-}12$.

G40206: SAR-estimated rate constant, $(k_{\text{ads}} + k_{\text{adt}}) \cdot \text{acoch3} = 6.46\text{E-}11$ where $k_{\text{ads}} = 3.0\text{E-}11$, $k_{\text{adt}} = 5.5\text{E-}11$, $\text{acoch3} = 0.76$

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard and Pascoe (2009).

G40212: Products from Rickard and Pascoe (2009).

G40232: Products from Capouet et al. (2008). BELV from Ehn et al. (2014). BLOV guess

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard and Pascoe (2009).

G40248: Alkyl nitrate formation neglected.

G40252a: Products from Vereecken and Peeters (2012).

G40252b: Products from Vereecken and Peeters (2012).

G40262: RO6R1OOH is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

G40267a: Products from Nguyen et al. (2009). BELV from Ehn et al. (2014). BLOV guess

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for RO6R1NO3 in G4085.

G40276: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)_2 .

G40277: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G40278: Theoretical keto-enol tautomerization catalyzed by formic acid (Grenfell et al., 2006).

G40282a: Products from Vereecken and Peeters (2012).

G40282b: Products from Vereecken and Peeters (2012).

G40283a: Products from Nguyen et al. (2009).

G40284: Products from Rickard and Pascoe (2009).

G40285a: Products from Vereecken and Peeters (2012).

G40285b: Products from Vereecken and Peeters (2012).

G40286a: Products from Nguyen et al. (2009).

G40287: Products from Rickard and Pascoe (2009).

G40400: DIET35TOL(from MCM) as representative of higher aromatics

G40401: Same products as for toluene.

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.

G6409: It is assumed that the reaction liberates all Cl atoms in the form of HCl.

G8102: Consistent with O'Dowd and Hoffmann (2005), 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 I + O_2 .

G8300: The rate coefficient is: $k_{\text{I_NO2}} = k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 3.\text{E-}31, 1., 6.6\text{E-}11, 0., 0.63)$.

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

G8401: The rate coefficient is from Dillon et al. (2006b), 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).

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

G40259a: ROO6R1OOH is produced but no sink for it.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
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_HNO3)	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HNO4)	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_CH3ON0)	Sander et al. (2014)
J41005	StTrGJN	$CH_3ONO_2 + h\nu \rightarrow CH_3O + NO_2$	jx(ip_CH3NO3)	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)
J42000	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J42001a	TrGJC	$CH_3CHO + h\nu \rightarrow CH_3 + HO_2 + CO$	jx(ip_CH3CHO)	Sander et al. (2014)
J42001b	TrGJC	$CH_3CHO + h\nu \rightarrow CH_2CHOH$	jx(ip_CH3CHO2VINY)	Clubb et al. (2012)
J42002	TrGJC	$CH_3C(O)OOH + h\nu \rightarrow CH_3 + OH + CO_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J42004	TrGJCN	$PAN + h\nu \rightarrow .7 CH_3C(O) + .7 NO_2 + .3 CH_3 + .3 CO_2 + .3 NO_3$	jx(ip_PAN)	Sander et al. (2014)*
J42005a	TrGJC	$HOCH_2CHO + h\nu \rightarrow HCHO + 2 HO_2 + CO$	jx(ip_HOCH2CHO)*0.83	Sander et al. (2014)*
J42005b	TrGJC	$HOCH_2CHO + h\nu \rightarrow OH + HCOCH_2O_2$	jx(ip_HOCH2CHO)*0.07	Sander et al. (2014)*
J42005c	TrGJC	$HOCH_2CHO + h\nu \rightarrow CH_3OH + CO$	jx(ip_HOCH2CHO)*0.10	Sander et al. (2014)*
J42006	TrGJC	$HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$	jx(ip_CH300H)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42007	TrGJCN	PHAN + $h\nu \rightarrow .7 \text{ HOCH}_2\text{CO} + .7 \text{ NO}_2 + .3 \text{ HCHO} + .3 \text{ HO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	see note*
J42008	TrGJC	GLYOX + $h\nu \rightarrow 2 \text{ CO} + 2 \text{ HO}_2$	jx(ip_GLYOX)	Sander et al. (2014)
J42009	TrGJC	HCOCO ₂ H + $h\nu \rightarrow 2 \text{ HO}_2 + \text{CO} + \text{CO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J42010	TrGJC	HCOCO ₃ H + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J42011	TrGJC	HYETHO2H + $h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J42012	TrGJCN	ETHOHNO ₃ + $h\nu \rightarrow \text{HO}_2 + 2 \text{ HCHO} + \text{NO}_2$	j_IC3H7N03	Rickard and Pascoe (2009)
J42013	TrGJC	HOCH2CO3H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	2*jx(ip_CH300H)	Sander et al. (2018)
J42014	TrGC	HOCH2CO2H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2$	jx(ip_CH300H)	Sander et al. (2018)
J42015	TrGC	CH2CO + $h\nu \rightarrow .4 \text{ CO}_2 + .8 \text{ H} + .34 \text{ CO} + .34 \text{ OH} + .34 \text{ HO}_2 + .16 \text{ HCHO} + .16 \text{ O}(^3\text{P}) + .1 \text{ HCOOH} + \text{CO}$	j_ketene* 0.36	Sander et al. (2018)
J42016	TrGC	CH3CHOHOOH + $h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	jx(ip_CH300H)	Sander et al. (2018)
J42017	TrGJCN	NO ₃ CH2CHO + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	(jx(ip_C2H5N03)+jx(ip_CH3CHO)) *(jx(ip_NOA)+1E-10)/(0.59*j_IC3H7N03+jx(ip_CH3COCH3)+1E-10)	Sander et al. (2018)*
J42018	TrGJC	HOCH2CHO + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Sander et al. (2018)
J42019	TrGJCN	C ₂ H ₅ ONO ₂ + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	jx(ip_C2H5N03)	Sander et al. (2018)
J42020	TrGJCN	NO ₃ CH2CHO + $h\nu \rightarrow .7 \text{ NO}_3\text{CH}_2\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ HCHO} + .3 \text{ NO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	Sander et al. (2018)*
J42021	StTrGJCN	C ₂ H ₅ O ₂ NO ₂ + $h\nu \rightarrow .667 \text{ NO}_2 + .667 \text{ C}_2\text{H}_5\text{O}_2 + .333 \text{ NO}_3 + .333 \text{ CH}_3\text{CHO} + .333 \text{ HO}_2$	jx(ip_CH302N02)	Sander et al. (2018)*
J43000	TrGJC	iC ₃ H ₇ OOH + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	von Kuhlmann (2001)
J43001	TrGJC	CH ₃ COCH ₃ + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{CH}_3$	jx(ip_CH3COCH3)	Sander et al. (2014)
J43002	TrGJC	CH ₃ COCH ₂ OH + $h\nu \rightarrow .5 \text{ CH}_3\text{C(O)} + .5 \text{ HCHO} + .5 \text{ HO}_2 + .5 \text{ HOCH}_2\text{CO} + .5 \text{ CH}_3$	j_ACETOL	Sander et al. (2014)*
J43003	TrGJC	MGLYOX + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Sander et al. (2014)
J43004	TrGJC	CH ₃ COCH ₂ O ₂ H + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Rickard and Pascoe (2009)
J43005	TrGJC	HOCH2COCH2OOH + $h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Sander et al. (2018)
J43006	TrGJCN	iC ₃ H ₇ ONO ₂ + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	j_IC3H7N03	von Kuhlmann et al. (2003)*
J43007	TrGJCN	NOA + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{NO}_2$	jx(ip_NOA)	Barnes et al. (1993)
J43009	TrGJC	HYPPO2H + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43010	TrGJCN	PR2O2HNO ₃ + $h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43011	TrGJC	HOCH2COCHO + $h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J43012	TrGJC	HCOCOCH ₂ OOH + $h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Sander et al. (2018)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43013	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2018)
J43014	TrGJTerC	$\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard and Pascoe (2009)
J43015	TrGJTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{HO}_2$	$\text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J43016	TrGJTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J43017	TrGJC	$\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$	$2 * \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2018)
J43018	TrGJC	$\text{CH}_3\text{COCO}_2\text{H} + h\nu \rightarrow .32 \text{ CH}_3\text{CHO} + .16 \text{ CH}_2\text{CHOH} + .54 \text{ CO}_2 + .38 \text{ CH}_3\text{C}(\text{O}) + .38 \text{ HO}_2 + .38 \text{ CO}_2 + .07 \text{ CH}_3\text{COOH} + .07 \text{ CO} + .05 \text{ CH}_3\text{C}(\text{O}) + .05 \text{ CO} + .05 \text{ OH}$	$\text{jx}(\text{IP_CH3COCOC}_2\text{H})$	Sander et al. (2018)*
J43019	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{CO}_2$	$\text{jx}(\text{IP_MGLYOX}) + \text{jx}(\text{ip_CH300H})$	Sander et al. (2018)
J43020	TrGC	$\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{j_ketene} * 0.36 * 2.$	Sander et al. (2018)
J43021	TrGCN	$\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	j_IC3H7NO_3	Sander et al. (2018)
J43022	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$	$\text{jx}(\text{ip_CH302NO}_2) + \text{jx}(\text{ip_CH3COC}_2\text{H})$	Sander et al. (2018)
J43023	TrGJC	$\text{C}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43024	TrGJCN	$\text{C}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{NO}_2 + \text{HO}_2$	$0.59 * \text{j_IC3H7NO}_3$	see note*
J43025a	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{HCO})$	see note*
J43025b	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$	$\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$	Andrews et al. (2012), Sander et al. (2018)*
J43026	TrGJCN	$\text{PPN} + h\nu \rightarrow .7 \text{ C}_2\text{H}_5\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ C}_2\text{H}_5\text{O}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2014)
J43027	TrGJC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43028a	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2018)
J43028b	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH300H})$	Sander et al. (2018)
J43200	TrGJTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J43400	TrGJAroC	$\text{C3DIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2 + \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J43401	TrGJAroC	$\text{C32OH13CO} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2$	Rickard and Pascoe (2009)
J43402	TrGJAroC	$\text{HCOCOCHCO}_3\text{H} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J44000a	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_p} / (\text{k_p} + \text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2018)
J44000b	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_s} / (\text{k_p} + \text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2018)
J44001	TrGJC	$\text{MVK} + h\nu \rightarrow .5 \text{ C}_3\text{H}_6 + .5 \text{ CH}_3\text{C}(\text{O}) + .5 \text{ HCHO} + \text{CO} + .5 \text{ HO}_2$	$\text{jx}(\text{ip_MVK})$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44002	TrGJC	MEK + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$	$0.42 * jx(ip_CHOH)$	von Kuhlmann et al. (2003)
J44003	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$	$jx(ip_CH300H) + 0.42 * jx(ip_CHOH)$	Sander et al. (2018)
J44004	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C}(\text{O})$	$2.15 * jx(ip_MGLYOX)$	see note*
J44005a	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$j_IC3H7N03*(k_p/(k_p+k_s))$	see note*
J44005b	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$	$j_IC3H7N03*(k_s/(k_p+k_s))$	see note*
J44006	TrGJCN	$\text{MPAN} + h\nu \rightarrow .7 \text{MACO}_3 + .7 \text{NO}_2 + .3 \text{MACO}_2 + .3 \text{NO}_3$	$jx(ip_PAN)$	see note*
J44007a	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J44007b	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HO}_2 + \text{HCOCO}_3\text{H}$	j_ACETOL	Rickard and Pascoe (2009)
J44008	TrGJC	$\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$	$jx(ip_MACR)$	Sander et al. (2014)
J44009	TrGJC	$\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$	$jx(ip_CH300H) + 2.77 * jx(ip_HOCH2CHO)$	Sander et al. (2018)*
J44010	TrGJC	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$2.77 * jx(ip_HOCH2CHO)$	see note*
J44011	TrGJC	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2018)
J44012	TrGJC	$\text{LHMVKABOOH} + h\nu \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{CH}_3\text{C}(\text{O}) + .88 \text{HOCH}_2\text{CHO} + .12 \text{HCHO} + \text{OH}$	$jx(ip_CH300H) + j_ACETOL$	Sander et al. (2018)
J44013	TrGJC	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$jx(ip_HOCH2CHO) + j_ACETOL$	Sander et al. (2018)
J44014	TrGJC	$\text{HO}_2\text{CO}_3\text{C}_4 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{HO}_2$	j_ACETOL	Rickard and Pascoe (2009)
J44015	TrGJC	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	$2.15 * jx(ip_MGLYOX)$	see note*
J44016	TrGC	$\text{HCOCCH}_3\text{CO} + h\nu \rightarrow .5 \text{OH} + .5 \text{CH}_3\text{CHO} + \text{CO} + .5 \text{CH}_3\text{CHCO} + .5 \text{CO}$	j_KETENE	Sander et al. (2018)
J44017a	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{CH}_3\text{COCO}_2\text{H} + .1848 \text{H}_2\text{O}_2 + .2208 \text{MGLYOX} + .36 \text{OH} + .36 \text{CO} + .56 \text{CH}_3\text{C}(\text{O}) + .2 \text{CH}_3\text{CHO} + .2 \text{CO}_2 + .2 \text{HCHO} + .2 \text{HO}_2 + \text{CO}$	$j_KETENE * 0.5$	Sander et al. (2018), Rickard and Pascoe (2009)*
J44017b	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$	$j_KETENE * 0.5$	Sander et al. (2018)
J44018a	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$	$jx(ip_MGLYOX)$	Sander et al. (2018)
J44018b	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$	$2.15 * jx(ip_MGLYOX)$	Sander et al. (2018)
J44019	TrGJC	$\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$	$3.15 * jx(ip_MGLYOX)$	Sander et al. (2018)
J44020a	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$	$jx(ip_CH300H) + j_ACETOL$	Rickard and Pascoe (2009)
J44020b	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$	$2.15 * jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J44021	TrGJTerC	$\text{C44OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J44022	TrGJTerC	$\text{C413COOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$	$jx(ip_CH300H) + jx(ip_HOCH2CHO) + j_ACETOL$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44023a	TrGJTerC	$C4CODIAL + h\nu \rightarrow HCOCOCH_2O_2 + HO_2 + CO$	$jx(ip_HOCH2CHO)$	Rickard and Pascoe (2009)
J44023b	TrGJTerC	$C4CODIAL + h\nu \rightarrow HCOCH_2CO_3 + HO_2 + CO$	$jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J44024	TrGJTerC	$C312COCO3H + h\nu \rightarrow HCOCOCH_2O_2 + CO_2 + OH$	$jx(ip_CH300H) + jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J44025	TrGJCN	$LMEKNO_3 + h\nu \rightarrow .62 CH_3C(O) + .62 CH_3CHO + .38 HCHO$ $+ .38 CO_2 + .38 HOCH_2CH_2O_2 + NO_2$	$jx(ip_MEKN03)$	Barnes et al. (1993), Sander et al. (2018)*
J44026	TrGJCN	$MVKNO_3 + h\nu \rightarrow CH_3C(O) + HOCH_2CHO + NO_2$	$jx(ip_MEKN03)$	Barnes et al. (1993), Sander et al. (2018)*
J44027	TrGJCN	$MACRNO_3 + h\nu \rightarrow CH_3COCH_2OH + CO + HO_2 + NO_2$	$(2.84*j_IC3H7N03 + jx(ip_CH3CHO))$ $*(jx(ip_MEKN03) + 1E-10) / (j_$ $IC3H7N03 + 0.42*jx(ip_CHOH) + 1E-10)$	Müller et al. (2014), Sander et al. (2018)*
J44028	TrGJCN	$TC4H9NO_3 + h\nu \rightarrow CH_3COCH_3 + CH_3 + NO_2$	$2.84*j_IC3H7N03$	Sander et al. (2018)
J44029	TrGJC	$TC_4H_9OOH + h\nu \rightarrow CH_3COCH_3 + CH_3 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44030	TrGJCN	$IBUTOLBNO_3 + h\nu \rightarrow CH_3COCH_3 + HCHO + HO_2 + NO_2$	$2.84*j_IC3H7N03$	Sander et al. (2018)
J44031	TrGJC	$IBUTOLBOOH + h\nu \rightarrow CH_3COCH_3 + HCHO + HO_2 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44032	TrGJC	$LBUT1ENOOH + h\nu \rightarrow C_2H_5CHO + HCHO + HO_2 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44033	TrGJCN	$LBUT1ENNO_3 + h\nu \rightarrow C_2H_5CHO + HCHO + HO_2 + NO_2$	$j_IC3H7N03$	Sander et al. (2018)
J44034	TrGJC	$BUT2OLOOH + h\nu \rightarrow 2 CH_3CHO + HO_2 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44035	TrGJCN	$BUT2OLNO_3 + h\nu \rightarrow 2 CH_3CHO + HO_2 + NO_2$	$j_IC3H7N03$	Sander et al. (2018)
J44036	TrGJC	$BUT2OLO + h\nu \rightarrow CH_3C(O) + HOCH_2CO$	j_ACETOL	Sander et al. (2018)
J44037a	TrGJC	$C_3H_7CHO + h\nu \rightarrow C_3H_7O_2 + CO + HO_2$	$jx(ip_C3H7CHO2HCO)$	Sander et al. (2018)
J44037b	TrGJC	$C_3H_7CHO + h\nu \rightarrow C_2H_4 + CH_2CHOH$	$jx(ip_C3H7CHO2VINY)$	Sander et al. (2018)*
J44038	TrGJC	$IPRCHO + h\nu \rightarrow iC_3H_7O_2 + CO + HO_2$	$jx(ip_IPRCHO2HCO)$	Sander et al. (2018)
J44039	TrGJCN	$IC4H9NO_3 + h\nu \rightarrow IPRCHO + NO_2$	$j_IC3H7N03$	Sander et al. (2018)
J44040	TrGJC	$IC_4H_9OOH + h\nu \rightarrow IPRCHO + HO_2 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44041	TrGJC	$PERIBUACID + h\nu \rightarrow iC_3H_7O_2 + CO_2 + OH$	$jx(ip_CH300H)$	Sander et al. (2018)
J44042	TrGJCN	$PIPNO_3 + h\nu \rightarrow .7 IPRCO_3 + .7 NO_2 + .3 iC_3H_7O_2 + .3 CO_2 +$ $.3 NO_3$	$jx(ip_PAN)$	Sander et al. (2018), Sander et al. (2014)
J44043	TrGJC	$HVMK + h\nu \rightarrow MGLYOX + CO + 2 OH$	$jx(ip_PeDIONE24)$	Sander et al. (2018), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	$HMAC + h\nu \rightarrow HCOCCH_3CO + 2 OH$	$jx(ip_PeDIONE24)$	Sander et al. (2018), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44045a	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_C2H5CHO2HCO})$	Rickard and Pascoe (2009)
J44045b	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$	$\text{jx}(\text{ip_C2H5CHO2ENOL})$	Andrews et al. (2012), Sander et al. (2018)
J44046a	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{jx}(\text{ip_C2H5CHO2HCO})*2.$	see note*
J44046b	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$	$\text{jx}(\text{ip_C2H5CHO2ENOL})*2.$	Andrews et al. (2012), Sander et al. (2018)
J44200	TrGJTerC	$\text{IBUTALOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{HO}_2 + \text{CO}$	j_ACETOL	Rickard and Pascoe (2009)
J44201	TrGJTerC	$\text{IPRHOCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J44400a	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{C}_3\text{OH13CO} + \text{CO} + \text{OH} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH2CHO})*2$	Rickard and Pascoe (2009)
J44400b	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44401	TrGJAroC	$\text{BZFUOOH} + h\nu \rightarrow \text{CO14O3CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44402	TrGJAroC	$\text{HOCOC4DIAL} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MGLYOX})+\text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44403	TrGJAroCN	$\text{NBZFUOOH} + h\nu \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard and Pascoe (2009)
J44404b	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow .6 \text{ MALANHY} + \text{HO}_2 + .4 \text{ GLYOX} + .4 \text{ CO} + .4 \text{ CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44405	TrGJAroC	$\text{EPXDLCO}_2\text{H} + h\nu \rightarrow \text{C3DIALO}_2 + \text{CO}_2 + \text{HO}_2$	$2.77*\text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44406	TrGJAroC	$\text{MALDIAL} + h\nu \rightarrow .4 \text{ BZFUONE} + .6 \text{ MALDIALCO}_3 + .6 \text{ HO}_2$	$\text{jx}(\text{ip_N02})*0.14$	Rickard and Pascoe (2009)
J44407	TrGJAroC	$\text{MALANHYOOH} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44408	TrGJAroC	$\text{EPXDLCO}_3\text{H} + h\nu \rightarrow \text{C3DIALO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H})+2.77*\text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44409	TrGJAroC	$\text{CO}_2\text{C}_4\text{DIAL} + h\nu \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{HO}_2 + \text{CO} + \text{CO}$	$\text{jx}(\text{ip_MGLYOX})*2$	Rickard and Pascoe (2009)
J44410	TrGJAroC	$\text{MALDALCO}_2\text{H} + h\nu \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard and Pascoe (2009)
J44411	TrGJAroC	$\text{EPXC4DIAL} + h\nu \rightarrow \text{C3DIALO}_2 + \text{CO} + \text{HO}_2$	$2.77*\text{jx}(\text{ip_HOCH2CHO})*2$	Rickard and Pascoe (2009)
J44412	TrGJAroC	$\text{CO14O3CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J44414	TrGJAroC	$\text{MECOACEOOH} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J45002	TrGJC	$\text{LISOPACOOH} + h\nu \rightarrow \text{LISOPACO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45003	TrGJCN	$\text{LISOPACNO}_3 + h\nu \rightarrow \text{LISOPACO} + \text{NO}_2$	$0.59*\text{j_IC3H7N03}$	see note*
J45004	TrGJC	$\text{ISOPBOOH} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45005	TrGJCN	$\text{ISOPBNO}_3 + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84*\text{j_IC3H7N03}$	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45006	TrGJC	ISOPDOOH + $h\nu$ → MACR + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45007	TrGJCN	ISOPDNO ₃ + $h\nu$ → MACR + HCHO + HO ₂ + NO ₂	j_IC3H7N03	see note*
J45008	TrGJCN	NISOPOOH + $h\nu$ → NC4CHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45009	TrGJCN	NC4CHO + $h\nu$ → LHC4ACCO ₃ + NO ₂	(.59*j_IC3H7N03+jx(ip_MACR)) *(jx(ip_MEKN03)+1E-10)/(j_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)	Müller et al. (2014), Sander et al. (2018)*
J45010	TrGJCN	LNISOOH + $h\nu$ → NOA + OH + .5 HOCHCHO + .5 CO + .5 HO ₂ + .5 CO ₂	jx(ip_CH300H)	Taraborrelli et al. (2009), Sander et al. (2018)
J45011	TrGJC	LHC4ACCHO + $h\nu$ → .5 LHC4ACCO ₃ + .5 HO ₂ + .5 CO + .5 OH + .25 MACRO ₂ + .25 LHMVKABO ₂	jx(ip_MACR)	Sander et al. (2018)
J45012	TrGJC	LC578OOH + $h\nu$ → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ + OH	jx(ip_CH300H)+ 2.77*jx(ip_HOCH2CHO)	Sander et al. (2018)
J45013	TrGJC	LHC4ACCO ₃ H + $h\nu$ → OH + .5 MACRO ₂ + .5 LHMVKABO ₂ + OH + CO ₂	j_HPALD	Sander et al. (2018)
J45014	TrGJCN	LC5PAN1719 + $h\nu$ → .7 LHC4ACCO ₃ + .7 NO ₂ + .15 MACRO ₂ + .15 LHMVKABO ₂ + .3 CO ₂ + .3 NO ₃	jx(ip_PAN)	Sander et al. (2018)
J45015	TrGJC	HCOC ₅ + $h\nu$ → .65 CH ₃ + .65 CO + .65 HCHO + .35 OH + .35 CH ₃ COCH ₂ O ₂ + HOCH ₂ CO	0.5*jx(ip_MVK)	Sander et al. (2018)*
J45016	TrGJC	C59OOH + $h\nu$ → CH ₃ COCH ₂ OH + HOCH ₂ CO + OH	j_ACETOL+jx(ip_CH300H)	Sander et al. (2018)
J45017	TrGJTerC	C511OOH + $h\nu$ → CH ₃ C(O) + HCOCH ₂ CHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018a	TrGJTerC	CO23C4CHO + $h\nu$ → CH ₃ COCOCH ₂ O ₂ + HO ₂ + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018b	TrGJTerC	CO23C4CHO + $h\nu$ → CH ₃ C(O) + HCOCH ₂ CO ₃	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45019	TrGJTerC	CO23C4CO ₃ H + $h\nu$ → CH ₃ COCOCH ₂ O ₂ + CO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45020	TrGJTerC	C512OOH + $h\nu$ → C513O ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45021	TrGJTerC	CO13C4CHO + $h\nu$ → CHOC ₃ COO ₂ + CO + HO ₂	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45022	TrGJTerC	C513OOH + $h\nu$ → GLYOX + HOC ₂ H ₄ CO ₃ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45023	TrGJTerC	C513CO + $h\nu$ → HOC ₂ H ₄ CO ₃ + HO ₂ + CO + CO	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45024	TrGJTerC	C514OOH + $h\nu$ → CO13C4CHO + HO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45025	TrGJTerCN	C514NO ₃ + $h\nu$ → CO13C4CHO + HO ₂ + NO ₂	j_IC3H7N03+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45026a	TrGJC	LZCODC23DBCOOH + $h\nu$ → OH + CO + HVMK + OH	j_HPALD*0.6*0.5	Sander et al. (2018), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	LZCODC23DBCOOH + $h\nu$ → OH + CO + CH ₃ C(O) + HOCH ₂ CHO	j_HPALD*0.6*0.5	Sander et al. (2018), Jenkin et al. (2015), Peeters et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45026c	TrGJC	LZCODC23DBCOOH + $h\nu$ → OH + CO + HMAc + OH	j_HPAlD*0.4*0.5	Sander et al. (2018), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	LZCODC23DBCOOH + $h\nu$ → OH + CO + CO + CH ₃ COCH ₂ OH + HO ₂	j_HPAlD*0.4*0.5	Sander et al. (2018), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	LZCO3HC23DBCOD + $h\nu$ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO ₂	j_HPAlD	Sander et al. (2018)
J45028a	TrGJC	C1OOHC2OOHC4OD + $h\nu$ → CH ₃ COCH ₂ O ₂ H + OH + 2 CO + HO ₂	2.77*jx(IP_HOCH2CHO)	Sander et al. (2018)
J45028b	TrGJC	C1OOHC2OOHC4OD + $h\nu$ → .5 CH ₃ COCH ₂ O ₂ H + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH	2.*jx(IP_CH300H)	Sander et al. (2018)
J45029	TrGC	DB1OOH + $h\nu$ → DB1O2 + OH	jx(IP_CH300H)	Sander et al. (2018)
J45030	TrGC	DB2OOH + $h\nu$ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH	jx(ip_CH300H)	Sander et al. (2018)
J45031a	TrGJC	C1ODC2OOHC4OD + $h\nu$ → MGLYOX + HOCHCHO + OH	jx(ip_CH300H)	Sander et al. (2018)
J45031b	TrGJC	C1ODC2OOHC4OD + $h\nu$ → CO2H3CHO + CO + HO ₂ + OH	2.*2.77*jx(IP_HOCH2CHO)	Sander et al. (2018)
J45032	TrGJC	C4MDIAL + $h\nu$ → .5 CH ₃ COCHCO + .5 HCOCCH ₃ CO + CO + HO ₂ + OH	jx(ip_N02)*0.1*0.5	Sander et al. (2018)*
J45033	TrGCN	DB1NO3 + $h\nu$ → DB1O2 + NO ₂	j_IC3H7N03	Sander et al. (2018)
J45034	TrGJTerC	CHOC3COOOH + $h\nu$ → CHOC3COO2 + CO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO) +j_ACETOL	Rickard and Pascoe (2009)
J45200a	TrGJTerC	LMBOABOOH + $h\nu$ → HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + OH	jx(ip_CH300H)*.67	Rickard and Pascoe (2009), Sander et al. (2018)
J45200b	TrGJTerC	LMBOABOOH + $h\nu$ → IBUTALOH + HCHO + HO ₂ + OH	jx(ip_CH300H)*.33	Rickard and Pascoe (2009), Sander et al. (2018)
J45201	TrGJTerC	MBOACO + $h\nu$ → HCHO + HO ₂ + IPRHOCO3	j_ACETOL	Rickard and Pascoe (2009)
J45202	TrGJTerC	MBOCOCO + $h\nu$ → CO + HO ₂ + IPRHOCO3	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45203a	TrGJTerCN	LNMBOABOOH + $h\nu$ → NO ₃ CH2CHO + CH ₃ COCH ₃ + HO ₂ + OH	jx(ip_CH300H)*.65	Rickard and Pascoe (2009), Sander et al. (2018)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45203b	TrGJTerCN	LNMBOABOOH + $h\nu$ → IBUTALOH + HCHO + NO ₂ + OH	jx(ip_CH300H)*.35	Rickard and Pascoe (2009), Sander et al. (2018)
J45204	TrGJTerCN	NC4OHCO3H + $h\nu$ → IBUTALOH + CO ₂ + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45400	TrGJAroC	C54CO + $h\nu$ → HO ₂ + CO + CO + CO + CH ₃ C(O)	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
J45401	TrGJAroC	C5134CO2OH + $h\nu$ → CH ₃ COCOCHO + HO ₂ + CO + HO ₂	jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45402	TrGJAroC	C5DIALOOH + $h\nu$ → MALDIAL + CO + HO ₂ + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)*
J45406	TrGJAroC	C5CO14OH + $h\nu$ → CH ₃ C(O) + HCOCO ₂ H + HO ₂ + CO	jx(ip_MVK)	Rickard and Pascoe (2009)
J45407	TrGJAroC	C5DICARB + $h\nu$ → .6 C5CO14O2 + .6 HO ₂ + .4 TLFUONE	jx(ip_N02)*0.2	Rickard and Pascoe (2009)*
J45408	TrGJAroC	MC3ODBCO2H + $h\nu$ → CH ₃ COCO ₂ H + HO ₂ + CO + HO ₂ + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J45409	TrGJAroC	ACCOMMECHO + $h\nu$ → MECOACETO2 + HO ₂ + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45410	TrGJAroC	MMALNHYOOH + $h\nu$ → CO2H3CO3 + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45411	TrGJAroC	C5DICAROOH + $h\nu$ → MGLYOX + GLYOX + HO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)+j_ACETOL	Rickard and Pascoe (2009)*
J45412	TrGJAroCN	NTLFUOOH + $h\nu$ → ACCOMECHO + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45414	TrGJAroC	C5CO14OOH + $h\nu$ → .83 MALANHY + .83 CH ₃ + .17 MGLYOX + .17 HO ₂ + .17 CO + .17 CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45415	TrGJAroC	TLFUOOH + $h\nu$ → ACCOMECHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45417	TrGJAroC	ACCOMECO3H + $h\nu$ → MECOACETO2 + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45418	TrGJAroC	C5DIALCO + $h\nu$ → MALDIALCO3 + CO + HO ₂	jx(ip_MGLYOX)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46200	TrGJTerCN	C614NO3 + $h\nu$ → CO23C4CHO + HCHO + HO ₂ + NO ₂	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46201	TrGJTerC	C614OOH + $h\nu$ → CO23C4CHO + HCHO + HO ₂ + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46202	TrGJTerC	CO235C5CHO + $h\nu$ → CO23C4CO3 + CO + HO ₂	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46203	TrGJTerC	CO235C6OOH + $h\nu$ → CO23C4CO3 + HCHO + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46400	TrGJAroC	PHENOOH + $h\nu$ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46401	TrGJAroC	C6CO4DB + $h\nu$ → C4CO2DBCO3 + HO ₂ + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46402	TrGJAroC	$C_5CO_2DCO_3H + h\nu \rightarrow CH_3C(O) + HCOCOCHO + CO_2 + OH$	$jx(ip_CH300H) + jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J46403	TrGJAroCN	$NDNPHENO_2H + h\nu \rightarrow NC_4DCO_2H + HNO_3 + CO + CO + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	$BZBIPERNO_3 + h\nu \rightarrow GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + NO_2$	$j_IC3H7N03$	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	$HOC_6H_4NO_2 + h\nu \rightarrow HONO + CPDKETENE$	$jx(ip_HOC_6H_4NO_2)$	Chen et al. (2011)*
J46406	TrGJAroC	$CPDKETENE + h\nu \rightarrow CO_2 + CO + 2 HO_2 + MALDIAL$	j_KETENE	see note*
J46407	TrGJAroC	$C_5COOHCO_3H + h\nu \rightarrow HOCOC_4DIAL + HO_2 + CO + CO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46408	TrGJAroC	$BZEPOXMUC + h\nu \rightarrow .5 C_5DIALO_2 + 1.5 HO_2 + 1.5 CO + .5 MALDIAL$	$4.E3*jx(ip_MVK)*0.1$	Rickard and Pascoe (2009)
J46409	TrGJAroCN	$NPHEN1OOH + h\nu \rightarrow NPHEN1O + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46410	TrGJAroC	$BZEMUCCO + h\nu \rightarrow HCOCO_2HCO_3 + C_3DIALO_2$	$jx(ip_HOCH_2CHO)*2 + j_ACETOL$	Rickard and Pascoe (2009)
J46411	TrGJAroC	$BZEMUCCO_2H + h\nu \rightarrow C_5DIALO_2 + CO_2 + HO_2$	$jx(ip_MACR)$	Rickard and Pascoe (2009)
J46412	TrGJAroCN	$NNCATECOOH + h\nu \rightarrow NC_4DCO_2H + HCOCO_2H + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46413	TrGJAroC	$C_615CO_2OOH + h\nu \rightarrow C_5DICARB + CO + HO_2 + OH$	$jx(ip_MVK) + jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46414	TrGJAroCN	$NPHENO_2H + h\nu \rightarrow MALDALCO_2H + GLYOX + OH + NO_2$	$j_IC3H7N03 + jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46415	TrGJAroCN	$NCATECOOH + h\nu \rightarrow NC_4DCO_2H + HCOCO_2H + HO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46416	TrGJAroC	$PBZQOOH + h\nu \rightarrow C_5CO_2OHCOC_3 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46417	TrGJAroC	$BZOBIPEROH + h\nu \rightarrow MALDIALCO_3 + GLYOX + HO_2$	j_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	$BZBIPERO_2H + h\nu \rightarrow GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	$NBZQOOH + h\nu \rightarrow C_6CO_4DB + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46420	TrGJAroC	$CATEC1OOH + h\nu \rightarrow CATEC1O + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46421	TrGJAroC	$C_6125CO + h\nu \rightarrow C_5CO_14O_2 + CO + HO_2$	$jx(ip_MGLYOX) + jx(ip_MVK)$	Rickard and Pascoe (2009)
J46422	TrGJAroCN	$DNPHENO_2H + h\nu \rightarrow NC_4DCO_2H + HCOCO_2H + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J46423	TrGJAroC	$BZEMUCCO_3H + h\nu \rightarrow C_5DIALO_2 + CO_2 + OH$	$jx(ip_CH300H) + jx(ip_MACR)$	Rickard and Pascoe (2009)
J46424	TrGJAroC	$C_6H_5OOH + h\nu \rightarrow C_6H_5O + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J46425	TrGJAroC	$BZEMUCOOH + h\nu \rightarrow .5 EPXC_4DIAL + .5 GLYOX + .5 HO_2 + .5 C_3DIALO_2 + .5 C_32OH13CO + OH$	$jx(ip_CH300H) + jx(ip_HOCH_2CHO)*2$	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46427	TrGJAroCN	BZEMUCNO ₃ + hν → EPXC4DIAL + NO ₂ + GLYOX + HO ₂	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J46428	TrGJAroCN	DNPEN + hν → HONO + NCPDKETENE	jx(ip_HOC6H4NO ₂)	Sander et al. (2018)
J46429	TrGJAroCN	NCPDKETENE + hν → CO ₂ + CO + 2 HO ₂ + NC4DCO ₂ H	j_KETENE	see note*
J47200	TrGJTerC	CO ₂ 35C6CHO + hν → CHOC3COCO ₃ + CH ₃ C(O)	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47201	TrGJTerC	C ₂ 35C6CO ₃ H + hν → CO ₂ 35C6O ₂ + CO ₂ + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47202	TrGJTerC	C ₇ 16OOH + hν → CO ₁₃ C ₄ CHO + CH ₃ C(O) + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J47203	TrGJTerC	C ₇ 21OOH + hν → C ₇ 22O ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47204	TrGJTerC	C ₇ 22OOH + hν → CH ₃ COCH ₃ + C ₄ 4O ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47400	TrGJAroC	TLEPOXMUC + hν → .5 C ₆ 15CO ₂ O ₂ + HO ₂ + CO + .5 EPXC4DIAL + .5 CH ₃ C(O)	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)
J47401	TrGJAroC	C ₆ H ₅ CH ₂ OOH + hν → BENZAL + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47402	TrGJAroCN	C ₆ H ₅ CH ₂ NO ₃ + hν → BENZAL + HO ₂ + NO ₂	0.59*j_IC3H7NO ₃	Rickard and Pascoe (2009)*
J47403	TrGJAroC	BENZAL + hν → HO ₂ + CO + C ₆ H ₅ O ₂	jx(ip_BENZAL)	Wallington et al. (2018)
J47404	TrGJAroC	TLBIPEROOH + hν → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C ₄ MDIAL + .2 C ₅ DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47405	TrGJAroCN	TLBIPERNO ₃ + hν → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C ₄ MDIAL + .2 C ₅ DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO ₂	j_IC3H7NO ₃	Rickard and Pascoe (2009)*
J47406	TrGJAroC	TLOBIPEROH + hν → C ₅ CO ₁₄ O ₂ + GLYOX + HO ₂	j_ACETOL	Rickard and Pascoe (2009)
J47407	TrGJAroC	CRESOOH + hν → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47408a	TrGJAroCN	NCRESOOH + hν → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH + NO ₂	j_IC3H7NO ₃	Rickard and Pascoe (2009)*
J47408b	TrGJAroCN	NCRESOOH + hν → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	TOL1OHNO ₂ + hν → HONO + MCPDKETENE	jx(ip_HOPh3Me2NO ₂)	see note*
J47410	TrGJAroC	TLEMUCCO ₂ H + hν → C ₆ 15CO ₂ O ₂ + CO ₂ + HO ₂	jx(ip_MACR)	Rickard and Pascoe (2009)
J47411	TrGJAroC	TLEMUCCO ₃ H + hν → C ₆ 15CO ₂ O ₂ + CO ₂ + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)
J47412	TrGJAroC	TLEMUCOOH + hν → .5 C ₃ DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)+j_ACETOL	Rickard and Pascoe (2009)*
J47413	TrGJAroCN	TLEMUCNO ₃ + hν → EPXC4DIAL + NO ₂ + CH ₃ C(O) + CO + HO ₂	2.77*jx(ip_HOCH2CHO)+j_ACETOL	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47414	TrGJAroC	$\text{TLEMUCCO} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{EPXC4DIAL} + \text{CO} + \text{HO}_2$	$2.77 * \text{jx(ip_HOCH2CHO)} + 2.15 * \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J47415	TrGJAroC	$\text{C6H5CO3H} + h\nu \rightarrow \text{C6H5O2} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47416	TrGJAroC	$\text{OXYL1OOH} + h\nu \rightarrow \text{TOL1O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47417	TrGJAroCN	$\text{MNCATECH} + h\nu \rightarrow \text{HONO} + \text{MCPDKETENE}$	$\text{jx(ip_HOPh3Me2N02)}$	see note*
J47418	TrGJAroC	$\text{MCPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{HO}_2 + \text{C4MDIAL}$	j_KETENE	see note*
J47419	TrGJAroCN	$\text{DNCREs} + h\nu \rightarrow \text{HONO} + \text{MNCPDKETENE}$	$\text{jx(ip_HOPh3Me2N02)}$	see note*
J47420	TrGJAroCN	$\text{MNCPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{HO}_2 + \text{NC4MDCO2HN}$	j_KETENE	see note*
J47421	TrGJAroC	$\text{MCATEC1OOH} + h\nu \rightarrow \text{MCATEC1O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47422	TrGJAroCN	$\text{NPTLQOOH} + h\nu \rightarrow \text{C7CO4DB} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47423	TrGJAroC	$\text{PTLQOOH} + h\nu \rightarrow \text{C6CO2OHCO3} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47424	TrGJAroCN	$\text{NCRES1OOH} + h\nu \rightarrow \text{NCRES1O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47425	TrGJAroCN	$\text{MNNCATCOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47426	TrGJAroCN	$\text{MNCATECOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47427	TrGJAroC	$\text{C7CO4DB} + h\nu \rightarrow \text{C5CO2DBCO3} + \text{HO}_2 + \text{CO}$	$\text{jx(ip_MGLYOX)} * 2$	Rickard and Pascoe (2009)
J47428	TrGJAroCN	$\text{NDNCRESOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47429	TrGJAroCN	$\text{DNCRESOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47430	TrGJAroC	$\text{C6COOHCO3H} + h\nu \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48200	TrGJTerC	$\text{C86OOH} + h\nu \rightarrow \text{C511O2} + \text{CH}_3\text{COCH}_3 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J48201	TrGJTerC	$\text{C812OOH} + h\nu \rightarrow \text{C813O2} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48202	TrGJTerC	$\text{C813OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J48203	TrGJTerC	$\text{C721CHO} + h\nu \rightarrow \text{C721O2} + \text{CO} + \text{HO}_2$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48204	TrGJTerC	$\text{C721CO3H} + h\nu \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48205	TrGJTerC	$\text{C8BCOOH} + h\nu \rightarrow \text{C89O2} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48206	TrGJTerC	$\text{C89OOH} + h\nu \rightarrow \text{C810O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J48207	TrGJTerCN	$\text{C89NO3} + h\nu \rightarrow \text{C810O2} + \text{NO}_2$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J48208	TrGJTerC	$\text{C810OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J48209	TrGJTerCN	$\text{C810NO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O}_2 + \text{NO}_2$	$2.84 \cdot j_{\text{IC3H7NO}_3} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J48210	TrGJTerCN	$\text{C8BCNO}_3 + h\nu \rightarrow \text{C89O}_2 + \text{NO}_2$	j_{IC3H7NO_3}	Rickard and Pascoe (2009)
J48211	TrGJTerC	$\text{C85OOH} + h\nu \rightarrow \text{C86O}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ACETOL}}$	Rickard and Pascoe (2009)
J48400	TrGJAroC	$\text{STYRENOOH} + h\nu \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL} + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)*
J49200	TrGJTerC	$\text{C96OOH} + h\nu \rightarrow \text{C97O}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ACETOL}}$	Rickard and Pascoe (2009)
J49201	TrGJTerC	$\text{C97OOH} + h\nu \rightarrow \text{C98O}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ACETOL}}$	Rickard and Pascoe (2009)
J49202	TrGJTerC	$\text{C98OOH} + h\nu \rightarrow \text{C614O}_2 + \text{CH}_3\text{COCH}_3 + \text{OH}$	$(j_{\text{ip_CH300H}} + 2.15 \cdot j_{\text{ip_MGLYOX}})$	Rickard and Pascoe (2009)
J49203a	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{C85O}_2 + \text{CO} + \text{HO}_2$	$j_{\text{ip_PINAL2HCO}}$	Rickard and Pascoe (2009), Sander et al. (2018)
J49203b	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{NORPINENOL}$	$j_{\text{ip_PINAL2ENOL}}$	Sander et al. (2018), Andrews et al. (2012)
J49204	TrGJTerC	$\text{C85CO}_3\text{H} + h\nu \rightarrow \text{C85O}_2 + \text{CO}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ACETOL}}$	Rickard and Pascoe (2009)
J49205	TrGJTerC	$\text{C89CO}_2\text{H} + h\nu \rightarrow .8 \text{ C811CO}_3 + .2 \text{ C89O}_2 + .2 \text{ CO}_2 + \text{HO}_2$	$j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J49206	TrGJTerC	$\text{C89CO}_3\text{H} + h\nu \rightarrow .8 \text{ C811CO}_3 + .2 \text{ C89O}_2 + .2 \text{ CO}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J49207	TrGJTerC	$\text{C811CO}_3\text{H} + h\nu \rightarrow \text{C811O}_2 + \text{CO}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)
J49208	TrGJTerC	$\text{NOPINDOOH} + h\nu \rightarrow \text{C89CO}_3 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)
J40200	TrGJTerC	$\text{LAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{HO}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)
J40201	TrGJTerC	$\text{MENTHEN6ONE} + h\nu \rightarrow \text{RO6R1O}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Vereecken et al. (2007)
J40202	TrGJTerC	$2\text{OHMENTHEN6ONE} + h\nu \rightarrow 10 \text{ L CARBON} + \text{OH}$	$j_{\text{ip_CH300H}}$	Vereecken et al. (2007)
J40203a	TrGJTerC	$\text{PINAL} + h\nu \rightarrow \text{C96O}_2 + \text{CO} + \text{HO}_2$	$j_{\text{ip_PINAL2HCO}}$	Rickard and Pascoe (2009)
J40203b	TrGJTerC	$\text{PINAL} + h\nu \rightarrow \text{PINEOL}$	$j_{\text{ip_PINAL2ENOL}}$	Sander et al. (2018), Andrews et al. (2012)*
J40204	TrGJTerC	$\text{PERPINONIC} + h\nu \rightarrow \text{C96O}_2 + \text{CO}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ACETOL}}$	Rickard and Pascoe (2009)
J40205	TrGJTerC	$\text{PINALOOH} + h\nu \rightarrow \text{C106O}_2 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40206	TrGJTerCN	$\text{PINALNO}_3 + h\nu \rightarrow \text{C106O}_2 + \text{NO}_2$	$j_{\text{IC3H7NO}_3} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40207	TrGJTerC	$\text{C106OOH} + h\nu \rightarrow \text{C716O}_2 + \text{CH}_3\text{COCH}_3 + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40208	TrGJTerCN	$\text{C106NO}_3 + h\nu \rightarrow \text{C716O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$j_{\text{IC3H7NO}_3} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40209	TrGJTerC	$\text{C109OOH} + h\nu \rightarrow \text{C89CO}_3 + \text{HCHO} + \text{OH}$	$j_{\text{ip_CH300H}} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40210	TrGJTerC	$\text{C109CO} + h\nu \rightarrow \text{C89CO}_3 + \text{CO} + \text{HO}_2$	$j_{\text{ip_MGLYOX}} + j_{\text{ip_HOCH}_2\text{CHO}}$	Rickard and Pascoe (2009)
J40211	TrGJTerCN	$\text{LNAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{NO}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)
J40212	TrGJTerC	$\text{BPINAOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)
J40213	TrGJTerCN	$\text{LNBPINABOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$j_{\text{ip_CH300H}}$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J40214	TrGJTerCN	$\text{ROO6R1NO3} + h\nu \rightarrow \text{ROO6R3O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$2.84 \cdot j_{\text{IC3H7N03}} + j_{\text{x(ip_CH300H)}}$	Sander et al. (2018)
J40215	TrGJTerCN	$\text{RO6R1NO3} + h\nu \rightarrow 9 \text{LCARBON} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 \cdot j_{\text{IC3H7N03}}$	Sander et al. (2018)
J6000	StTrGJCl	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$j_{\text{x(ip_Cl2)}}$	Sander et al. (2014)
J6100	StTrGJCl	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2 \text{Cl}$	$j_{\text{x(ip_Cl2O2)}}$	Sander et al. (2014)
J6101	StTrGJCl	$\text{OCIO} + h\nu \rightarrow \text{ClO} + \text{O}(^3\text{P})$	$j_{\text{x(ip_OCIO)}}$	Sander et al. (2014)
J6201	StTrGJCl	$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$	$j_{\text{x(ip_HOC1)}}$	Sander et al. (2014)
J6300	TrGJCIN	$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$	$j_{\text{x(ip_ClNO2)}}$	Sander et al. (2014)
J6301a	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	$j_{\text{x(ip_ClNO3)}}$	Sander et al. (2014)
J6301b	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$j_{\text{x(ip_ClON02)}}$	Sander et al. (2014)
J8000	TrGJI	$\text{I}_2 + h\nu \rightarrow \text{I} + \text{I}$	$j_{\text{x(ip_I2)}}$	Sander et al. (2014)
J8100	TrGJI	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}(^3\text{P})$	$j_{\text{x(ip_IO)}}$	Sander et al. (2014)
J8200	TrGJI	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	$j_{\text{x(ip_HOI)}}$	Sander et al. (2014)
J8300	TrGJIN	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$	$j_{\text{x(ip_INO2)}}$	Sander et al. (2014)
J8301	TrGJIN	$\text{INO}_3 + h\nu \rightarrow \text{I} + \text{NO}_3$	$j_{\text{x(ip_INO3)}}$	Sander et al. (2014)
J8400	TrGJI	$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2 \text{I} + 2 \text{HO}_2 + \text{CO}$	$j_{\text{x(ip_CH2I2)}}$	Sander et al. (2014)
J8401	TrGJI	$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3$	$j_{\text{x(ip_CH3I)}}$	Sander et al. (2014)
J8402	TrGJCI	$\text{CH}_3\text{CHICH}_3 + h\nu \rightarrow 2 \text{LCARBON} + \text{I} + \text{CH}_3$	$j_{\text{x(ip_C3H7I)}}$	Sander et al. (2014)
J8403	TrGJCII	$\text{CH}_2\text{CII} + h\nu \rightarrow \text{I} + \text{Cl} + 2 \text{HO}_2 + \text{CO}$	$j_{\text{x(ip_CH2CII)}}$	Sander et al. (2014)
J8600	TrGJCII	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	$j_{\text{x(ip_ICl)}}$	Sander et al. (2014)
J8101SR	TrGJI	$\text{OIO} + h\nu \rightarrow \text{I} + \text{O}_2$	$j_{\text{x(ip_OIO)}}$	Sander et al. (2014)
J8102SR	TrGJI	$\text{I}_2\text{O}_2 + h\nu \rightarrow \text{I} + \text{OIO}$	$j_{\text{x(ip_I2O2)}}$	Sander et al. (2014)
J8103SR	TrGJI	$\text{I}_2\text{O}_4 + h\nu \rightarrow 2 \text{OIO}$	$j_{\text{x(ip_I2O4)}}$	Sander et al. (2014)
J8104SR	TrGJI	$\text{I}_2\text{O}_3 + h\nu \rightarrow \text{OIO} + \text{IO}$	$j_{\text{x(ip_I2O3)}}$	Sander et al. (2014)
J8302SR	TrGJIN	$\text{INO} + h\nu \rightarrow \text{I} + \text{NO}$	$j_{\text{x(ip_INO)}}$	Sander et al. (2014)
J4200MK	TrGAJCN	$\text{H2NCH2CHO} + h\nu \rightarrow \text{MMAO2} + \text{HCHO}$	$j_{\text{x(ip_CH3CHO)}}$	Karl et al. (2012a)
J4201MK	TrGAJCN	$\text{H2NCOCHO} + h\nu \rightarrow \text{H2NCHO} + \text{HCHO}$	$j_{\text{x(ip_CH3CHO)}}$	Karl et al. (2012a)
J4202MK	TrGAJCN	$\text{MEANNO} + h\nu \rightarrow \text{MEAN} + \text{NO}$	$0.33 \cdot j_{\text{x(ip_N02)}}$	Karl et al. (2012a)
J4203MK	TrGAJCN	$\text{NDMA} + h\nu \rightarrow \text{CH3NCH3} + \text{NO}$	$0.25 \cdot j_{\text{x(ip_N02)}}$	Karl et al. (2012a)
J4300MK	TrGJCN	$\text{IPN} + h\nu \rightarrow \text{CH3CHOCH3} + \text{NO}$	$0.08 \cdot j_{\text{x(ip_N02)}}$	Karl (2012)
J4400MK	TrGAJCN	$\text{NDELA} + h\nu \rightarrow \text{HOETNETOH} + \text{NO}$	$0.33 \cdot j_{\text{x(ip_N02)}}$	Karl et al. (2012a)
J4401MK	TrGAJCN	$\text{NAMP} + h\nu \rightarrow \text{AMPN} + \text{NO}$	$0.34 \cdot j_{\text{x(ip_N02)}}$	Nielsen and Schade (2012)
J4402MK	TrGAJCN	$\text{DMOCNH2MOH} + h\nu \rightarrow \text{CH3CNH2MOH} + \text{HCHO}$	$j_{\text{x(ip_CH3CHO)}}$	Karl (2012)
J4403MK	TrGAJCN	$\text{DMCNH2CHO} + h\nu \rightarrow \text{DMCNH2} + \text{HCHO}$	$j_{\text{x(ip_CH3CHO)}}$	Karl (2012)
J4600MK	TrGJC	$\text{CHEXONE} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{C}_3\text{H}_6 + \text{CO}$	$0.42 \cdot j_{\text{x(ip_CHOH)}}$	von Kuhlmann et al. (2003)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH (aqueous)				
PH11000_a01	TrAa01JFe	$\text{FeOH}^{2+}(\text{a01}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a01}) + \text{OH}(\text{a01})$	$\text{xaer}(\text{01}) * 4.51\text{E-}3 * 0.312$	Herrmann et al. (2000)
PH11001_a01	TrAa01JFe	$\text{Fe}(\text{OH})_2^+(\text{a01}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a01}) + \text{OH}(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * 5.77\text{E-}3 * 0.255$	Herrmann et al. (2000)
PH11003_a01	TrAa01JFeS	$\text{FeSO}_4^+(\text{a01}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a01}) + \text{SO}_4^-(\text{a01})$	$\text{xaer}(\text{01}) * 6.43\text{E-}3 * 7.9\text{E-}3$	Herrmann et al. (2000)
PH2100_a01	TrAa01J	$\text{H}_2\text{O}_2(\text{a01}) + h\nu \rightarrow 2 \text{OH}(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_H202}) * 7.11\text{E-}1$	Ervens et al. (2003)
PH3200_a01	TrAa01JN	$\text{NO}_3^-(\text{a01}) + h\nu \rightarrow \text{NO}_2(\text{a01}) + \text{OH}(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N020}) * 1.91\text{E-}6$	Ervens et al. (2003)
PH3201_a01	TrAa01JN	$\text{NO}_2^-(\text{a01}) + h\nu \rightarrow \text{NO}(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 2.50\text{E-}3$	Ervens et al. (2003)
PH4101_a01	TrAa01AmiJN	$\text{MMNNO}_2(\text{a01}) + h\nu \rightarrow \text{NO}_2(\text{a01}) + \text{CH}_3\text{NH}_2^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH4102_a01	TrAa01AmiJCN	$\text{MEANNO}_2(\text{a01}) + h\nu \rightarrow \text{NO}_2(\text{a01}) + \text{HOCH}_2\text{CH}_2\text{NH}_2^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH4201_a01	TrAa01AmiJCN	$\text{NDMA}(\text{a01}) + h\nu \rightarrow \text{NO}(\text{a01}) + (\text{CH}_3)_2\text{NH}^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 1.30\text{E-}1 * \text{xaqcnno}$	Karl et al. (2012b)
PH4202_a01	TrAa01AmiJCN	$\text{DMNNO}_2(\text{a01}) + h\nu \rightarrow \text{NO}_2(\text{a01}) + (\text{CH}_3)_2\text{NH}^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH4203_a01	TrAa01AmiJCN	$\text{MEANNO}(\text{a01}) + h\nu \rightarrow \text{NO}(\text{a01}) + \text{HOCH}_2\text{CH}_2\text{NH}_2^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 1.30\text{E-}1 * \text{xaqcnno}$	Karl et al. (2012b)
PH4401_a01	TrAa01AmiJCN	$\text{NDELA}(\text{a01}) + h\nu \rightarrow \text{NO}(\text{a01}) + (\text{HOET})_2\text{NH}^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}2 * \text{xaqcnno}$	Karl et al. (2012b)
PH4402_a01	TrAa01AmiJCN	$\text{DEANNO}_2(\text{a01}) + h\nu \rightarrow \text{NO}_2(\text{a01}) + (\text{HOET})_2\text{NH}^+(\text{a01}) + \text{OH}^-(\text{a01})$	$\text{xaer}(\text{01}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH11000_a02	TrAa02JFe	$\text{FeOH}^{2+}(\text{a02}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a02}) + \text{OH}(\text{a02})$	$\text{xaer}(\text{02}) * 4.51\text{E-}3 * 0.312$	Herrmann et al. (2000)
PH11001_a02	TrAa02JFe	$\text{Fe}(\text{OH})_2^+(\text{a02}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a02}) + \text{OH}(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * 5.77\text{E-}3 * 0.255$	Herrmann et al. (2000)
PH11003_a02	TrAa02JFeS	$\text{FeSO}_4^+(\text{a02}) + h\nu \rightarrow \text{Fe}^{2+}(\text{a02}) + \text{SO}_4^-(\text{a02})$	$\text{xaer}(\text{02}) * 6.43\text{E-}3 * 7.9\text{E-}3$	Herrmann et al. (2000)
PH2100_a02	TrAa02J	$\text{H}_2\text{O}_2(\text{a02}) + h\nu \rightarrow 2 \text{OH}(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_H202}) * 7.11\text{E-}1$	Ervens et al. (2003)
PH3200_a02	TrAa02JN	$\text{NO}_3^-(\text{a02}) + h\nu \rightarrow \text{NO}_2(\text{a02}) + \text{OH}(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N020}) * 1.91\text{E-}6$	Ervens et al. (2003)
PH3201_a02	TrAa02JN	$\text{NO}_2^-(\text{a02}) + h\nu \rightarrow \text{NO}(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N02}) * 2.50\text{E-}3$	Ervens et al. (2003)
PH4101_a02	TrAa02AmiJN	$\text{MMNNO}_2(\text{a02}) + h\nu \rightarrow \text{NO}_2(\text{a02}) + \text{CH}_3\text{NH}_2^+(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH4102_a02	TrAa02AmiJCN	$\text{MEANNO}_2(\text{a02}) + h\nu \rightarrow \text{NO}_2(\text{a02}) + \text{HOCH}_2\text{CH}_2\text{NH}_2^+(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)
PH4201_a02	TrAa02AmiJCN	$\text{NDMA}(\text{a02}) + h\nu \rightarrow \text{NO}(\text{a02}) + (\text{CH}_3)_2\text{NH}^+(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N02}) * 1.30\text{E-}1 * \text{xaqcnno}$	Karl et al. (2012b)
PH4202_a02	TrAa02AmiJCN	$\text{DMNNO}_2(\text{a02}) + h\nu \rightarrow \text{NO}_2(\text{a02}) + (\text{CH}_3)_2\text{NH}^+(\text{a02}) + \text{OH}^-(\text{a02})$	$\text{xaer}(\text{02}) * \text{jx}(\text{ip_N02}) * 5.3\text{E-}3 * \text{xaqcnno}$	Karl et al. (2012b)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH4203_a02	TrAa02AmiJCN	MEANNO(a02) + $h\nu$ → NO(a02) + HOCH ₂ CH ₂ NH ₂ ⁺ (a02) + OH ⁻ (a02)	xaer(02)*jx(ip_N02) *1.30E-1 *xaqcnno	Karl et al. (2012b)
PH4401_a02	TrAa02AmiJCN	NDELA(a02) + $h\nu$ → NO(a02) + (HOET) ₂ NH ⁺ (a02) + OH ⁻ (a02)	xaer(02)*jx(ip_N02) *5.3E-2 *xaqcnno	Karl et al. (2012b)
PH4402_a02	TrAa02AmiJCN	DEANNO2(a02) + $h\nu$ → NO ₂ (a02) + (HOET) ₂ NH ⁺ (a02) + OH ⁻ (a02)	xaer(02)*jx(ip_N02) *5.3E-3 *xaqcnno	Karl et al. (2012b)
PH11000_a03	TrAa03JFe	FeOH ²⁺ (a03) + $h\nu$ → Fe ²⁺ (a03) + OH(a03)	xaer(03)*4.51E-3*0.312	Herrmann et al. (2000)
PH11001_a03	TrAa03JFe	Fe(OH) ₂ ⁺ (a03) + $h\nu$ → Fe ²⁺ (a03) + OH(a03) + OH ⁻ (a03)	xaer(03)*5.77E-3*0.255	Herrmann et al. (2000)
PH11003_a03	TrAa03JFeS	FeSO ₄ ⁺ (a03) + $h\nu$ → Fe ²⁺ (a03) + SO ₄ ⁻ (a03)	xaer(03)*6.43E-3*7.9E-3	Herrmann et al. (2000)
PH2100_a03	TrAa03J	H ₂ O ₂ (a03) + $h\nu$ → 2 OH(a03)	xaer(03)*jx(ip_H2O2) *7.11E-1	Ervens et al. (2003)
PH3200_a03	TrAa03JN	NO ₃ ⁻ (a03) + $h\nu$ → NO ₂ (a03) + OH(a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N020) *1.91E-6	Ervens et al. (2003)
PH3201_a03	TrAa03JN	NO ₂ ⁻ (a03) + $h\nu$ → NO(a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *2.50E-3	Ervens et al. (2003)
PH4101_a03	TrAa03AmiJN	MMNNO2(a03) + $h\nu$ → NO ₂ (a03) + CH ₃ NH ₂ ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *5.3E-3 *xaqcnno	Karl et al. (2012b)
PH4102_a03	TrAa03AmiJCN	MEANNO2(a03) + $h\nu$ → NO ₂ (a03) + HOCH ₂ CH ₂ NH ₂ ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *5.3E-3 *xaqcnno	Karl et al. (2012b)
PH4201_a03	TrAa03AmiJCN	NDMA(a03) + $h\nu$ → NO(a03) + (CH ₃) ₂ NH ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *1.30E-1 *xaqcnno	Karl et al. (2012b)
PH4202_a03	TrAa03AmiJCN	DMNNO2(a03) + $h\nu$ → NO ₂ (a03) + (CH ₃) ₂ NH ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *5.3E-3 *xaqcnno	Karl et al. (2012b)
PH4203_a03	TrAa03AmiJCN	MEANNO(a03) + $h\nu$ → NO(a03) + HOCH ₂ CH ₂ NH ₂ ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *1.30E-1 *xaqcnno	Karl et al. (2012b)
PH4401_a03	TrAa03AmiJCN	NDELA(a03) + $h\nu$ → NO(a03) + (HOET) ₂ NH ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *5.3E-2 *xaqcnno	Karl et al. (2012b)
PH4402_a03	TrAa03AmiJCN	DEANNO2(a03) + $h\nu$ → NO ₂ (a03) + (HOET) ₂ NH ⁺ (a03) + OH ⁻ (a03)	xaer(03)*jx(ip_N02) *5.3E-3 *xaqcnno	Karl et al. (2012b)

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(34) → jx(ip_MGLYOX)
j(12) → jx(ip_CHOH)	j(41) → jx(ip_CH3OOH)
j(15) → jx(ip_HOCH2CHO)	j(53) → j(isopropyl nitrate)
j(18) → jx(ip_MACR)	j(54) → j(isopropyl nitrate)
j(22) → jx(ip_ACETOL)	j(55) → j(isopropyl nitrate)
j(23)+j(24) → jx(ip_MVK)	j(56)+j(57) → jx(ip_NOA)
j(31)+j(32)+j(33) → jx(ip_GLYOX)	

Specific notes

J41006: product distribution as for HNO₄

J42004: Quantum yields from Burkholder et al. (2015).

J42005a: Quantum yields from Burkholder et al. (2015).

J42005b: Quantum yields from Burkholder et al. (2015).

J42005c: Quantum yields from Burkholder et al. (2015).

J42007: It is assumed that J(PHAN) is the same as J(PAN).

J42017: Enhancement of j according to Müller et al. (2014).

J42020: It is assumed that $j(\text{NO}_3\text{CH}_2\text{CHO})$ is the same as $j(\text{PAN})$.

J42021: In analogy to what is assumed for $\text{CH}_3\text{O}_2\text{NO}_2$ photolysis as in (Sander et al., 2014).

J43002: Following von Kuhlmann et al. (2003), we use $j(\text{CH}_3\text{COCH}_2\text{OH}) = 0.11 \cdot j_x(\text{ip_CHOH})$. As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a).

J43006: Following von Kuhlmann et al. (2003), we use $J(\text{iC}_3\text{H}_7\text{ONO}_2) = 3.7 \cdot j_x(\text{ip_PAN})$.

J43018: One third of the acetaldehyde channel is considered to be CH_2CHOH according to Hjorth (2002) EUPHORE Report.

J43024: Assuming $J(\text{C}_3\text{H}_7\text{ONO}_2) = 0.59 \times J(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J43025a: Photolysis frequencies very similar to the ones of CH_3CHO .

J43025b: Photolysis frequencies very similar to the ones of CH_3CHO .

J43400: $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

J44004: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44005a: It is assumed that J(LC4H9NO₃) is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J44005b: It is assumed that J(LC4H9NO₃) is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J44006: It is assumed that J(MPAN) is the same as J(PAN).

J44009: It is assumed that J(MACROOH) is 2.77 times larger than J(HOCH_2CHO), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44010: It is assumed that J(MACROH) is 2.77 times larger than J(HOCH_2CHO), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44015: It is assumed that J(BIACETOH) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44017a: CO-channel yielding CH_3COCH which upon reaction with O_2 produces an excited Criegee Intermediate assumed to be similar to MGLOOA in MCM. MGLOOA is produced also in other reactions and is substituted by its decomposition products. Furthermore, the stabilized Criegee Intermediate is assumed to solely react with water.

J44025: J values only for the secondary nitrate.

J44026: Like for LMEKNO₃ photolysis

J44027: $2.84 \cdot J_{\text{IC3H7NO3}}$ like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to Müller et al. (2014).

J44037b: Channel which produces just vinyl alcohol and not a larger enol via keto-enol photo-tautomerization.

J44043: The resulting vinyl peroxy radical is assumed to mostly form with HO_2 a labile hydroperoxide (see ketene formation). The products are further simplified.

J44044: 1,5-H-shift for the resulting vinyl peroxy radical assumed to be dominant.

J44046a: Simplified oxidation.

J44400b: $\text{KDEC MALDIALO} \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2$

J44401: $\text{KDEC BZFUO} \rightarrow \text{CO14O3CHO} + \text{HO}_2$

J44403: $\text{KDEC NBZFUO} \rightarrow 0.5 \text{ CO14O3CHO} + 0.5 \text{ NO}_2 + 0.5 \text{ NBZFUONE} + 0.5 \text{ HO}_2$

J44404b: $\text{KDEC MALDIALCO}_2 \rightarrow 0.6 \text{ MALANHY} + \text{HO}_2 + 0.4 \text{ GLYOX} + 0.4 \text{ CO}$

J44407: $\text{KDEC MALANHYO} \rightarrow \text{HCOCOHC}_3\text{O}_3$

J44414: $\text{KDEC MECOACETO} \rightarrow \text{CH}_3\text{CO}_3 + \text{HCHO}$

J45003: It is assumed that $J(\text{LISOPACNO}_3) = 0.59 \times J(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that $J(\text{ISOPBNO}_3) = 2.84 \times J(\text{iC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that J(ISOPDNO₃) is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J45009: $0.59 \cdot J_{\text{IC3H7NO3}}$ like for other primary alkyl nitrates (see J4503). Enhancement of J according to Müller et al. (2014).

J45015: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that J(HCOC5) is half as large as J(MVK). With exception of HOCH₂CO the products of MACO₂ decomposition without CO₂.

J45032: approximation with 4-oxo-pentenal photolysis combining results of Thüner et al(2004) and Xiang et al(2007)

J45402: KDEC C5DIALO → MALDIAL + CO + HO₂

J45407: KDEC TLFUONE → 0.6 C5CO₁₄OH + 0.6 HO₂ + 0.4 TLFUONE

J45410: KDEC MMALANHYO → CO₂H₃CO₃

J45411: KDEC C5DICARBO → MGLYOX + GLYOX + HO₂

J45412: KDEC NTLFUO → ACCOMECHO + NO₂

J45414: KDEC C5CO₁₄CO₂ → 0.83 MALANHY + 0.83 CH₃ + .17 MGLYOX + .17 HO₂ + .17 CO + .17 CO₂

J45415: KDEC TLFUO → ACCOMECHO + HO₂

J46400: KDEC PHENO → 0.71 MALDALCO₂H + 0.71 GLYOX + 0.29 PBZQONE + HO₂

J46403: KDEC NDNPHENO → NC₄D₂CO₂H + HNO₃ + CO + CO + NO₂

J46404: KDEC BZBIPERO → GLYOX + HO₂ + 0.5 BZFUONE + 0.5 BZFUONE

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO → NC₄D₂CO₂H + HCOCO₂H + NO₂

J46415: KDEC NCATECO → NC₄D₂CO₂H + HCOCO₂H + HO₂

J46416: KDEC PBZQO → C₅CO₂OHCO₃

J46418: KDEC BZBIPERO → GLYOX + HO₂ + 0.5 BZFUONE + 0.5 BZFUONE

J46419: KDEC NBZQO → C₆CO₄DB + NO₂

J46422: KDEC DNPHEO → NC₄D₂CO₂H + HCOCO₂H + NO₂

J46425: KDEC BZEMUCO → 0.5 EPXC₄DIAL + .5 GLYOX + .5 HO₂ + .5 C₃DIALO₂ + .5 C₃OH₁₃CO

J46429: new channel

J47401: KROPRIM*O₂ fast reaction C₆H₅CH₂O = BENZAL + HO₂

J47402: KROPRIM*O₂ fast reaction C₆H₅CH₂O = BENZAL + HO₂

J47404: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO₂ + 0.2 C₄MDIAL + 0.2 C₅DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47405: KDEC TLBIPERO → 0.6 GLYOX + 0.4 MGLYOX + HO₂ + 0.2 C₄MDIAL + 0.2 C₅DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47407: KDEC CRESO → 0.68 C₅CO₁₄OH + 0.68 GLYOX + HO₂ + 0.32 PTLQONE

J47408a: KDEC CRESO → 0.68 C₅CO₁₄OH + 0.68 GLYOX + HO₂ + 0.32 PTLQONE

J47408b: KDEC NCRESO → C₅CO₁₄OH + GLYOX + NO₂

J47409: Using J for 3-methyl-2-nitrophenol.

J47412: KDEC TLEMUCO → 0.5 C₃DIALO₂ + 0.5 CO₂H₃CHO + 0.5 EPXC₄DIAL + 0.5 MGLYOX + 0.5 HO₂

J47417: Using J for 3-methyl-2-nitrophenol.

J47418: new channel

J47419: Using J for 3-methyl-2-nitrophenol.

J47420: new channel

J47422: KDEC NPTLQO → C₇CO₄DB + NO₂

J47423: KDEC PTLQO → C₆CO₂OHCO₃

J47425: KDEC MNNCATECO → NC₄MDCO₂H + HCOCO₂H + NO₂

J47426: KDEC MNCATECO → NC₄MDCO₂H + HCOCO₂H + HO₂

J47428: KDEC NDNCRESO → NC₄MDCO₂H + HNO₃ + CO + CO + NO₂

J47429: KDEC DNCRESO → NC₄MDCO₂H + HCOCO₂H + NO₂

J48400: KDEC STYRENO → HO₂ + HCHO + BENZAL

J40203b: Substituted vinyl alcohol in analogy to CH₃CHO photolysis.

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

#	labels	reaction	rate coefficient	reference
H1000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(a01)$	$k_{\text{exf}}(01, \text{ind}_{O2})$	see general notes*
H1000b_a01	TrAa01Sc	$O_2(a01) \rightarrow O_2$	$k_{\text{exb}}(01, \text{ind}_{O2})$	see general notes*
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(a01)$	$k_{\text{exf}}(01, \text{ind}_{O3})$	see general notes*
H1001b_a01	TrAa01MblScScm	$O_3(a01) \rightarrow O_3$	$k_{\text{exb}}(01, \text{ind}_{O3})$	see general notes*
H2100f_a01	TrAa01Sc	$OH \rightarrow OH(a01)$	$k_{\text{exf}}(01, \text{ind}_{OH})$	see general notes*
H2100b_a01	TrAa01Sc	$OH(a01) \rightarrow OH$	$k_{\text{exb}}(01, \text{ind}_{OH})$	see general notes*
H2101f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(a01)$	$k_{\text{exf}}(01, \text{ind}_{HO2})$	see general notes*
H2101b_a01	TrAa01Sc	$HO_2(a01) \rightarrow HO_2$	$k_{\text{exb}}(01, \text{ind}_{HO2})$	see general notes*
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(a01)$	$k_{\text{exf}}(01, \text{ind}_{H2O2})$	see general notes*
H2102b_a01	TrAa01MblScScm	$H_2O_2(a01) \rightarrow H_2O_2$	$k_{\text{exb}}(01, \text{ind}_{H2O2})$	see general notes*
H3101f_a01	TrAa01ScN	$NO_2 \rightarrow NO_2(a01)$	$k_{\text{exf}}(01, \text{ind}_{NO2})$	see general notes*
H3101b_a01	TrAa01ScN	$NO_2(a01) \rightarrow NO_2$	$k_{\text{exb}}(01, \text{ind}_{NO2})$	see general notes*
H3102f_a01	TrAa01ScN	$NO_3 \rightarrow NO_3(a01)$	$k_{\text{exf}}(01, \text{ind}_{NO3})$	see general notes*
H3102b_a01	TrAa01ScN	$NO_3(a01) \rightarrow NO_3$	$k_{\text{exb}}(01, \text{ind}_{NO3})$	see general notes*
H3200f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(a01)$	$k_{\text{exf}}(01, \text{ind}_{NH3})$	see general notes*
H3200b_a01	TrAa01MblScScmN	$NH_3(a01) \rightarrow NH_3$	$k_{\text{exb}}(01, \text{ind}_{NH3})$	see general notes*
H3201_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow HNO_3(a01) + HNO_3(a01)$	$k_{\text{exf}}_{N2O5}(01) * C(\text{ind}_{H2O_a01})$	Behnke et al. (1994), Behnke et al. (1997)
H3202f_a01	TrAa01ScN	$HONO \rightarrow HONO(a01)$	$k_{\text{exf}}(01, \text{ind}_{HONO})$	see general notes*
H3202b_a01	TrAa01ScN	$HONO(a01) \rightarrow HONO$	$k_{\text{exb}}(01, \text{ind}_{HONO})$	see general notes*
H3203f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(a01)$	$k_{\text{exf}}(01, \text{ind}_{HNO3})$	see general notes*
H3203b_a01	TrAa01MblScScmN	$HNO_3(a01) \rightarrow HNO_3$	$k_{\text{exb}}(01, \text{ind}_{HNO3})$	see general notes*
H3204f_a01	TrAa01ScN	$HNO_4 \rightarrow HNO_4(a01)$	$k_{\text{exf}}(01, \text{ind}_{HNO4})$	see general notes*
H3204b_a01	TrAa01ScN	$HNO_4(a01) \rightarrow HNO_4$	$k_{\text{exb}}(01, \text{ind}_{HNO4})$	see general notes*
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(a01)$	$k_{\text{exf}}(01, \text{ind}_{CO2})$	see general notes*
H4100b_a01	TrAa01MblScScm	$CO_2(a01) \rightarrow CO_2$	$k_{\text{exb}}(01, \text{ind}_{CO2})$	see general notes*
H4101f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(a01)$	$k_{\text{exf}}(01, \text{ind}_{HCHO})$	see general notes*
H4101b_a01	TrAa01ScScm	$HCHO(a01) \rightarrow HCHO$	$k_{\text{exb}}(01, \text{ind}_{HCHO})$	see general notes*
H4102f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(a01)$	$k_{\text{exf}}(01, \text{ind}_{CH3O2})$	see general notes*
H4102b_a01	TrAa01Sc	$CH_3OO(a01) \rightarrow CH_3O_2$	$k_{\text{exb}}(01, \text{ind}_{CH3O2})$	see general notes*
H4103f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(a01)$	$k_{\text{exf}}(01, \text{ind}_{HCOOH})$	see general notes*
H4103b_a01	TrAa01ScScm	$HCOOH(a01) \rightarrow HCOOH$	$k_{\text{exb}}(01, \text{ind}_{HCOOH})$	see general notes*
H4104f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(a01)$	$k_{\text{exf}}(01, \text{ind}_{CH3OOH})$	see general notes*
H4104b_a01	TrAa01ScScm	$CH_3OOH(a01) \rightarrow CH_3OOH$	$k_{\text{exb}}(01, \text{ind}_{CH3OOH})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H6000f_a01	TrAa01MblScCl	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{a01})$	$k_{\text{exf}}(01, \text{ind_Cl2})$	see general notes*
H6000b_a01	TrAa01MblScCl	$\text{Cl}_2(\text{a01}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(01, \text{ind_Cl2})$	see general notes*
H6200f_a01	TrAa01MblScScmCl	$\text{HCl} \rightarrow \text{HCl}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_HCl})$	see general notes*
H6200b_a01	TrAa01MblScScmCl	$\text{HCl}(\text{a01}) \rightarrow \text{HCl}$	$k_{\text{exb}}(01, \text{ind_HCl})$	see general notes*
H6201f_a01	TrAa01MblScCl	$\text{HOCl} \rightarrow \text{HOCl}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_HOCl})$	see general notes*
H6201b_a01	TrAa01MblScCl	$\text{HOCl}(\text{a01}) \rightarrow \text{HOCl}$	$k_{\text{exb}}(01, \text{ind_HOCl})$	see general notes*
H6300_a01	TrAa01MblClN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{a01}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{a01})$	$k_{\text{exf_N205}}(01) * 5.\text{E}2$	Behnke et al. (1994), Behnke et al. (1997)
H6301_a01	TrAa01MblClN	$\text{ClNO}_3 \rightarrow \text{HOCl}(\text{a01}) + \text{HNO}_3(\text{a01})$	$k_{\text{exf_ClN03}}(01) * \text{C}(\text{ind_H2O_a01})$	see general notes*
H6302_a01	TrAa01MblClN	$\text{ClNO}_3 + \text{Cl}^-(\text{a01}) \rightarrow \text{Cl}_2(\text{a01}) + \text{NO}_3^-(\text{a01})$	$k_{\text{exf_ClN03}}(01) * 5.\text{E}2$	see general notes*
H8000f_a01	TrAa01ScI	$\text{I}_2 \rightarrow \text{I}_2(\text{a01})$	$k_{\text{exf}}(01, \text{ind_I2})$	see general notes*
H8000b_a01	TrAa01ScI	$\text{I}_2(\text{a01}) \rightarrow \text{I}_2$	$k_{\text{exb}}(01, \text{ind_I2})$	see general notes*
H8100f_a01	TrAa01MblScI	$\text{IO} \rightarrow \text{IO}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_IO})$	see general notes*
H8100b_a01	TrAa01MblScI	$\text{IO}(\text{a01}) \rightarrow \text{IO}$	$k_{\text{exb}}(01, \text{ind_IO})$	see general notes*
H8101_a01	TrAa01I	$\text{OIO} \rightarrow \text{HOI}(\text{a01}) + \text{HO}_2(\text{a01})$	$k_{\text{exf}}(01, \text{ind_OIO})$	see general notes*
H8102_a01	TrAa01I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI}(\text{a01}) + \text{H}^+(\text{a01}) + \text{IO}_2^-(\text{a01})$	$k_{\text{exf}}(01, \text{ind_I202})$	see general notes*
H8200f_a01	TrAa01MblScI	$\text{HOI} \rightarrow \text{HOI}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_HOI})$	see general notes*
H8200b_a01	TrAa01MblScI	$\text{HOI}(\text{a01}) \rightarrow \text{HOI}$	$k_{\text{exb}}(01, \text{ind_HOI})$	see general notes*
H8201_a01	TrAa01MblScI	$\text{HI} \rightarrow \text{H}^+(\text{a01}) + \text{I}^-(\text{a01})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see general notes*
H8202_a01	TrAa01ScI	$\text{HIO}_3 \rightarrow \text{IO}_3^-(\text{a01}) + \text{H}^+(\text{a01})$	$k_{\text{mt}}(\text{HIO}_3) \cdot lwc$	see general notes*
H8300_a01	TrAa01IN	$\text{INO}_2 \rightarrow \text{HOI}(\text{a01}) + \text{HONO}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_INO2})$	see general notes*
H8301_a01	TrAa01MblIN	$\text{INO}_3 \rightarrow \text{HOI}(\text{a01}) + \text{HNO}_3(\text{a01})$	$k_{\text{exf}}(01, \text{ind_INO3})$	see general notes*
H8600f_a01	TrAa01MblScClI	$\text{ICl} \rightarrow \text{ICl}(\text{a01})$	$k_{\text{exf}}(01, \text{ind_ICl})$	see general notes*
H8600b_a01	TrAa01MblScClI	$\text{ICl}(\text{a01}) \rightarrow \text{ICl}$	$k_{\text{exb}}(01, \text{ind_ICl})$	see general notes*
H9100f_a01	TrAa01MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{a01})$	$xnom7so2 * k_{\text{exf}}(01, \text{ind_S02})$	see general notes*
H9100b_a01	TrAa01MblScScmS	$\text{SO}_2(\text{a01}) \rightarrow \text{SO}_2$	$xnom7so2 * k_{\text{exb}}(01, \text{ind_S02})$	see general notes*
H9200_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{a01})$	$xnom7sulf * k_{\text{exf}}(01, \text{ind_H2S04})$	see general notes*
H9400f_a01	TrAa01CS	$\text{DMSO} \rightarrow \text{DMSO}(\text{a01})$	$xnom7dms * k_{\text{exf}}(01, \text{ind_DMS0})$	see general notes*
H9400b_a01	TrAa01CS	$\text{DMSO}(\text{a01}) \rightarrow \text{DMSO}$	$xnom7dms * k_{\text{exb}}(01, \text{ind_DMS0})$	see general notes*
H9401_a01	TrAa01MblS	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{a01}) + \text{H}^+(\text{a01})$	$xnom7dms * k_{\text{exf}}(01, \text{ind_CH3S03H})$	see general notes*
H9402f_a01	TrAa01CS	$\text{DMS} \rightarrow \text{DMS}(\text{a01})$	$xnom7dms * k_{\text{exf}}(01, \text{ind_DMS})$	see general notes*
H9402b_a01	TrAa01CS	$\text{DMS}(\text{a01}) \rightarrow \text{DMS}$	$xnom7dms * k_{\text{exb}}(01, \text{ind_DMS})$	see general notes*
H3103f_a01MK	TrAa01ScN	$\text{N}_2\text{O}_3 \rightarrow \text{N}_2\text{O}_3(\text{a01})$	$xnom7nox * k_{\text{exf}}(01, \text{ind_N203})$	Karl et al. (2012b)
H3103b_a01MK	TrAa01ScN	$\text{N}_2\text{O}_3(\text{a01}) \rightarrow \text{N}_2\text{O}_3$	$xnom7nox * k_{\text{exb}}(01, \text{ind_N203})$	Karl et al. (2012b)

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

#	labels	reaction	rate coefficient	reference
H3104f_a01MK	TrAa01ScN	$\text{N}_2\text{O}_4 \rightarrow \text{N}_2\text{O}_4(\text{a01})$	$\text{xnom7nox*k_exf}(01, \text{ind_N2O4})$	Karl et al. (2012b)
H3104b_a01MK	TrAa01ScN	$\text{N}_2\text{O}_4(\text{a01}) \rightarrow \text{N}_2\text{O}_4$	$\text{xnom7nox*k_exb}(01, \text{ind_N2O4})$	Karl et al. (2012b)
H4106f_a01MK	TrAa01AmiScN	$\text{MMA} \rightarrow \text{MMA}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_MMA})$	Karl et al. (2012b)
H4106b_a01MK	TrAa01AmiScN	$\text{MMA}(\text{a01}) \rightarrow \text{MMA}$	$\text{xnom7amin*k_exb}(01, \text{ind_MMA})$	Karl et al. (2012b)
H4107f_a01MK	TrAa01AmiScN	$\text{MMNNO}_2 \rightarrow \text{MMNNO}_2(\text{a01})$	$\text{xnom7nno*k_exf}(01, \text{ind_MMNNO}_2)$	Karl et al. (2012b)
H4107b_a01MK	TrAa01AmiScN	$\text{MMNNO}_2(\text{a01}) \rightarrow \text{MMNNO}_2$	$\text{xnom7nno*k_exb}(01, \text{ind_MMNNO}_2)$	Karl et al. (2012b)
H4108f_a01MK	TrAa01AmiScN	$\text{HNCO} \rightarrow \text{HNCO}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_HNCO})$	Karl et al. (2012b)
H4108b_a01MK	TrAa01AmiScN	$\text{HNCO}(\text{a01}) \rightarrow \text{HNCO}$	$\text{xnom7amin*k_exb}(01, \text{ind_HNCO})$	Karl et al. (2012b)
H4109f_a01MK	TrAa01AmiScN	$\text{H}_2\text{NCHO} \rightarrow \text{H}_2\text{NCHO}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_H}_2\text{NCHO})$	Karl et al. (2012b)
H4109b_a01MK	TrAa01AmiScN	$\text{H}_2\text{NCHO}(\text{a01}) \rightarrow \text{H}_2\text{NCHO}$	$\text{xnom7amin*k_exb}(01, \text{ind_H}_2\text{NCHO})$	Karl et al. (2012b)
H4203f_a01MK	TrAa01ScC	$\text{HOCH}_2\text{CHO} \rightarrow \text{HOCH}_2\text{CHO}(\text{a01})$	$\text{xnom7co2*k_exf}(01, \text{ind_HOCH}_2\text{CHO})$	Ervens et al. (2004)
H4203b_a01MK	TrAa01ScC	$\text{HOCH}_2\text{CHO}(\text{a01}) \rightarrow \text{HOCH}_2\text{CHO}$	$\text{xnom7co2*k_exb}(01, \text{ind_HOCH}_2\text{CHO})$	Ervens et al. (2004)
H4204f_a01MK	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOCH}_2\text{CO}_2\text{H}(\text{a01})$	$\text{xnom7co2*k_exf}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	Ervens et al. (2004)
H4204b_a01MK	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H}(\text{a01}) \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$\text{xnom7co2*k_exb}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	Ervens et al. (2004)
H4205f_a01MK	TrAa01ScC	$\text{HCOCO}_2\text{H} \rightarrow \text{HCOCO}_2\text{H}(\text{a01})$	$\text{xnom7co2*k_exf}(01, \text{ind_HCOCO}_2\text{H})$	Ervens et al. (2004)
H4205b_a01MK	TrAa01ScC	$\text{HCOCO}_2\text{H}(\text{a01}) \rightarrow \text{HCOCO}_2\text{H}$	$\text{xnom7co2*k_exb}(01, \text{ind_HCOCO}_2\text{H})$	Ervens et al. (2004)
H4206f_a01MK	TrAa01ScC	$\text{GLYOX} \rightarrow \text{GLYOX}(\text{a01})$	$\text{xnom7co2*k_exf}(01, \text{ind_GLYOX})$	Ervens et al. (2004)
H4206b_a01MK	TrAa01ScC	$\text{GLYOX}(\text{a01}) \rightarrow \text{GLYOX}$	$\text{xnom7co2*k_exb}(01, \text{ind_GLYOX})$	Ervens et al. (2004)
H4207f_a01MK	TrAa01AmiScCN	$\text{DMA} \rightarrow \text{DMA}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_DMA})$	Karl et al. (2012b)
H4207b_a01MK	TrAa01AmiScCN	$\text{DMA}(\text{a01}) \rightarrow \text{DMA}$	$\text{xnom7amin*k_exb}(01, \text{ind_DMA})$	Karl et al. (2012b)
H4208f_a01MK	TrAa01AmiScCN	$\text{MEA} \rightarrow \text{MEA}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_MEA})$	Karl et al. (2012b)
H4208b_a01MK	TrAa01AmiScCN	$\text{MEA}(\text{a01}) \rightarrow \text{MEA}$	$\text{xnom7amin*k_exb}(01, \text{ind_MEA})$	Karl et al. (2012b)
H4209f_a01MK	TrAa01AmiScCN	$\text{MEANNO} \rightarrow \text{MEANNO}(\text{a01})$	$\text{xnom7nno*k_exf}(01, \text{ind_MEANNO})$	Karl et al. (2012b)
H4209b_a01MK	TrAa01AmiScCN	$\text{MEANNO}(\text{a01}) \rightarrow \text{MEANNO}$	$\text{xnom7nno*k_exb}(01, \text{ind_MEANNO})$	Karl et al. (2012b)
H4210f_a01MK	TrAa01AmiScCN	$\text{MEANNO}_2 \rightarrow \text{MEANNO}_2(\text{a01})$	$\text{xnom7nno*k_exf}(01, \text{ind_MEANNO}_2)$	Karl et al. (2012b)
H4210b_a01MK	TrAa01AmiScCN	$\text{MEANNO}_2(\text{a01}) \rightarrow \text{MEANNO}_2$	$\text{xnom7nno*k_exb}(01, \text{ind_MEANNO}_2)$	Karl et al. (2012b)
H4211f_a01MK	TrAa01AmiScCN	$\text{NDMA} \rightarrow \text{NDMA}(\text{a01})$	$\text{xnom7nno*k_exf}(01, \text{ind_NDMA})$	Karl et al. (2012b)
H4211b_a01MK	TrAa01AmiScCN	$\text{NDMA}(\text{a01}) \rightarrow \text{NDMA}$	$\text{xnom7nno*k_exb}(01, \text{ind_NDMA})$	Karl et al. (2012b)
H4212f_a01MK	TrAa01AmiScCN	$\text{DMNNO}_2 \rightarrow \text{DMNNO}_2(\text{a01})$	$\text{xnom7nno*k_exf}(01, \text{ind_DMNNO}_2)$	Karl et al. (2012b)
H4212b_a01MK	TrAa01AmiScCN	$\text{DMNNO}_2(\text{a01}) \rightarrow \text{DMNNO}_2$	$\text{xnom7nno*k_exb}(01, \text{ind_DMNNO}_2)$	Karl et al. (2012b)
H4213f_a01MK	TrAa01AmiScCN	$\text{H}_2\text{NCOCH}_2\text{OH} \rightarrow \text{H}_2\text{NCOCH}_2\text{OH}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_H}_2\text{NCOCH}_2\text{OH})$	Karl et al. (2012b)
H4213b_a01MK	TrAa01AmiScCN	$\text{H}_2\text{NCOCH}_2\text{OH}(\text{a01}) \rightarrow \text{H}_2\text{NCOCH}_2\text{OH}$	$\text{xnom7amin*k_exb}(01, \text{ind_H}_2\text{NCOCH}_2\text{OH})$	Karl et al. (2012b)
H4214f_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCHO} \rightarrow \text{CH}_3\text{NHCHO}(\text{a01})$	$\text{xnom7amin*k_exf}(01, \text{ind_CH}_3\text{NHCHO})$	Karl et al. (2012b)

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

#	labels	reaction	rate coefficient	reference
H4214b_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCHO(a01)} \rightarrow \text{CH}_3\text{NHCHO}$	$\text{xnom7amin*k_exb(01,ind_CH}_3\text{NHCHO)}$	Karl et al. (2012b)
H4301f_a01MK	TrAa01ScC	$\text{MGLYOX} \rightarrow \text{MGLYOX(a01)}$	$\text{xnom7co2*k_exf(01,ind_MGLYOX)}$	Ervens et al. (2004)
H4301b_a01MK	TrAa01ScC	$\text{MGLYOX(a01)} \rightarrow \text{MGLYOX}$	$\text{xnom7co2*k_exb(01,ind_MGLYOX)}$	Ervens et al. (2004)
H4302f_a01MK	TrAa01ScC	$\text{MGLYOAC} \rightarrow \text{MGLYOAC(a01)}$	$\text{xnom7co2*k_exf(01,ind_MGLYOAC)}$	Ervens et al. (2004)
H4302b_a01MK	TrAa01ScC	$\text{MGLYOAC(a01)} \rightarrow \text{MGLYOAC}$	$\text{xnom7co2*k_exb(01,ind_MGLYOAC)}$	Ervens et al. (2004)
H4303f_a01MK	TrAa01AmiScCN	$\text{TMA} \rightarrow \text{TMA(a01)}$	$\text{xnom7amin*k_exf(01,ind_TMA)}$	Karl et al. (2012b)
H4303b_a01MK	TrAa01AmiScCN	$\text{TMA(a01)} \rightarrow \text{TMA}$	$\text{xnom7amin*k_exb(01,ind_TMA)}$	Karl et al. (2012b)
H4304f_a01MK	TrAa01AmiScCN	$\text{DMNCHO} \rightarrow \text{DMNCHO(a01)}$	$\text{xnom7amin*k_exf(01,ind_DMNCHO)}$	Karl et al. (2012b)
H4304b_a01MK	TrAa01AmiScCN	$\text{DMNCHO(a01)} \rightarrow \text{DMNCHO}$	$\text{xnom7amin*k_exb(01,ind_DMNCHO)}$	Karl et al. (2012b)
H4400f_a01MK	TrAa01AmiScCN	$\text{DEA} \rightarrow \text{DEA(a01)}$	$\text{xnom7amin*k_exf(01,ind_DEA)}$	Karl et al. (2012b)
H4400b_a01MK	TrAa01AmiScCN	$\text{DEA(a01)} \rightarrow \text{DEA}$	$\text{xnom7amin*k_exb(01,ind_DEA)}$	Karl et al. (2012b)
H4401f_a01MK	TrAa01AmiScCN	$\text{NDELA} \rightarrow \text{NDELA(a01)}$	$\text{xnom7nno*k_exf(01,ind_NDELA)}$	Karl et al. (2012b)
H4401b_a01MK	TrAa01AmiScCN	$\text{NDELA(a01)} \rightarrow \text{NDELA}$	$\text{xnom7nno*k_exb(01,ind_NDELA)}$	Karl et al. (2012b)
H4402f_a01MK	TrAa01AmiScCN	$\text{DEANNO2} \rightarrow \text{DEANNO2(a01)}$	$\text{xnom7nno*k_exf(01,ind_DEANNO2)}$	Karl et al. (2012b)
H4402b_a01MK	TrAa01AmiScCN	$\text{DEANNO2(a01)} \rightarrow \text{DEANNO2}$	$\text{xnom7nno*k_exb(01,ind_DEANNO2)}$	Karl et al. (2012b)
H4403f_a01MK	TrAa01Sc	$\text{BSOV} \rightarrow \text{SUCCAC(a01)}$	$\text{xnom7co2*k_exf(01,ind_BSOV)}$	Ervens et al. (2004)
H4403b_a01MK	TrAa01Sc	$\text{SUCCAC(a01)} \rightarrow \text{BSOV}$	$\text{xnom7co2*k_exb(01,ind_BSOV)}$	Ervens et al. (2004)
H4600f_a01MK	TrAa01AmiScCN	$\text{TEA} \rightarrow \text{TEA(a01)}$	$\text{xnom7amin*k_exf(01,ind_TEA)}$	Karl et al. (2012b)
H4600b_a01MK	TrAa01AmiScCN	$\text{TEA(a01)} \rightarrow \text{TEA}$	$\text{xnom7amin*k_exb(01,ind_TEA)}$	Karl et al. (2012b)
H4601f_a01MK	TrAa01Sc	$\text{BLOV} \rightarrow \text{ADIPAC(a01)}$	$\text{xnom7co2*k_exf(01,ind_BLOV)}$	Ervens et al. (2004)
H4601b_a01MK	TrAa01Sc	$\text{ADIPAC(a01)} \rightarrow \text{BLOV}$	$\text{xnom7co2*k_exb(01,ind_BLOV)}$	Ervens et al. (2004)
H9403f_a01MK	TrAa01S	$\text{CH}_3\text{SOOH} \rightarrow \text{MSIA(a01)}$	$\text{xnom7dmso*k_exf(01,ind_CH}_3\text{SOOH)}$	Hoffmann et al. (2016)
H9403b_a01MK	TrAa01S	$\text{MSIA(a01)} \rightarrow \text{CH}_3\text{SOOH}$	$\text{xnom7dmso*k_exb(01,ind_CH}_3\text{SOOH)}$	Hoffmann et al. (2016)
H9404f_a01MK	TrAa01CS	$\text{HPMTF} \rightarrow \text{HPMTF(a01)}$	$\text{xnom7dmso*k_exf(01,ind_HPMTF)}$	Wollesen de Jonge et al. (2021)
H9404b_a01MK	TrAa01CS	$\text{HPMTF(a01)} \rightarrow \text{HPMTF}$	$\text{xnom7dmso*k_exb(01,ind_HPMTF)}$	Wollesen de Jonge et al. (2021)
H9405f_a01MK	TrAa01CS	$\text{HOOCH}_2\text{SCO} \rightarrow \text{HOOCH}_2\text{SCO(a01)}$	$\text{xnom7dmso*k_exf(01,ind_HOOCH}_2\text{SCO)}$	Wollesen de Jonge et al. (2021)
H9405b_a01MK	TrAa01CS	$\text{HOOCH}_2\text{SCO(a01)} \rightarrow \text{HOOCH}_2\text{SCO}$	$\text{xnom7dmso*k_exb(01,ind_HOOCH}_2\text{SCO)}$	Wollesen de Jonge et al. (2021)
H1000f_a02	TrAa02Sc	$\text{O}_2 \rightarrow \text{O}_2(\text{a02})$	$\text{k_exf(02,ind_O}_2\text{)}$	see general notes*
H1000b_a02	TrAa02Sc	$\text{O}_2(\text{a02}) \rightarrow \text{O}_2$	$\text{k_exb(02,ind_O}_2\text{)}$	see general notes*
H1001f_a02	TrAa02MblScScm	$\text{O}_3 \rightarrow \text{O}_3(\text{a02})$	$\text{k_exf(02,ind_O}_3\text{)}$	see general notes*
H1001b_a02	TrAa02MblScScm	$\text{O}_3(\text{a02}) \rightarrow \text{O}_3$	$\text{k_exb(02,ind_O}_3\text{)}$	see general notes*
H2100f_a02	TrAa02Sc	$\text{OH} \rightarrow \text{OH(a02)}$	k_exf(02,ind_OH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H2100b_a02	TrAa02Sc	$\text{OH(a02)} \rightarrow \text{OH}$	$k_{\text{exb}}(02, \text{ind_OH})$	see general notes*
H2101f_a02	TrAa02Sc	$\text{HO}_2 \rightarrow \text{HO}_2(\text{a02})$	$k_{\text{exf}}(02, \text{ind_H02})$	see general notes*
H2101b_a02	TrAa02Sc	$\text{HO}_2(\text{a02}) \rightarrow \text{HO}_2$	$k_{\text{exb}}(02, \text{ind_H02})$	see general notes*
H2102f_a02	TrAa02MblScScm	$\text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2(\text{a02})$	$k_{\text{exf}}(02, \text{ind_H202})$	see general notes*
H2102b_a02	TrAa02MblScScm	$\text{H}_2\text{O}_2(\text{a02}) \rightarrow \text{H}_2\text{O}_2$	$k_{\text{exb}}(02, \text{ind_H202})$	see general notes*
H3101f_a02	TrAa02ScN	$\text{NO}_2 \rightarrow \text{NO}_2(\text{a02})$	$k_{\text{exf}}(02, \text{ind_N02})$	see general notes*
H3101b_a02	TrAa02ScN	$\text{NO}_2(\text{a02}) \rightarrow \text{NO}_2$	$k_{\text{exb}}(02, \text{ind_N02})$	see general notes*
H3102f_a02	TrAa02ScN	$\text{NO}_3 \rightarrow \text{NO}_3(\text{a02})$	$k_{\text{exf}}(02, \text{ind_N03})$	see general notes*
H3102b_a02	TrAa02ScN	$\text{NO}_3(\text{a02}) \rightarrow \text{NO}_3$	$k_{\text{exb}}(02, \text{ind_N03})$	see general notes*
H3200f_a02	TrAa02MblScScmN	$\text{NH}_3 \rightarrow \text{NH}_3(\text{a02})$	$k_{\text{exf}}(02, \text{ind_NH3})$	see general notes*
H3200b_a02	TrAa02MblScScmN	$\text{NH}_3(\text{a02}) \rightarrow \text{NH}_3$	$k_{\text{exb}}(02, \text{ind_NH3})$	see general notes*
H3201_a02	TrAa02MblScScmN	$\text{N}_2\text{O}_5 \rightarrow \text{HNO}_3(\text{a02}) + \text{HNO}_3(\text{a02})$	$k_{\text{exf_N205}}(02) * C(\text{ind_H20_a02})$	Behnke et al. (1994), Behnke et al. (1997)
H3202f_a02	TrAa02ScN	$\text{HONO} \rightarrow \text{HONO(a02)}$	$k_{\text{exf}}(02, \text{ind_HONO})$	see general notes*
H3202b_a02	TrAa02ScN	$\text{HONO(a02)} \rightarrow \text{HONO}$	$k_{\text{exb}}(02, \text{ind_HONO})$	see general notes*
H3203f_a02	TrAa02MblScScmN	$\text{HNO}_3 \rightarrow \text{HNO}_3(\text{a02})$	$k_{\text{exf}}(02, \text{ind_HNO3})$	see general notes*
H3203b_a02	TrAa02MblScScmN	$\text{HNO}_3(\text{a02}) \rightarrow \text{HNO}_3$	$k_{\text{exb}}(02, \text{ind_HNO3})$	see general notes*
H3204f_a02	TrAa02ScN	$\text{HNO}_4 \rightarrow \text{HNO}_4(\text{a02})$	$k_{\text{exf}}(02, \text{ind_HNO4})$	see general notes*
H3204b_a02	TrAa02ScN	$\text{HNO}_4(\text{a02}) \rightarrow \text{HNO}_4$	$k_{\text{exb}}(02, \text{ind_HNO4})$	see general notes*
H4100f_a02	TrAa02MblScScm	$\text{CO}_2 \rightarrow \text{CO}_2(\text{a02})$	$k_{\text{exf}}(02, \text{ind_C02})$	see general notes*
H4100b_a02	TrAa02MblScScm	$\text{CO}_2(\text{a02}) \rightarrow \text{CO}_2$	$k_{\text{exb}}(02, \text{ind_C02})$	see general notes*
H4101f_a02	TrAa02ScScm	$\text{HCHO} \rightarrow \text{HCHO(a02)}$	$k_{\text{exf}}(02, \text{ind_HCHO})$	see general notes*
H4101b_a02	TrAa02ScScm	$\text{HCHO(a02)} \rightarrow \text{HCHO}$	$k_{\text{exb}}(02, \text{ind_HCHO})$	see general notes*
H4102f_a02	TrAa02Sc	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OO(a02)}$	$k_{\text{exf}}(02, \text{ind_CH302})$	see general notes*
H4102b_a02	TrAa02Sc	$\text{CH}_3\text{OO(a02)} \rightarrow \text{CH}_3\text{O}_2$	$k_{\text{exb}}(02, \text{ind_CH302})$	see general notes*
H4103f_a02	TrAa02ScScm	$\text{HCOOH} \rightarrow \text{HCOOH(a02)}$	$k_{\text{exf}}(02, \text{ind_HCOOH})$	see general notes*
H4103b_a02	TrAa02ScScm	$\text{HCOOH(a02)} \rightarrow \text{HCOOH}$	$k_{\text{exb}}(02, \text{ind_HCOOH})$	see general notes*
H4104f_a02	TrAa02ScScm	$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH(a02)}$	$k_{\text{exf}}(02, \text{ind_CH300H})$	see general notes*
H4104b_a02	TrAa02ScScm	$\text{CH}_3\text{OOH(a02)} \rightarrow \text{CH}_3\text{OOH}$	$k_{\text{exb}}(02, \text{ind_CH300H})$	see general notes*
H6000f_a02	TrAa02MblScCl	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{a02})$	$k_{\text{exf}}(02, \text{ind_Cl2})$	see general notes*
H6000b_a02	TrAa02MblScCl	$\text{Cl}_2(\text{a02}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(02, \text{ind_Cl2})$	see general notes*
H6200f_a02	TrAa02MblScScmCl	$\text{HCl} \rightarrow \text{HCl(a02)}$	$k_{\text{exf}}(02, \text{ind_HCl})$	see general notes*
H6200b_a02	TrAa02MblScScmCl	$\text{HCl(a02)} \rightarrow \text{HCl}$	$k_{\text{exb}}(02, \text{ind_HCl})$	see general notes*
H6201f_a02	TrAa02MblScCl	$\text{HOCl} \rightarrow \text{HOCl(a02)}$	$k_{\text{exf}}(02, \text{ind_HOCl})$	see general notes*
H6201b_a02	TrAa02MblScCl	$\text{HOCl(a02)} \rightarrow \text{HOCl}$	$k_{\text{exb}}(02, \text{ind_HOCl})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H6300_a02	TrAa02MblClN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{a02}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{a02})$	$k_{\text{exf_N2O5}}(\text{02}) * 5.\text{E2}$	Behnke et al. (1994), Behnke et al. (1997)
H6301_a02	TrAa02MblClN	$\text{ClNO}_3 \rightarrow \text{HOCl}(\text{a02}) + \text{HNO}_3(\text{a02})$	$k_{\text{exf_ClNO3}}(\text{02}) * \text{C}(\text{ind_H2O_a02})$	see general notes*
H6302_a02	TrAa02MblClN	$\text{ClNO}_3 + \text{Cl}^-(\text{a02}) \rightarrow \text{Cl}_2(\text{a02}) + \text{NO}_3^-(\text{a02})$	$k_{\text{exf_ClNO3}}(\text{02}) * 5.\text{E2}$	see general notes*
H8000f_a02	TrAa02ScI	$\text{I}_2 \rightarrow \text{I}_2(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_I2})$	see general notes*
H8000b_a02	TrAa02ScI	$\text{I}_2(\text{a02}) \rightarrow \text{I}_2$	$k_{\text{exb}}(\text{02}, \text{ind_I2})$	see general notes*
H8100f_a02	TrAa02MblScI	$\text{IO} \rightarrow \text{IO}(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_IO})$	see general notes*
H8100b_a02	TrAa02MblScI	$\text{IO}(\text{a02}) \rightarrow \text{IO}$	$k_{\text{exb}}(\text{02}, \text{ind_IO})$	see general notes*
H8101_a02	TrAa02I	$\text{OIO} \rightarrow \text{HOI}(\text{a02}) + \text{HO}_2(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_OIO})$	see general notes*
H8102_a02	TrAa02I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI}(\text{a02}) + \text{H}^+(\text{a02}) + \text{IO}_2^-(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_I2O2})$	see general notes*
H8200f_a02	TrAa02MblScI	$\text{HOI} \rightarrow \text{HOI}(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_HOI})$	see general notes*
H8200b_a02	TrAa02MblScI	$\text{HOI}(\text{a02}) \rightarrow \text{HOI}$	$k_{\text{exb}}(\text{02}, \text{ind_HOI})$	see general notes*
H8201_a02	TrAa02MblScI	$\text{HI} \rightarrow \text{H}^+(\text{a02}) + \text{I}^-(\text{a02})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see general notes*
H8202_a02	TrAa02ScI	$\text{HIO}_3 \rightarrow \text{IO}_3^-(\text{a02}) + \text{H}^+(\text{a02})$	$k_{\text{mt}}(\text{HIO}_3) \cdot lwc$	see general notes*
H8300_a02	TrAa02IN	$\text{INO}_2 \rightarrow \text{HOI}(\text{a02}) + \text{HONO}(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_INO2})$	see general notes*
H8301_a02	TrAa02MblIN	$\text{INO}_3 \rightarrow \text{HOI}(\text{a02}) + \text{HNO}_3(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_INO3})$	see general notes*
H8600f_a02	TrAa02MblScClI	$\text{ICl} \rightarrow \text{ICl}(\text{a02})$	$k_{\text{exf}}(\text{02}, \text{ind_ICl})$	see general notes*
H8600b_a02	TrAa02MblScClI	$\text{ICl}(\text{a02}) \rightarrow \text{ICl}$	$k_{\text{exb}}(\text{02}, \text{ind_ICl})$	see general notes*
H9100f_a02	TrAa02MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{a02})$	$xnom7so2 * k_{\text{exf}}(\text{02}, \text{ind_SO2})$	see general notes*
H9100b_a02	TrAa02MblScScmS	$\text{SO}_2(\text{a02}) \rightarrow \text{SO}_2$	$xnom7so2 * k_{\text{exb}}(\text{02}, \text{ind_SO2})$	see general notes*
H9200_a02	TrAa02MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{a02})$	$xnom7sulf * k_{\text{exf}}(\text{02}, \text{ind_H2SO4})$	see general notes*
H9400f_a02	TrAa02CS	$\text{DMSO} \rightarrow \text{DMSO}(\text{a02})$	$xnom7dms * k_{\text{exf}}(\text{02}, \text{ind_DMSO})$	see general notes*
H9400b_a02	TrAa02CS	$\text{DMSO}(\text{a02}) \rightarrow \text{DMSO}$	$xnom7dms * k_{\text{exb}}(\text{02}, \text{ind_DMSO})$	see general notes*
H9401_a02	TrAa02MblS	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{a02}) + \text{H}^+(\text{a02})$	$xnom7dms * k_{\text{exf}}(\text{02}, \text{ind_CH3SO3H})$	see general notes*
H9402f_a02	TrAa02CS	$\text{DMS} \rightarrow \text{DMS}(\text{a02})$	$xnom7dms * k_{\text{exf}}(\text{02}, \text{ind_DMS})$	see general notes*
H9402b_a02	TrAa02CS	$\text{DMS}(\text{a02}) \rightarrow \text{DMS}$	$xnom7dms * k_{\text{exb}}(\text{02}, \text{ind_DMS})$	see general notes*
H3103f_a02MK	TrAa02ScN	$\text{N}_2\text{O}_3 \rightarrow \text{N}_2\text{O}_3(\text{a02})$	$xnom7nox * k_{\text{exf}}(\text{02}, \text{ind_N2O3})$	Karl et al. (2012b)
H3103b_a02MK	TrAa02ScN	$\text{N}_2\text{O}_3(\text{a02}) \rightarrow \text{N}_2\text{O}_3$	$xnom7nox * k_{\text{exb}}(\text{02}, \text{ind_N2O3})$	Karl et al. (2012b)
H3104f_a02MK	TrAa02ScN	$\text{N}_2\text{O}_4 \rightarrow \text{N}_2\text{O}_4(\text{a02})$	$xnom7nox * k_{\text{exf}}(\text{02}, \text{ind_N2O4})$	Karl et al. (2012b)
H3104b_a02MK	TrAa02ScN	$\text{N}_2\text{O}_4(\text{a02}) \rightarrow \text{N}_2\text{O}_4$	$xnom7nox * k_{\text{exb}}(\text{02}, \text{ind_N2O4})$	Karl et al. (2012b)
H4106f_a02MK	TrAa02AmiScN	$\text{MMA} \rightarrow \text{MMA}(\text{a02})$	$xnom7amin * k_{\text{exf}}(\text{02}, \text{ind_MMA})$	Karl et al. (2012b)
H4106b_a02MK	TrAa02AmiScN	$\text{MMA}(\text{a02}) \rightarrow \text{MMA}$	$xnom7amin * k_{\text{exb}}(\text{02}, \text{ind_MMA})$	Karl et al. (2012b)
H4107f_a02MK	TrAa02AmiScN	$\text{MMNNO}_2 \rightarrow \text{MMNNO}_2(\text{a02})$	$xnom7nno * k_{\text{exf}}(\text{02}, \text{ind_MMNNO2})$	Karl et al. (2012b)
H4107b_a02MK	TrAa02AmiScN	$\text{MMNNO}_2(\text{a02}) \rightarrow \text{MMNNO}_2$	$xnom7nno * k_{\text{exb}}(\text{02}, \text{ind_MMNNO2})$	Karl et al. (2012b)

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

#	labels	reaction	rate coefficient	reference
H4108f_a02MK	TrAa02AmiScN	$\text{HNCO} \rightarrow \text{HNCO(a02)}$	$\text{xnom7amin*k_exf(02,ind_HNCO)}$	Karl et al. (2012b)
H4108b_a02MK	TrAa02AmiScN	$\text{HNCO(a02)} \rightarrow \text{HNCO}$	$\text{xnom7amin*k_exb(02,ind_HNCO)}$	Karl et al. (2012b)
H4109f_a02MK	TrAa02AmiScN	$\text{H2NCHO} \rightarrow \text{H2NCHO(a02)}$	$\text{xnom7amin*k_exf(02,ind_H2NCHO)}$	Karl et al. (2012b)
H4109b_a02MK	TrAa02AmiScN	$\text{H2NCHO(a02)} \rightarrow \text{H2NCHO}$	$\text{xnom7amin*k_exb(02,ind_H2NCHO)}$	Karl et al. (2012b)
H4203f_a02MK	TrAa02ScC	$\text{HOCH}_2\text{CHO} \rightarrow \text{HOCH}_2\text{CHO(a02)}$	$\text{xnom7co2*k_exf(02,ind_HOCH2CHO)}$	Ervens et al. (2004)
H4203b_a02MK	TrAa02ScC	$\text{HOCH}_2\text{CHO(a02)} \rightarrow \text{HOCH}_2\text{CHO}$	$\text{xnom7co2*k_exb(02,ind_HOCH2CHO)}$	Ervens et al. (2004)
H4204f_a02MK	TrAa02ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOCH}_2\text{CO}_2\text{H(a02)}$	$\text{xnom7co2*k_exf(02,ind_HOCH2CO2H)}$	Ervens et al. (2004)
H4204b_a02MK	TrAa02ScC	$\text{HOCH}_2\text{CO}_2\text{H(a02)} \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$\text{xnom7co2*k_exb(02,ind_HOCH2CO2H)}$	Ervens et al. (2004)
H4205f_a02MK	TrAa02ScC	$\text{HCOCO}_2\text{H} \rightarrow \text{HCOCO}_2\text{H(a02)}$	$\text{xnom7co2*k_exf(02,ind_HCOCO2H)}$	Ervens et al. (2004)
H4205b_a02MK	TrAa02ScC	$\text{HCOCO}_2\text{H(a02)} \rightarrow \text{HCOCO}_2\text{H}$	$\text{xnom7co2*k_exb(02,ind_HCOCO2H)}$	Ervens et al. (2004)
H4206f_a02MK	TrAa02ScC	$\text{GLYOX} \rightarrow \text{GLYOX(a02)}$	$\text{xnom7co2*k_exf(02,ind_GLYOX)}$	Ervens et al. (2004)
H4206b_a02MK	TrAa02ScC	$\text{GLYOX(a02)} \rightarrow \text{GLYOX}$	$\text{xnom7co2*k_exb(02,ind_GLYOX)}$	Ervens et al. (2004)
H4207f_a02MK	TrAa02AmiScCN	$\text{DMA} \rightarrow \text{DMA(a02)}$	$\text{xnom7amin*k_exf(02,ind_DMA)}$	Karl et al. (2012b)
H4207b_a02MK	TrAa02AmiScCN	$\text{DMA(a02)} \rightarrow \text{DMA}$	$\text{xnom7amin*k_exb(02,ind_DMA)}$	Karl et al. (2012b)
H4208f_a02MK	TrAa02AmiScCN	$\text{MEA} \rightarrow \text{MEA(a02)}$	$\text{xnom7amin*k_exf(02,ind_MEA)}$	Karl et al. (2012b)
H4208b_a02MK	TrAa02AmiScCN	$\text{MEA(a02)} \rightarrow \text{MEA}$	$\text{xnom7amin*k_exb(02,ind_MEA)}$	Karl et al. (2012b)
H4209f_a02MK	TrAa02AmiScCN	$\text{MEANNO} \rightarrow \text{MEANNO(a02)}$	$\text{xnom7nno*k_exf(02,ind_MEANNO)}$	Karl et al. (2012b)
H4209b_a02MK	TrAa02AmiScCN	$\text{MEANNO(a02)} \rightarrow \text{MEANNO}$	$\text{xnom7nno*k_exb(02,ind_MEANNO)}$	Karl et al. (2012b)
H4210f_a02MK	TrAa02AmiScCN	$\text{MEANNO2} \rightarrow \text{MEANNO2(a02)}$	$\text{xnom7nno*k_exf(02,ind_MEANNO2)}$	Karl et al. (2012b)
H4210b_a02MK	TrAa02AmiScCN	$\text{MEANNO2(a02)} \rightarrow \text{MEANNO2}$	$\text{xnom7nno*k_exb(02,ind_MEANNO2)}$	Karl et al. (2012b)
H4211f_a02MK	TrAa02AmiScCN	$\text{NDMA} \rightarrow \text{NDMA(a02)}$	$\text{xnom7nno*k_exf(02,ind_NDMA)}$	Karl et al. (2012b)
H4211b_a02MK	TrAa02AmiScCN	$\text{NDMA(a02)} \rightarrow \text{NDMA}$	$\text{xnom7nno*k_exb(02,ind_NDMA)}$	Karl et al. (2012b)
H4212f_a02MK	TrAa02AmiScCN	$\text{DMNNO2} \rightarrow \text{DMNNO2(a02)}$	$\text{xnom7nno*k_exf(02,ind_DMNNO2)}$	Karl et al. (2012b)
H4212b_a02MK	TrAa02AmiScCN	$\text{DMNNO2(a02)} \rightarrow \text{DMNNO2}$	$\text{xnom7nno*k_exb(02,ind_DMNNO2)}$	Karl et al. (2012b)
H4213f_a02MK	TrAa02AmiScCN	$\text{H2NCOCH2OH} \rightarrow \text{H2NCOCH2OH(a02)}$	$\text{xnom7amin*k_exf(02,ind_H2NCOCH2OH)}$	Karl et al. (2012b)
H4213b_a02MK	TrAa02AmiScCN	$\text{H2NCOCH2OH(a02)} \rightarrow \text{H2NCOCH2OH}$	$\text{xnom7amin*k_exb(02,ind_H2NCOCH2OH)}$	Karl et al. (2012b)
H4214f_a02MK	TrAa02AmiScCN	$\text{CH}_3\text{NHCHO} \rightarrow \text{CH}_3\text{NHCHO(a02)}$	$\text{xnom7amin*k_exf(02,ind_CH3NHCHO)}$	Karl et al. (2012b)
H4214b_a02MK	TrAa02AmiScCN	$\text{CH}_3\text{NHCHO(a02)} \rightarrow \text{CH}_3\text{NHCHO}$	$\text{xnom7amin*k_exb(02,ind_CH3NHCHO)}$	Karl et al. (2012b)
H4301f_a02MK	TrAa02ScC	$\text{MGLYOX} \rightarrow \text{MGLYOX(a02)}$	$\text{xnom7co2*k_exf(02,ind_MGLYOX)}$	Ervens et al. (2004)
H4301b_a02MK	TrAa02ScC	$\text{MGLYOX(a02)} \rightarrow \text{MGLYOX}$	$\text{xnom7co2*k_exb(02,ind_MGLYOX)}$	Ervens et al. (2004)
H4302f_a02MK	TrAa02ScC	$\text{MGLYOAC} \rightarrow \text{MGLYOAC(a02)}$	$\text{xnom7co2*k_exf(02,ind_MGLYOAC)}$	Ervens et al. (2004)
H4302b_a02MK	TrAa02ScC	$\text{MGLYOAC(a02)} \rightarrow \text{MGLYOAC}$	$\text{xnom7co2*k_exb(02,ind_MGLYOAC)}$	Ervens et al. (2004)
H4303f_a02MK	TrAa02AmiScCN	$\text{TMA} \rightarrow \text{TMA(a02)}$	$\text{xnom7amin*k_exf(02,ind_TMA)}$	Karl et al. (2012b)

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

#	labels	reaction	rate coefficient	reference
H4303b_a02MK	TrAa02AmiScCN	TMA(a02) \rightarrow TMA	$xnom7amin*k_exb(02,ind_TMA)$	Karl et al. (2012b)
H4304f_a02MK	TrAa02AmiScCN	DMNCHO \rightarrow DMNCHO(a02)	$xnom7amin*k_exf(02,ind_DMNCHO)$	Karl et al. (2012b)
H4304b_a02MK	TrAa02AmiScCN	DMNCHO(a02) \rightarrow DMNCHO	$xnom7amin*k_exb(02,ind_DMNCHO)$	Karl et al. (2012b)
H4400f_a02MK	TrAa02AmiScCN	DEA \rightarrow DEA(a02)	$xnom7amin*k_exf(02,ind_DEA)$	Karl et al. (2012b)
H4400b_a02MK	TrAa02AmiScCN	DEA(a02) \rightarrow DEA	$xnom7amin*k_exb(02,ind_DEA)$	Karl et al. (2012b)
H4401f_a02MK	TrAa02AmiScCN	NDELA \rightarrow NDELA(a02)	$xnom7nno*k_exf(02,ind_NDELA)$	Karl et al. (2012b)
H4401b_a02MK	TrAa02AmiScCN	NDELA(a02) \rightarrow NDELA	$xnom7nno*k_exb(02,ind_NDELA)$	Karl et al. (2012b)
H4402f_a02MK	TrAa02AmiScCN	DEANNO2 \rightarrow DEANNO2(a02)	$xnom7nno*k_exf(02,ind_DEANNO2)$	Karl et al. (2012b)
H4402b_a02MK	TrAa02AmiScCN	DEANNO2(a02) \rightarrow DEANNO2	$xnom7nno*k_exb(02,ind_DEANNO2)$	Karl et al. (2012b)
H4403f_a02MK	TrAa02Sc	BSOV \rightarrow SUCCAC(a02)	$xnom7co2*k_exf(02,ind_BSOV)$	Ervens et al. (2004)
H4403b_a02MK	TrAa02Sc	SUCCAC(a02) \rightarrow BSOV	$xnom7co2*k_exb(02,ind_BSOV)$	Ervens et al. (2004)
H4600f_a02MK	TrAa02AmiScCN	TEA \rightarrow TEA(a02)	$xnom7amin*k_exf(02,ind_TEA)$	Karl et al. (2012b)
H4600b_a02MK	TrAa02AmiScCN	TEA(a02) \rightarrow TEA	$xnom7amin*k_exb(02,ind_TEA)$	Karl et al. (2012b)
H4601f_a02MK	TrAa02Sc	BLOV \rightarrow ADIPAC(a02)	$xnom7co2*k_exf(02,ind_BLOV)$	Ervens et al. (2004)
H4601b_a02MK	TrAa02Sc	ADIPAC(a02) \rightarrow BLOV	$xnom7co2*k_exb(02,ind_BLOV)$	Ervens et al. (2004)
H9403f_a02MK	TrAa02S	CH ₃ SOOH \rightarrow MSIA(a02)	$xnom7dmso*k_exf(02,ind_CH3SOOH)$	Hoffmann et al. (2016)
H9403b_a02MK	TrAa02S	MSIA(a02) \rightarrow CH ₃ SOOH	$xnom7dmso*k_exb(02,ind_CH3SOOH)$	Hoffmann et al. (2016)
H9404f_a02MK	TrAa02CS	HPMTF \rightarrow HPMTF(a02)	$xnom7dmso*k_exf(02,ind_HPMTF)$	Wollesen de Jonge et al. (2021)
H9404b_a02MK	TrAa02CS	HPMTF(a02) \rightarrow HPMTF	$xnom7dmso*k_exb(02,ind_HPMTF)$	Wollesen de Jonge et al. (2021)
H9405f_a02MK	TrAa02CS	HOOCH ₂ SCO \rightarrow HOOCH ₂ SCO(a02)	$xnom7dmso*k_exf(02,ind_HOOCH2SCO)$	Wollesen de Jonge et al. (2021)
H9405b_a02MK	TrAa02CS	HOOCH ₂ SCO(a02) \rightarrow HOOCH ₂ SCO	$xnom7dmso*k_exb(02,ind_HOOCH2SCO)$	Wollesen de Jonge et al. (2021)
H1000f_a03	TrAa03Sc	O ₂ \rightarrow O ₂ (a03)	$k_exf(03,ind_O2)$	see general notes*
H1000b_a03	TrAa03Sc	O ₂ (a03) \rightarrow O ₂	$k_exb(03,ind_O2)$	see general notes*
H1001f_a03	TrAa03MblScScm	O ₃ \rightarrow O ₃ (a03)	$k_exf(03,ind_O3)$	see general notes*
H1001b_a03	TrAa03MblScScm	O ₃ (a03) \rightarrow O ₃	$k_exb(03,ind_O3)$	see general notes*
H2100f_a03	TrAa03Sc	OH \rightarrow OH(a03)	$k_exf(03,ind_OH)$	see general notes*
H2100b_a03	TrAa03Sc	OH(a03) \rightarrow OH	$k_exb(03,ind_OH)$	see general notes*
H2101f_a03	TrAa03Sc	HO ₂ \rightarrow HO ₂ (a03)	$k_exf(03,ind_H02)$	see general notes*
H2101b_a03	TrAa03Sc	HO ₂ (a03) \rightarrow HO ₂	$k_exb(03,ind_H02)$	see general notes*
H2102f_a03	TrAa03MblScScm	H ₂ O ₂ \rightarrow H ₂ O ₂ (a03)	$k_exf(03,ind_H202)$	see general notes*
H2102b_a03	TrAa03MblScScm	H ₂ O ₂ (a03) \rightarrow H ₂ O ₂	$k_exb(03,ind_H202)$	see general notes*
H3101f_a03	TrAa03ScN	NO ₂ \rightarrow NO ₂ (a03)	$k_exf(03,ind_N02)$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H3101b_a03	TrAa03ScN	$\text{NO}_2(\text{a03}) \rightarrow \text{NO}_2$	$k_{\text{exb}}(03, \text{ind_NO2})$	see general notes*
H3102f_a03	TrAa03ScN	$\text{NO}_3 \rightarrow \text{NO}_3(\text{a03})$	$k_{\text{exf}}(03, \text{ind_NO3})$	see general notes*
H3102b_a03	TrAa03ScN	$\text{NO}_3(\text{a03}) \rightarrow \text{NO}_3$	$k_{\text{exb}}(03, \text{ind_NO3})$	see general notes*
H3200f_a03	TrAa03MblScScmN	$\text{NH}_3 \rightarrow \text{NH}_3(\text{a03})$	$k_{\text{exf}}(03, \text{ind_NH3})$	see general notes*
H3200b_a03	TrAa03MblScScmN	$\text{NH}_3(\text{a03}) \rightarrow \text{NH}_3$	$k_{\text{exb}}(03, \text{ind_NH3})$	see general notes*
H3201_a03	TrAa03MblScScmN	$\text{N}_2\text{O}_5 \rightarrow \text{HNO}_3(\text{a03}) + \text{HNO}_3(\text{a03})$	$k_{\text{exf_N2O5}}(03) * C(\text{ind_H2O_a03})$	Behnke et al. (1994), Behnke et al. (1997)
H3202f_a03	TrAa03ScN	$\text{HONO} \rightarrow \text{HONO}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HONO})$	see general notes*
H3202b_a03	TrAa03ScN	$\text{HONO}(\text{a03}) \rightarrow \text{HONO}$	$k_{\text{exb}}(03, \text{ind_HONO})$	see general notes*
H3203f_a03	TrAa03MblScScmN	$\text{HNO}_3 \rightarrow \text{HNO}_3(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HNO3})$	see general notes*
H3203b_a03	TrAa03MblScScmN	$\text{HNO}_3(\text{a03}) \rightarrow \text{HNO}_3$	$k_{\text{exb}}(03, \text{ind_HNO3})$	see general notes*
H3204f_a03	TrAa03ScN	$\text{HNO}_4 \rightarrow \text{HNO}_4(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HNO4})$	see general notes*
H3204b_a03	TrAa03ScN	$\text{HNO}_4(\text{a03}) \rightarrow \text{HNO}_4$	$k_{\text{exb}}(03, \text{ind_HNO4})$	see general notes*
H4100f_a03	TrAa03MblScScm	$\text{CO}_2 \rightarrow \text{CO}_2(\text{a03})$	$k_{\text{exf}}(03, \text{ind_CO2})$	see general notes*
H4100b_a03	TrAa03MblScScm	$\text{CO}_2(\text{a03}) \rightarrow \text{CO}_2$	$k_{\text{exb}}(03, \text{ind_CO2})$	see general notes*
H4101f_a03	TrAa03ScScm	$\text{HCHO} \rightarrow \text{HCHO}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HCHO})$	see general notes*
H4101b_a03	TrAa03ScScm	$\text{HCHO}(\text{a03}) \rightarrow \text{HCHO}$	$k_{\text{exb}}(03, \text{ind_HCHO})$	see general notes*
H4102f_a03	TrAa03Sc	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OO}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_CH3O2})$	see general notes*
H4102b_a03	TrAa03Sc	$\text{CH}_3\text{OO}(\text{a03}) \rightarrow \text{CH}_3\text{O}_2$	$k_{\text{exb}}(03, \text{ind_CH3O2})$	see general notes*
H4103f_a03	TrAa03ScScm	$\text{HCOOH} \rightarrow \text{HCOOH}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HCOOH})$	see general notes*
H4103b_a03	TrAa03ScScm	$\text{HCOOH}(\text{a03}) \rightarrow \text{HCOOH}$	$k_{\text{exb}}(03, \text{ind_HCOOH})$	see general notes*
H4104f_a03	TrAa03ScScm	$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_CH3OOH})$	see general notes*
H4104b_a03	TrAa03ScScm	$\text{CH}_3\text{OOH}(\text{a03}) \rightarrow \text{CH}_3\text{OOH}$	$k_{\text{exb}}(03, \text{ind_CH3OOH})$	see general notes*
H6000f_a03	TrAa03MblScCl	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{a03})$	$k_{\text{exf}}(03, \text{ind_Cl2})$	see general notes*
H6000b_a03	TrAa03MblScCl	$\text{Cl}_2(\text{a03}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(03, \text{ind_Cl2})$	see general notes*
H6200f_a03	TrAa03MblScScmCl	$\text{HCl} \rightarrow \text{HCl}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HCl})$	see general notes*
H6200b_a03	TrAa03MblScScmCl	$\text{HCl}(\text{a03}) \rightarrow \text{HCl}$	$k_{\text{exb}}(03, \text{ind_HCl})$	see general notes*
H6201f_a03	TrAa03MblScCl	$\text{HOCl} \rightarrow \text{HOCl}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HOCl})$	see general notes*
H6201b_a03	TrAa03MblScCl	$\text{HOCl}(\text{a03}) \rightarrow \text{HOCl}$	$k_{\text{exb}}(03, \text{ind_HOCl})$	see general notes*
H6300_a03	TrAa03MblClN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{a03}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{a03})$	$k_{\text{exf_N2O5}}(03) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)
H6301_a03	TrAa03MblClN	$\text{ClNO}_3 \rightarrow \text{HOCl}(\text{a03}) + \text{HNO}_3(\text{a03})$	$k_{\text{exf_ClNO3}}(03) * C(\text{ind_H2O_a03})$	see general notes*
H6302_a03	TrAa03MblClN	$\text{ClNO}_3 + \text{Cl}^-(\text{a03}) \rightarrow \text{Cl}_2(\text{a03}) + \text{NO}_3^-(\text{a03})$	$k_{\text{exf_ClNO3}}(03) * 5.E2$	see general notes*
H8000f_a03	TrAa03ScI	$\text{I}_2 \rightarrow \text{I}_2(\text{a03})$	$k_{\text{exf}}(03, \text{ind_I2})$	see general notes*
H8000b_a03	TrAa03ScI	$\text{I}_2(\text{a03}) \rightarrow \text{I}_2$	$k_{\text{exb}}(03, \text{ind_I2})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H8100f_a03	TrAa03MblScI	$\text{IO} \rightarrow \text{IO}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_IO})$	see general notes*
H8100b_a03	TrAa03MblScI	$\text{IO}(\text{a03}) \rightarrow \text{IO}$	$k_{\text{exb}}(03, \text{ind_IO})$	see general notes*
H8101_a03	TrAa03I	$\text{OIO} \rightarrow \text{HOI}(\text{a03}) + \text{HO}_2(\text{a03})$	$k_{\text{exf}}(03, \text{ind_OIO})$	see general notes*
H8102_a03	TrAa03I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI}(\text{a03}) + \text{H}^+(\text{a03}) + \text{IO}_2^-(\text{a03})$	$k_{\text{exf}}(03, \text{ind_I2O2})$	see general notes*
H8200f_a03	TrAa03MblScI	$\text{HOI} \rightarrow \text{HOI}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_HOI})$	see general notes*
H8200b_a03	TrAa03MblScI	$\text{HOI}(\text{a03}) \rightarrow \text{HOI}$	$k_{\text{exb}}(03, \text{ind_HOI})$	see general notes*
H8201_a03	TrAa03MblScI	$\text{HI} \rightarrow \text{H}^+(\text{a03}) + \text{I}^-(\text{a03})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see general notes*
H8202_a03	TrAa03ScI	$\text{HIO}_3 \rightarrow \text{IO}_3^-(\text{a03}) + \text{H}^+(\text{a03})$	$k_{\text{mt}}(\text{HIO}_3) \cdot lwc$	see general notes*
H8300_a03	TrAa03IN	$\text{INO}_2 \rightarrow \text{HOI}(\text{a03}) + \text{HONO}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_INO2})$	see general notes*
H8301_a03	TrAa03MblIN	$\text{INO}_3 \rightarrow \text{HOI}(\text{a03}) + \text{HNO}_3(\text{a03})$	$k_{\text{exf}}(03, \text{ind_INO3})$	see general notes*
H8600f_a03	TrAa03MblScClI	$\text{ICl} \rightarrow \text{ICl}(\text{a03})$	$k_{\text{exf}}(03, \text{ind_ICl})$	see general notes*
H8600b_a03	TrAa03MblScClI	$\text{ICl}(\text{a03}) \rightarrow \text{ICl}$	$k_{\text{exb}}(03, \text{ind_ICl})$	see general notes*
H9100f_a03	TrAa03MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{a03})$	$\text{xnom7so2} * k_{\text{exf}}(03, \text{ind_SO2})$	see general notes*
H9100b_a03	TrAa03MblScScmS	$\text{SO}_2(\text{a03}) \rightarrow \text{SO}_2$	$\text{xnom7so2} * k_{\text{exb}}(03, \text{ind_SO2})$	see general notes*
H9200_a03	TrAa03MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{a03})$	$\text{xnom7sulf} * k_{\text{exf}}(03, \text{ind_H2SO4})$	see general notes*
H9400f_a03	TrAa03CS	$\text{DMSO} \rightarrow \text{DMSO}(\text{a03})$	$\text{xnom7dmsO} * k_{\text{exf}}(03, \text{ind_DMSO})$	see general notes*
H9400b_a03	TrAa03CS	$\text{DMSO}(\text{a03}) \rightarrow \text{DMSO}$	$\text{xnom7dmsO} * k_{\text{exb}}(03, \text{ind_DMSO})$	see general notes*
H9401_a03	TrAa03MblS	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{a03}) + \text{H}^+(\text{a03})$	$\text{xnom7dmsO} * k_{\text{exf}}(03, \text{ind_CH3SO3H})$	see general notes*
H9402f_a03	TrAa03CS	$\text{DMS} \rightarrow \text{DMS}(\text{a03})$	$\text{xnom7dmsO} * k_{\text{exf}}(03, \text{ind_DMS})$	see general notes*
H9402b_a03	TrAa03CS	$\text{DMS}(\text{a03}) \rightarrow \text{DMS}$	$\text{xnom7dmsO} * k_{\text{exb}}(03, \text{ind_DMS})$	see general notes*
H3103f_a03MK	TrAa03ScN	$\text{N}_2\text{O}_3 \rightarrow \text{N}_2\text{O}_3(\text{a03})$	$\text{xnom7nox} * k_{\text{exf}}(03, \text{ind_N2O3})$	Karl et al. (2012b)
H3103b_a03MK	TrAa03ScN	$\text{N}_2\text{O}_3(\text{a03}) \rightarrow \text{N}_2\text{O}_3$	$\text{xnom7nox} * k_{\text{exb}}(03, \text{ind_N2O3})$	Karl et al. (2012b)
H3104f_a03MK	TrAa03ScN	$\text{N}_2\text{O}_4 \rightarrow \text{N}_2\text{O}_4(\text{a03})$	$\text{xnom7nox} * k_{\text{exf}}(03, \text{ind_N2O4})$	Karl et al. (2012b)
H3104b_a03MK	TrAa03ScN	$\text{N}_2\text{O}_4(\text{a03}) \rightarrow \text{N}_2\text{O}_4$	$\text{xnom7nox} * k_{\text{exb}}(03, \text{ind_N2O4})$	Karl et al. (2012b)
H4106f_a03MK	TrAa03AmiScN	$\text{MMA} \rightarrow \text{MMA}(\text{a03})$	$\text{xnom7amin} * k_{\text{exf}}(03, \text{ind_MMA})$	Karl et al. (2012b)
H4106b_a03MK	TrAa03AmiScN	$\text{MMA}(\text{a03}) \rightarrow \text{MMA}$	$\text{xnom7amin} * k_{\text{exb}}(03, \text{ind_MMA})$	Karl et al. (2012b)
H4107f_a03MK	TrAa03AmiScN	$\text{MMNNO}_2 \rightarrow \text{MMNNO}_2(\text{a03})$	$\text{xnom7nno} * k_{\text{exf}}(03, \text{ind_MMNNO2})$	Karl et al. (2012b)
H4107b_a03MK	TrAa03AmiScN	$\text{MMNNO}_2(\text{a03}) \rightarrow \text{MMNNO}_2$	$\text{xnom7nno} * k_{\text{exb}}(03, \text{ind_MMNNO2})$	Karl et al. (2012b)
H4108f_a03MK	TrAa03AmiScN	$\text{HNCO} \rightarrow \text{HNCO}(\text{a03})$	$\text{xnom7amin} * k_{\text{exf}}(03, \text{ind_HNCO})$	Karl et al. (2012b)
H4108b_a03MK	TrAa03AmiScN	$\text{HNCO}(\text{a03}) \rightarrow \text{HNCO}$	$\text{xnom7amin} * k_{\text{exb}}(03, \text{ind_HNCO})$	Karl et al. (2012b)
H4109f_a03MK	TrAa03AmiScN	$\text{H}_2\text{NCHO} \rightarrow \text{H}_2\text{NCHO}(\text{a03})$	$\text{xnom7amin} * k_{\text{exf}}(03, \text{ind_H2NCHO})$	Karl et al. (2012b)
H4109b_a03MK	TrAa03AmiScN	$\text{H}_2\text{NCHO}(\text{a03}) \rightarrow \text{H}_2\text{NCHO}$	$\text{xnom7amin} * k_{\text{exb}}(03, \text{ind_H2NCHO})$	Karl et al. (2012b)
H4203f_a03MK	TrAa03ScC	$\text{HOCH}_2\text{CHO} \rightarrow \text{HOCH}_2\text{CHO}(\text{a03})$	$\text{xnom7co2} * k_{\text{exf}}(03, \text{ind_HOCH2CHO})$	Ervens et al. (2004)
H4203b_a03MK	TrAa03ScC	$\text{HOCH}_2\text{CHO}(\text{a03}) \rightarrow \text{HOCH}_2\text{CHO}$	$\text{xnom7co2} * k_{\text{exb}}(03, \text{ind_HOCH2CHO})$	Ervens et al. (2004)

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

#	labels	reaction	rate coefficient	reference
H4204f_a03MK	TrAa03ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOCH}_2\text{CO}_2\text{H(a03)}$	$\text{xnom7co2*k_exf(03,ind_HOCH}_2\text{CO}_2\text{H)}$	Ervens et al. (2004)
H4204b_a03MK	TrAa03ScC	$\text{HOCH}_2\text{CO}_2\text{H(a03)} \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$\text{xnom7co2*k_exb(03,ind_HOCH}_2\text{CO}_2\text{H)}$	Ervens et al. (2004)
H4205f_a03MK	TrAa03ScC	$\text{HCOCO}_2\text{H} \rightarrow \text{HCOCO}_2\text{H(a03)}$	$\text{xnom7co2*k_exf(03,ind_HCOCO}_2\text{H)}$	Ervens et al. (2004)
H4205b_a03MK	TrAa03ScC	$\text{HCOCO}_2\text{H(a03)} \rightarrow \text{HCOCO}_2\text{H}$	$\text{xnom7co2*k_exb(03,ind_HCOCO}_2\text{H)}$	Ervens et al. (2004)
H4206f_a03MK	TrAa03ScC	$\text{GLYOX} \rightarrow \text{GLYOX(a03)}$	$\text{xnom7co2*k_exf(03,ind_GLYOX)}$	Ervens et al. (2004)
H4206b_a03MK	TrAa03ScC	$\text{GLYOX(a03)} \rightarrow \text{GLYOX}$	$\text{xnom7co2*k_exb(03,ind_GLYOX)}$	Ervens et al. (2004)
H4207f_a03MK	TrAa03AmiScCN	$\text{DMA} \rightarrow \text{DMA(a03)}$	$\text{xnom7amin*k_exf(03,ind_DMA)}$	Karl et al. (2012b)
H4207b_a03MK	TrAa03AmiScCN	$\text{DMA(a03)} \rightarrow \text{DMA}$	$\text{xnom7amin*k_exb(03,ind_DMA)}$	Karl et al. (2012b)
H4208f_a03MK	TrAa03AmiScCN	$\text{MEA} \rightarrow \text{MEA(a03)}$	$\text{xnom7amin*k_exf(03,ind_MEA)}$	Karl et al. (2012b)
H4208b_a03MK	TrAa03AmiScCN	$\text{MEA(a03)} \rightarrow \text{MEA}$	$\text{xnom7amin*k_exb(03,ind_MEA)}$	Karl et al. (2012b)
H4209f_a03MK	TrAa03AmiScCN	$\text{MEANNO} \rightarrow \text{MEANNO(a03)}$	$\text{xnom7nno*k_exf(03,ind_MEANNO)}$	Karl et al. (2012b)
H4209b_a03MK	TrAa03AmiScCN	$\text{MEANNO(a03)} \rightarrow \text{MEANNO}$	$\text{xnom7nno*k_exb(03,ind_MEANNO)}$	Karl et al. (2012b)
H4210f_a03MK	TrAa03AmiScCN	$\text{MEANNO}_2 \rightarrow \text{MEANNO}_2\text{(a03)}$	$\text{xnom7nno*k_exf(03,ind_MEANNO}_2\text{)}$	Karl et al. (2012b)
H4210b_a03MK	TrAa03AmiScCN	$\text{MEANNO}_2\text{(a03)} \rightarrow \text{MEANNO}_2$	$\text{xnom7nno*k_exb(03,ind_MEANNO}_2\text{)}$	Karl et al. (2012b)
H4211f_a03MK	TrAa03AmiScCN	$\text{NDMA} \rightarrow \text{NDMA(a03)}$	$\text{xnom7nno*k_exf(03,ind_NDMA)}$	Karl et al. (2012b)
H4211b_a03MK	TrAa03AmiScCN	$\text{NDMA(a03)} \rightarrow \text{NDMA}$	$\text{xnom7nno*k_exb(03,ind_NDMA)}$	Karl et al. (2012b)
H4212f_a03MK	TrAa03AmiScCN	$\text{DMNNO}_2 \rightarrow \text{DMNNO}_2\text{(a03)}$	$\text{xnom7nno*k_exf(03,ind_DMNNO}_2\text{)}$	Karl et al. (2012b)
H4212b_a03MK	TrAa03AmiScCN	$\text{DMNNO}_2\text{(a03)} \rightarrow \text{DMNNO}_2$	$\text{xnom7nno*k_exb(03,ind_DMNNO}_2\text{)}$	Karl et al. (2012b)
H4213f_a03MK	TrAa03AmiScCN	$\text{H}_2\text{NCOCH}_2\text{OH} \rightarrow \text{H}_2\text{NCOCH}_2\text{OH(a03)}$	$\text{xnom7amin*k_exf(03,ind_H}_2\text{NCOCH}_2\text{OH)}$	Karl et al. (2012b)
H4213b_a03MK	TrAa03AmiScCN	$\text{H}_2\text{NCOCH}_2\text{OH(a03)} \rightarrow \text{H}_2\text{NCOCH}_2\text{OH}$	$\text{xnom7amin*k_exb(03,ind_H}_2\text{NCOCH}_2\text{OH)}$	Karl et al. (2012b)
H4214f_a03MK	TrAa03AmiScCN	$\text{CH}_3\text{NHCHO} \rightarrow \text{CH}_3\text{NHCHO(a03)}$	$\text{xnom7amin*k_exf(03,ind_CH}_3\text{NHCHO)}$	Karl et al. (2012b)
H4214b_a03MK	TrAa03AmiScCN	$\text{CH}_3\text{NHCHO(a03)} \rightarrow \text{CH}_3\text{NHCHO}$	$\text{xnom7amin*k_exb(03,ind_CH}_3\text{NHCHO)}$	Karl et al. (2012b)
H4301f_a03MK	TrAa03ScC	$\text{MGLYOX} \rightarrow \text{MGLYOX(a03)}$	$\text{xnom7co2*k_exf(03,ind_MGLYOX)}$	Ervens et al. (2004)
H4301b_a03MK	TrAa03ScC	$\text{MGLYOX(a03)} \rightarrow \text{MGLYOX}$	$\text{xnom7co2*k_exb(03,ind_MGLYOX)}$	Ervens et al. (2004)
H4302f_a03MK	TrAa03ScC	$\text{MGLYOAC} \rightarrow \text{MGLYOAC(a03)}$	$\text{xnom7co2*k_exf(03,ind_MGLYOAC)}$	Ervens et al. (2004)
H4302b_a03MK	TrAa03ScC	$\text{MGLYOAC(a03)} \rightarrow \text{MGLYOAC}$	$\text{xnom7co2*k_exb(03,ind_MGLYOAC)}$	Ervens et al. (2004)
H4303f_a03MK	TrAa03AmiScCN	$\text{TMA} \rightarrow \text{TMA(a03)}$	$\text{xnom7amin*k_exf(03,ind_TMA)}$	Karl et al. (2012b)
H4303b_a03MK	TrAa03AmiScCN	$\text{TMA(a03)} \rightarrow \text{TMA}$	$\text{xnom7amin*k_exb(03,ind_TMA)}$	Karl et al. (2012b)
H4304f_a03MK	TrAa03AmiScCN	$\text{DMNCHO} \rightarrow \text{DMNCHO(a03)}$	$\text{xnom7amin*k_exf(03,ind_DMNCHO)}$	Karl et al. (2012b)
H4304b_a03MK	TrAa03AmiScCN	$\text{DMNCHO(a03)} \rightarrow \text{DMNCHO}$	$\text{xnom7amin*k_exb(03,ind_DMNCHO)}$	Karl et al. (2012b)
H4400f_a03MK	TrAa03AmiScCN	$\text{DEA} \rightarrow \text{DEA(a03)}$	$\text{xnom7amin*k_exf(03,ind_DEA)}$	Karl et al. (2012b)
H4400b_a03MK	TrAa03AmiScCN	$\text{DEA(a03)} \rightarrow \text{DEA}$	$\text{xnom7amin*k_exb(03,ind_DEA)}$	Karl et al. (2012b)
H4401f_a03MK	TrAa03AmiScCN	$\text{NDELA} \rightarrow \text{NDELA(a03)}$	$\text{xnom7nno*k_exf(03,ind_NDELA)}$	Karl et al. (2012b)

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

#	labels	reaction	rate coefficient	reference
H4401b_a03MK	TrAa03AmiScCN	NDELA(a03) \rightarrow NDELA	xnom7nno*k_exb(03,ind_NDELA)	Karl et al. (2012b)
H4402f_a03MK	TrAa03AmiScCN	DEANNO2 \rightarrow DEANNO2(a03)	xnom7nno*k_exf(03,ind_DEANNO2)	Karl et al. (2012b)
H4402b_a03MK	TrAa03AmiScCN	DEANNO2(a03) \rightarrow DEANNO2	xnom7nno*k_exb(03,ind_DEANNO2)	Karl et al. (2012b)
H4403f_a03MK	TrAa03Sc	BSOV \rightarrow SUCCAC(a03)	xnom7co2*k_exf(03,ind_BSOV)	Ervens et al. (2004)
H4403b_a03MK	TrAa03Sc	SUCCAC(a03) \rightarrow BSOV	xnom7co2*k_exb(03,ind_BSOV)	Ervens et al. (2004)
H4600f_a03MK	TrAa03AmiScCN	TEA \rightarrow TEA(a03)	xnom7amin*k_exf(03,ind_TEA)	Karl et al. (2012b)
H4600b_a03MK	TrAa03AmiScCN	TEA(a03) \rightarrow TEA	xnom7amin*k_exb(03,ind_TEA)	Karl et al. (2012b)
H4601f_a03MK	TrAa03Sc	BLOV \rightarrow ADIPAC(a03)	xnom7co2*k_exf(03,ind_BLOV)	Ervens et al. (2004)
H4601b_a03MK	TrAa03Sc	ADIPAC(a03) \rightarrow BLOV	xnom7co2*k_exb(03,ind_BLOV)	Ervens et al. (2004)
H9403f_a03MK	TrAa03S	CH ₃ SOOH \rightarrow MSIA(a03)	xnom7dmsa*k_exf(03,ind_CH3SOOH)	Hoffmann et al. (2016)
H9403b_a03MK	TrAa03S	MSIA(a03) \rightarrow CH ₃ SOOH	xnom7dmsa*k_exb(03,ind_CH3SOOH)	Hoffmann et al. (2016)
H9404f_a03MK	TrAa03CS	HPMTF \rightarrow HPMTF(a03)	xnom7dmsa*k_exf(03,ind_HPMTF)	Wollesen de Jonge et al. (2021)
H9404b_a03MK	TrAa03CS	HPMTF(a03) \rightarrow HPMTF	xnom7dmsa*k_exb(03,ind_HPMTF)	Wollesen de Jonge et al. (2021)
H9405f_a03MK	TrAa03CS	HOOCH ₂ SCO \rightarrow HOOCH ₂ SCO(a03)	xnom7dmsa*k_exf(03,ind_	Wollesen de Jonge et al. (2021)
			HOOCH ₂ SCO)	
H9405b_a03MK	TrAa03CS	HOOCH ₂ SCO(a03) \rightarrow HOOCH ₂ SCO	xnom7dmsa*k_exb(03,ind_	Wollesen de Jonge et al. (2021)
			HOOCH ₂ SCO)	

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
---	--------	----------	------------------	-----------

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
EQ20_a01	TrAa01Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
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)
EQ31_a01	TrAa01ScN	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a01	TrAa01MblScScmN	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a01	TrAa01ScN	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ40_a01	TrAa01MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a01	TrAa01ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ60_a01	TrAa01Cl	$\text{Cl}_2 \rightleftharpoons \text{Cl} + \text{Cl}^-$	7.3E-6		Yu (2004)
EQ61_a01	TrAa01MblScScmCl	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a01	TrAa01ScCl	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ80_a01	TrAa01MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
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)
EQ110_a01	TrAa01Fe	$\text{Fe}^{3+} \rightleftharpoons \text{FeOH}^{2+} + \text{H}^+$	2.34E-3		de Laat and Le (2006)*
EQ111_a01	TrAa01Fe	$\text{FeOH}^{2+} \rightleftharpoons \text{Fe}(\text{OH})_2^+ + \text{H}^+$	2E-4		de Laat and Le (2006)*
EQ112_a01	TrAa01Fe	$\text{Fe}^{3+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{FeHO}_2^{2+} + \text{H}^+$	3.1E-3		de Laat and Le (2006)
EQ113_a01	TrAa01Fe	$\text{FeOH}^{2+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{Fe}(\text{OH})(\text{HO}_2)^+ + \text{H}^+$	2E-4		de Laat and Le (2006)
EQ114_a01	TrAa01ClFe	$\text{Fe}^{3+} + \text{Cl}^- \rightleftharpoons \text{FeCl}^{2+}$	6.61		de Laat and Le (2006)*
EQ115_a01	TrAa01ClFe	$\text{FeCl}^{2+} + \text{Cl}^- \rightleftharpoons \text{FeCl}_2^+$	1.6		de Laat and Le (2006)*
EQ116_a01	TrAa01FeS	$\text{Fe}^{3+} + \text{SO}_4^{2-} \rightleftharpoons \text{FeSO}_4^+$	120		Brand and van Eldik (1995)*
EQ117_a01	TrAa01FeS	$\text{FeOH}^{2+} + \text{HSO}_3^- \rightleftharpoons \text{FeSO}_3^+$	8.25E2		Warneck (2018)*
EQ118_a01	TrAa01FeS	$\text{Fe}^{2+} + \text{SO}_3^- \rightleftharpoons \text{FeSO}_3^+$	1.6E7		Warneck (2018)
EQ43_a01MK	TrAa01ScC	$\text{HCOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{HCOCOO}^-$	6.6E-4		Ervens et al. (2004)
EQ44_a01MK	TrAa01ScC	$\text{MGLYOAC} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COCOO}^-$	4.07E-3		Ervens et al. (2004)
EQ45_a01MK	TrAa01Sc	$\text{OXALAC} \rightleftharpoons \text{H}^+ + \text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)
EQ46_a01MK	TrAa01Sc	$\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ47_a01MK	TrAa01Sc	$\text{SUCCAC} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)
EQ48_a01MK	TrAa01Sc	$\text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ120_a01MK	TrAa01AmiScN	$\text{MMA}^+ \rightleftharpoons \text{H}^+ + \text{MMA}$	2.19E-11		Ge et al. (2011)
EQ121_a01MK	TrAa01AmiScCN	$\text{DMA}^+ \rightleftharpoons \text{H}^+ + \text{DMA}$	1.86E-11		Ge et al. (2011)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ122_a01MK	TrAa01AmiScCN	$\text{TMA}^+ \rightleftharpoons \text{H}^+ + \text{TMA}$	1.74E-10		Das and von Sonntag (1986)
EQ123_a01MK	TrAa01AmiScCN	$\text{MEA}^+ \rightleftharpoons \text{H}^+ + \text{MEA}$	3.98E-10		Kishore et al. (2004)
EQ124_a01MK	TrAa01AmiScCN	$\text{DEA}^+ \rightleftharpoons \text{H}^+ + \text{DEA}$	1.17E-9		Kishore et al. (2004)
EQ125_a01MK	TrAa01AmiScCN	$\text{TEA}^+ \rightleftharpoons \text{H}^+ + \text{TEA}$	1.66E-8		Kishore et al. (2004)
EQ126_a01MK	TrAa01AmiScCN	$(\text{CH}_3)_2\text{NH}^+\text{CH}_2 \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ127_a01MK	TrAa01AmiScCN	$(\text{CH}_3)_3\text{N}^+ \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ128_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NH}_2^+\text{CH}_2 \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ129_a01MK	TrAa01AmiScCN	$(\text{CH}_3)_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ130_a01MK	TrAa01AmiScN	$\text{CH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	4.00E3		Das and von Sonntag (1986)
EQ131_a01MK	TrAa01AmiScN	$\text{CH}_3\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	5.71E7		Das and von Sonntag (1986)
EQ132_a01MK	TrAa01AmiScCN	$\text{HOCHCH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ133_a01MK	TrAa01AmiScCN	$\text{HOCH}_2\text{CH}_2\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ134_a01MK	TrAa01AmiScCN	$\text{HOETNH}_2\text{CH}_2\text{CHOH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ135_a01MK	TrAa01AmiScCN	$(\text{HOET})_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ136_a01MK	TrAa01AmiScCN	$(\text{HOET})_2\text{NH}^+\text{CH}_2\text{CHOH} \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ137_a01MK	TrAa01AmiScCN	$(\text{HOET})_3\text{N}^+ \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ138_a01MK	TrAa01AmiScN	$\text{HNCO} \rightleftharpoons \text{H}^+ + \text{NCO}^-$	2.0E-4		Roberts et al. (2011)
EQ20_a02	TrAa02Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a02	TrAa02MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a02	TrAa02MblScScmN	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ31_a02	TrAa02ScN	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a02	TrAa02MblScScmN	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a02	TrAa02ScN	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ40_a02	TrAa02MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a02	TrAa02ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ60_a02	TrAa02Cl	$\text{Cl}_2 \rightleftharpoons \text{Cl} + \text{Cl}^-$	7.3E-6		Yu (2004)
EQ61_a02	TrAa02MblScScmCl	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a02	TrAa02ScCl	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ80_a02	TrAa02MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ90_a02	TrAa02MblScScmS	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a02	TrAa02MblScScmS	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a02	TrAa02MblScScmS	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ93_a02	TrAa02MblScScmS	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ110_a02	TrAa02Fe	$\text{Fe}^{3+} \rightleftharpoons \text{FeOH}^{2+} + \text{H}^+$	2.34E-3		de Laat and Le (2006)*
EQ111_a02	TrAa02Fe	$\text{FeOH}^{2+} \rightleftharpoons \text{Fe}(\text{OH})_2^+ + \text{H}^+$	2E-4		de Laat and Le (2006)*
EQ112_a02	TrAa02Fe	$\text{Fe}^{3+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{FeHO}_2^{2+} + \text{H}^+$	3.1E-3		de Laat and Le (2006)
EQ113_a02	TrAa02Fe	$\text{FeOH}^{2+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{Fe}(\text{OH})(\text{HO}_2)^+ + \text{H}^+$	2E-4		de Laat and Le (2006)
EQ114_a02	TrAa02ClFe	$\text{Fe}^{3+} + \text{Cl}^- \rightleftharpoons \text{FeCl}^{2+}$	6.61		de Laat and Le (2006)*
EQ115_a02	TrAa02ClFe	$\text{FeCl}^{2+} + \text{Cl}^- \rightleftharpoons \text{FeCl}_2^+$	1.6		de Laat and Le (2006)*
EQ116_a02	TrAa02FeS	$\text{Fe}^{3+} + \text{SO}_4^{2-} \rightleftharpoons \text{FeSO}_4^+$	120		Brand and van Eldik (1995)*
EQ117_a02	TrAa02FeS	$\text{FeOH}^{2+} + \text{HSO}_3^- \rightleftharpoons \text{FeSO}_3^+$	8.25E2		Warneck (2018)*
EQ118_a02	TrAa02FeS	$\text{Fe}^{2+} + \text{SO}_3^- \rightleftharpoons \text{FeSO}_3^+$	1.6E7		Warneck (2018)
EQ43_a02MK	TrAa02ScC	$\text{HCOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{HCOCOO}^-$	6.6E-4		Ervens et al. (2004)
EQ44_a02MK	TrAa02ScC	$\text{MGLYOAC} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COCOO}^-$	4.07E-3		Ervens et al. (2004)
EQ45_a02MK	TrAa02Sc	$\text{OXALAC} \rightleftharpoons \text{H}^+ + \text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)
EQ46_a02MK	TrAa02Sc	$\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ47_a02MK	TrAa02Sc	$\text{SUCCAC} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)
EQ48_a02MK	TrAa02Sc	$\text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ120_a02MK	TrAa02AmiScN	$\text{MMA}^+ \rightleftharpoons \text{H}^+ + \text{MMA}$	2.19E-11		Ge et al. (2011)
EQ121_a02MK	TrAa02AmiScCN	$\text{DMA}^+ \rightleftharpoons \text{H}^+ + \text{DMA}$	1.86E-11		Ge et al. (2011)
EQ122_a02MK	TrAa02AmiScCN	$\text{TMA}^+ \rightleftharpoons \text{H}^+ + \text{TMA}$	1.74E-10		Das and von Sonntag (1986)
EQ123_a02MK	TrAa02AmiScCN	$\text{MEA}^+ \rightleftharpoons \text{H}^+ + \text{MEA}$	3.98E-10		Kishore et al. (2004)
EQ124_a02MK	TrAa02AmiScCN	$\text{DEA}^+ \rightleftharpoons \text{H}^+ + \text{DEA}$	1.17E-9		Kishore et al. (2004)
EQ125_a02MK	TrAa02AmiScCN	$\text{TEA}^+ \rightleftharpoons \text{H}^+ + \text{TEA}$	1.66E-8		Kishore et al. (2004)
EQ126_a02MK	TrAa02AmiScCN	$(\text{CH}_3)_2\text{NH}^+\text{CH}_2 \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ127_a02MK	TrAa02AmiScCN	$(\text{CH}_3)_3\text{N}^+ \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ128_a02MK	TrAa02AmiScCN	$\text{CH}_3\text{NH}_2^+\text{CH}_2 \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ129_a02MK	TrAa02AmiScCN	$(\text{CH}_3)_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ130_a02MK	TrAa02AmiScN	$\text{CH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	4.00E3		Das and von Sonntag (1986)
EQ131_a02MK	TrAa02AmiScN	$\text{CH}_3\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	5.71E7		Das and von Sonntag (1986)
EQ132_a02MK	TrAa02AmiScCN	$\text{HOCHCH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ133_a02MK	TrAa02AmiScCN	$\text{HOCH}_2\text{CH}_2\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ134_a02MK	TrAa02AmiScCN	$\text{HOETNH}_2\text{CH}_2\text{CHOH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ135_a02MK	TrAa02AmiScCN	$(\text{HOET})_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ136_a02MK	TrAa02AmiScCN	$(\text{HOET})_2\text{NH}^+\text{CH}_2\text{CHOH} \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ137_a02MK	TrAa02AmiScCN	$(\text{HOET})_3\text{N}^+ \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ138_a02MK	TrAa02AmiScN	$\text{HNCO} \rightleftharpoons \text{H}^+ + \text{NCO}^-$	2.0E-4		Roberts et al. (2011)
EQ20_a03	TrAa03Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a03	TrAa03MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a03	TrAa03MblScScmN	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ31_a03	TrAa03ScN	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a03	TrAa03MblScScmN	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a03	TrAa03ScN	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ40_a03	TrAa03MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a03	TrAa03ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ60_a03	TrAa03Cl	$\text{Cl}_2^- \rightleftharpoons \text{Cl} + \text{Cl}^-$	7.3E-6		Yu (2004)
EQ61_a03	TrAa03MblScScmCl	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a03	TrAa03ScCl	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ80_a03	TrAa03MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ90_a03	TrAa03MblScScmS	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a03	TrAa03MblScScmS	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a03	TrAa03MblScScmS	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a03	TrAa03MblScScmS	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ110_a03	TrAa03Fe	$\text{Fe}^{3+} \rightleftharpoons \text{FeOH}^{2+} + \text{H}^+$	2.34E-3		de Laat and Le (2006)*
EQ111_a03	TrAa03Fe	$\text{FeOH}^{2+} \rightleftharpoons \text{Fe}(\text{OH})_2^+ + \text{H}^+$	2E-4		de Laat and Le (2006)*
EQ112_a03	TrAa03Fe	$\text{Fe}^{3+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{FeHO}_2^{2+} + \text{H}^+$	3.1E-3		de Laat and Le (2006)
EQ113_a03	TrAa03Fe	$\text{FeOH}^{2+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{Fe}(\text{OH})(\text{HO}_2)^+ + \text{H}^+$	2E-4		de Laat and Le (2006)
EQ114_a03	TrAa03ClFe	$\text{Fe}^{3+} + \text{Cl}^- \rightleftharpoons \text{FeCl}^{2+}$	6.61		de Laat and Le (2006)*
EQ115_a03	TrAa03ClFe	$\text{FeCl}^{2+} + \text{Cl}^- \rightleftharpoons \text{FeCl}_2^+$	1.6		de Laat and Le (2006)*
EQ116_a03	TrAa03FeS	$\text{Fe}^{3+} + \text{SO}_4^{2-} \rightleftharpoons \text{FeSO}_4^+$	120		Brand and van Eldik (1995)*
EQ117_a03	TrAa03FeS	$\text{FeOH}^{2+} + \text{HSO}_3^- \rightleftharpoons \text{FeSO}_3^+$	8.25E2		Warneck (2018)*
EQ118_a03	TrAa03FeS	$\text{Fe}^{2+} + \text{SO}_3^- \rightleftharpoons \text{FeSO}_3^+$	1.6E7		Warneck (2018)
EQ43_a03MK	TrAa03ScC	$\text{HCOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{HCOCOO}^-$	6.6E-4		Ervens et al. (2004)
EQ44_a03MK	TrAa03ScC	$\text{MGLYOAC} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COCOO}^-$	4.07E-3		Ervens et al. (2004)
EQ45_a03MK	TrAa03Sc	$\text{OXALAC} \rightleftharpoons \text{H}^+ + \text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)
EQ46_a03MK	TrAa03Sc	$\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ47_a03MK	TrAa03Sc	$\text{SUCCAC} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^-$	6.4E-2		Ervens et al. (2004)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ48_a03MK	TrAa03Sc	$\text{CH}_2\text{CH}_2\text{HC}_2\text{O}_4^- \rightleftharpoons \text{H}^+ + \text{CH}_2\text{CH}_2\text{C}_2\text{O}_4^{2-}$	5.25E-5		Ervens et al. (2004)
EQ120_a03MK	TrAa03AmiScN	$\text{MMA}^+ \rightleftharpoons \text{H}^+ + \text{MMA}$	2.19E-11		Ge et al. (2011)
EQ121_a03MK	TrAa03AmiScCN	$\text{DMA}^+ \rightleftharpoons \text{H}^+ + \text{DMA}$	1.86E-11		Ge et al. (2011)
EQ122_a03MK	TrAa03AmiScCN	$\text{TMA}^+ \rightleftharpoons \text{H}^+ + \text{TMA}$	1.74E-10		Das and von Sonntag (1986)
EQ123_a03MK	TrAa03AmiScCN	$\text{MEA}^+ \rightleftharpoons \text{H}^+ + \text{MEA}$	3.98E-10		Kishore et al. (2004)
EQ124_a03MK	TrAa03AmiScCN	$\text{DEA}^+ \rightleftharpoons \text{H}^+ + \text{DEA}$	1.17E-9		Kishore et al. (2004)
EQ125_a03MK	TrAa03AmiScCN	$\text{TEA}^+ \rightleftharpoons \text{H}^+ + \text{TEA}$	1.66E-8		Kishore et al. (2004)
EQ126_a03MK	TrAa03AmiScCN	$(\text{CH}_3)_2\text{NH}^+\text{CH}_2 \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ127_a03MK	TrAa03AmiScCN	$(\text{CH}_3)_3\text{N}^+ \rightleftharpoons \text{H}^+ + (\text{CH}_3)_2\text{NCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ128_a03MK	TrAa03AmiScCN	$\text{CH}_3\text{NH}_2^+\text{CH}_2 \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	4.00E3		Das and von Sonntag (1986)
EQ129_a03MK	TrAa03AmiScCN	$(\text{CH}_3)_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{CH}_3\text{NHCH}_2$	5.71E7		Das and von Sonntag (1986)
EQ130_a03MK	TrAa03AmiScN	$\text{CH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	4.00E3		Das and von Sonntag (1986)
EQ131_a03MK	TrAa03AmiScN	$\text{CH}_3\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{CH}_2\text{NH}_2$	5.71E7		Das and von Sonntag (1986)
EQ132_a03MK	TrAa03AmiScCN	$\text{HOCHCH}_2\text{NH}_3^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ133_a03MK	TrAa03AmiScCN	$\text{HOCH}_2\text{CH}_2\text{NH}_2^+ \rightleftharpoons \text{H}^+ + \text{NH}_2\text{CH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ134_a03MK	TrAa03AmiScCN	$\text{HOETNH}_2\text{CH}_2\text{CHOH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ135_a03MK	TrAa03AmiScCN	$(\text{HOET})_2\text{NH}^+ \rightleftharpoons \text{H}^+ + \text{HOETNHCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ136_a03MK	TrAa03AmiScCN	$(\text{HOET})_2\text{NH}^+\text{CH}_2\text{CHOH} \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	4.00E3		Das and von Sonntag (1986)
EQ137_a03MK	TrAa03AmiScCN	$(\text{HOET})_3\text{N}^+ \rightleftharpoons \text{H}^+ + \text{DENCH}_2\text{CHOH}$	5.71E7		Das and von Sonntag (1986)
EQ138_a03MK	TrAa03AmiScN	$\text{HNCO} \rightleftharpoons \text{H}^+ + \text{NCO}^-$	2.0E-4		Roberts et al. (2011)

Specific notes

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

EQ110_a01: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ111_a01: Equilibrium calculated from K_1 and K_2 in Tab. 1 of de Laat and Le (2006). Rate constant for back reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ114_a01: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ115_a01: Equilibrium calculated from K_{29} and K_{30} in Tab. 2 of de Laat and Le (2006). Rate constant for forward reaction assumed. See also K values listed in

Tab. 2.5 of Brand and van Eldik (1995).

EQ116_a01: Equilibrium at $I = 1$ M. Rate constant for back reaction assumed.

EQ117_a01: Rate of equilibration assumed.

EQ40_a02: For $pK_a(\text{CO}_2)$, see also Dickson and Millero (1987).

EQ110_a02: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ111_a02: Equilibrium calculated from K_1 and K_2 in Tab. 1 of de Laat and Le (2006). Rate constant for back reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ114_a02: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ115_a02: Equilibrium calculated from K_{29} and K_{30} in Tab. 2 of de Laat and Le (2006). Rate constant for forward reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ116_a02: Equilibrium at $I = 1$ M. Rate constant for back reaction assumed.

EQ117_a02: Rate of equilibration assumed.

EQ40_a03: For $pK_a(\text{CO}_2)$, see also Dickson and Millero (1987).

EQ110_a03: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ111_a03: Equilibrium calculated from K_1 and K_2 in Tab. 1 of de Laat and Le (2006). Rate constant for back reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ114_a03: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ115_a03: Equilibrium calculated from K_{29} and K_{30} in Tab. 2 of de Laat and Le (2006). Rate constant for forward reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ116_a03: Equilibrium at $I = 1$ M. Rate constant for back reaction assumed.

EQ117_a03: Rate of equilibration assumed.

Table 6: Aqueous phase reactions

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A1000_a01	TrAa01Sc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9		Sehested et al. (1983)
A2100_a01	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A2101_a01	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A2102_a01	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A2103_a01	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A2104_a01	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A2105_a01	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A3100_a01	TrAa01ScN	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A3101_a01	TrAa01ScN	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A3102_a01	TrAa01ScN	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A3200_a01	TrAa01ScN	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A3201_a01	TrAa01ScN	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A3202_a01	TrAa01ScN	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A3203_a01	TrAa01ScN	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A3204_a01	TrAa01ScN	$HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$	4.6E3	-6800	Damschen and Martin (1983)
A4100_a01	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A4101_a01	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A4102_a01	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2 HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A4103_a01	TrAa01Sc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A4104_a01	TrAa01Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A4105_a01	TrAa01Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A4106_a01	TrAa01Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A4107_a01	TrAa01Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A4108_a01	TrAa01Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A4109_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8		Buxton et al. (1988)
A4110a_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715	Jacob (1986)
A4110b_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715	Jacob (1986)
A6000_a01	TrAa01Cl	$Cl + Cl \rightarrow Cl_2$	8.8E7		Wu et al. (1980)
A6001_a01	TrAa01Cl	$Cl_2^- + Cl_2^- \rightarrow Cl_2 + 2 Cl^-$	3.5E9		Yu (2004)
A6100_a01	TrAa01Cl	$Cl^- + O_3 \rightarrow ClO^-$	3.0E-3		Hoigné et al. (1985)
A6101_a01	TrAa01Cl	$Cl_2 + O_2^- \rightarrow Cl_2^-$	1.0E9		Bjergbakke et al. (1981)
A6102_a01	TrAa01Cl	$Cl_2^- + O_2^- \rightarrow 2 Cl^-$	1.0E9		Jacobi (1996)*
A6200_a01	TrAa01Cl	$Cl \rightarrow H^+ + ClOH^-$	1.8E5		Yu (2004)
A6201_a01	TrAa01Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A6202_a01	TrAa01Cl	$Cl^- + OH^- \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a01	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a01	TrAa01MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a01	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a01	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a01	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a01	TrAa01MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a01	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH^-$	6.0E9		Yu (2004)
A6210_a01	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a01	TrAa01ClN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a01	TrAa01ClN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a01	TrAa01ClN	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a01	TrAa01Cl	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
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)
A8201_a01	TrAa01I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
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	TrAa01MblClII	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601_a01	TrAa01MblClII	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8602_a01	TrAa01ClII	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A8603_a01	TrAa01MblClII	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8604_a01	TrAa01ClII	$HOI + Cl_2 \rightarrow IO_2^- + 2 Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A8605_a01	TrAa01ClII	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2 H^+$	5.0E5		Citri and Epstein (1988)
A8606_a01	TrAa01ClII	$ICl + I^- \rightarrow I_2 + Cl^-$	1.1E9		Margerum et al. (1986)
A9100_a01	TrAa01ScS	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101_a01	TrAa01MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a01	TrAa01ScS	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a01	TrAa01ScS	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a01	TrAa01ScS	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105_a01	TrAa01S	$SO_5^- + SO_3^{2-} \rightarrow .72 SO_4^- + .72 SO_4^{2-} + .28 SO_3^- + .28 HSO_5^- + .28 OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A9106_a01	TrAa01S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + LSULFUR$	1.0E8		Ross et al. (1992)*

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9200_a01	TrAa01ScS	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201_a01	TrAa01ScS	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202_a01	TrAa01ScS	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203_a01	TrAa01ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a01	TrAa01ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205_a01	TrAa01ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note*
A9206_a01	TrAa01MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a01	TrAa01ScS	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208_a01	TrAa01ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note*
A9209_a01	TrAa01MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a01	TrAa01ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211_a01	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75 SO_4^- + .75 SO_4^{2-} + .75 H^+ + .25 SO_3^- + .25 HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212_a01	TrAa01ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2 HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A9301_a01	TrAa01ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302_a01	TrAa01ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Løgager et al. (1993)
A9304_a01	TrAa01ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a01	TrAa01ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400_a01	TrAa01ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OH SO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)*
A9401_a01	TrAa01ScS	$SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402_a01	TrAa01ScS	$HSO_3^- + HCHO \rightarrow CH_2OH SO_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A9403_a01	TrAa01ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404_a01	TrAa01ScS	$CH_2OH SO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600_a01	TrAa01ClS	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2 Cl^-$	6.2E7		Jacobi et al. (1996)
A9601_a01	TrAa01MblClS	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a01	TrAa01ClS	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603_a01	TrAa01ClS	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604_a01	TrAa01ClS	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2 Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a01	TrAa01MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A9606_a01	TrAa01ClS	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9800_a01	TrAa01IS	$HSO_3^- + I_2 \rightarrow 2 I^- + HSO_4^- + 2 H^+$	1.7E9		Yiin and Margerum (1990)
A11101_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11102_a01	TrAa01Fe	$Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$	5E7		de Laat and Le (2006)
A11103_a01	TrAa01Fe	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	8.2E5		Løgager et al. (1992)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A11201a_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$	2.7E8		de Laat and Le (2006)
A11201b_a01	TrAa01Fe	$FeOH^+ + OH \rightarrow Fe^{3+} + 2 OH^-$	2.7E8		de Laat and Le (2006)
A11202a_a01	TrAa01Fe	$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$	5.5E1		de Laat and Le (2006)
A11202b_a01	TrAa01Fe	$FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2 OH^-$	5.9E6		de Laat and Le (2006)
A11203_a01	TrAa01Fe	$FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$	2.3E-3		de Laat and Le (2006)
A11204_a01	TrAa01Fe	$Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$	2.3E-3		de Laat and Le (2006)
A11206_a01	TrAa01Fe	$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO_2^-$	1.2E6		de Laat and Le (2006)
A11208a_a01	TrAa01Fe	$FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$	1.5E8		Rush and Bielski (1985)
A11208b_a01	TrAa01Fe	$Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2 OH^-$	1.5E8		Rush and Bielski (1985)
A11209_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2 OH^-$	1.0E7		Rush and Bielski (1985)
A11210_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow FeOH^{2+}$	4.3E8		Christensen and Sehested (1981)
A11211_a01	TrAa01Fe	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	9.5E3		Løgager et al. (1992)
A11212_a01	TrAa01Fe	$FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$	1.3E-2		Løgager et al. (1992)
A11213_a01	TrAa01Fe	$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	2.0E6		Løgager et al. (1992)
A11214_a01	TrAa01Fe	$FeO^{2+} + OH \rightarrow Fe^{3+} + HO_2^-$	1.0E7		Løgager et al. (1992)
A11215_a01	TrAa01Fe	$FeO^{2+} + Fe^{2+} \rightarrow 2 Fe^{3+} + 2 OH^-$	1.4E5		Løgager et al. (1992)
A11216_a01	TrAa01Fe	$FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+}$	1.8E4		Jacobsen et al. (1997)
A11217_a01	TrAa01Fe	$Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2 Fe^{3+} + OH^-$	2.0		Jacobsen et al. (1997)
A11218_a01	TrAa01Fe	$Fe(OH)_2Fe^{4+} \rightarrow 2 Fe^{3+} + 2 OH^-$	0.49		Jacobsen et al. (1997)
A11301_a01	TrAa01FeN	$FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$	1.1E4		Jacobsen et al. (1998)
A11302_a01	TrAa01FeN	$Fe^{2+} + NO_3 \rightarrow Fe^{3+} + NO_3^-$	8.0E6		Herrmann et al. (2000)*
A11601_a01	TrAa01ClFe	$Fe^{2+} + Cl \rightarrow Fe^{3+} + Cl^-$	5.9E9		Jayson et al. (1973)
A11602a_a01	TrAa01ClFe	$Fe^{2+} + Cl_2^- \rightarrow Fe^{3+} + 2 Cl^-$	1E7		Thornton and Laurence (1973)
A11602b_a01	TrAa01ClFe	$Fe^{2+} + Cl_2^- \rightarrow FeCl^{2+} + Cl^-$	4E6		Thornton and Laurence (1973)
A11603a_a01	TrAa01ClFe	$FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO_2^-$	1.2E6		de Laat and Le (2006)
A11603b_a01	TrAa01ClFe	$FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11604a_a01	TrAa01ClFe	$FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604b_a01	TrAa01ClFe	$FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2 Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604c_a01	TrAa01ClFe	$FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$	5E7		de Laat and Le (2006)
A11604d_a01	TrAa01ClFe	$FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2 Cl^- + O_2$	5E7		de Laat and Le (2006)
A11605_a01	TrAa01ClFe	$FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2 OH^-$	1E2		Jacobsen et al. (1998)*
A11901_a01	TrAa01FeS	$FeO^{2+} + SO_2 \rightarrow Fe^{3+} + SO_3^-$	4.5E5		Jacobsen et al. (1998)*
A11902_a01	TrAa01FeS	$FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH^-$	2.5E5		Jacobsen et al. (1998)*
A11903_a01	TrAa01FeS	$FeOH^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	30		Ziajka et al. (1994)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A11904_a01	TrAa01FeS	$Fe^{2+} + SO_5^- \rightarrow FeOH^{2+} + HSO_5^-$	8E5		Ziajka et al. (1994)*
A11905_a01	TrAa01FeS	$Fe^{2+} + HSO_5^- \rightarrow FeOH^{2+} + SO_4^-$	3.0E4		Gilbert and Stell (1990)
A11906_a01	TrAa01FeS	$Fe^{2+} + SO_4^- \rightarrow FeSO_4^+$	3.6E7		McElroy and Waygood (1990)*
A11907_a01	TrAa01FeS	$FeOH^{2+} + SO_3^- \rightarrow Fe^{2+} + HSO_4^-$	3E7		Warneck (2018)
A11908_a01	TrAa01FeS	$FeSO_3^+ + SO_3^- \rightarrow Fe^{2+} + SO_4^{2-} + SO_2$	2.16E6		Warneck (2018)*
A3103_a01MK	TrAa01ScN	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	6.4E6		Pires et al. (1994)
A3104_a01MK	TrAa01ScN	$NO_2 + NO_2 \rightarrow N_2O_4$	4.5E8		Mack and Bolton (1999)
A3105_a01MK	TrAa01ScN	$NO + NO_2 \rightarrow N_2O_3$	1.1E9		Mack and Bolton (1999)
A3106_a01MK	TrAa01ScN	$NO_2 + O_2^- \rightarrow O_2 + NO_2^-$	1.0E8		Ervens et al. (2003)
A3107_a01MK	TrAa01ScN	$NO_2 + O_2^- \rightarrow NO_4^-$	4.5E9		Ervens et al. (2003)
A3109_a01MK	TrAa01ScN	$N_2O_3 \rightarrow 2 NO_2^- + 2 H^+$	1.6E3		Licht et al. (1988)
A3205_a01MK	TrAa01ScN	$NO + OH \rightarrow HONO$	1.0E10		Mack and Bolton (1999)
A3206_a01MK	TrAa01ScN	$HONO + HONO \rightarrow N_2O_3 + H_2O$	5.6		Schwartz (1983)
A4111_a01MK	TrAa01Sc	$CH_3OO + CH_3OO \rightarrow HCHO + CH_3OH + HO_2$	1.7E8	-2200	Ervens et al. (2004)
A4112_a01MK	TrAa01Sc	$CH_3OH + OH \rightarrow CH_2(OH)_2 + HO_2$	1.0E9		Ervens et al. (2004)
A4113_a01MK	TrAa01Sc	$CH_3OOH + OH \rightarrow HCOOH + HO_2$	6.0E6	-1715	Ervens et al. (2004)
A4114_a01MK	TrAa01Sc	$CH_2(OH)_2 + OH \rightarrow HCOOH + HO_2$	1.0E9		Ervens et al. (2004)
A4120_a01MK	TrAa01AmiScN	$MMA + N_2O_4 \rightarrow 0.3 MMNNO_2 + 0.7 CH_2NH_2 + 1.7 HONO$	4.0E7		Challis and Kyrtopoulos (1979)
A4121_a01MK	TrAa01AmiScN	$MMA + OH \rightarrow 0.5 CH_2NH_2 + 0.5 CH_3NH_2^+ + 0.5 OH^- + H_2O$	6.9E9		Simić et al. (1971)
A4122_a01MK	TrAa01AmiScN	$CH_2NH_2 + O_2 \rightarrow CH_2NH_2^+ + O_2^-$	3.5E9		Duff et al. (2003)
A4123_a01MK	TrAa01AmiScN	$CH_2NH_2^+ \rightarrow NH_3 + HCHO + H^+$	4.0		Duff et al. (2003)
A4124_a01MK	TrAa01AmiScN	$CH_2NH_2 + CH_2NH_2 \rightarrow NH_2CH_2CH_2NH_2$	2.0E9		Simić et al. (1971)
A4125_a01MK	TrAa01AmiScN	$CH_3NH_2^+ + CH_3NH_2^+ \rightarrow CH_3NHNHCH_3 + 2 H^+$	2.0E9		Simić et al. (1971)
A4126_a01MK	TrAa01AmiScN	$MMA^+ + OH \rightarrow 0.275 CH_2NH_3^+ + 0.725 CH_3NH_2^+ + H_2O$	1.1E8		Simić et al. (1971)
A4127_a01MK	TrAa01AmiScN	$HNCO \rightarrow NH_3 + CO_2$	7.83E-4		Roberts et al. (2011)
A4128_a01MK	TrAa01AmiScN	$H_2NCHO + OH \rightarrow HNCO + H_2O$	3.7E8		Munoz et al. (2000)
A4129_a01MK	TrAa01AScN	$MMNNO_2 + OH \rightarrow NH_4^+ + HCHO + OH^- + NO_2$	5.44E8		Fuller-Rowell (1993)
A4200_a01MK	TrAa01ScC	$GLYOX + OH \rightarrow HCOCO_2H + HO_2$	1.1E9	-1516	Ervens et al. (2004)
A4201_a01MK	TrAa01ScC	$HCOCO_2H + OH \rightarrow OXALAC + HO_2 + 2 CO_2$	3.6E8	-1000	Ervens et al. (2004)
A4202_a01MK	TrAa01ScC	$HCOCOO^- + OH \rightarrow HC_2O_4^- + HO_2 + 2 CO_2$	2.9E9	-4300	Ervens et al. (2004)
A4203_a01MK	TrAa01ScC	$HOCH_2CHO + OH \rightarrow GLYOX + HO_2$	1.2E9		Ervens et al. (2004)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A4204_a01MK	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH}^- \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2$	1.2E9		Ervens et al. (2004)
A4205_a01MK	TrAa01Sc	$\text{C}_2\text{O}_4^{2-} + \text{OH}^- \rightarrow \text{OH}^- + \text{O}_2^-$	1.6E8	-4300	Ervens et al. (2004)
A4206_a01MK	TrAa01Sc	$\text{HC}_2\text{O}_4^- + \text{OH}^- \rightarrow \text{OH}^- + \text{HO}_2$	1.9E8	-2800	Ervens et al. (2004)
A4207_a01MK	TrAa01Sc	$\text{OXALAC} + \text{OH}^- \rightarrow \text{H}_2\text{O} + \text{HO}_2$	1.4E6		Ervens et al. (2004)
A4208_a01MK	TrAa01ScC	$\text{CH}_3\text{COO}^- + \text{OH}^- \rightarrow \text{HO}_2 + \text{OH}^- + \text{CH}_3\text{COO}_2$	1.0E8	-1800	Ervens et al. (2004)
A4209_a01MK	TrAa01ScC	$\text{CH}_3\text{COOH} + \text{OH}^- \rightarrow \text{HO}_2 + \text{H}_2\text{O} + \text{CH}_3\text{COO}_2$	1.5E7	-1330	Ervens et al. (2004)
A4210_a01MK	TrAa01AmiScCN	$\text{DMA} + \text{N}_2\text{O}_3 \rightarrow \text{NDMA} + \text{HONO}$	4.29E7		Mirvish (1975)
A4211_a01MK	TrAa01AmiScCN	$\text{DMA} + \text{N}_2\text{O}_4 \rightarrow 0.4 \text{ DMNNO}_2 + 0.4 \text{ NDMA} + 0.2 \text{ CH}_3\text{NHCH}_2 + 0.6 \text{ HONO} + 0.6 \text{ HNO}_3$	4.0E7		Challis and Kyrtopoulos (1979)
A4212_a01MK	TrAa01AmiScCN	$\text{DMA} + \text{HONO} \rightarrow \text{NDMA} + \text{H}_2\text{O}$	0.1		Anastasio and Chu (2009)
A4213_a01MK	TrAa01AmiScCN	$\text{DMA} + \text{NO}_2^- \rightarrow \text{NDMA} + \text{OH}^-$	0.1		Anastasio and Chu (2009)
A4214_a01MK	TrAa01AmiScCN	$(\text{CH}_3)_2\text{NH}^+ + \text{NO}_2 \rightarrow \text{DMNNO}_2 + \text{H}^+$	1.0E4		Fell et al. (1990)
A4215_a01MK	TrAa01AmiScCN	$\text{DMA} + \text{OH}^- \rightarrow 0.5 \text{ CH}_3\text{NHCH}_2 + 0.5 (\text{CH}_3)_2\text{NH}^+ + 0.5 \text{ OH}^- + \text{H}_2\text{O}$	8.9E9		Lee et al. (2007a)
A4216_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{NH}^+\text{CH}_2 + \text{O}_2^-$	3.5E9		Duff et al. (2003)
A4217_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NH}^+\text{CH}_2 \rightarrow \text{MMA} + \text{HCHO} + \text{H}^+$	4.0		Duff et al. (2003)
A4218_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCH}_2 + \text{CH}_3\text{NHCH}_2 \rightarrow \text{DMA} + \text{CH}_3\text{NH}^+\text{CH}_2 + \text{OH}^-$	2.0E9		Das and von Sonntag (1986)
A4219_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCH}_2 + (\text{CH}_3)_2\text{NH}^+ \rightarrow \text{DMA} + \text{CH}_3\text{NH}^+\text{CH}_2$	2.0E9		Das and von Sonntag (1986)
A4220_a01MK	TrAa01AmiScCN	$\text{DMA}^+ + \text{OH}^- \rightarrow 0.275 \text{ CH}_3\text{NH}_2^+\text{CH}_2 + 0.725 (\text{CH}_3)_2\text{NH}^+ + \text{H}_2\text{O}$	6.0E7		Lee et al. (2007a)
A4221_a01MK	TrAa01AmiScCN	$\text{MEA} + \text{N}_2\text{O}_4 \rightarrow 0.3 \text{ MEANNO}_2 + 0.7 \text{ NH}_2\text{CH}_2\text{CHOH} + 1.7 \text{ HONO}$	4.0E7		Challis and Kyrtopoulos (1979)
A4222_a01MK	TrAa01AmiScCN	$\text{MEA} + \text{OH}^- \rightarrow 0.5 \text{ NH}_2\text{CH}_2\text{CHOH} + 0.5 \text{ HOCH}_2\text{CH}_2\text{NH}_2^+ + 0.5 \text{ OH}^- + \text{H}_2\text{O}$	2.9E9		Kishore et al. (2004)
A4223_a01MK	TrAa01AmiScCN	$\text{NH}_2\text{CH}_2\text{CHOH} + \text{OH}^- \rightarrow \text{CH}_2\text{NH}_2 + \text{HCHO}$	1.0E9		Kishore et al. (2004)
A4224_a01MK	TrAa01AmiScCN	$\text{MEA}^+ + \text{OH}^- \rightarrow 0.275 \text{ HOCHCH}_2\text{NH}_3^+ + 0.725 \text{ HOCH}_2\text{CH}_2\text{NH}_2^+ + \text{H}_2\text{O}$	3.0E8		Kishore et al. (2004)
A4225_a01MK	TrAa01AmiScCN	$\text{H}_2\text{NCOCH}_2\text{OH} + \text{OH}^- \rightarrow \text{HNCO} + \text{HCHO} + \text{HO}_2$	1.9E8		Roble (1995)
A4226_a01MK	TrAa01AmiScCN	$\text{CH}_3\text{NHCHO} + \text{OH}^- \rightarrow \text{HNCO} + \text{HCHO} + \text{HO}_2$	1.2E9		Roble (1995)
A4227_a01MK	TrAa01AmiScCN	$\text{NDMA} + \text{OH}^- \rightarrow \text{MMA}^+ + \text{HCHO} + \text{OH}^- + \text{NO}$	4.5E8		Lee et al. (2007b)
A4228_a01MK	TrAa01AmiScCN	$\text{DMNNO}_2 + \text{OH}^- \rightarrow \text{MMA}^+ + \text{HCHO} + \text{OH}^- + \text{NO}_2$	5.44E8		Fuller-Rowell (1993)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4229_a01MK	TrAa01AmiScCN	MEANNO + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO	4.5E8		Lee et al. (2007b)
A4230_a01MK	TrAa01AmiScCN	MEANNO ₂ + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO ₂	5.44E8		Fuller-Rowell (1993)
A4231_a01MK	TrAa01AmiScCN	CH ₃ NCO \rightarrow MMA + CO ₂	7.83E-4		Roberts et al. (2011)
A4300_a01MK	TrAa01ScC	MGLYOX + OH \rightarrow MGLYOAC + HO ₂	1.1E9	-1600	Ervens et al. (2004)
A4301_a01MK	TrAa01ScC	CH ₃ COCOO ⁻ + OH \rightarrow CH ₃ COO ₂ + HO ₂ + CO ₂ + O ₂ ⁻	7.0E8		Ervens et al. (2004)
A4302_a01MK	TrAa01ScC	MGLYOAC + OH \rightarrow CH ₃ CHO + HO ₂ + H ₂ O + CO ₂	1.2E8		Ervens et al. (2004)
A4303_a01MK	TrAa01Sc	DOC + OH \rightarrow DOCO + HO ₂	4.1E8		Barth (1992)
A4304_a01MK	TrAa01Sc	MALONAC + OH \rightarrow OXALAC + HO ₂	5.0E7		Ervens et al. (2004)
A4310_a01MK	TrAa01AmiScCN	TMA + N ₂ O ₃ \rightarrow 0.075 NDMA + 1.9 HONO + 0.95 (CH ₃) ₂ NCH ₂	4.0E7		Challis and Kyrtopoulos (1979)
A4311_a01MK	TrAa01AmiScCN	TMA + N ₂ O ₄ \rightarrow 0.05 DMNNO ₂ + 0.1 NDMA + 0.90 (CH ₃) ₂ NCH ₂ + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4312_a01MK	TrAa01AmiScCN	TMA + OH \rightarrow 0.5 (CH ₃) ₂ NCH ₂ + 0.5 (CH ₃) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	1.2E10		Das and von Sonntag (1986)
A4313_a01MK	TrAa01AmiScCN	(CH ₃) ₂ NCH ₂ + O ₂ \rightarrow (CH ₃) ₂ N ⁺ CH ₂ + O ₂ ⁻	3.5E9		Duff et al. (2003)
A4314_a01MK	TrAa01AmiScCN	(CH ₃) ₂ N ⁺ CH ₂ \rightarrow DMA + HCHO + H ⁺	4.0		Duff et al. (2003)
A4315_a01MK	TrAa01AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₂ NCH ₂ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂ + OH ⁻	2.0E9		Das and von Sonntag (1986)
A4316_a01MK	TrAa01AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₃ N ⁺ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂	2.0E9		Das and von Sonntag (1986)
A4317_a01MK	TrAa01AmiScCN	TMA ⁺ + OH \rightarrow 0.275 (CH ₃) ₂ NH ⁺ CH ₂ + 0.725 (CH ₃) ₃ N ⁺ + H ₂ O	4.0E8		Das and von Sonntag (1986)
A4318_a01MK	TrAa01AmiScCN	DMNCHO + OH \rightarrow CH ₃ NCO + HCHO + HO ₂	1.7E9		Roble (1995)
A4400_a01MK	TrAa01Sc	SUCCAC + OH \rightarrow MALONAC + HO ₂	5.0E7		Ervens et al. (2004)
A4410_a01MK	TrAa01AmiScCN	DEA + N ₂ O ₃ \rightarrow NDELA + HONO	1.0E7		Mitch and Herckes (2012)
A4411_a01MK	TrAa01AmiScCN	DEA + N ₂ O ₄ \rightarrow 0.4 DEANNO ₂ + 0.4 NDELA + 0.2 HOETNHCH ₂ CHOH + 0.6 HONO + 0.6 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4412_a01MK	TrAa01AmiScCN	DEA + HONO \rightarrow NDELA + H ₂ O	0.1		Anastasio and Chu (2009)
A4413_a01MK	TrAa01AmiScCN	DEA + NO ₂ ⁻ \rightarrow NDELA + OH ⁻	0.1		Anastasio and Chu (2009)
A4414_a01MK	TrAa01AmiScCN	(HOET) ₂ NH ⁺ + NO ₂ \rightarrow DEANNO ₂ + H ⁺	0.0		Fell et al. (1990)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4415_a01MK	TrAa01AmiScCN	DEA + OH \rightarrow 0.5 HOETNHCH ₂ CHOH + 0.5 (HOET) ₂ NH ⁺ + 0.5 OH ⁻ + H ₂ O	8.0E9		Kishore et al. (2004)
A4416_a01MK	TrAa01AmiScCN	HOETNHCH ₂ CHOH + OH \rightarrow MEA + 2 HCHO	1.0E9		Kishore et al. (2004)
A4417_a01MK	TrAa01AmiScCN	DEA ⁺ + OH \rightarrow 0.275 HOETNH ₂ CH ₂ CHOH ⁺ + 0.725 (HOET) ₂ NH ⁺ + H ₂ O	4.5E8		Kishore et al. (2004)
A4418_a01MK	TrAa01AmiScCN	NDELA + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO	6.99E8		Fuller-Rowell (1993)
A4419_a01MK	TrAa01AmiScCN	DEANNO ₂ + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO ₂	8.67E8		Fuller-Rowell (1993)
A4500_a01MK	TrAa01Sc	GLUTARAC + OH \rightarrow SUCCAC + HO ₂	1.0E7		Ervens et al. (2004)
A4600_a01MK	TrAa01Sc	ADIPAC + OH \rightarrow GLUTARAC + HO ₂	1.0E7		Ervens et al. (2004)
A4610_a01MK	TrAa01AmiScCN	TEA + OH \rightarrow 0.5 DENCH ₂ CHOH + 0.5 (HOET) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	2.0E10		Kishore et al. (2004)
A4611_a01MK	TrAa01AmiScCN	DENCH ₂ CHOH + OH \rightarrow (HOET) ₂ N ⁺ CH ₂ CH ₂ OH + OH ⁻	3.18E9		Das and von Sonntag (1986)
A4612_a01MK	TrAa01AmiScCN	(HOET) ₂ N ⁺ CH ₂ CH ₂ OH \rightarrow DEA + HOCH ₂ CHO + H ⁺	3.0E6		Das and von Sonntag (1986)
A4613_a01MK	TrAa01AmiScCN	(HOET) ₃ N ⁺ + DENCH ₂ CHOH \rightarrow TEA + (HOET) ₂ N ⁺ CH ₂ CH ₂ OH	2.0E9		Das and von Sonntag (1986)
A4614_a01MK	TrAa01AmiScCN	TEA ⁺ + OH \rightarrow 0.275 (HOET) ₂ NH ⁺ CH ₂ CHOH + 0.725 (HOET) ₃ N ⁺ + H ₂ O	2.0E9		Kishore et al. (2004)
A4615_a01MK	TrAa01AmiScCN	TEA + N ₂ O ₃ \rightarrow 0.075 NDELA + 0.95 DENCH ₂ CHOH + 1.9 HONO	2.9E5		Mitch and Herckes (2012)
A4616_a01MK	TrAa01AmiScCN	TEA + N ₂ O ₄ \rightarrow 0.05 DEANNO ₂ + 0.1 NDELA + 0.9 DENCH ₂ CHOH + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A9405_a01MK	TrAa01MblScS	HSO ₃ ⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OHSO ₃ ⁻	0.436	-2990	Ervens et al. (2004)
A9406a_a01MK	TrAa01MblScS	CH ₂ OHSO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + HSO ₃ ⁻	1.22E-7		Ervens et al. (2004)
A9406b_a01MK	TrAa01MblScS	CH ₂ OHSO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + SO ₃ ²⁻ + H ⁺	3.8E-6	-5530	Ervens et al. (2004)
A9407_a01MK	TrAa01MblScS	SO ₃ ²⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OHSO ₃ ⁻ + O ₂ ⁻	1.36E5	-2450	Ervens et al. (2004)
A9408_a01MK	TrAa01MblScS	CH ₂ OHSO ₃ ⁻ + OH \rightarrow HCOOH + HO ₂ + HSO ₃ ⁻	3.0E8		Ervens et al. (2004)
A9409_a01MK	TrAa01MblScCS	DMS + O ₃ \rightarrow DMSO	8.61E8	-2600	Hoffmann et al. (2016)
A9410_a01MK	TrAa01MblScCS	DMS + OH \rightarrow DMSO + HO ₂	1.9E10		Hoffmann et al. (2016)
A9411_a01MK	TrAa01MblScCS	DMSO + OH \rightarrow MSIA + HO ₂ + CO ₂	6.65E9	-1270	Hoffmann et al. (2016)
A9412_a01MK	TrAa01MblScS	MSIA + O ₃ \rightarrow CH ₃ SO ₃ ⁻ + H ⁺	3.5E7		Hoffmann et al. (2016)
A9413_a01MK	TrAa01MblScS	MSIA + OH \rightarrow CH ₃ SO ₃ ⁻ + H ⁺ + HO ₂	6.0E9		Hoffmann et al. (2016)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n} s^{-1}$]	$-E_a/R[K]$	reference
A9414_a01MK	TrAa01MblScCS	HPMTF + OH \rightarrow HOOCH ₂ SCO	1.0E10		Wollesen de Jonge et al. (2021)
A1000_a02	TrAa02Sc	O ₃ + O ₂ ⁻ \rightarrow OH + OH ⁻	1.5E9		Sehested et al. (1983)
A2100_a02	TrAa02Sc	OH + O ₂ ⁻ \rightarrow OH ⁻	1.0E10		Sehested et al. (1968)
A2101_a02	TrAa02Sc	OH + OH \rightarrow H ₂ O ₂	5.5E9		Buxton et al. (1988)
A2102_a02	TrAa02Sc	HO ₂ + O ₂ ⁻ \rightarrow H ₂ O ₂ + OH ⁻	1.0E8	-900	Christensen and Sehested (1988)
A2103_a02	TrAa02Sc	HO ₂ + OH \rightarrow H ₂ O	7.1E9		Sehested et al. (1968)
A2104_a02	TrAa02Sc	HO ₂ + HO ₂ \rightarrow H ₂ O ₂	9.7E5	-2500	Christensen and Sehested (1988)
A2105_a02	TrAa02Sc	H ₂ O ₂ + OH \rightarrow HO ₂	2.7E7	-1684	Christensen et al. (1982)
A3100_a02	TrAa02ScN	NO ₂ ⁻ + O ₃ \rightarrow NO ₃ ⁻	5.0E5	-6950	Damschen and Martin (1983)
A3101_a02	TrAa02ScN	NO ₂ + NO ₂ \rightarrow HNO ₃ + HONO	1.0E8		Lee and Schwartz (1981)
A3102_a02	TrAa02ScN	NO ₄ ⁻ \rightarrow NO ₂ ⁻	8.0E1		Warneck (1999)
A3200_a02	TrAa02ScN	NO ₂ + HO ₂ \rightarrow HNO ₄	1.8E9		Warneck (1999)
A3201_a02	TrAa02ScN	NO ₂ ⁻ + OH \rightarrow NO ₂ + OH ⁻	1.0E10		Wingenter et al. (1999)
A3202_a02	TrAa02ScN	NO ₃ + OH ⁻ \rightarrow NO ₃ ⁻ + OH	8.2E7	-2700	Exner et al. (1992)
A3203_a02	TrAa02ScN	HONO + OH \rightarrow NO ₂	1.0E10		Barker et al. (1970)
A3204_a02	TrAa02ScN	HONO + H ₂ O ₂ + H ⁺ \rightarrow HNO ₃ + H ⁺	4.6E3	-6800	Damschen and Martin (1983)
A4100_a02	TrAa02Sc	CO ₃ ⁻ + O ₂ ⁻ \rightarrow HCO ₃ ⁻ + OH ⁻	6.5E8		Ross et al. (1992)
A4101_a02	TrAa02Sc	CO ₃ ⁻ + H ₂ O ₂ \rightarrow HCO ₃ ⁻ + HO ₂	4.3E5		Ross et al. (1992)
A4102_a02	TrAa02Sc	HCOO ⁻ + CO ₃ ⁻ \rightarrow 2 HCO ₃ ⁻ + HO ₂	1.5E5		Ross et al. (1992)
A4103_a02	TrAa02Sc	HCOO ⁻ + OH \rightarrow OH ⁻ + HO ₂ + CO ₂	3.1E9	-1240	Chin and Wine (1994)
A4104_a02	TrAa02Sc	HCO ₃ ⁻ + OH \rightarrow CO ₃ ⁻	8.5E6		Ross et al. (1992)
A4105_a02	TrAa02Sc	HCHO + OH \rightarrow HCOOH + HO ₂	7.7E8	-1020	Chin and Wine (1994)
A4106_a02	TrAa02Sc	HCOOH + OH \rightarrow HO ₂ + CO ₂	1.1E8	-991	Chin and Wine (1994)
A4107_a02	TrAa02Sc	CH ₃ OO + O ₂ ⁻ \rightarrow CH ₃ OOH + OH ⁻	5.0E7		Jacob (1986)
A4108_a02	TrAa02Sc	CH ₃ OO + HO ₂ \rightarrow CH ₃ OOH	4.3E5		Jacob (1986)
A4109_a02	TrAa02Sc	CH ₃ OH + OH \rightarrow HCHO + HO ₂	9.7E8		Buxton et al. (1988)
A4110a_a02	TrAa02Sc	CH ₃ OOH + OH \rightarrow CH ₃ OO	2.7E7	-1715	Jacob (1986)
A4110b_a02	TrAa02Sc	CH ₃ OOH + OH \rightarrow HCHO + OH	1.1E7	-1715	Jacob (1986)
A6000_a02	TrAa02Cl	Cl + Cl \rightarrow Cl ₂	8.8E7		Wu et al. (1980)
A6001_a02	TrAa02Cl	Cl ₂ ⁻ + Cl ₂ ⁻ \rightarrow Cl ₂ + 2 Cl ⁻	3.5E9		Yu (2004)
A6100_a02	TrAa02Cl	Cl ⁻ + O ₃ \rightarrow ClO ⁻	3.0E-3		Hoigné et al. (1985)
A6101_a02	TrAa02Cl	Cl ₂ + O ₂ ⁻ \rightarrow Cl ₂ ⁻	1.0E9		Bjergbakke et al. (1981)
A6102_a02	TrAa02Cl	Cl ₂ ⁻ + O ₂ ⁻ \rightarrow 2 Cl ⁻	1.0E9		Jacobi (1996)*
A6200_a02	TrAa02Cl	Cl \rightarrow H ⁺ + ClOH ⁻	1.8E5		Yu (2004)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A6201_a02	TrAa02Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)
A6202_a02	TrAa02Cl	$Cl^- + OH \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a02	TrAa02Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a02	TrAa02MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a02	TrAa02Cl	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a02	TrAa02Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a02	TrAa02Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a02	TrAa02MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a02	TrAa02Cl	$ClOH^- \rightarrow Cl^- + OH$	6.0E9		Yu (2004)
A6210_a02	TrAa02Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a02	TrAa02ClN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a02	TrAa02ClN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a02	TrAa02ClN	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a02	TrAa02Cl	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A8100_a02	TrAa02MblI	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a02	TrAa02MblI	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A8200_a02	TrAa02MblI	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A8201_a02	TrAa02I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
A8202_a02	TrAa02MblI	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A8203_a02	TrAa02MblI	$IO_2^- + I^- + H^+ \rightarrow 2 HOI + OH^-$	2.0E10		Edblom et al. (1987)
A8600_a02	TrAa02MblClII	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601_a02	TrAa02MblClII	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8602_a02	TrAa02ClII	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A8603_a02	TrAa02MblClII	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8604_a02	TrAa02ClII	$HOI + Cl_2 \rightarrow IO_2^- + 2 Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A8605_a02	TrAa02ClII	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2 H^+$	5.0E5		Citri and Epstein (1988)
A8606_a02	TrAa02ClII	$ICl + I^- \rightarrow I_2 + Cl^-$	1.1E9		Margerum et al. (1986)
A9100_a02	TrAa02ScS	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101_a02	TrAa02MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a02	TrAa02ScS	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a02	TrAa02ScS	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a02	TrAa02ScS	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105_a02	TrAa02S	$SO_5^- + SO_3^{2-} \rightarrow .72 SO_4^- + .72 SO_4^{2-} + .28 SO_3^- + .28 HSO_5^- + .28 OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9106_a02	TrAa02S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + \text{LSULFUR}$	1.0E8		Ross et al. (1992)*
A9200_a02	TrAa02ScS	$SO_3^- + OH^- \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201_a02	TrAa02ScS	$SO_4^- + OH^- \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202_a02	TrAa02ScS	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203_a02	TrAa02ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH^-$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a02	TrAa02ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205_a02	TrAa02ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH^-$	3.0E3		see note*
A9206_a02	TrAa02MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a02	TrAa02ScS	$HSO_3^- + OH^- \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208_a02	TrAa02ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH^- + H^+$	3.0E3		see note*
A9209_a02	TrAa02MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a02	TrAa02ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211_a02	TrAa02S	$HSO_3^- + SO_5^- \rightarrow .75 SO_4^- + .75 SO_4^{2-} + .75 H^+ + .25 SO_3^- + .25 HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212_a02	TrAa02ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2 HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A9301_a02	TrAa02ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302_a02	TrAa02ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Løgager et al. (1993)
A9304_a02	TrAa02ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a02	TrAa02ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400_a02	TrAa02ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OH SO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)*
A9401_a02	TrAa02ScS	$SO_3^- + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402_a02	TrAa02ScS	$HSO_3^- + HCHO \rightarrow CH_2OH SO_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A9403_a02	TrAa02ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404_a02	TrAa02ScS	$CH_2OH SO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600_a02	TrAa02ClS	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2 Cl^-$	6.2E7		Jacobi et al. (1996)
A9601_a02	TrAa02MblClS	$SO_3^- + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a02	TrAa02ClS	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603_a02	TrAa02ClS	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604_a02	TrAa02ClS	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2 Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a02	TrAa02MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A9606_a02	TrAa02ClS	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9800_a02	TrAa02IS	$HSO_3^- + I_2 \rightarrow 2 I^- + HSO_4^- + 2 H^+$	1.7E9		Yiin and Margerum (1990)
A11101_a02	TrAa02Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11102_a02	TrAa02Fe	$Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$	5E7		de Laat and Le (2006)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A11103_a02	TrAa02Fe	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	8.2E5		Løgager et al. (1992)
A11201a_a02	TrAa02Fe	$Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$	2.7E8		de Laat and Le (2006)
A11201b_a02	TrAa02Fe	$FeOH^+ + OH \rightarrow Fe^{3+} + 2 OH^-$	2.7E8		de Laat and Le (2006)
A11202a_a02	TrAa02Fe	$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$	5.5E1		de Laat and Le (2006)
A11202b_a02	TrAa02Fe	$FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2 OH^-$	5.9E6		de Laat and Le (2006)
A11203_a02	TrAa02Fe	$FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$	2.3E-3		de Laat and Le (2006)
A11204_a02	TrAa02Fe	$Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$	2.3E-3		de Laat and Le (2006)
A11206_a02	TrAa02Fe	$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO_2^-$	1.2E6		de Laat and Le (2006)
A11208a_a02	TrAa02Fe	$FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$	1.5E8		Rush and Bielski (1985)
A11208b_a02	TrAa02Fe	$Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2 OH^-$	1.5E8		Rush and Bielski (1985)
A11209_a02	TrAa02Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2 OH^-$	1.0E7		Rush and Bielski (1985)
A11210_a02	TrAa02Fe	$Fe^{2+} + OH \rightarrow FeOH^{2+}$	4.3E8		Christensen and Sehested (1981)
A11211_a02	TrAa02Fe	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	9.5E3		Løgager et al. (1992)
A11212_a02	TrAa02Fe	$FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$	1.3E-2		Løgager et al. (1992)
A11213_a02	TrAa02Fe	$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	2.0E6		Løgager et al. (1992)
A11214_a02	TrAa02Fe	$FeO^{2+} + OH \rightarrow Fe^{3+} + HO_2^-$	1.0E7		Løgager et al. (1992)
A11215_a02	TrAa02Fe	$FeO^{2+} + Fe^{2+} \rightarrow 2 Fe^{3+} + 2 OH^-$	1.4E5		Løgager et al. (1992)
A11216_a02	TrAa02Fe	$FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+}$	1.8E4		Jacobsen et al. (1997)
A11217_a02	TrAa02Fe	$Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2 Fe^{3+} + OH^-$	2.0		Jacobsen et al. (1997)
A11218_a02	TrAa02Fe	$Fe(OH)_2Fe^{4+} \rightarrow 2 Fe^{3+} + 2 OH^-$	0.49		Jacobsen et al. (1997)
A11301_a02	TrAa02FeN	$FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$	1.1E4		Jacobsen et al. (1998)
A11302_a02	TrAa02FeN	$Fe^{2+} + NO_3 \rightarrow Fe^{3+} + NO_3^-$	8.0E6		Herrmann et al. (2000)*
A11601_a02	TrAa02ClFe	$Fe^{2+} + Cl \rightarrow Fe^{3+} + Cl^-$	5.9E9		Jayson et al. (1973)
A11602a_a02	TrAa02ClFe	$Fe^{2+} + Cl_2^- \rightarrow Fe^{3+} + 2 Cl^-$	1E7		Thornton and Laurence (1973)
A11602b_a02	TrAa02ClFe	$Fe^{2+} + Cl_2^- \rightarrow FeCl^{2+} + Cl^-$	4E6		Thornton and Laurence (1973)
A11603a_a02	TrAa02ClFe	$FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO_2^-$	1.2E6		de Laat and Le (2006)
A11603b_a02	TrAa02ClFe	$FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11604a_a02	TrAa02ClFe	$FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604b_a02	TrAa02ClFe	$FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2 Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604c_a02	TrAa02ClFe	$FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$	5E7		de Laat and Le (2006)
A11604d_a02	TrAa02ClFe	$FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2 Cl^- + O_2$	5E7		de Laat and Le (2006)
A11605_a02	TrAa02ClFe	$FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2 OH^-$	1E2		Jacobsen et al. (1998)*
A11901_a02	TrAa02FeS	$FeO^{2+} + SO_2 \rightarrow Fe^{3+} + SO_3^-$	4.5E5		Jacobsen et al. (1998)*
A11902_a02	TrAa02FeS	$FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH^-$	2.5E5		Jacobsen et al. (1998)*

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A11903_a02	TrAa02FeS	$FeOH^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	30		Ziajka et al. (1994)
A11904_a02	TrAa02FeS	$Fe^{2+} + SO_5^- \rightarrow FeOH^{2+} + HSO_5^-$	8E5		Ziajka et al. (1994)*
A11905_a02	TrAa02FeS	$Fe^{2+} + HSO_5^- \rightarrow FeOH^{2+} + SO_4^-$	3.0E4		Gilbert and Stell (1990)
A11906_a02	TrAa02FeS	$Fe^{2+} + SO_4^- \rightarrow FeSO_4^+$	3.6E7		McElroy and Waygood (1990)*
A11907_a02	TrAa02FeS	$FeOH^{2+} + SO_3^- \rightarrow Fe^{2+} + HSO_4^-$	3E7		Warneck (2018)
A11908_a02	TrAa02FeS	$FeSO_3^+ + SO_3^- \rightarrow Fe^{2+} + SO_4^{2-} + SO_2$	2.16E6		Warneck (2018)*
A3103_a02MK	TrAa02ScN	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	6.4E6		Pires et al. (1994)
A3104_a02MK	TrAa02ScN	$NO_2 + NO_2 \rightarrow N_2O_4$	4.5E8		Mack and Bolton (1999)
A3105_a02MK	TrAa02ScN	$NO + NO_2 \rightarrow N_2O_3$	1.1E9		Mack and Bolton (1999)
A3106_a02MK	TrAa02ScN	$NO_2 + O_2^- \rightarrow O_2 + NO_2^-$	1.0E8		Ervens et al. (2003)
A3107_a02MK	TrAa02ScN	$NO_2 + O_2^- \rightarrow NO_4^-$	4.5E9		Ervens et al. (2003)
A3109_a02MK	TrAa02ScN	$N_2O_3 \rightarrow 2 NO_2^- + 2 H^+$	1.6E3		Licht et al. (1988)
A3205_a02MK	TrAa02ScN	$NO + OH \rightarrow HONO$	1.0E10		Mack and Bolton (1999)
A3206_a02MK	TrAa02ScN	$HONO + HONO \rightarrow N_2O_3 + H_2O$	5.6		Schwartz (1983)
A4111_a02MK	TrAa02Sc	$CH_3OO + CH_3OO \rightarrow HCHO + CH_3OH + HO_2$	1.7E8	-2200	Ervens et al. (2004)
A4112_a02MK	TrAa02Sc	$CH_3OH + OH \rightarrow CH_2(OH)_2 + HO_2$	1.0E9		Ervens et al. (2004)
A4113_a02MK	TrAa02Sc	$CH_3OOH + OH \rightarrow HCOOH + HO_2$	6.0E6	-1715	Ervens et al. (2004)
A4114_a02MK	TrAa02Sc	$CH_2(OH)_2 + OH \rightarrow HCOOH + HO_2$	1.0E9		Ervens et al. (2004)
A4120_a02MK	TrAa02AmiScN	$MMA + N_2O_4 \rightarrow 0.3 MMNNO_2 + 0.7 CH_2NH_2 + 1.7 HONO$	4.0E7		Challis and Kyrtopoulos (1979)
A4121_a02MK	TrAa02AmiScN	$MMA + OH \rightarrow 0.5 CH_2NH_2 + 0.5 CH_3NH_2^+ + 0.5 OH^- + H_2O$	6.9E9		Simić et al. (1971)
A4122_a02MK	TrAa02AmiScN	$CH_2NH_2 + O_2 \rightarrow CH_2NH_2^+ + O_2^-$	3.5E9		Duff et al. (2003)
A4123_a02MK	TrAa02AmiScN	$CH_2NH_2^+ \rightarrow NH_3 + HCHO + H^+$	4.0		Duff et al. (2003)
A4124_a02MK	TrAa02AmiScN	$CH_2NH_2 + CH_2NH_2 \rightarrow NH_2CH_2CH_2NH_2$	2.0E9		Simić et al. (1971)
A4125_a02MK	TrAa02AmiScN	$CH_3NH_2^+ + CH_3NH_2^+ \rightarrow CH_3NHNHCH_3 + 2 H^+$	2.0E9		Simić et al. (1971)
A4126_a02MK	TrAa02AmiScN	$MMA^+ + OH \rightarrow 0.275 CH_2NH_3^+ + 0.725 CH_3NH_2^+ + H_2O$	1.1E8		Simić et al. (1971)
A4127_a02MK	TrAa02AmiScN	$HNCO \rightarrow NH_3 + CO_2$	7.83E-4		Roberts et al. (2011)
A4128_a02MK	TrAa02AmiScN	$H_2NCHO + OH \rightarrow HNCO + H_2O$	3.7E8		Munoz et al. (2000)
A4129_a02MK	TrAa02AScN	$MMNNO_2 + OH \rightarrow NH_4^+ + HCHO + OH^- + NO_2$	5.44E8		Fuller-Rowell (1993)
A4200_a02MK	TrAa02ScC	$GLYOX + OH \rightarrow HCOCO_2H + HO_2$	1.1E9	-1516	Ervens et al. (2004)
A4201_a02MK	TrAa02ScC	$HCOCO_2H + OH \rightarrow OXALAC + HO_2 + 2 CO_2$	3.6E8	-1000	Ervens et al. (2004)
A4202_a02MK	TrAa02ScC	$HCOCOO^- + OH \rightarrow HC_2O_4^- + HO_2 + 2 CO_2$	2.9E9	-4300	Ervens et al. (2004)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4203_a02MK	TrAa02ScC	$HOCH_2CHO + OH \rightarrow GLYOX + HO_2$	1.2E9		Ervens et al. (2004)
A4204_a02MK	TrAa02ScC	$HOCH_2CO_2H + OH \rightarrow HCOCO_2H + HO_2$	1.2E9		Ervens et al. (2004)
A4205_a02MK	TrAa02Sc	$C_2O_4^{2-} + OH \rightarrow OH^- + O_2^-$	1.6E8	-4300	Ervens et al. (2004)
A4206_a02MK	TrAa02Sc	$HC_2O_4^- + OH \rightarrow OH^- + HO_2$	1.9E8	-2800	Ervens et al. (2004)
A4207_a02MK	TrAa02Sc	$OXALAC + OH \rightarrow H_2O + HO_2$	1.4E6		Ervens et al. (2004)
A4208_a02MK	TrAa02ScC	$CH_3COO^- + OH \rightarrow HO_2 + OH^- + CH_3COO_2$	1.0E8	-1800	Ervens et al. (2004)
A4209_a02MK	TrAa02ScC	$CH_3COOH + OH \rightarrow HO_2 + H_2O + CH_3COO_2$	1.5E7	-1330	Ervens et al. (2004)
A4210_a02MK	TrAa02AmiScCN	$DMA + N_2O_3 \rightarrow NDMA + HONO$	4.29E7		Mirvish (1975)
A4211_a02MK	TrAa02AmiScCN	$DMA + N_2O_4 \rightarrow 0.4 DMNNO_2 + 0.4 NDMA + 0.2 CH_3NHCH_2 + 0.6 HONO + 0.6 HNO_3$	4.0E7		Challis and Kyrtopoulos (1979)
A4212_a02MK	TrAa02AmiScCN	$DMA + HONO \rightarrow NDMA + H_2O$	0.1		Anastasio and Chu (2009)
A4213_a02MK	TrAa02AmiScCN	$DMA + NO_2^- \rightarrow NDMA + OH^-$	0.1		Anastasio and Chu (2009)
A4214_a02MK	TrAa02AmiScCN	$(CH_3)_2NH^+ + NO_2 \rightarrow DMNNO_2 + H^+$	1.0E4		Fell et al. (1990)
A4215_a02MK	TrAa02AmiScCN	$DMA + OH \rightarrow 0.5 CH_3NHCH_2 + 0.5 (CH_3)_2NH^+ + 0.5 OH^- + H_2O$	8.9E9		Lee et al. (2007a)
A4216_a02MK	TrAa02AmiScCN	$CH_3NHCH_2 + O_2 \rightarrow CH_3NH^+CH_2 + O_2^-$	3.5E9		Duff et al. (2003)
A4217_a02MK	TrAa02AmiScCN	$CH_3NH^+CH_2 \rightarrow MMA + HCHO + H^+$	4.0		Duff et al. (2003)
A4218_a02MK	TrAa02AmiScCN	$CH_3NHCH_2 + CH_3NHCH_2 \rightarrow DMA + CH_3NH^+CH_2 + OH^-$	2.0E9		Das and von Sonntag (1986)
A4219_a02MK	TrAa02AmiScCN	$CH_3NHCH_2 + (CH_3)_2NH^+ \rightarrow DMA + CH_3NH^+CH_2$	2.0E9		Das and von Sonntag (1986)
A4220_a02MK	TrAa02AmiScCN	$DMA^+ + OH \rightarrow 0.275 CH_3NH_2^+CH_2 + 0.725 (CH_3)_2NH^+ + H_2O$	6.0E7		Lee et al. (2007a)
A4221_a02MK	TrAa02AmiScCN	$MEA + N_2O_4 \rightarrow 0.3 MEANNO_2 + 0.7 NH_2CH_2CHOH + 1.7 HONO$	4.0E7		Challis and Kyrtopoulos (1979)
A4222_a02MK	TrAa02AmiScCN	$MEA + OH \rightarrow 0.5 NH_2CH_2CHOH + 0.5 HOCH_2CH_2NH_2^+ + 0.5 OH^- + H_2O$	2.9E9		Kishore et al. (2004)
A4223_a02MK	TrAa02AmiScCN	$NH_2CH_2CHOH + OH \rightarrow CH_2NH_2 + HCHO$	1.0E9		Kishore et al. (2004)
A4224_a02MK	TrAa02AmiScCN	$MEA^+ + OH \rightarrow 0.275 HOCHCH_2NH_3^+ + 0.725 HOCH_2CH_2NH_2^+ + H_2O$	3.0E8		Kishore et al. (2004)
A4225_a02MK	TrAa02AmiScCN	$H_2NCOCH_2OH + OH \rightarrow HNCO + HCHO + HO_2$	1.9E8		Roble (1995)
A4226_a02MK	TrAa02AmiScCN	$CH_3NHCHO + OH \rightarrow HNCO + HCHO + HO_2$	1.2E9		Roble (1995)
A4227_a02MK	TrAa02AmiScCN	$NDMA + OH \rightarrow MMA^+ + HCHO + OH^- + NO$	4.5E8		Lee et al. (2007b)
A4228_a02MK	TrAa02AmiScCN	$DMNNO_2 + OH \rightarrow MMA^+ + HCHO + OH^- + NO_2$	5.44E8		Fuller-Rowell (1993)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4229_a02MK	TrAa02AmiScCN	MEANNO + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO	4.5E8		Lee et al. (2007b)
A4230_a02MK	TrAa02AmiScCN	MEANNO ₂ + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO ₂	5.44E8		Fuller-Rowell (1993)
A4231_a02MK	TrAa02AmiScCN	CH ₃ NCO \rightarrow MMA + CO ₂	7.83E-4		Roberts et al. (2011)
A4300_a02MK	TrAa02ScC	MGLYOX + OH \rightarrow MGLYOAC + HO ₂	1.1E9	-1600	Ervens et al. (2004)
A4301_a02MK	TrAa02ScC	CH ₃ COCOO ⁻ + OH \rightarrow CH ₃ COO ₂ + HO ₂ + CO ₂ + O ₂ ⁻	7.0E8		Ervens et al. (2004)
A4302_a02MK	TrAa02ScC	MGLYOAC + OH \rightarrow CH ₃ CHO + HO ₂ + H ₂ O + CO ₂	1.2E8		Ervens et al. (2004)
A4303_a02MK	TrAa02Sc	DOC + OH \rightarrow DOCO + HO ₂	4.1E8		Barth (1992)
A4304_a02MK	TrAa02Sc	MALONAC + OH \rightarrow OXALAC + HO ₂	5.0E7		Ervens et al. (2004)
A4310_a02MK	TrAa02AmiScCN	TMA + N ₂ O ₃ \rightarrow 0.075 NDMA + 1.9 HONO + 0.95 (CH ₃) ₂ NCH ₂	4.0E7		Challis and Kyrtopoulos (1979)
A4311_a02MK	TrAa02AmiScCN	TMA + N ₂ O ₄ \rightarrow 0.05 DMNNO ₂ + 0.1 NDMA + 0.90 (CH ₃) ₂ NCH ₂ + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4312_a02MK	TrAa02AmiScCN	TMA + OH \rightarrow 0.5 (CH ₃) ₂ NCH ₂ + 0.5 (CH ₃) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	1.2E10		Das and von Sonntag (1986)
A4313_a02MK	TrAa02AmiScCN	(CH ₃) ₂ NCH ₂ + O ₂ \rightarrow (CH ₃) ₂ N ⁺ CH ₂ + O ₂ ⁻	3.5E9		Duff et al. (2003)
A4314_a02MK	TrAa02AmiScCN	(CH ₃) ₂ N ⁺ CH ₂ \rightarrow DMA + HCHO + H ⁺	4.0		Duff et al. (2003)
A4315_a02MK	TrAa02AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₂ NCH ₂ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂ + OH ⁻	2.0E9		Das and von Sonntag (1986)
A4316_a02MK	TrAa02AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₃ N ⁺ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂	2.0E9		Das and von Sonntag (1986)
A4317_a02MK	TrAa02AmiScCN	TMA ⁺ + OH \rightarrow 0.275 (CH ₃) ₂ NH ⁺ CH ₂ + 0.725 (CH ₃) ₃ N ⁺ + H ₂ O	4.0E8		Das and von Sonntag (1986)
A4318_a02MK	TrAa02AmiScCN	DMNCHO + OH \rightarrow CH ₃ NCO + HCHO + HO ₂	1.7E9		Roble (1995)
A4400_a02MK	TrAa02Sc	SUCCAC + OH \rightarrow MALONAC + HO ₂	5.0E7		Ervens et al. (2004)
A4410_a02MK	TrAa02AmiScCN	DEA + N ₂ O ₃ \rightarrow NDELA + HONO	1.0E7		Mitch and Herckes (2012)
A4411_a02MK	TrAa02AmiScCN	DEA + N ₂ O ₄ \rightarrow 0.4 DEANNO ₂ + 0.4 NDELA + 0.2 HOETNHCH ₂ CHOH + 0.6 HONO + 0.6 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4412_a02MK	TrAa02AmiScCN	DEA + HONO \rightarrow NDELA + H ₂ O	0.1		Anastasio and Chu (2009)
A4413_a02MK	TrAa02AmiScCN	DEA + NO ₂ ⁻ \rightarrow NDELA + OH ⁻	0.1		Anastasio and Chu (2009)
A4414_a02MK	TrAa02AmiScCN	(HOET) ₂ NH ⁺ + NO ₂ \rightarrow DEANNO ₂ + H ⁺	0.0		Fell et al. (1990)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4415_a02MK	TrAa02AmiScCN	DEA + OH \rightarrow 0.5 HOETNHCH ₂ CHOH + 0.5 (HOET) ₂ NH ⁺ + 0.5 OH ⁻ + H ₂ O	8.0E9		Kishore et al. (2004)
A4416_a02MK	TrAa02AmiScCN	HOETNHCH ₂ CHOH + OH \rightarrow MEA + 2 HCHO	1.0E9		Kishore et al. (2004)
A4417_a02MK	TrAa02AmiScCN	DEA ⁺ + OH \rightarrow 0.275 HOETNH ₂ CH ₂ CHOH ⁺ + 0.725 (HOET) ₂ NH ⁺ + H ₂ O	4.5E8		Kishore et al. (2004)
A4418_a02MK	TrAa02AmiScCN	NDELA + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO	6.99E8		Fuller-Rowell (1993)
A4419_a02MK	TrAa02AmiScCN	DEANNO ₂ + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO ₂	8.67E8		Fuller-Rowell (1993)
A4500_a02MK	TrAa02Sc	GLUTARAC + OH \rightarrow SUCCAC + HO ₂	1.0E7		Ervens et al. (2004)
A4600_a02MK	TrAa02Sc	ADIPAC + OH \rightarrow GLUTARAC + HO ₂	1.0E7		Ervens et al. (2004)
A4610_a02MK	TrAa02AmiScCN	TEA + OH \rightarrow 0.5 DENCH ₂ CHOH + 0.5 (HOET) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	2.0E10		Kishore et al. (2004)
A4611_a02MK	TrAa02AmiScCN	DENCH ₂ CHOH + OH \rightarrow (HOET) ₂ N ⁺ CH ₂ CH ₂ OH + OH ⁻	3.18E9		Das and von Sonntag (1986)
A4612_a02MK	TrAa02AmiScCN	(HOET) ₂ N ⁺ CH ₂ CH ₂ OH \rightarrow DEA + HOCH ₂ CHO + H ⁺	3.0E6		Das and von Sonntag (1986)
A4613_a02MK	TrAa02AmiScCN	(HOET) ₃ N ⁺ + DENCH ₂ CHOH \rightarrow TEA + (HOET) ₂ N ⁺ CH ₂ CH ₂ OH	2.0E9		Das and von Sonntag (1986)
A4614_a02MK	TrAa02AmiScCN	TEA ⁺ + OH \rightarrow 0.275 (HOET) ₂ NH ⁺ CH ₂ CHOH + 0.725 (HOET) ₃ N ⁺ + H ₂ O	2.0E9		Kishore et al. (2004)
A4615_a02MK	TrAa02AmiScCN	TEA + N ₂ O ₃ \rightarrow 0.075 NDELA + 0.95 DENCH ₂ CHOH + 1.9 HONO	2.9E5		Mitch and Herckes (2012)
A4616_a02MK	TrAa02AmiScCN	TEA + N ₂ O ₄ \rightarrow 0.05 DEANNO ₂ + 0.1 NDELA + 0.9 DENCH ₂ CHOH + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A9405_a02MK	TrAa02MblScS	HSO ₃ ⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OH SO ₃ ⁻	0.436	-2990	Ervens et al. (2004)
A9406a_a02MK	TrAa02MblScS	CH ₂ OH SO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + HSO ₃ ⁻	1.22E-7		Ervens et al. (2004)
A9406b_a02MK	TrAa02MblScS	CH ₂ OH SO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + SO ₃ ²⁻ + H ⁺	3.8E-6	-5530	Ervens et al. (2004)
A9407_a02MK	TrAa02MblScS	SO ₃ ²⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OH SO ₃ ⁻ + O ₂ ⁻	1.36E5	-2450	Ervens et al. (2004)
A9408_a02MK	TrAa02MblScS	CH ₂ OH SO ₃ ⁻ + OH \rightarrow HCOOH + HO ₂ + HSO ₃ ⁻	3.0E8		Ervens et al. (2004)
A9409_a02MK	TrAa02MblScCS	DMS + O ₃ \rightarrow DMSO	8.61E8	-2600	Hoffmann et al. (2016)
A9410_a02MK	TrAa02MblScCS	DMS + OH \rightarrow DMSO + HO ₂	1.9E10		Hoffmann et al. (2016)
A9411_a02MK	TrAa02MblScCS	DMSO + OH \rightarrow MSIA + HO ₂ + CO ₂	6.65E9	-1270	Hoffmann et al. (2016)
A9412_a02MK	TrAa02MblScS	MSIA + O ₃ \rightarrow CH ₃ SO ₃ ⁻ + H ⁺	3.5E7		Hoffmann et al. (2016)
A9413_a02MK	TrAa02MblScS	MSIA + OH \rightarrow CH ₃ SO ₃ ⁻ + H ⁺ + HO ₂	6.0E9		Hoffmann et al. (2016)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n} s^{-1}$]	$-E_a/R[K]$	reference
A9414_a02MK	TrAa02MblScCS	HPMTF + OH \rightarrow HOOCH2SCO	1.0E10		Wollesen de Jonge et al. (2021)
A1000_a03	TrAa03Sc	O ₃ + O ₂ ⁻ \rightarrow OH + OH ⁻	1.5E9		Sehested et al. (1983)
A2100_a03	TrAa03Sc	OH + O ₂ ⁻ \rightarrow OH ⁻	1.0E10		Sehested et al. (1968)
A2101_a03	TrAa03Sc	OH + OH \rightarrow H ₂ O ₂	5.5E9		Buxton et al. (1988)
A2102_a03	TrAa03Sc	HO ₂ + O ₂ ⁻ \rightarrow H ₂ O ₂ + OH ⁻	1.0E8	-900	Christensen and Sehested (1988)
A2103_a03	TrAa03Sc	HO ₂ + OH \rightarrow H ₂ O	7.1E9		Sehested et al. (1968)
A2104_a03	TrAa03Sc	HO ₂ + HO ₂ \rightarrow H ₂ O ₂	9.7E5	-2500	Christensen and Sehested (1988)
A2105_a03	TrAa03Sc	H ₂ O ₂ + OH \rightarrow HO ₂	2.7E7	-1684	Christensen et al. (1982)
A3100_a03	TrAa03ScN	NO ₂ ⁻ + O ₃ \rightarrow NO ₃ ⁻	5.0E5	-6950	Damschen and Martin (1983)
A3101_a03	TrAa03ScN	NO ₂ + NO ₂ \rightarrow HNO ₃ + HONO	1.0E8		Lee and Schwartz (1981)
A3102_a03	TrAa03ScN	NO ₄ ⁻ \rightarrow NO ₂ ⁻	8.0E1		Warneck (1999)
A3200_a03	TrAa03ScN	NO ₂ + HO ₂ \rightarrow HNO ₄	1.8E9		Warneck (1999)
A3201_a03	TrAa03ScN	NO ₂ ⁻ + OH \rightarrow NO ₂ + OH ⁻	1.0E10		Wingenter et al. (1999)
A3202_a03	TrAa03ScN	NO ₃ + OH ⁻ \rightarrow NO ₃ ⁻ + OH	8.2E7	-2700	Exner et al. (1992)
A3203_a03	TrAa03ScN	HONO + OH \rightarrow NO ₂	1.0E10		Barker et al. (1970)
A3204_a03	TrAa03ScN	HONO + H ₂ O ₂ + H ⁺ \rightarrow HNO ₃ + H ⁺	4.6E3	-6800	Damschen and Martin (1983)
A4100_a03	TrAa03Sc	CO ₃ ⁻ + O ₂ ⁻ \rightarrow HCO ₃ ⁻ + OH ⁻	6.5E8		Ross et al. (1992)
A4101_a03	TrAa03Sc	CO ₃ ⁻ + H ₂ O ₂ \rightarrow HCO ₃ ⁻ + HO ₂	4.3E5		Ross et al. (1992)
A4102_a03	TrAa03Sc	HCOO ⁻ + CO ₃ ⁻ \rightarrow 2 HCO ₃ ⁻ + HO ₂	1.5E5		Ross et al. (1992)
A4103_a03	TrAa03Sc	HCOO ⁻ + OH \rightarrow OH ⁻ + HO ₂ + CO ₂	3.1E9	-1240	Chin and Wine (1994)
A4104_a03	TrAa03Sc	HCO ₃ ⁻ + OH \rightarrow CO ₃ ⁻	8.5E6		Ross et al. (1992)
A4105_a03	TrAa03Sc	HCHO + OH \rightarrow HCOOH + HO ₂	7.7E8	-1020	Chin and Wine (1994)
A4106_a03	TrAa03Sc	HCOOH + OH \rightarrow HO ₂ + CO ₂	1.1E8	-991	Chin and Wine (1994)
A4107_a03	TrAa03Sc	CH ₃ OO + O ₂ ⁻ \rightarrow CH ₃ OOH + OH ⁻	5.0E7		Jacob (1986)
A4108_a03	TrAa03Sc	CH ₃ OO + HO ₂ \rightarrow CH ₃ OOH	4.3E5		Jacob (1986)
A4109_a03	TrAa03Sc	CH ₃ OH + OH \rightarrow HCHO + HO ₂	9.7E8		Buxton et al. (1988)
A4110a_a03	TrAa03Sc	CH ₃ OOH + OH \rightarrow CH ₃ OO	2.7E7	-1715	Jacob (1986)
A4110b_a03	TrAa03Sc	CH ₃ OOH + OH \rightarrow HCHO + OH	1.1E7	-1715	Jacob (1986)
A6000_a03	TrAa03Cl	Cl + Cl \rightarrow Cl ₂	8.8E7		Wu et al. (1980)
A6001_a03	TrAa03Cl	Cl ₂ ⁻ + Cl ₂ ⁻ \rightarrow Cl ₂ + 2 Cl ⁻	3.5E9		Yu (2004)
A6100_a03	TrAa03Cl	Cl ⁻ + O ₃ \rightarrow ClO ⁻	3.0E-3		Hoigné et al. (1985)
A6101_a03	TrAa03Cl	Cl ₂ + O ₂ ⁻ \rightarrow Cl ₂ ⁻	1.0E9		Bjergbakke et al. (1981)
A6102_a03	TrAa03Cl	Cl ₂ ⁻ + O ₂ ⁻ \rightarrow 2 Cl ⁻	1.0E9		Jacobi (1996)*
A6200_a03	TrAa03Cl	Cl \rightarrow H ⁺ + ClOH ⁻	1.8E5		Yu (2004)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A6201_a03	TrAa03Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)
A6202_a03	TrAa03Cl	$Cl^- + OH \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a03	TrAa03Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a03	TrAa03MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a03	TrAa03Cl	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a03	TrAa03Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a03	TrAa03Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a03	TrAa03MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a03	TrAa03Cl	$ClOH^- \rightarrow Cl^- + OH$	6.0E9		Yu (2004)
A6210_a03	TrAa03Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a03	TrAa03ClN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a03	TrAa03ClN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a03	TrAa03ClN	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a03	TrAa03Cl	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A8100_a03	TrAa03MblI	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a03	TrAa03MblI	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A8200_a03	TrAa03MblI	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A8201_a03	TrAa03I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
A8202_a03	TrAa03MblI	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A8203_a03	TrAa03MblI	$IO_2^- + I^- + H^+ \rightarrow 2 HOI + OH^-$	2.0E10		Edblom et al. (1987)
A8600_a03	TrAa03MblClII	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601_a03	TrAa03MblClII	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8602_a03	TrAa03ClII	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A8603_a03	TrAa03MblClII	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8604_a03	TrAa03ClII	$HOI + Cl_2 \rightarrow IO_2^- + 2 Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A8605_a03	TrAa03ClII	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2 H^+$	5.0E5		Citri and Epstein (1988)
A8606_a03	TrAa03ClII	$ICl + I^- \rightarrow I_2 + Cl^-$	1.1E9		Margerum et al. (1986)
A9100_a03	TrAa03ScS	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101_a03	TrAa03MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a03	TrAa03ScS	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a03	TrAa03ScS	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a03	TrAa03ScS	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105_a03	TrAa03S	$SO_5^- + SO_3^{2-} \rightarrow .72 SO_4^- + .72 SO_4^{2-} + .28 SO_3^- + .28 HSO_5^- + .28 OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9106_a03	TrAa03S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + \text{LSULFUR}$	1.0E8		Ross et al. (1992)*
A9200_a03	TrAa03ScS	$SO_3^- + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201_a03	TrAa03ScS	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202_a03	TrAa03ScS	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203_a03	TrAa03ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a03	TrAa03ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A9205_a03	TrAa03ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note*
A9206_a03	TrAa03MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a03	TrAa03ScS	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208_a03	TrAa03ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note*
A9209_a03	TrAa03MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a03	TrAa03ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211_a03	TrAa03S	$HSO_3^- + SO_5^- \rightarrow .75 SO_4^- + .75 SO_4^{2-} + .75 H^+ + .25 SO_3^- + .25 HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212_a03	TrAa03ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2 HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A9301_a03	TrAa03ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302_a03	TrAa03ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Løgager et al. (1993)
A9304_a03	TrAa03ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a03	TrAa03ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400_a03	TrAa03ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OH SO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)*
A9401_a03	TrAa03ScS	$SO_3^- + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402_a03	TrAa03ScS	$HSO_3^- + HCHO \rightarrow CH_2OH SO_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A9403_a03	TrAa03ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404_a03	TrAa03ScS	$CH_2OH SO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600_a03	TrAa03ClS	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2 Cl^-$	6.2E7		Jacobi et al. (1996)
A9601_a03	TrAa03MblClS	$SO_3^- + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a03	TrAa03ClS	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603_a03	TrAa03ClS	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604_a03	TrAa03ClS	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2 Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a03	TrAa03MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A9606_a03	TrAa03ClS	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9800_a03	TrAa03IS	$HSO_3^- + I_2 \rightarrow 2 I^- + HSO_4^- + 2 H^+$	1.7E9		Yiin and Margerum (1990)
A11101_a03	TrAa03Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11102_a03	TrAa03Fe	$Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$	5E7		de Laat and Le (2006)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A11103_a03	TrAa03Fe	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	8.2E5		Løgager et al. (1992)
A11201a_a03	TrAa03Fe	$Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$	2.7E8		de Laat and Le (2006)
A11201b_a03	TrAa03Fe	$FeOH^+ + OH \rightarrow Fe^{3+} + 2 OH^-$	2.7E8		de Laat and Le (2006)
A11202a_a03	TrAa03Fe	$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$	5.5E1		de Laat and Le (2006)
A11202b_a03	TrAa03Fe	$FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2 OH^-$	5.9E6		de Laat and Le (2006)
A11203_a03	TrAa03Fe	$FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$	2.3E-3		de Laat and Le (2006)
A11204_a03	TrAa03Fe	$Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$	2.3E-3		de Laat and Le (2006)
A11206_a03	TrAa03Fe	$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO_2^-$	1.2E6		de Laat and Le (2006)
A11208a_a03	TrAa03Fe	$FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$	1.5E8		Rush and Bielski (1985)
A11208b_a03	TrAa03Fe	$Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2 OH^-$	1.5E8		Rush and Bielski (1985)
A11209_a03	TrAa03Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2 OH^-$	1.0E7		Rush and Bielski (1985)
A11210_a03	TrAa03Fe	$Fe^{2+} + OH \rightarrow FeOH^{2+}$	4.3E8		Christensen and Sehested (1981)
A11211_a03	TrAa03Fe	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	9.5E3		Løgager et al. (1992)
A11212_a03	TrAa03Fe	$FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$	1.3E-2		Løgager et al. (1992)
A11213_a03	TrAa03Fe	$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	2.0E6		Løgager et al. (1992)
A11214_a03	TrAa03Fe	$FeO^{2+} + OH \rightarrow Fe^{3+} + HO_2^-$	1.0E7		Løgager et al. (1992)
A11215_a03	TrAa03Fe	$FeO^{2+} + Fe^{2+} \rightarrow 2 Fe^{3+} + 2 OH^-$	1.4E5		Løgager et al. (1992)
A11216_a03	TrAa03Fe	$FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+}$	1.8E4		Jacobsen et al. (1997)
A11217_a03	TrAa03Fe	$Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2 Fe^{3+} + OH^-$	2.0		Jacobsen et al. (1997)
A11218_a03	TrAa03Fe	$Fe(OH)_2Fe^{4+} \rightarrow 2 Fe^{3+} + 2 OH^-$	0.49		Jacobsen et al. (1997)
A11301_a03	TrAa03FeN	$FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$	1.1E4		Jacobsen et al. (1998)
A11302_a03	TrAa03FeN	$Fe^{2+} + NO_3 \rightarrow Fe^{3+} + NO_3^-$	8.0E6		Herrmann et al. (2000)*
A11601_a03	TrAa03ClFe	$Fe^{2+} + Cl \rightarrow Fe^{3+} + Cl^-$	5.9E9		Jayson et al. (1973)
A11602a_a03	TrAa03ClFe	$Fe^{2+} + Cl_2^- \rightarrow Fe^{3+} + 2 Cl^-$	1E7		Thornton and Laurence (1973)
A11602b_a03	TrAa03ClFe	$Fe^{2+} + Cl_2^- \rightarrow FeCl^{2+} + Cl^-$	4E6		Thornton and Laurence (1973)
A11603a_a03	TrAa03ClFe	$FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO_2^-$	1.2E6		de Laat and Le (2006)
A11603b_a03	TrAa03ClFe	$FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A11604a_a03	TrAa03ClFe	$FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604b_a03	TrAa03ClFe	$FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2 Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A11604c_a03	TrAa03ClFe	$FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$	5E7		de Laat and Le (2006)
A11604d_a03	TrAa03ClFe	$FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2 Cl^- + O_2$	5E7		de Laat and Le (2006)
A11605_a03	TrAa03ClFe	$FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2 OH^-$	1E2		Jacobsen et al. (1998)*
A11901_a03	TrAa03FeS	$FeO^{2+} + SO_2 \rightarrow Fe^{3+} + SO_3^-$	4.5E5		Jacobsen et al. (1998)*
A11902_a03	TrAa03FeS	$FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH^-$	2.5E5		Jacobsen et al. (1998)*

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A11903_a03	TrAa03FeS	$FeOH^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	30		Ziajka et al. (1994)
A11904_a03	TrAa03FeS	$Fe^{2+} + SO_5^- \rightarrow FeOH^{2+} + HSO_5^-$	8E5		Ziajka et al. (1994)*
A11905_a03	TrAa03FeS	$Fe^{2+} + HSO_5^- \rightarrow FeOH^{2+} + SO_4^-$	3.0E4		Gilbert and Stell (1990)
A11906_a03	TrAa03FeS	$Fe^{2+} + SO_4^- \rightarrow FeSO_4^+$	3.6E7		McElroy and Waygood (1990)*
A11907_a03	TrAa03FeS	$FeOH^{2+} + SO_3^- \rightarrow Fe^{2+} + HSO_4^-$	3E7		Warneck (2018)
A11908_a03	TrAa03FeS	$FeSO_3^+ + SO_3^- \rightarrow Fe^{2+} + SO_4^{2-} + SO_2$	2.16E6		Warneck (2018)*
A3103_a03MK	TrAa03ScN	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	6.4E6		Pires et al. (1994)
A3104_a03MK	TrAa03ScN	$NO_2 + NO_2 \rightarrow N_2O_4$	4.5E8		Mack and Bolton (1999)
A3105_a03MK	TrAa03ScN	$NO + NO_2 \rightarrow N_2O_3$	1.1E9		Mack and Bolton (1999)
A3106_a03MK	TrAa03ScN	$NO_2 + O_2^- \rightarrow O_2 + NO_2^-$	1.0E8		Ervens et al. (2003)
A3107_a03MK	TrAa03ScN	$NO_2 + O_2^- \rightarrow NO_4^-$	4.5E9		Ervens et al. (2003)
A3109_a03MK	TrAa03ScN	$N_2O_3 \rightarrow 2 NO_2^- + 2 H^+$	1.6E3		Licht et al. (1988)
A3205_a03MK	TrAa03ScN	$NO + OH \rightarrow HONO$	1.0E10		Mack and Bolton (1999)
A3206_a03MK	TrAa03ScN	$HONO + HONO \rightarrow N_2O_3 + H_2O$	5.6		Schwartz (1983)
A4111_a03MK	TrAa03Sc	$CH_3OO + CH_3OO \rightarrow HCHO + CH_3OH + HO_2$	1.7E8	-2200	Ervens et al. (2004)
A4112_a03MK	TrAa03Sc	$CH_3OH + OH \rightarrow CH_2(OH)_2 + HO_2$	1.0E9		Ervens et al. (2004)
A4113_a03MK	TrAa03Sc	$CH_3OOH + OH \rightarrow HCOOH + HO_2$	6.0E6	-1715	Ervens et al. (2004)
A4114_a03MK	TrAa03Sc	$CH_2(OH)_2 + OH \rightarrow HCOOH + HO_2$	1.0E9		Ervens et al. (2004)
A4120_a03MK	TrAa03AmiScN	$MMA + N_2O_4 \rightarrow 0.3 MMNNO_2 + 0.7 CH_2NH_2 + 1.7 HONO$	4.0E7		Challis and Kyrtopoulos (1979)
A4121_a03MK	TrAa03AmiScN	$MMA + OH \rightarrow 0.5 CH_2NH_2 + 0.5 CH_3NH_2^+ + 0.5 OH^- + H_2O$	6.9E9		Simić et al. (1971)
A4122_a03MK	TrAa03AmiScN	$CH_2NH_2 + O_2 \rightarrow CH_2NH_2^+ + O_2^-$	3.5E9		Duff et al. (2003)
A4123_a03MK	TrAa03AmiScN	$CH_2NH_2^+ \rightarrow NH_3 + HCHO + H^+$	4.0		Duff et al. (2003)
A4124_a03MK	TrAa03AmiScN	$CH_2NH_2 + CH_2NH_2 \rightarrow NH_2CH_2CH_2NH_2$	2.0E9		Simić et al. (1971)
A4125_a03MK	TrAa03AmiScN	$CH_3NH_2^+ + CH_3NH_2^+ \rightarrow CH_3NHNHCH_3 + 2 H^+$	2.0E9		Simić et al. (1971)
A4126_a03MK	TrAa03AmiScN	$MMA^+ + OH \rightarrow 0.275 CH_2NH_3^+ + 0.725 CH_3NH_2^+ + H_2O$	1.1E8		Simić et al. (1971)
A4127_a03MK	TrAa03AmiScN	$HNCO \rightarrow NH_3 + CO_2$	7.83E-4		Roberts et al. (2011)
A4128_a03MK	TrAa03AmiScN	$H_2NCHO + OH \rightarrow HNCO + H_2O$	3.7E8		Munoz et al. (2000)
A4129_a03MK	TrAa03AScN	$MMNNO_2 + OH \rightarrow NH_4^+ + HCHO + OH^- + NO_2$	5.44E8		Fuller-Rowell (1993)
A4200_a03MK	TrAa03ScC	$GLYOX + OH \rightarrow HCOCO_2H + HO_2$	1.1E9	-1516	Ervens et al. (2004)
A4201_a03MK	TrAa03ScC	$HCOCO_2H + OH \rightarrow OXALAC + HO_2 + 2 CO_2$	3.6E8	-1000	Ervens et al. (2004)
A4202_a03MK	TrAa03ScC	$HCOCOO^- + OH \rightarrow HC_2O_4^- + HO_2 + 2 CO_2$	2.9E9	-4300	Ervens et al. (2004)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4203_a03MK	TrAa03ScC	$HOCH_2CHO + OH \rightarrow GLYOX + HO_2$	1.2E9		Ervens et al. (2004)
A4204_a03MK	TrAa03ScC	$HOCH_2CO_2H + OH \rightarrow HCOCO_2H + HO_2$	1.2E9		Ervens et al. (2004)
A4205_a03MK	TrAa03Sc	$C_2O_4^{2-} + OH \rightarrow OH^- + O_2^-$	1.6E8	-4300	Ervens et al. (2004)
A4206_a03MK	TrAa03Sc	$HC_2O_4^- + OH \rightarrow OH^- + HO_2$	1.9E8	-2800	Ervens et al. (2004)
A4207_a03MK	TrAa03Sc	$OXALAC + OH \rightarrow H_2O + HO_2$	1.4E6		Ervens et al. (2004)
A4208_a03MK	TrAa03ScC	$CH_3COO^- + OH \rightarrow HO_2 + OH^- + CH_3COO_2$	1.0E8	-1800	Ervens et al. (2004)
A4209_a03MK	TrAa03ScC	$CH_3COOH + OH \rightarrow HO_2 + H_2O + CH_3COO_2$	1.5E7	-1330	Ervens et al. (2004)
A4210_a03MK	TrAa03AmiScCN	$DMA + N_2O_3 \rightarrow NDMA + HONO$	4.29E7		Mirvish (1975)
A4211_a03MK	TrAa03AmiScCN	$DMA + N_2O_4 \rightarrow 0.4 DMNNO_2 + 0.4 NDMA + 0.2 CH_3NHCH_2 + 0.6 HONO + 0.6 HNO_3$	4.0E7		Challis and Kyrtopoulos (1979)
A4212_a03MK	TrAa03AmiScCN	$DMA + HONO \rightarrow NDMA + H_2O$	0.1		Anastasio and Chu (2009)
A4213_a03MK	TrAa03AmiScCN	$DMA + NO_2^- \rightarrow NDMA + OH^-$	0.1		Anastasio and Chu (2009)
A4214_a03MK	TrAa03AmiScCN	$(CH_3)_2NH^+ + NO_2 \rightarrow DMNNO_2 + H^+$	1.0E4		Fell et al. (1990)
A4215_a03MK	TrAa03AmiScCN	$DMA + OH \rightarrow 0.5 CH_3NHCH_2 + 0.5 (CH_3)_2NH^+ + 0.5 OH^- + H_2O$	8.9E9		Lee et al. (2007a)
A4216_a03MK	TrAa03AmiScCN	$CH_3NHCH_2 + O_2 \rightarrow CH_3NH^+CH_2 + O_2^-$	3.5E9		Duff et al. (2003)
A4217_a03MK	TrAa03AmiScCN	$CH_3NH^+CH_2 \rightarrow MMA + HCHO + H^+$	4.0		Duff et al. (2003)
A4218_a03MK	TrAa03AmiScCN	$CH_3NHCH_2 + CH_3NHCH_2 \rightarrow DMA + CH_3NH^+CH_2 + OH^-$	2.0E9		Das and von Sonntag (1986)
A4219_a03MK	TrAa03AmiScCN	$CH_3NHCH_2 + (CH_3)_2NH^+ \rightarrow DMA + CH_3NH^+CH_2$	2.0E9		Das and von Sonntag (1986)
A4220_a03MK	TrAa03AmiScCN	$DMA^+ + OH \rightarrow 0.275 CH_3NH_2^+CH_2 + 0.725 (CH_3)_2NH^+ + H_2O$	6.0E7		Lee et al. (2007a)
A4221_a03MK	TrAa03AmiScCN	$MEA + N_2O_4 \rightarrow 0.3 MEANNO_2 + 0.7 NH_2CH_2CHOH + 1.7 HONO$	4.0E7		Challis and Kyrtopoulos (1979)
A4222_a03MK	TrAa03AmiScCN	$MEA + OH \rightarrow 0.5 NH_2CH_2CHOH + 0.5 HOCH_2CH_2NH_2^+ + 0.5 OH^- + H_2O$	2.9E9		Kishore et al. (2004)
A4223_a03MK	TrAa03AmiScCN	$NH_2CH_2CHOH + OH \rightarrow CH_2NH_2 + HCHO$	1.0E9		Kishore et al. (2004)
A4224_a03MK	TrAa03AmiScCN	$MEA^+ + OH \rightarrow 0.275 HOCHCH_2NH_3^+ + 0.725 HOCH_2CH_2NH_2^+ + H_2O$	3.0E8		Kishore et al. (2004)
A4225_a03MK	TrAa03AmiScCN	$H_2NCOCH_2OH + OH \rightarrow HNCO + HCHO + HO_2$	1.9E8		Roble (1995)
A4226_a03MK	TrAa03AmiScCN	$CH_3NHCHO + OH \rightarrow HNCO + HCHO + HO_2$	1.2E9		Roble (1995)
A4227_a03MK	TrAa03AmiScCN	$NDMA + OH \rightarrow MMA^+ + HCHO + OH^- + NO$	4.5E8		Lee et al. (2007b)
A4228_a03MK	TrAa03AmiScCN	$DMNNO_2 + OH \rightarrow MMA^+ + HCHO + OH^- + NO_2$	5.44E8		Fuller-Rowell (1993)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4229_a03MK	TrAa03AmiScCN	MEANNO + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO	4.5E8		Lee et al. (2007b)
A4230_a03MK	TrAa03AmiScCN	MEANNO ₂ + OH \rightarrow CH ₂ NH ₃ ⁺ + HCHO + OH ⁻ + NO ₂	5.44E8		Fuller-Rowell (1993)
A4231_a03MK	TrAa03AmiScCN	CH ₃ NCO \rightarrow MMA + CO ₂	7.83E-4		Roberts et al. (2011)
A4300_a03MK	TrAa03ScC	MGLYOX + OH \rightarrow MGLYOAC + HO ₂	1.1E9	-1600	Ervens et al. (2004)
A4301_a03MK	TrAa03ScC	CH ₃ COCOO ⁻ + OH \rightarrow CH ₃ COO ₂ + HO ₂ + CO ₂ + O ₂ ⁻	7.0E8		Ervens et al. (2004)
A4302_a03MK	TrAa03ScC	MGLYOAC + OH \rightarrow CH ₃ CHO + HO ₂ + H ₂ O + CO ₂	1.2E8		Ervens et al. (2004)
A4303_a03MK	TrAa03Sc	DOC + OH \rightarrow DOCO + HO ₂	4.1E8		Barth (1992)
A4304_a03MK	TrAa03Sc	MALONAC + OH \rightarrow OXALAC + HO ₂	5.0E7		Ervens et al. (2004)
A4310_a03MK	TrAa03AmiScCN	TMA + N ₂ O ₃ \rightarrow 0.075 NDMA + 1.9 HONO + 0.95 (CH ₃) ₂ NCH ₂	4.0E7		Challis and Kyrtopoulos (1979)
A4311_a03MK	TrAa03AmiScCN	TMA + N ₂ O ₄ \rightarrow 0.05 DMNNO ₂ + 0.1 NDMA + 0.90 (CH ₃) ₂ NCH ₂ + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4312_a03MK	TrAa03AmiScCN	TMA + OH \rightarrow 0.5 (CH ₃) ₂ NCH ₂ + 0.5 (CH ₃) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	1.2E10		Das and von Sonntag (1986)
A4313_a03MK	TrAa03AmiScCN	(CH ₃) ₂ NCH ₂ + O ₂ \rightarrow (CH ₃) ₂ N ⁺ CH ₂ + O ₂ ⁻	3.5E9		Duff et al. (2003)
A4314_a03MK	TrAa03AmiScCN	(CH ₃) ₂ N ⁺ CH ₂ \rightarrow DMA + HCHO + H ⁺	4.0		Duff et al. (2003)
A4315_a03MK	TrAa03AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₂ NCH ₂ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂ + OH ⁻	2.0E9		Das and von Sonntag (1986)
A4316_a03MK	TrAa03AmiScCN	(CH ₃) ₂ NCH ₂ + (CH ₃) ₃ N ⁺ \rightarrow TMA + (CH ₃) ₂ N ⁺ CH ₂	2.0E9		Das and von Sonntag (1986)
A4317_a03MK	TrAa03AmiScCN	TMA ⁺ + OH \rightarrow 0.275 (CH ₃) ₂ NH ⁺ CH ₂ + 0.725 (CH ₃) ₃ N ⁺ + H ₂ O	4.0E8		Das and von Sonntag (1986)
A4318_a03MK	TrAa03AmiScCN	DMNCHO + OH \rightarrow CH ₃ NCO + HCHO + HO ₂	1.7E9		Roble (1995)
A4400_a03MK	TrAa03Sc	SUCCAC + OH \rightarrow MALONAC + HO ₂	5.0E7		Ervens et al. (2004)
A4410_a03MK	TrAa03AmiScCN	DEA + N ₂ O ₃ \rightarrow NDELA + HONO	1.0E7		Mitch and Herckes (2012)
A4411_a03MK	TrAa03AmiScCN	DEA + N ₂ O ₄ \rightarrow 0.4 DEANNO ₂ + 0.4 NDELA + 0.2 HOETNHCH ₂ CHOH + 0.6 HONO + 0.6 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A4412_a03MK	TrAa03AmiScCN	DEA + HONO \rightarrow NDELA + H ₂ O	0.1		Anastasio and Chu (2009)
A4413_a03MK	TrAa03AmiScCN	DEA + NO ₂ ⁻ \rightarrow NDELA + OH ⁻	0.1		Anastasio and Chu (2009)
A4414_a03MK	TrAa03AmiScCN	(HOET) ₂ NH ⁺ + NO ₂ \rightarrow DEANNO ₂ + H ⁺	0.0		Fell et al. (1990)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A4415_a03MK	TrAa03AmiScCN	DEA + OH \rightarrow 0.5 HOETNHCH ₂ CHOH + 0.5 (HOET) ₂ NH ⁺ + 0.5 OH ⁻ + H ₂ O	8.0E9		Kishore et al. (2004)
A4416_a03MK	TrAa03AmiScCN	HOETNHCH ₂ CHOH + OH \rightarrow MEA + 2 HCHO	1.0E9		Kishore et al. (2004)
A4417_a03MK	TrAa03AmiScCN	DEA ⁺ + OH \rightarrow 0.275 HOETNH ₂ CH ₂ CHOH ⁺ + 0.725 (HOET) ₂ NH ⁺ + H ₂ O	4.5E8		Kishore et al. (2004)
A4418_a03MK	TrAa03AmiScCN	NDELA + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO	6.99E8		Fuller-Rowell (1993)
A4419_a03MK	TrAa03AmiScCN	DEANNO ₂ + OH \rightarrow MEA ⁺ + 2 HCHO + OH ⁻ + NO ₂	8.67E8		Fuller-Rowell (1993)
A4500_a03MK	TrAa03Sc	GLUTARAC + OH \rightarrow SUCCAC + HO ₂	1.0E7		Ervens et al. (2004)
A4600_a03MK	TrAa03Sc	ADIPAC + OH \rightarrow GLUTARAC + HO ₂	1.0E7		Ervens et al. (2004)
A4610_a03MK	TrAa03AmiScCN	TEA + OH \rightarrow 0.5 DENCH ₂ CHOH + 0.5 (HOET) ₃ N ⁺ + 0.5 OH ⁻ + H ₂ O	2.0E10		Kishore et al. (2004)
A4611_a03MK	TrAa03AmiScCN	DENCH ₂ CHOH + OH \rightarrow (HOET) ₂ N ⁺ CH ₂ CH ₂ OH + OH ⁻	3.18E9		Das and von Sonntag (1986)
A4612_a03MK	TrAa03AmiScCN	(HOET) ₂ N ⁺ CH ₂ CH ₂ OH \rightarrow DEA + HOCH ₂ CHO + H ⁺	3.0E6		Das and von Sonntag (1986)
A4613_a03MK	TrAa03AmiScCN	(HOET) ₃ N ⁺ + DENCH ₂ CHOH \rightarrow TEA + (HOET) ₂ N ⁺ CH ₂ CH ₂ OH	2.0E9		Das and von Sonntag (1986)
A4614_a03MK	TrAa03AmiScCN	TEA ⁺ + OH \rightarrow 0.275 (HOET) ₂ NH ⁺ CH ₂ CHOH + 0.725 (HOET) ₃ N ⁺ + H ₂ O	2.0E9		Kishore et al. (2004)
A4615_a03MK	TrAa03AmiScCN	TEA + N ₂ O ₃ \rightarrow 0.075 NDELA + 0.95 DENCH ₂ CHOH + 1.9 HONO	2.9E5		Mitch and Herckes (2012)
A4616_a03MK	TrAa03AmiScCN	TEA + N ₂ O ₄ \rightarrow 0.05 DEANNO ₂ + 0.1 NDELA + 0.9 DENCH ₂ CHOH + 0.9 HONO + 0.9 HNO ₃	4.0E7		Challis and Kyrtopoulos (1979)
A9405_a03MK	TrAa03MblScS	HSO ₃ ⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OH SO ₃ ⁻	0.436	-2990	Ervens et al. (2004)
A9406a_a03MK	TrAa03MblScS	CH ₂ OH SO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + HSO ₃ ⁻	1.22E-7		Ervens et al. (2004)
A9406b_a03MK	TrAa03MblScS	CH ₂ OH SO ₃ ⁻ \rightarrow CH ₂ (OH) ₂ + SO ₃ ²⁻ + H ⁺	3.8E-6	-5530	Ervens et al. (2004)
A9407_a03MK	TrAa03MblScS	SO ₃ ²⁻ + CH ₂ (OH) ₂ \rightarrow CH ₂ OH SO ₃ ⁻ + O ₂ ⁻	1.36E5	-2450	Ervens et al. (2004)
A9408_a03MK	TrAa03MblScS	CH ₂ OH SO ₃ ⁻ + OH \rightarrow HCOOH + HO ₂ + HSO ₃ ⁻	3.0E8		Ervens et al. (2004)
A9409_a03MK	TrAa03MblScCS	DMS + O ₃ \rightarrow DMSO	8.61E8	-2600	Hoffmann et al. (2016)
A9410_a03MK	TrAa03MblScCS	DMS + OH \rightarrow DMSO + HO ₂	1.9E10		Hoffmann et al. (2016)
A9411_a03MK	TrAa03MblScCS	DMSO + OH \rightarrow MSIA + HO ₂ + CO ₂	6.65E9	-1270	Hoffmann et al. (2016)
A9412_a03MK	TrAa03MblScS	MSIA + O ₃ \rightarrow CH ₃ SO ₃ ⁻ + H ⁺	3.5E7		Hoffmann et al. (2016)
A9413_a03MK	TrAa03MblScS	MSIA + OH \rightarrow CH ₃ SO ₃ ⁻ + H ⁺ + HO ₂	6.0E9		Hoffmann et al. (2016)

Table 6: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A9414_a03MK	TrAa03MblScCs	HPMTF + OH \rightarrow HOOCH2SCO	1.0E10		Wollesen de Jonge et al. (2021)

Specific notes

A6102_a01: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A6301_a01: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A9105_a01: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9106_a01: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^- , it will have an effect. However, we currently assume only the stable $\text{S}_2\text{O}_8^{2-}$ as product. Since $\text{S}_2\text{O}_8^{2-}$ is not treated explicitly in the mechanism, SO_4^{2-} is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.

A9205_a01: D. Sedlak, pers. comm. (1993).

A9208_a01: D. Sedlak, pers. comm. (1993).

A9400_a01: Product $2.48 \times 10^7 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9402_a01: Product $790 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9605_a01: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOCl}$.

A11302_a01: value from Pikaev et al. (1974)

A11605_a01: products assumed

A11901_a01: products assumed

A11902_a01: products assumed

A11904_a01: Assumed. Note that CAPRAM 2.4 lists $k=4.3\text{E}7$ from Herrmann Air Pollution Research Report 57 and it also lists $k=2.65\text{E}7$ from Williams PhD 1996 <http://lib.leeds.ac.uk/record=b1835184~S5>. Brand and van Eldik (1995) also list $k=3.56\text{E}4$ from Waygood EUROTRAC 1992 report.

A11906_a01: $3\text{E}8*6500/(48000+6500)$

A11908_a01: Assuming that the intermediate $\text{S}_2\text{O}_6^{2-}$ dissociates quickly.

A6102_a02: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A6301_a02: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A9105_a02: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9106_a02: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^- , it will have an effect. However, we currently assume only the stable $\text{S}_2\text{O}_8^{2-}$ as product. Since $\text{S}_2\text{O}_8^{2-}$ is not treated explicitly in the mechanism, SO_4^{2-} is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.

A9205_a02: D. Sedlak, pers. comm. (1993).

A9208_a02: D. Sedlak, pers. comm. (1993).

A9400_a02: Product $2.48 \times 10^7 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9402_a02: Product $790 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9605_a02: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOCl}$.

A11302_a02: value from Pikaev et al. (1974)

A11605_a02: products assumed

A11901_a02: products assumed

A11902_a02: products assumed

A11904_a02: Assumed. Note that CAPRAM 2.4 lists $k=4.3\text{E}7$ from Herrmann Air Pollution Research Report 57 and it also lists $k=2.65\text{E}7$ from Williams PhD 1996 <http://lib.leeds.ac.uk/record=b1835184~S5>. Brand and van Eldik (1995) also list $k=3.56\text{E}4$ from Waygood EUROTRAC 1992 report.

A11906_a02: $3\text{E}8*6500/(48000+6500)$

A11908_a02: Assuming that the intermediate $\text{S}_2\text{O}_6^{2-}$ dissociates quickly.

A6102_a03: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A6301_a03: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A9105_a03: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9106_a03: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^- , it will have an effect. However, we currently assume only the stable

$\text{S}_2\text{O}_8^{2-}$ as product. Since $\text{S}_2\text{O}_8^{2-}$ is not treated explicitly in the mechanism, SO_4^{2-} is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.

A9205_a03: D. Sedlak, pers. comm. (1993).

A9208_a03: D. Sedlak, pers. comm. (1993).

A9400_a03: Product $2.48 \times 10^7 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9402_a03: Product $790 \times 5.5 \times 10^{-4}$ considering the hydrated form of HCHO.

A9605_a03: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOCl}$.

A11302_a03: value from Pikaev et al. (1974)

A11605_a03: products assumed

A11901_a03: products assumed

A11902_a03: products assumed

A11904_a03: Assumed. Note that CAPRAM 2.4 lists $k=4.3\text{E}7$ from Herrmann Air Pollution Re-

search Report 57 and it also lists $k=2.65\text{E}7$ from Williams PhD 1996 <http://lib.leeds.ac.uk/record=b1835184~S5>. Brand and van Eldik (1995) also list $k=3.56\text{E}4$ from Waygood EUROTRAC 1992 report.

A11906_a03: $3\text{E}8*6500/(48000+6500)$

A11908_a03: Assuming that the intermediate $\text{S}_2\text{O}_6^{2-}$ dissociates quickly.

References

- Albaladejo, J., Jiménez, E., Notario, A., Cabañas, B., and Martínez, E.: CH_3O yield in the $\text{CH}_3 + \text{O}_3$ reaction using the LP/LIF technique at room temperature, *J. Phys. Chem. A*, 106, 2512–2519, doi:10.1021/jp012249o, 2002.
- Anastasio, C. and Chu, L.: Photochemistry of nitrous acid (HONO) and nitrous acidium ion (H_2ONO^+ in aqueous solution and ice, *Environ. Sci. Technol.*, 43, 1108–1114, 2009.
- Anderson, L. C. and Fahey, D. W.: Studies with ClONO_2 : Thermal dissociation rate and catalytic conversion to NO using an NO/ O_3 chemiluminescence detector, *J. Phys. Chem.*, 94, 644–652, doi:10.1021/J100365A027, 1990.
- Andrews, D. U., Heazlewood, B. R., Maccarone, A. T., Conroy, T., Payne, R. J., Jordan, M. J. T., and Kable, S. H.: Photo-tautomerization of acetaldehyde to vinyl alcohol: a potential route to tropospheric acids, *Science*, 337, 1203–1206, doi:10.1126/science.1220712, 2012.
- Aschmann, S. M., Nishino, N., Arey, J., and Atkinson, R.: Products of the OH radical-initiated reactions of furan, 2- and 3-methylfuran, and 2,3- and 2,5-dimethylfuran in the presence of NO, *J. Phys. Chem. A*, 118, 457–466, doi:10.1021/jp410345k, 2014.
- Atkinson, R.: Gas-phase tropospheric chemistry of volatile organic compounds: 1. Alkanes and alkenes, *J. Phys. Chem. Ref. Data*, 26, 215–290, doi:10.1063/1.556012, 1997.
- Atkinson, R.: Kinetics of the gas-phase reactions of OH radicals with alkanes and cycloalkanes, *Atmos. Chem. Phys.*, 3, 2233–2307, doi:10.5194/ACP-3-2233-2003, 2003.
- Atkinson, R. and Arey, J.: Atmospheric degradation of volatile organic compounds, *Chem. Rev.*, 103, 4605–4638, doi:10.1021/cr0206420, 2003.
- Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume I – gas phase reactions of O_x , HO_x , NO_x and SO_x species, *Atmos. Chem. Phys.*, 4, 1461–1738, doi:10.5194/ACP-4-1461-2004, 2004.
- Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and IUPAC Subcommittee: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II – gas phase reactions of organic species, *Atmos. Chem. Phys.*, 6, 3625–4055, doi:10.5194/ACP-6-3625-2006, 2006.
- Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume III – gas phase reactions of inorganic halogens, *Atmos. Chem. Phys.*, 7, 981–1191, doi:10.5194/ACP-7-981-2007, 2007.
- Baeza-Romero, M. T., Glowacki, D. R., Blitz, M. A., Heard, D., Pilling, M. J., Rickard, A. R., and Seakins, P. W.: A combined experimental and theoretical study of the reaction between methylglyoxal and OH/OD radical: OH regeneration, *Phys. Chem. Chem. Phys.*, 9, 4114–4128, doi:10.1039/b702916k, 2007.
- Bale, C. S. E., Canosa-Mas, C. E., Shallcross, D. E., and Wayne, R. P.: A discharge-flow study of the kinetics of the reactions of IO with CH_3O_2 and CF_3O_2 , *Phys. Chem. Chem. Phys.*, 7, 2164–2172, doi:10.1039/B501903F, 2005.
- Banic, C. M., Beauchamp, S. T., Tordon, R. J., Schroeder, W. H., Steffen, A., Anlauf, K. A., and Wong, H. K. T.: Vertical distribution of gaseous elemental mercury in Canada, *J. Geophys. Res.*, 108D, 4264, doi:10.1029/2002JD002116, 2003.
- Barker, G. C., Fowles, P., and Stringer, B.: Pulse radiolytic induced transient electrical conductance in liquid solutions, *Trans. Faraday Soc.*, 66, 1509–1519, doi:10.1039/TF9706601509, 1970.
- Barnes, I., Becker, K. H., Fink, E. H., Reimer, A., Zabel, F., and Niki, H.: FTIR spectroscopic study of the gas-phase reaction of HO_2 with H_2CO , *Chem. Phys. Lett.*, 115, 1–8, doi:10.1016/0009-2614(85)80091-9, 1985.
- Barnes, I., Becker, K. H., and Zhu, T.: Near UV absorption-spectra and photolysis products of difunctional organic nitrates - possible importance as NO_x reservoirs, *J. Atmos. Chem.*, 17, 353–373, doi:10.1007/BF00696854, 1993.
- Barth, C. A.: Nitric oxide in the lower thermosphere, *Planet. Space Sci.*, 40, 315–336, doi:10.1016/0032-0633(92)90067-X, 1992.
- Bates, K. H., Crounse, J. D., St. Clair, J. M., Bennett, N. B., Nguyen, T. B., Seinfeld, J. H., Stoltz, B. M., and Wennberg, P. O.: Gas phase production and loss of isoprene epoxydiols, *J. Phys. Chem. A*, 118, 1237–1246, doi:10.1021/jp4107958, 2014.
- Baulch, D. L., Bowman, C. T., Cobos, C. J., Cox, R. A., Just, T., Kerr, J. A., Pilling, M. J., Stocker, D., Troe, J., Tsang, W., Walker, R. W., and Warnatz, J.: Evaluated kinetic data for combustion modeling: Supple-

- ment II, *J. Phys. Chem. Ref. Data*, 34, 757–1397, doi:10.1063/1.1748524, 2005.
- Becker, K. H., Kurtenbach, R., Schmidt, F., and Wiesen, P.: Kinetics of the NCO radical reacting with atoms and selected molecules, *Combust. Flame*, 120, 570–577, doi:10.1016/S0010-2180(99)00108-X, 2000.
- Behnke, W., Scheer, V., and Zetzsch, C.: Production of BrNO₂, Br₂ and ClNO₂ from the reaction between sea spray aerosol and N₂O₅, *J. Aerosol Sci.*, 25, S277–S278, doi:10.1016/0021-8502(94)90369-7, 1994.
- Behnke, W., George, C., Scheer, V., and Zetzsch, C.: Production and decay of ClNO₂ from the reaction of gaseous N₂O₅ with NaCl solution: Bulk and aerosol experiments, *J. Geophys. Res.*, 102D, 3795–3804, doi:10.1029/96JD03057, 1997.
- Betterton, E. A. and Hoffmann, M. R.: Oxidation of aqueous SO₂ by peroxymonosulfate, *J. Phys. Chem.*, 92, 5962–5965, doi:10.1021/J100332A025, 1988.
- Beyersdorf, A. J., Blake, D. R., Swanson, A., Meinardi, S., Rowland, F. S., and Davis, D.: Abundances and variability of tropospheric volatile organic compounds at the South Pole and other Antarctic locations, *Atmos. Environ.*, 44, 4565–4574, doi:10.1016/j.atmosenv.2010.08.025, 2010.
- Birdsall, A. W., Andreoni, J. F., and Elrod, M. J.: Investigation of the role of bicyclic peroxy radicals in the oxidation mechanism of toluene, *J. Phys. Chem. A*, 114, 10 655–10 663, doi:10.1021/jp105467e, 2010.
- Bjergbakke, E., Navartnam, S., Parsons, B. J., and Swallow, A. J.: Reaction between HO₂· and chlorine in aqueous solution, *J. Am. Chem. Soc.*, 103, 5926–5928, doi:10.1021/JA00409A059, 1981.
- Bossolasco, A., Faragó, E. P., Schoemaeker, C., and Fittschen, C.: Rate constant of the reaction between CH₃O₂ and OH radicals, *Chem. Phys. Lett.*, 593, 7–13, doi:10.1016/j.cplett.2013.12.052, 2014.
- Boyce, S. D. and Hoffmann, M. R.: Kinetics and mechanism of the formation of hydroxymethanesulfonic acid at low pH, *J. Phys. Chem.*, 88, 4740–4746, doi:10.1021/j150664a059, 1984.
- Brand, C. and van Eldik, R.: Transition metal-catalyzed oxidation of sulfur(IV)oxides. Atmospheric relevant processes and mechanisms, *Chem. Rev.*, 95, 119–190, doi:10.1021/cr00033a006, 1995.
- Buras, Z. J., Elsamra, R. M. I., and Green, W. H.: Direct determination of the simplest Criegee intermediate (CH₂OO) self reaction rate, *J. Phys. Chem. Lett.*, 5, 2224–2228, doi:10.1021/jz5008406, 2014.
- Burkholder, J. B., Sander, S. P., Abbatt, J., Barker, J. R., Huie, R. E., Kolb, C. E., Kurylo, M. J., Orkin, V. L., Wilmouth, D. M., and Wine, P. H.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 18, JPL Publication 15-10, Jet Propulsion Laboratory, Pasadena, <http://jpldataeval.jpl.nasa.gov>, 2015.
- Butkovskaya, N., Kukui, A., and Le Bras, G.: Pressure and temperature dependence of ethyl nitrate formation in the C₂H₅O₂ + NO reaction, *J. Phys. Chem. A*, 114, 956–964, doi:10.1021/jp910003a, 2010.
- Butkovskaya, N., Kukui, A., and Le Bras, G.: Pressure and temperature dependence of methyl nitrate formation in the CH₃O₂ + NO reaction, *J. Phys. Chem. A*, 116, 5972–5980, doi:10.1021/jp210710d, 2012.
- Buxton, G. V., Kilner, C., and Sellers, R. M.: Pulse radiolysis of HOI and IO⁻ in aqueous solution. Formation and characterization of I(II), *Proc. Tihany Symp. Radiat. Chem.*, 6, 155–159, 1986.
- Buxton, G. V., Greenstock, C. L., Helman, W. P., and Ross, A. B.: Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (·OH/·O⁻) in aqueous solution, *J. Phys. Chem. Ref. Data*, 17, 513–886, doi:10.1063/1.555805, 1988.
- Buxton, G. V., McGowan, S., Salmon, G. A., Williams, J. E., and Wood, N. D.: A study of the spectra and reactivity of oxysulphur-radical anions involved in the chain oxidation of S(IV): A pulse and γ-radiolysis study, *Atmos. Environ.*, 30, 2483–2493, doi:10.1016/1352-2310(95)00473-4, 1996.
- Buxton, G. V., Bydder, M., and Salmon, G. A.: The reactivity of chlorine atoms in aqueous solution: Part II. The equilibrium SO₄⁻ + Cl⁻ ⇌ Cl· + SO₄²⁻, *Phys. Chem. Chem. Phys.*, 1, 269–273, doi:10.1039/A807808D, 1999a.
- Buxton, G. V., Salmon, G. A., and Wang, J. Q.: The equilibrium NO₃ + Cl⁻ ⇌ NO₃⁻ + Cl·: A laser flash photolysis and pulse radiolysis study of the reactivity of NO₃ with chloride ion in aqueous solution, *Phys. Chem. Chem. Phys.*, 1, 3589–3593, doi:10.1039/A903286J, 1999b.
- Cala, B. A., Archer-Nicholls, S., Weber, J., Abraham, N. L., Griffiths, P. T., Jacob, L., Shin, Y. M., Revell, L. E., Woodhouse, M., and Archibald, A. T.: Development, intercomparison, and evaluation of an improved mechanism for the oxidation of dimethyl sulfide in the UKCA model, *Atmos. Chem. Phys.*, pp. 14 735–14 760, doi:10.5194/acp-23-14735-2023, 2023.
- Canosa-Mas, C. E., King, M. D., Lopez, R., Percival, C. J., Wayne, R. P., Shallcross, D. E., Pyle, J. A.,

- and Daele, V.: Is the reaction between $\text{CH}_3(\text{O})\text{O}_2$ and NO_3 important in the night-time troposphere?, *J. Chem. Soc. Faraday Trans.*, 92, 2211–2222, doi:10.1039/FT9969202211, 1996.
- Capouet, M., Müller, J.-F., Ceulemans, K., Compernelle, S., Vereecken, L., and Peeters, J.: Modeling aerosol formation in alpha-pinene photo-oxidation experiments, *J. Geophys. Res.*, 113D, doi:10.1029/2007JD008995, 2008.
- Carl, S. A. and Crowley, J. N.: 298 K rate coefficients for the reaction of OH with $i\text{-C}_3\text{H}_7\text{I}$, $n\text{-C}_3\text{H}_7\text{I}$ and C_3H_8 , *Atmos. Chem. Phys.*, 1, 1–7, doi:10.5194/acp-1-1-2001, 2001.
- Carlton, A. G., Bhawe, P. V., Napelenok, S. L., Edney, E. O., Sarwar, G., Pinder, R. W., Pouliot, G. A., and Houyoux, M.: Model representation of secondary organic aerosol in CMAQv4.7, *Environ. Sci. Technol.*, 44, 8553–8560, 2010.
- Carter, W. P. L.: Reactivity estimates for selected consumer product compounds, Final report to the California Air Resources Board, Tech. Rep. Contract No. 06-408, Center for Environmental Research and Technology, University of California, Riverside, CA, U.S.A., 2008.
- Chai, J., Hu, H., Dibble, T. S., Tyndall, G. S., and Orlando, J. J.: Rate constants and kinetic isotope effects for methoxy radical reacting with NO_2 and O_2 , *J. Phys. Chem. A*, 118, 3552–3563, doi:10.1021/jp501205d, 2014.
- Challis, B. C. and Kyrtopoulos, S. A.: Chemistry of Nitroso-Compounds. 11. Nitrosation of Amines by the 2-Phase Interaction of Amines in Solution with Gaseous Oxides of Nitrogen., *Journal of the Chemical Society- Perkin Transactions 1*, 2, 299–304, 1979.
- Chameides, W. L.: The photochemistry of a remote marine stratiform cloud, *J. Geophys. Res.*, 89D, 4739–4755, doi:10.1029/JD089ID03P04739, 1984.
- Chao, W., Hsieh, J.-T., Chang, C.-H., and Lin, J. J.-M.: Direct kinetic measurement of the reaction of the simplest Criegee intermediate with water vapor, *Science*, 347, 751–754, doi:10.1126/science.1261549, 2015.
- Chen, J., Wenger, J. C., and Venables, D. S.: Near-ultraviolet absorption cross sections of nitrophenols and their potential influence on tropospheric oxidation capacity, *J. Phys. Chem. A*, 115, 12 235–12 242, doi:10.1021/jp206929r, 2011.
- Chin, M. and Wine, P. H.: A temperature-dependent competitive kinetics study of the aqueous-phase reactions of OH radicals with formate, formic acid, acetate, acetic acid, and hydrated formaldehyde, in: *Aquatic and Surface Photochemistry*, edited by Helz, G. R., Zepp, R. G., and Crosby, D. G., pp. 85–96, A. F. Lewis, NY, 1994.
- Chinake, C. R. and Simoyi, R. H.: Kinetics and mechanism of the complex bromate-iodine reaction, *J. Phys. Chem.*, 100, 1643–1656, doi:10.1021/JP951956C, 1996.
- Christensen, H. and Sehested, K.: Pulse radiolysis at high temperatures and high pressures, *Radiat. Phys. Chem.*, 18, 723–231, doi:10.1016/0146-5724(81)90195-3, 1981.
- Christensen, H. and Sehested, K.: HO_2 and O_2^- radicals at elevated temperatures, *J. Phys. Chem.*, 92, 3007–3011, doi:10.1021/J100321A060, 1988.
- Christensen, H., Sehested, K., and Corfitzen, H.: Reactions of hydroxyl radicals with hydrogen peroxide at ambient and elevated temperatures, *J. Phys. Chem.*, 86, 1588–1590, doi:10.1021/J100206A023, 1982.
- Citri, O. and Epstein, I. R.: Mechanistic study of a coupled chemical oscillator: the bromate-chlorite-iodide reaction, *J. Phys. Chem.*, 92, 1865–1871, doi:10.1021/J100318A034, 1988.
- Clubb, A. E., Jordan, M. J. T., Kable, S. H., and Osborn, D. L.: Phototautomerization of acetaldehyde to vinyl alcohol: a primary process in UV-irradiated acetaldehyde from 295 to 335 nm, *J. Phys. Chem. Lett.*, 3, 3522–3526, doi:10.1021/jz301701x, 2012.
- Conn, J. B., Kistiakowsky, G. B., Roberts, R. M., and Smith, E. A.: Heats of organic reactions. XIII. Heats of hydrolysis of some acid anhydrides, *Journal of the American Chemical Society*, 64, 1747–1752, doi:10.1021/ja01260a001, 1942.
- da Silva, G.: Carboxylic acid catalyzed keto-enol tautomerizations in the gas phase, *Angew. Chem.*, 122, 7685–7687, doi:10.1002/ange.201003530, 2010.
- Damschen, D. E. and Martin, L. R.: Aqueous aerosol oxidation of nitrous acid by O_2 , O_3 and H_2O_2 , *Atmos. Environ.*, 17, 2005–2011, doi:10.1016/0004-6981(83)90357-8, 1983.
- Das, S. and von Sonntag, C.: The oxidation of trimethylamine by OH radicals in aqueous solution, as studied by pulse radiolysis, ESR, and product analysis. The reactions of the alkylamine radical cation, the aminoalkyl radical, and the protonated aminoalkyl radical, *Z. Naturforschung*, 41B, 505–513, 1986.
- Davis, D., Chen, G., Kasibhatla, P., Jefferson, A., Tanner, D., Eisele, F., Lenschow, D., Neff, W., and Berresheim, H.: DMS oxidation in the Antarctic marine boundary layer: Comparison of model simulations and field observations of DMS, DMSO, DMSO_2 ,

- H₂SO₄(g), MSA(g), and MSA(p), *J. Geophys. Res.*, 103D, 1657–1678, doi:10.1029/97JD03452, 1998.
- Davis, Jr., W. and de Bruin, H. J.: New activity coefficients of 0–100 per cent aqueous nitric acid, *J. Inorg. Nucl. Chem.*, 26, 1069–1083, doi:10.1016/0022-1902(64)80268-2, 1964.
- de Laat, J. and Le, T. G.: Effects of chloride ions on the iron(III)-catalyzed decomposition of hydrogen peroxide and on the efficiency of the Fenton-like oxidation process, *Appl. Catal. B: Environ.*, 66, 137–146, doi:10.1016/j.apcatb.2006.03.008, 2006.
- Deister, U. and Warneck, P.: Photooxidation of SO₃²⁻ in aqueous solution, *J. Phys. Chem.*, 94, 2191–2198, doi:10.1021/J100368A084, 1990.
- Dickson, A. G. and Millero, F. J.: A comparison of the equilibrium constants for the dissociation of carbonic acid in seawater media, *Deep-Sea Res. A*, 34, 1733–1743, 1987.
- Dillon, T. J., Karunanandan, R., and Crowley, J. N.: The reaction of IO with CH₃SCH₃: Products and temperature dependent rate coefficients by laser induced fluorescence, *Phys. Chem. Chem. Phys.*, 8, 847–855, doi:10.1039/B514718B, 2006a.
- Dillon, T. J., Tucceri, M. E., and Crowley, J. N.: Laser induced fluorescence studies of iodine oxide chemistry. Part II. The reactions of IO with CH₃O₂, CF₃O₂ and O₃, *Phys. Chem. Chem. Phys.*, 8, 5185–5198, doi:10.1039/B611116E, 2006b.
- Dillon, T. J., Tucceri, M. E., Sander, R., and Crowley, J. N.: LIF studies of iodine oxide chemistry, part 3. Reactions IO + NO₃ → OIO + NO₂, I + NO₃ → IO + NO₂, and CH₂I + O₂ → (products): Implications for the chemistry of the marine atmosphere at night., *Phys. Chem. Chem. Phys.*, 10, 1540–1554, doi:10.1039/B717386E, 2008.
- Duff, J. W., Dothe, H., and Sharma, R. D.: On the rate coefficient of the N(²D)+O₂ → NO+O reaction in the terrestrial thermosphere, *Geophys. Res. Lett.*, 30, 1259–1263, 2003.
- Dulitz, K., Amedro, D., Dillon, T. J., Pozzer, A., and Crowley, J. N.: Temperature (208–318 K) and pressure (18–696 Torr) dependent rate coefficients for the reaction between OH and HNO₃, *Atmos. Chem. Phys.*, 18, 2381–2394, doi:10.5194/acp-18-2381-2018, 2018.
- Edblom, E. C., Györgyi, L., Orbán, M., and Epstein, I. R.: A mechanism for dynamical behavior in the Landolt reaction with ferrocyanide, *J. Am. Chem. Soc.*, 109, 4876–4880, doi:10.1021/JA00250A020, 1987.
- Ehn, M., Thornton, J. A., Kleist, E., Sipila, M., Junninen, H., Pullinen, I., Springer, M., Rubach, F., Tillmann, R., Lee, B., Lopez-Hilfiker, F., Andres, S., Acir, I.-H., Rissanen, M., Jokinen, T., Schobesberger, S., Kangasluoma, J., Kontkanen, J., Nieminen, T., Kurten, T., Nielsen, L. B., Jorgensen, S., Kjaergaard, H. G., Canagaratna, M., Maso, M. D., Berndt, T., Petaja, T., Wahner, A., Kerminen, V.-M., Kulmala, M., Worsnop, D. R., Wildt, J., and Mentel, T. F.: A large source of low-volatility secondary organic aerosol, *Nature*, 506, 476–486, doi:10.1038/nature13032, 2014.
- Eigen, M. and Kustin, K.: The kinetics of halogen hydrolysis, *J. Am. Chem. Soc.*, 84, 1355–1361, doi:10.1021/JA00867A005, 1962.
- Ervens, B., George, C., Williams, J. E., Buxton, G. V., Salmon, G. A., Bydder, M., Wilkinson, F., Dentener, F., Mirabel, P., Wolke, R., and Herrmann, H.: CAPRAM2.4 (MODAC mechanism): An extended and condensed tropospheric aqueous phase mechanism and its application, *J. Geophys. Res.*, 108D, 4426, doi:10.1029/2002JD002202, 2003.
- Ervens, B., Feingold, G., Frost, G. J., and Kreidenweis, S. M.: A modeling study of aqueous production of dicarboxylic acids: 1. Chemical pathways and speciated organic mass production, *J. Geophys. Res.*, 109D, 15205, doi:10.1029/2003JD004387, 2004.
- Exner, M., Herrmann, H., and Zellner, R.: Laser-based studies of reactions of the nitrate radical in aqueous solution, *Ber. Bunsenges. Phys. Chem.*, 96, 470–477, doi:10.1002/BBPC.19920960347, 1992.
- Feierabend, K. J., Zhu, L., Talukdar, R. K., and Burkholder, J. B.: Rate coefficients for the OH + HC(O)C(O)H (glyoxal) reaction between 210 and 390 K, *J. Phys. Chem. A*, 112, 73–82, doi:10.1021/JP0768571, 2008.
- Fell, C., Steinfeld, J. I., and Miller, S.: Quenching of N(²D) by O(³P), *J. Chem. Phys.*, 92, 4768–4777, doi:10.1063/1.457694, 1990.
- Finkbeiner, M., Crowley, J. N., Horie, O., Müller, R., Moortgat, G. K., and Crutzen, P. J.: Reaction between HO₂ and ClO: Product formation between 210 and 300 K, *J. Phys. Chem.*, 99, 16 264–16 275, doi:10.1021/J100044A011, 1995.
- Flocke, F., Atlas, E., Madronich, S., Schauffler, S. M., Aikin, K., Margitan, J. J., and Bui, T. P.: Observations of methyl nitrate in the lower stratosphere during STRAT: implications for its gas phase production mechanisms, *Geophys. Res. Lett.*, 25, 1891–1894, doi:10.1029/98GL01417, 1998.

- Fogelman, K. D., Walker, D. M., and Margerum, D. W.: Non-metal redox kinetics: Hypochlorite and hypochlorous acid reactions with sulfite, *Inorg. Chem.*, 28, 986–993, doi:10.1021/IC00305A002, 1989.
- Fortnum, D. H., Battaglia, C. J., Cohen, S. R., and Edwards, J. O.: The kinetics of the oxidation of halide ions by monosubstituted peroxides, *J. Am. Chem. Soc.*, 82, 778–782, doi:10.1021/JA01489A004, 1960.
- Francisco-Marquez, M., Alvarez-Idaboy, J. R., Galano, A., and Vivier-Bunge, A.: Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions, *Phys. Chem. Chem. Phys.*, 5, 1392–1399, doi:10.1039/B211185C, 2003.
- Fuller-Rowell, T. J.: Modeling the solar cycle change in nitric oxide in the thermosphere and upper mesosphere, *J. Geophys. Res.*, 98A, 1559–1570, doi:10.1029/92JA02201, 1993.
- Furrow, S.: Reactions of iodine intermediates in iodate-hydrogen peroxide oscillators, *J. Phys. Chem.*, 91, 2129–2135, doi:10.1021/J100292A031, 1987.
- Ganzeveld, L., Klemm, O., Rappenglück, B., and Valverde-Canossa, J.: Evaluation of meteorological parameters over a coniferous forest in a single-column chemistry-climate model, *Atmos. Environ.*, 40, S21–S27, doi:10.1016/J.ATMOSENV.2006.01.061, 2006.
- Ge, X., Wexler, A. S., and Clegg, S. L.: Atmospheric amines - Part II. Thermodynamic properties and gas/particle partitioning, *Atmos. Environ.*, 45, 561–577, 2011.
- Gilbert, B. C. and Stell, J. K.: Mechanisms of peroxide decomposition. An ESR study of the reactions of the peroxomonosulphate anion (HOOSO_3^-) with Ti(III) , Fe(II) , and α -oxygen-substituted radicals, *J. Chem. Soc. Perkin Trans. 2*, pp. 1281–1288, doi:10.1039/P29900001281, 1990.
- Gill, K. J. and Hites, R. A.: Rate constants for the gas-phase reactions of the hydroxyl radical with isoprene, α - and β -pinene, and limonene as a function of temperature, *J. Phys. Chem. A*, 106, 2538–2544, doi:10.1021/jp013532q, 2002.
- Glowacki, D. R., Lockhart, J., Blitz, M. A., Klippenstein, S. J., Pilling, M. J., Robertson, S. H., and Seakins, P. W.: Interception of excited vibrational quantum states by O_2 in atmospheric association reactions, *Science*, 337, 1066–1069, doi:10.1126/science.1224106, 2012.
- Grenfell, J. L., Lehmann, R., Mieth, P., Langematz, U., and Steil, B.: Chemical reaction pathways affecting stratospheric and mesospheric ozone, *J. Geophys. Res.*, 111D, doi:10.1029/2004JD005713, 2006.
- Groß, C. B. M., Dillon, T. J., Schuster, G., Lelieveld, J., and Crowley, J. N.: Direct kinetic study of OH and O_3 formation in the reaction of $\text{CH}_3\text{C}(\text{O})\text{O}_2$ with HO_2 , *J. Phys. Chem. A*, 1, 974–985, doi:10.1021/jp412380z, 2014.
- Gruzdev, A. N., Elokhov, A. S., Makarov, O. V., and Mokhov, I. I.: Some recent results of Russian measurements of surface ozone in Antarctica. A meteorological interpretation, *Tellus*, 45B, 99–105, doi:10.3402/TELLUSB.V45I2.15584, 1993.
- Harris, G. W. and J. N. Pitts, J.: Rates of reaction of hydroxyl radicals with 2-(Dimethylamino)ethanol and 2-Amino-2-methyl-1-propanol in the gas phase at 300+2K, *Environ. Sci. Technol.*, 17, 50–51, 1983.
- Hatakeyama, S., Honda, S., and Akimoto, H.: Rate constants and mechanism for reactions of ketenes with OH radicals in air at 299 ± 2 K, *Bull. Chem. Soc. Jpn.*, 58, 2157–2162, doi:10.1246/BCSJ.58.2157, 1985.
- Hermans, I., Müller, J.-F., Nguyen, T. L., Jacobs, P. A., and Peeters, J.: Kinetics of α -hydroxy-alkylperoxyl radicals in oxidation processes. HO_2 -initiated oxidation of ketones/aldehydes near the tropopause, *J. Phys. Chem. A*, 109, 4303–4311, doi:10.1021/jp044080v, 2005.
- Herrmann, H., Reese, A., and Zellner, R.: Time resolved UV/VIS diode array absorption spectroscopy of SO_x^- ($x=3, 4, 5$) radical anions in aqueous solution, *J. Mol. Struct.*, 348, 183–186, doi:10.1016/0022-2860(95)08619-7, 1995.
- Herrmann, H., Ervens, B., Jacobi, H.-W., Wolke, R., Nowacki, P., and Zellner, R.: CAPRAM2.3: A chemical aqueous phase radical mechanism for tropospheric chemistry, *J. Atmos. Chem.*, 36, 231–284, doi:10.1023/A:1006318622743, 2000.
- Hoffmann, E. H., Tilgner, A., Schrodner, R., Brauer, P., Wolke, R., and Herrmann, H.: An advanced modeling study on the impacts and atmospheric implications of multiphase dimethyl sulfide chemistry, *Proc. Natl. Acad. Sci. USA*, 113, 11 776–11 781, doi:10.1073/pnas.1606320113, 2016.
- Hoffmann, M. R.: On the kinetics and mechanism of oxidation of aquated sulfur dioxide by ozone, *Atmos. Environ.*, 20, 1145–1154, doi:10.1016/0004-6981(86)90147-2, 1986.
- Hoigné, J., Bader, H., Haag, W. R., and Staehelin, J.: Rate constants of reactions of ozone with organic and inorganic compounds in water – III Inorganic compounds and radicals, *Wat. Res.*, 19, 993–1004, doi:10.1016/0043-1354(85)90368-9, 1985.

- Huie, R. E. and Neta, P.: Rate constants for some oxidations of S(IV) by radicals in aqueous solutions, *Atmos. Environ.*, 21, 1743–1747, doi:10.1016/0004-6981(87)90113-2, 1987.
- Hynes, A. J. and Wine, P. H.: The atmospheric chemistry of dimethylsulfoxide (DMSO) kinetics and mechanism of the OH + DMSO reaction, *J. Atmos. Chem.*, 24, 23–37, doi:10.1007/BF00053821, 1996.
- Jacob, D. J.: Chemistry of OH in remote clouds and its role in the production of formic acid and peroxy-monosulfate, *J. Geophys. Res.*, 91D, 9807–9826, doi:10.1029/JD091ID09P09807, 1986.
- Jacobi, H.-W.: Kinetische Untersuchungen und Modellrechnungen zur troposphärischen Chemie von Radikalanionen und Ozon in wässriger Phase, Ph.D. thesis, Universität GH Essen, Germany, 1996.
- Jacobi, H.-W., Herrmann, H., and Zellner, R.: Kinetic investigation of the Cl_2^- radical in the aqueous phase, in: *Air Pollution Research Report 57: Homogeneous and heterogeneous chemical Processes in the Troposphere*, edited by Mirabel, P., pp. 172–176, Office for official Publications of the European Communities, Luxembourg, 1996.
- Jacobsen, F., Holcman, J., and Sehested, K.: Activation parameters of ferryl ion reactions in aqueous acid solutions, *Int. J. Chem. Kinetics*, 29, 17–24, doi:10.1002/(SICI)1097-4601(1997)29:1<17::AID-KIN3>3.0.CO;2-O, 1997.
- Jacobsen, F., Holcman, J., and Sehested, K.: Reactions of the ferryl ion with some compounds found in cloud water, *Int. J. Chem. Kinetics*, 30, 215–221, doi:10.1002/(SICI)1097-4601(1998)30:3<215::AID-KIN7>3.0.CO;2-V, 1998.
- Jagiella, S. and Zabel, F.: Reaction of phenylperoxy radicals with NO_2 at 298 K, *Phys. Chem. Chem. Phys.*, 9, 5036–5051, doi:10.1039/B705193J, 2007.
- Jayson, G. G., Parsons, B. J., and Swallow, A. J.: Some simple, highly reactive, inorganic chlorine derivatives in aqueous solution, *J. Chem. Soc. Faraday Trans. 1*, 69, 1597–1607, doi:10.1039/F19736901597, 1973.
- Jenkin, M., Saunders, S. M., and Pilling, M. J.: The tropospheric degradation of volatile organic compounds: A protocol for mechanism development, *Atmos. Environ.*, 31, 81–104, doi:10.1016/S1352-2310(96)00105-7, 1997.
- Jenkin, M. E., Young, J. C., and Rickard, A. R.: The MCM v3.3.1 degradation scheme for isoprene, *Atmos. Chem. Phys.*, 15, 11 433–11 459, doi:10.5194/acp-15-11433-2015, 2015.
- Jiang, P.-Y., Katsumura, Y., Nagaishi, R., Domae, M., Ishikawa, K., Ishigure, K., and Yoshida, Y.: Pulse radiolysis study of concentrated sulfuric acid solutions. Formation mechanism, yield and reactivity of sulfate radicals, *J. Chem. Soc. Faraday Trans.*, 88, 1653–1658, doi:10.1039/FT9928801653, 1992.
- Kaltsoyannis, N. and Plane, J. M. C.: Quantum chemical calculations on a selection of iodine-containing species (IO , OIO , INO_3 , $(\text{IO})_2$, I_2O_3 , I_2O_4 and I_2O_5) of importance in the atmosphere, *Phys. Chem. Chem. Phys.*, 10, 1723–1733, doi:10.1039/B715687C, 2008.
- Karl, M.: Unpublished data, 2012.
- Karl, M., Gross, A., Leck, C., and Pirjola, L.: Intercomparison of dimethylsulfide oxidation mechanisms for the marine boundary layer: Gaseous and particulate sulfur constituents, *J. Geophys. Res.*, 112, doi:10.1029/2006JD007914, 2007.
- Karl, M., Dye, C., Schmidbauer, N., Wisthaler, A., Mikoviny, T., and coauthors: Study of OH-initiated degradation of 2-aminoethanol, *Atmos. Chem. Phys.*, 12, 1181–1901, 2012a.
- Karl, M., Herckes, P., Mitch, W., and da Silva, E. F.: Atmospheric Chemistry - Aqueous Phase Chemistry, Project 257430193, Final Report., 2012b.
- Kirchner, F., Mayer-Figge, A., Zabel, F., and Becker, K. H.: Thermal stability of peroxy-nitrates, *Int. J. Chem. Kinetics*, 31, 127–144, doi:10.1002/(SICI)1097-4601(1999)31:2<127::AID-KIN6>3.0.CO;2-L, 1999.
- Kishore, K., Dey, G. R., and Mukherjee, T.: OH radical reactions with ethanolamines: Formation of reducing as well as oxidizing radicals, *Res. Chem. Intermed.*, 30, 837–845, 2004.
- Kleinböhl, A., Toon, G. C., Sen, B., Blavier, J.-F. L., Weisenstein, D. K., Strekowski, R. S., Nicovich, J. M., Wine, P. H., and Wennberg, P. O.: On the stratospheric chemistry of hydrogen cyanide, *Geophys. Res. Lett.*, 33, doi:10.1029/2006GL026015, 2006.
- Kohlmann, J.-P. and Poppe, D.: The tropospheric gas-phase degradation of NH_3 and its impact on the formation of N_2O and NO_x , *J. Atmos. Chem.*, 32, 397–415, doi:10.1023/A:1006162910279, 1999.
- Lambe, A. T., Miracolo, M. A., Hennigan, C. J., Robinson, A. L., and Donahue, N. M.: Effective rate constants and uptake coefficients for the reactions of organic molecular markers (n-alkanes, hopanes, and steranes) in motor oil and diesel primary organic aerosols with hydroxyl radicals, *Environ. Sci. Technol.*, 43(23), 8794–8800, doi:10.1021/es9014745h, 2009.

- Lax, E.: Taschenbuch für Chemiker und Physiker, Springer Verlag, Berlin, 1969.
- Lazarou, Y. G., Kambanis, K. G., and Papagianakopoulos, P.: Gas-phase reactions of $(\text{CH}_3)_2\text{N}$ radicals with NO and NO_2 , *J. Phys. Chem.*, 98, 2110–2115, 1994.
- Lee, C., Schmidt, C., Yoon, J., and von Gunten, U.: Oxidation of N-nitrosodimethylamine (NDMA) precursors with ozone and chlorine dioxide: Kinetics and effect on NDMA formation potential, *Environ. Sci. Technol.*, 41, 2056–2063, 2007a.
- Lee, C., Yoon, J., and Gunten, U. V.: Oxidative degradation of N-nitrosodimethylamine by conventional ozonation and the advanced oxidation process ozone/hydrogen peroxide, *Wat. Res.*, 41, 581–590, 2007b.
- Lee, Y.-N. and Schwartz, S. E.: Reaction kinetics of nitrogen dioxide with liquid water at low partial pressure, *J. Phys. Chem.*, 85, 840–848, doi:10.1021/J150607A022, 1981.
- Lengyel, I., Li, J., Kustin, K., and Epstein, I. R.: Rate constants for reactions between iodine- and chlorine-containing species: A detailed mechanism of the chlorine dioxine/chlorite reaction, *J. Am. Chem. Soc.*, 118, 3708–3719, doi:10.1021/JA953938E, 1996.
- Lewis, T. R., Blitz, M. A., Heard, D. E., and Seakins, P. W.: Direct evidence for a substantive reaction between the Criegee intermediate, CH_2OO , and the water vapour dimer, *Phys. Chem. Chem. Phys.*, 17, 4859–4863, doi:10.1039/C4CP04750H, 2015.
- Licht, W. R., Tannenbaum, S. R., and Deen, W. M.: Use of ascorbic acid to inhibit nitrosation: kinetic and mass transfer considerations for an in vitro system, *Carcinogenesis*, 9, 365–372, 1988.
- Liljegren, J. A. and Stevens, P. S.: Measurements of the kinetics of the reaction of OH radicals with 3-methylfuran at low pressure, *Int. J. Chem. Kinetics*, 45, 787–794, doi:10.1002/KIN.20814, 2013.
- Lim, Y. B. and Ziemann, P. J.: Effects of molecular structure on aerosol yields from OH radical-initiated reactions of linear, branched, and cyclic alkanes in the presence of NO_x , *Environ. Sci. Technol.*, 43, 2328–2334, doi:10.1021/es100636q, 2009.
- Lind, J. A., Lazrus, A. L., and Kok, G. L.: Aqueous phase oxidation of sulfur(IV) by hydrogen peroxide, methylhydroperoxide, and peroxyacetic acid, *J. Geophys. Res.*, 92D, 4171–4177, doi:10.1029/JD092ID04P04171, 1987.
- Lockhart, J., Blitz, M., Heard, D., Seakins, P., and Shannon, R.: Kinetic study of the OH + glyoxal reaction: experimental evidence and quantification of direct OH recycling, *J. Phys. Chem. A*, 117, 11 027–11 037, doi:10.1021/jp4076806, 2013.
- Lockwood, A. L., Shepson, P. B., Fiddler, M. N., and Alaghmand, M.: Isoprene nitrates: preparation, separation, identification, yields, and atmospheric chemistry, *Atmos. Chem. Phys.*, 10, 6169–6178, doi:10.5194/acp-10-6169-2010, 2010.
- Løgager, T., Holcman, J., Sehested, K., and Pedersen, T.: Oxidation of ferrous ions by ozone in acidic solutions, *Inorg. Chem.*, 31, 3523–3529, doi:10.1021/ic00043a009, 1992.
- Løgager, T., Sehested, K., and Holcman, J.: Rate constants of the equilibrium reactions $\text{SO}_4 + \text{HNO}_3 \rightleftharpoons \text{HSO}_4^- + \text{NO}_3$ and $\text{SO}_4 + \text{NO}_3 \rightleftharpoons \text{SO}_4^{2-} + \text{NO}_3$, *Radiat. Phys. Chem.*, 41, 539–543, doi:10.1016/0969-806X(93)90017-O, 1993.
- Long, C. A. and Bielski, B. H. J.: Rate of reaction of superoxide radical with chloride-containing species, *J. Phys. Chem.*, 84, 555–557, doi:10.1021/J100442A023, 1980.
- Mack, J. and Bolton, J. R.: Photochemistry of nitrite and nitrate in aqueous solution: A review, *J. Photochem. Photobiol. A: Chem.*, 128, 1–13, 1999.
- Magi, L., Schweitzer, F., Pallares, C., Cherif, S., Mirabel, P., and George, C.: Investigation of the uptake rate of ozone and methyl hydroperoxide by water surfaces, *J. Phys. Chem. A*, 101, 4943–4949, doi:10.1021/JP970646M, 1997.
- Margerum, D. W., Dickson, P. N., Nagy, J. C., Kumar, K., Bowers, C. P., and Fogelman, K. D.: Kinetics of the iodine monochloride reaction with iodide measured by the pulsed-accelerated-flow method, *Inorg. Chem.*, 25, 4900–4904, doi:10.1021/IC00247A025, 1986.
- Marsh, A. R. W. and McElroy, W. J.: The dissociation constant and Henry's law constant of HCl in aqueous solution, *Atmos. Environ.*, 19, 1075–1080, doi:10.1016/0004-6981(85)90192-1, 1985.
- Martin, L. R. and Damschen, D. E.: Aqueous oxidation of sulfur dioxide by hydrogen peroxide at low pH, *Atmos. Environ.*, 15, 1615–1621, doi:10.1016/0004-6981(81)90146-3, 1981.
- McCabe, D. C., Gierczak, T., Talukdar, R. K., and Ravishankara, A. R.: Kinetics of the reaction $\text{OH} + \text{CO}$ under atmospheric conditions, *Geophys. Res. Lett.*, 28, 3135–3138, doi:10.1029/2000GL012719, 2001.
- McElroy, W. J. and Waygood, S. J.: Kinetics of the reactions of the SO_4^- radical with SO_4^- , $\text{S}_2\text{O}_8^{2-}$, H_2O and Fe^{2+} , *J. Chem. Soc. Faraday Trans.*, 86, 2557–2564, doi:10.1039/FT9908602557, 1990.

- Mellouki, A. and Mu, Y.: On the atmospheric degradation of pyruvic acid in the gas phase, *J. Photochem. Photobiol. A: Chem.*, 157, doi:10.1016/S1010-6030(03)00070-4, 2003.
- Messaadia, L., Dib, G. E., Ferhati, A., and Chakir, A.: UV-visible spectra and gas-phase rate coefficients for the reaction of 2,3-pentanedione and 2,4-pentanedione with OH radicals, *Chem. Phys. Lett.*, 626, 73–79, doi:10.1016/j.cplett.2015.02.032, 2015.
- Mirvish, S. S.: Formation of N-Nitroso Compounds: Chemistry, kinetics, and in vivo occurrence, *Toxicology and Applied Pharmacology*, 31, 325–351, 1975.
- Mitch, W. and Herckes, P.: Literature Review and Experiments on Nitrosamine and Nitramine Formation Chemistry Relevant to Carbon Capture., Tech. rep., SINTEF, Norway, 2012.
- Müller, J.-F., Peeters, J., and Stavrou, T.: Fast photolysis of carbonyl nitrates from isoprene, *Atmos. Chem. Phys.*, 14, 2497–2508, doi:10.5194/acp-14-2497-2014, 2014.
- Munger, J. W., Jacob, D. J., Fan, S.-M., Colman, A. S., and Dibb, J. E.: Concentrations and snow-atmosphere fluxes of reactive nitrogen at Summit, Greenland, *J. Geophys. Res.*, 104D, 13 721–13 734, doi:10.1029/1999JD900192, 1999.
- Munoz, F., Schuchmann, M. N., Olbrich, G., and von Sonntag, C.: Common intermediates in the OH-radical-induced oxidation of cyanide and formamide, *J. Chem. Soc. Faraday Trans. 2*, pp. 655–659, 2000.
- Nagy, J. C., Kumar, K., and Margerum, D. W.: Non-metal redox kinetics: Oxidation of iodide by hypochlorous acid and by nitrogen trichloride measured by the pulsed-accelerated-flow method, *Inorg. Chem.*, 27, 2773–2780, doi:10.1021/IC00289A007, 1988.
- Nakanishi, H., Morita, H., and Nagakura, S.: Electronic structures and spectra of the keto and enol forms of acetylacetone, *Bull. Chem. Soc. Jpn.*, 50, 2255–2261, doi:10.1246/bcsj.50.2255, 1977.
- Nakano, Y., Ishiwata, T., and Kawasaki, M.: Rate constants of the reaction of NO₃ with CH₃I measured with use of cavity ring-down spectroscopy, *J. Phys. Chem. A*, 109, 6527–6531, doi:10.1021/JP051817N, 2005.
- Nguyen, T. L., Peeters, J., and Vereecken, L.: Theoretical study of the gas-phase ozonolysis of β -pinene (C₁₀H₁₆), *Phys. Chem. Chem. Phys.*, 11, 5643–5656, doi:10.1039/b822984h, 2009.
- Nielsen, C. J. and Schade, G.: Atmospheric Chemistry of AMP. A theoretical study of the OH initiated atmospheric photo-oxidation of AMP, Tech. Rep. for TCM, confidential, University of Oslo, Oslo, Norway, 2012.
- Nielsen, C. J., D’Anna, B., Karl, M., Aursnes, M., Boreave, A., and coauthors: Atmospheric Degradation of Amines. Summary Report: Photo-oxidation of methylamine, dimethylamine and trimethylamine, CLIMIT project no. 201604, NILU Report OR 2/2011, Norwegian Institute for Air Research, Kjeller, Norway, <http://www.nilu.no>, 2011.
- Nielsen, O. J., Sidebottom, H. W., Donlon, M., and Treacy, J.: Rate constants for the gas-phase reactions of OH radicals and Cl atoms with *n*-alkyl nitrites at atmospheric pressure and 298 K, *Int. J. Chem. Kinetics*, 23, 1095–1109, doi:10.1002/kin.550231204, 1991.
- O’Dowd, C. D. and Hoffmann, T.: Coastal new particle formation: a review of the current state-of-the-art, *Environ. Chem.*, 2, 245–255, doi:10.1071/EN05077, 2005.
- Ogryzlo, E. A., Paltenghi, R., and Bayes, K. D.: The rate of reaction of methyl radicals with ozone, *Int. J. Chem. Kinetics*, 13, 667–675, doi:10.1002/kin.550130707, 1981.
- Olzmann, M., Kraka, E., Cremer, D., Gutbrod, R., and Andersson, S.: Energetics, kinetics, and product distributions of the reactions of ozone with ethene and 2,3-dimethyl-2-butene, *J. Phys. Chem. A*, 101, 9421–9429, doi:10.1021/JP971663E, 1997.
- Orlando, J. J. and Tyndall, G. S.: The atmospheric chemistry of the HC(O)CO radical, *Int. J. Chem. Kinetics*, 33, 149–156, doi:10.1002/1097-4601(200103)33:3<149::AID-KIN1008>3.0.CO;2-1, 2001.
- Orlando, J. J. and Tyndall, G. S.: Laboratory studies of organic peroxy radical chemistry: an overview with emphasis on recent issues of atmospheric significance, *Chem. Soc. Rev.*, 41, 6294–6317, doi:10.1039/C2CS35166H, 2012.
- Orlando, J. J., Tyndall, G. S., Bilde, M., Ferronato, C., Wallington, T. J., Vereecken, L., and Peeters, J.: Laboratory and theoretical study of the oxy radicals in the OH- and Cl-initiated oxidation of ethene, *J. Phys. Chem. A*, 102, 8116–8123, doi:10.1021/JP981937D, 1998.
- Orlando, J. J., Tyndall, G. S., Fracheboud, J. M., Estupinan, E. G., Haberkorn, S., and Zimmer, A.: The rate and mechanism of the gas-phase oxidation of hydroxyacetone, *Atmos. Environ.*, 33, 1621–1629, doi:10.1016/S1352-2310(98)00386-0, 1999a.
- Orlando, J. J., Tyndall, G. S., and Paulson, S. E.: Mechanism of the OH-initiated oxidation of

- methacrolein, *Geophys. Res. Lett.*, 26, 2191–2194, doi:10.1029/1999GL900453, 1999b.
- Orlando, J. J., Tyndall, G. S., Bertman, S. B., Chen, W., and Burkholder, J. B.: Rate coefficient for the reaction of OH with $\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{O})\text{OONO}_2$ (MPAN), *Atmos. Environ.*, 36, 1895–1900, doi:10.1016/S1352-2310(02)00090-0, 2002.
- Ouyang, B., McLeod, M. W., Jones, R. L., and Bloss, W. J.: NO_3 radical production from the reaction between the Criegee intermediate CH_2OO and NO_2 , *Phys. Chem. Chem. Phys.*, 15, 17 070–17 075, doi:10.1039/c3cp53024h, 2013.
- Paulot, F., Crounse, J. D., Kjaergaard, H. G., Kroll, J. H., Seinfeld, J. H., and Wennberg, P. O.: Isoprene photooxidation: new insights into the production of acids and organic nitrates, *Atmos. Chem. Phys.*, 9, 1479–1501, doi:10.5194/ACP-9-1479-2009, 2009a.
- Paulot, F., Crounse, J. D., Kjaergaard, H. G., Kürten, A., St. Clair, J. M., Seinfeld, J. H., and Wennberg, P. O.: Unexpected epoxide formation in the gas-phase photooxidation of isoprene, *Science*, 325, doi:10.1126/science.1172910, 2009b.
- Paulot, F., Wunch, D., Crounse, J. D., Toon, G. C., Millet, D. B., DeCarlo, P. F., Vigouroux, C., Deutscher, N. M., González Abad, G., Notholt, J., Warneke, T., Hannigan, J. W., Warneke, C., de Gouw, J. A., Dunlea, E. J., De Mazière, M., Griffith, D. W. T., Bernath, P., Jimenez, J. L., and Wennberg, P. O.: Importance of secondary sources in the atmospheric budgets of formic and acetic acids, *Atmos. Chem. Phys.*, 11, 1989–2013, doi:10.5194/acp-11-1989-2011, 2011.
- Peeters, J. and Nguyen, T. L.: Unusually fast 1,6-H shifts of enolic hydrogens in peroxy radicals: formation of the first-generation C_2 and C_3 carbonyls in the oxidation of isoprene, *J. Phys. Chem. A*, 116, 6134–6141, doi:10.1021/jp211447q, 2012.
- Peeters, J., Müller, J.-F., Stavrou, T., and Nguyen, V. S.: Hydroxyl radical recycling in isoprene oxidation driven by hydrogen bonding and hydrogen tunneling: the upgraded LIM1 mechanism, *J. Phys. Chem. A*, 118, 8625–8643, doi:10.1021/jp5033146, 2014.
- Pires, M., Rossi, M. J., and Ross, D. S.: Kinetic and mechanistic aspects of the NO oxidation by O_2 in aqueous phase, *Int. J. Chem. Kinetics*, 26, 1207–1227, 1994.
- Plane, J. M. C., Joseph, D. M., Allan, B. J., Ashworth, S. H., and Francisco, J. S.: An experimental and theoretical study of the reactions $\text{OIO} + \text{NO}$ and $\text{OIO} + \text{OH}$, *J. Phys. Chem. A*, 110, 93–100, doi:10.1021/JP055364Y, 2006.
- Platz, J., Nielsen, O. J., Wallington, T. J., Ball, J. C., Hurley, M. D., Straccia, A. M., Schneider, W. F., and Sehested, J.: Atmospheric chemistry of the phenoxy radical, $\text{C}_6\text{H}_5\text{O}(\cdot)$: UV spectrum and kinetics of its reaction with NO, NO_2 , and O_2 , *J. Phys. Chem. A*, 102, 7964–7974, doi:10.1021/jp982221l, 1998.
- Reiner, T. and Arnold, F.: Laboratory flow reactor measurements of the reaction $\text{SO}_3 + \text{H}_2\text{O} + \text{M} \rightarrow \text{H}_2\text{SO}_4 + \text{M}$: Implications for gaseous H_2SO_4 and aerosol formation in the plumes of jet aircraft, *Geophys. Res. Lett.*, 20(23), 2659–2662, 1993.
- Rickard, A. and Pascoe, S.: The Master Chemical Mechanism (MCM), <http://mcm.leeds.ac.uk>, 2009.
- Rickard, A. R., Johnson, D., McGill, C. D., and Marston, G.: OH yields in the gas-phase reactions of ozone with alkenes, *J. Phys. Chem. A*, 103, 7656–7664, doi:10.1021/JP9916992, 1999.
- Riffault, V., Bedjanian, Y., and Poulet, G.: Kinetic and mechanistic study of the reactions of OH with IBr and HOI, *J. Photochem. Photobiol. A: Chem.*, 176, 155–161, doi:10.1016/j.jphotochem.2005.09.002, 2005.
- Roberts, J. M., Veres, P. R., Cochran, A. K., Warneke, C., Burling, I. R., Yokelson, R. J., Lerner, B., Gilman, J. B., Kuster, W. C., Fall, R., and de Gouw, J.: Isocyanic acid in the atmosphere and its possible link to smoke-related health effects, *Proc. Natl. Acad. Sci. USA*, 108, 8966–8971, 2011.
- Roble, R. G.: Energetics of the mesosphere and thermosphere, in: *The upper Mesosphere and Lower Thermosphere: A Review of Experiment and Theory*, Geophysical Monograph 87, edited by Johnson, R. M. and Killeen, T. L., pp. 1–23, American Geophysical Union, Washington, DC, USA, 1995.
- Ross, A. B., Mallard, W. G., Helman, W. P., Bielski, B. H. J., Buxton, G. V., Cabelli, D. E., Greenstock, C. L., Huie, R. E., and Neta, P.: NDRL-NIST Solution Kinetics Database: - Ver. 1, National Institute of Standards and Technology, Gaithersburg, MD, 1992.
- Roth, E., Chakir, A., and Ferhati, A.: Study of a benzoylperoxy radical in the gas phase: ultraviolet spectrum and $\text{C}_6\text{H}_5\text{C}(\text{O})\text{O}_2 + \text{HO}_2$ reaction between 295 and 357 K, *J. Phys. Chem. A*, 114, 10 367–10 379, doi:10.1021/jp1021467, 2010.
- Rush, J. D. and Bielski, B. H. J.: Pulse radiolytic studies of the reaction of HO_2/O_2^- with $\text{Fe}(\text{II})/\text{Fe}(\text{III})$ ions. The reactivity of HO_2/O_2^- with ferric ions and its implication on the occurrence of the Haber-Weiss reaction, *J. Phys. Chem.*, 89, 5062–5066, doi:10.1021/j100269a035, 1985.

- Sander, R., Jöckel, P., Kirner, O., Kunert, A. T., Landgraf, J., and Pozzer, A.: The photolysis module JVAL-14, compatible with the MESSy standard, and the JVal PreProcessor (JVPP), *Geosci. Model Dev.*, 7, 2653–2662, doi:10.5194/GMD-7-2653-2014, 2014.
- Sander, R., Baumgaertner, A., Cabrera-Perez, D., Frank, F., Grooß, J.-U., Gromov, S., Harder, H., Huijnen, V., Jöckel, P., Karydis, V. A., Niemeyer, K., Pozzer, A., Riede, H., Schultz, M., Taraborrelli, D., and Tauer, S.: The atmospheric chemistry box model CAABA/MECCA-4.0gmdd, *Geosci. Model Dev. Discuss.*, doi:10.5194/gmd-2018-201, 2018.
- Sander, S. P., Friedl, R. R., Golden, D. M., Kurylo, M. J., Moortgat, G. K., Keller-Rudek, H., Wine, P. H., Ravishankara, A. R., Kolb, C. E., Molina, M. J., Finlayson-Pitts, B. J., Huie, R. E., and Orkin, V. L.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 15, JPL Publication 06-2, Jet Propulsion Laboratory, Pasadena, CA, <http://jpldataeval.jpl.nasa.gov>, 2006.
- Schwartz, S. E.: *Advances in Environmental Science and Technology*, John Wiley & Sons, New York, 1983.
- Schwartz, S. E. and White, W. H.: Solubility equilibria of the nitrogen oxides and oxyacids in dilute aqueous solution, in: *Advances in Environmental Science and Engineering*, edited by Pfafflin, J. R. and Ziegler, E. N., vol. 4, pp. 1–45, Gordon and Breach Science Publishers, NY, 1981.
- Scribano, Y., Goldman, N., Saykally, R. J., and Leforestier, C.: Water dimers in the atmosphere III: Equilibrium constant from a flexible potential, *J. Phys. Chem. A*, 110, 5411–5419, doi:10.1021/jp056759k, 2006.
- Sehested, J., Christensen, L. K., Nielsen, O. J., Bilde, M., Wallington, T. J., Schneider, W. F., Orlando, J. J., and Tyndall, G. S.: Atmospheric chemistry of acetone: Kinetic study of the $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2 + \text{NO}/\text{NO}_2$ reactions and decomposition of $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2\text{NO}_2$, *Int. J. Chem. Kinetics*, 30, 475–489, doi:10.1002/(SICI)1097-4601(1998)30:7<475::AID-KIN4>3.0.CO;2-P, 1998.
- Sehested, K., Rasmussen, O. L., and Fricke, H.: Rate constants of OH with HO_2 , O_2^- , and H_2O_2^+ from hydrogen peroxide formation in pulse-irradiated oxygenated water, *J. Phys. Chem.*, 72, 626–631, doi:10.1021/J100848A040, 1968.
- Sehested, K., Holcman, J., and Hart, E. J.: Rate constants and products of the reactions of e_{aq}^- , O_2^- and H with ozone in aqueous solutions, *J. Phys. Chem.*, 87, 1951–1954, doi:10.1021/J100234A024, 1983.
- Seinfeld, J. H. and Pandis, S. N.: *Atmospheric Chemistry and Physics*, John Wiley & Sons, Inc., 1998.
- Shoute, L. C. T., Alfassi, Z. B., Neta, P., and Huie, R. E.: Temperature dependence of the rate constants for reaction of dihalide and azide radicals with inorganic reductants, *J. Phys. Chem.*, 95, 3238–3242, doi:10.1021/J100161A050, 1991.
- Simić, M., Neta, P., and Hayon, E.: Pulse radiolytic investigation of aliphatic amines in aqueous solution, *Int. J. Radiat. Phys. Chem.*, 3, 309–320, 1971.
- Sivakumaran, V., Hölscher, D., Dillon, T. J., and Crowley, J. N.: Reaction between OH and HCHO: temperature dependent rate coefficients (202–399 K) and product pathways (298 K), *Phys. Chem. Chem. Phys.*, 5, 4821–4827, doi:10.1039/B306859E, 2003.
- So, S., Wille, U., and da Silva, G.: Atmospheric chemistry of enols: a theoretical study of the vinyl alcohol + OH + O_2 reaction mechanism, *Environ. Sci. Technol.*, 48, 6694–6701, doi:10.1021/es500319q, 2014.
- Sokolov, O., Hurley, M. D., Ball, J. C., Wallington, T. J., Nelsen, W., Barnes, I., and Becker, K. H.: Kinetics of the reactions of chlorine atoms with CH_3ONO and CH_3ONO_2 , *Int. J. Chem. Kinetics*, 31, 357–359, doi:10.1002/(SICI)1097-4601(1999)31:5<357::AID-KIN5>3.0.CO;2-6, 1999.
- Solberg, S., Stordal, F., and Hov, Ø.: Tropospheric ozone at high latitudes in clean and polluted air masses, a climatological study, *J. Atmos. Chem.*, 28, 111–123, doi:10.1023/A:1005766612853, 1997.
- Stone, D., Blitz, M., Daubney, L., Howes, N. U. M., and Seakins, P.: Kinetics of CH_2OO reactions with SO_2 , NO_2 , NO , H_2O and CH_3CHO as a function of pressure, *Phys. Chem. Chem. Phys.*, 16, 1139–1149, doi:10.1039/c3cp54391a, 2014.
- Strekowski, R. S., Nicovich, J. M., and Wine, P. H.: Kinetic and mechanistic study of the Reactions of $\text{O}(^1\text{D}_2)$ with HCN and CH_3CN , *Chem. Phys. Chem.*, 11, 3942–3955, doi:10.1002/cphc.201000550, 2010.
- Tao, Z. and Li, Z.: A kinetics study on reactions of $\text{C}_6\text{H}_5\text{O}$ with $\text{C}_6\text{H}_5\text{O}$ and O_3 at 298 K, *Int. J. Chem. Kinetics*, 31, 65–72, doi:10.1002/(SICI)1097-4601(1999)31:1<65::AID-KIN8>3.0.CO;2-J, 1999.
- Taraborrelli, D.: Isoprene oxidation and its impacts on the atmospheric composition, Ph.D. thesis, Johannes Gutenberg-Universität, Mainz, Germany, <http://d-nb.info/1003538770/34>, 2010.
- Taraborrelli, D., Lawrence, M. G., Butler, T. M., Sander, R., and Lelieveld, J.: Mainz Isoprene Mechanism 2 (MIM2): an isoprene oxidation mechanism for regional and global atmospheric modelling,

- Atmos. Chem. Phys., 9, 2751–2777, doi:10.5194/ACP-9-2751-2009, 2009.
- Thornton, A. T. and Laurence, G. S.: Kinetics of oxidation of transition-metal ions by halogen radical anions. Part I. The oxidation of iron(II) by dibromide and dichloride ions generated by flash photolysis, *J. Chem. Soc. Dalton Trans.*, pp. 804–813, doi:10.1039/DT9730000804, 1973.
- Tsimpidi, A. P., Karydis, V. A., Zavala, M., Lei, W., Molina, L., Ulbrich, I. M., Jimenez, J. L., and Pandis, S. N.: Evaluation of the volatility basis-set approach for the simulation of organic aerosol formation in the Mexico City metropolitan area, *Atmos. Chem. Phys.*, 10, 525–546, 2010.
- Tyndall, G. S., Staffelbach, T. A., Orlando, J. J., and Calvert, J. G.: Rate coefficients for the reactions of OH radicals with methylglyoxal and acetaldehyde, *Int. J. Chem. Kinetics*, 27, 1009–1020, doi:10.1002/KIN.550271006, 1995.
- Tyndall, G. S., Orlando, J. J., Wallington, T. J., Sehested, J., and Nielsen, O. J.: Kinetics of the reactions of acetonitrile with chlorine and fluorine atoms, *J. Phys. Chem.*, 100, 660–668, doi:10.1021/jp9521417, 1996.
- Tyndall, G. S., Cox, R. A., Granier, C., Lesclaux, R., Moortgat, G. K., Pilling, M. J., Ravishankara, A. R., and Wallington, T. J.: The atmospheric chemistry of small organic peroxy radicals, *J. Geophys. Res.*, 106D, 12 157–12 182, doi:10.1029/2000JD900746, 2001a.
- Tyndall, G. S., Orlando, J. J., Wallington, T. J., and Hurley, M. D.: Products of the chlorine-atom- and hydroxyl-radical-initiated oxidation of CH₃CN, *J. Phys. Chem. A*, 105, 5380–5384, doi:10.1021/jp004318p, 2001b.
- van den Bergh, H. and Troe, J.: Kinetic and thermodynamic properties of INO and INO₂ intermediate complexes in iodine recombination, *J. Chem. Phys.*, 64, 736–742, doi:10.1063/1.432220, 1976.
- Vereecken, L. and Francisco, J. S.: Theoretical studies of atmospheric reaction mechanisms in the troposphere, *Chem. Soc. Rev.*, 41, 6259–6293, doi:10.1039/c2cs35070j, 2012.
- Vereecken, L. and Peeters, J.: A theoretical study of the OH-initiated gas-phase oxidation mechanism of β -pinene (C₁₀H₁₆): first generation products, *Phys. Chem. Chem. Phys.*, 14, 3802–3815, doi:10.1039/c2cp23711c, 2012.
- Vereecken, L., Müller, J.-F., and Peeters, J.: Low-volatility poly-oxygenates in the OH-initiated atmospheric oxidation of α -pinene: impact of non-traditional peroxy radical chemistry, *Phys. Chem. Chem. Phys.*, 9, 5241–5248, doi:10.1039/b708023a, 2007.
- Vereecken, L., Harder, H., and Novelli, A.: The reaction of Criegee intermediates with NO, RO₂, and SO₂, and their fate in the atmosphere, *Phys. Chem. Chem. Phys.*, 14, 14 682–14 695, doi:10.1039/c2cp42300f, 2012.
- Vereecken, L., Harder, H., and Novelli, A.: The reactions of Criegee intermediates with alkenes, ozone, and carbonyl oxides, *Phys. Chem. Chem. Phys.*, 16, 4039–4049, doi:10.1039/c3cp54514h, 2014.
- Veres, P. R., Neuman, J. A., Bertram, T. H., Asaf, E., Wolfe, G. M., Williamson, C. J., Weinzierl, B., Tilmes, S., Thompson, C. R., Thames, A. B., Schroder, J. C., Saiz-Lopez, A., Rollins, A. W., Roberts, J. M., Price, D., Peischl, J., Nault, B. A., Möller, K. H., Miller, D. O., Meinardi, S., Li, Q., Lamarque, J. F., Kupc, A., Kjaergaard, H. G., Kinnison, D., Jimenez, J. L., Jernigan, C. M., Hornbrook, R. S., Hills, A., Dollner, M., Day, D. A., Cuevas, C. A., Campuzano-Jost, P., Burkholder, J., Bui, T. P., Brune, W. H., Brown, S. S., Brock, C. A., Bourgeois, I., Blake, D. R., Apel, E. C., and Ryerson, T. B.: Global airborne sampling reveals a previously unobserved dimethyl sulfide oxidation mechanism in the marine atmosphere, *Proc. Natl. Acad. Sci. USA*, 117, 4505–4510, doi:10.1073/pnas.1919344117, 2020.
- von Glasow, R., Sander, R., Bott, A., and Crutzen, P. J.: Modeling halogen chemistry in the marine boundary layer, 1. Cloud-free MBL, *J. Geophys. Res.*, 107D, 4341, doi:10.1029/2001JD000942, 2002.
- von Kuhlmann, R.: Tropospheric photochemistry of ozone, its precursors and the hydroxyl radical: A 3D-modeling study considering non-methane hydrocarbons, Ph.D. thesis, Johannes Gutenberg-Universität, Mainz, Germany, 2001.
- von Kuhlmann, R., Lawrence, M. G., Crutzen, P. J., and Rasch, P. J.: A model for studies of tropospheric ozone and nonmethane hydrocarbons: Model description and ozone results, *J. Geophys. Res.*, 108D, 4294, doi:10.1029/2002JD002893, 2003.
- Wallington, T. J., Ammann, M., Cox, R. A., Crowley, J. N., Herrmann, H., Jenkin, M. E., McNeill, V., Mellouki, A., Rossi, M. J., and Troe, J.: IUPAC Task group on atmospheric chemical kinetic data evaluation: Evaluated kinetic data, <http://iupac.pole-ether.fr>, 2018.
- Wang, T. X. and Margerum, D. W.: Kinetics of reversible chlorine hydrolysis: Temperature

- dependence and general-acid/base-assisted mechanisms, *Inorg. Chem.*, 33, 1050–1055, doi:10.1021/IC00084A014, 1994.
- Wang, Y. L., Nagy, J. C., and Margerum, D. W.: Kinetics of hydrolysis of iodine monochloride measured by the pulsed-accelerated-flow method, *J. Am. Chem. Soc.*, 111, 7838–7844, doi:10.1021/JA00202A026, 1989.
- Warneck, P.: Chemical reactions in clouds, *Frese-
nius J. Anal. Chem.*, 340, 585–590, doi:10.1007/
BF00322434, 1991.
- Warneck, P.: The relative importance of various path-
ways for the oxidation of sulfur dioxide and nitro-
gen dioxide in sunlit continental fair weather clouds,
Phys. Chem. Chem. Phys., 1, 5471–5483, doi:10.
1039/A906558J, 1999.
- Warneck, P.: The oxidation of sulfur(IV) by reac-
tion with iron(III): a critical review and data anal-
ysis, *Phys. Chem. Chem. Phys.*, 20, 4020–4037, doi:
10.1039/c7cp07584g, 2018.
- Wayne, R. P., Barnes, I., Biggs, P., Burrows, J. P.,
Canosa-Mas, C. E., Hjorth, J., Le Bras, G., Moort-
gat, G. K., Perner, D., Poulet, G., Restelli, G., and
Sidebottom, H.: The nitrate radical: Physics, chem-
istry, and the atmosphere, *Atmos. Environ.*, 25A, 1–
203, doi:10.1016/0960-1686(91)90192-A, 1991.
- Weast, R. C., ed.: *CRC Handbook of Chemistry and
Physics*, 61st Edition, CRC Press, Inc., Boca Raton,
FL, 1980.
- Weinstein-Lloyd, J. and Schwartz, S. E.: Low-intensity
radiolysis study of free-radical reactions in cloudwa-
ter: H_2O_2 production and destruction, *Environ. Sci.
Technol.*, 25, 791–800, doi:10.1021/ES00016A027,
1991.
- Welz, O., Savee, J. D., Osborn, D. L., Vasu, S. S., Per-
cival, C. J., Shallcross, D. E., and Taatjes, C. A.:
Direct kinetic measurements of Criegee intermedi-
ate (CH_2OO) formed by reaction of CH_2I with O_2 ,
Science, 335, 204–207, doi:10.1126/science.1213229,
2012.
- Welz, O., Eskola, A. J., Sheps, L., Rotavera, B., Savee,
J. D., Scheer, A. M., Osborn, D. L., Lowe, D.,
Booth, A. M., Xiao, P., Khan, M. A. H., Percival,
C. J., Shallcross, D. E., and Taatjes, C. A.: Rate
coefficients of C1 and C2 Criegee intermediate re-
actions with formic and acetic acid near the colli-
sion limit: Direct kinetics measurements and atmo-
spheric implications, *Angew. Chem.*, 126, 4635–4638,
doi:10.1002/ange.201400964, 2014.
- Wine, P. H., Tang, Y., Thorn, R. P., Wells, J. R., and
Davis, D. D.: Kinetics of aqueous phase reactions of
the SO_4^- radical with potential importance in cloud
chemistry, *J. Geophys. Res.*, 94D, 1085–1094, doi:
10.1029/JD094ID01P01085, 1989.
- Wingenter, O. W., Sive, B. C., Blake, N. J., and Row-
land, F. S.: Atomic chlorine concentrations deter-
mined from ethane and hydroxyl measurements made
over the Central Pacific Ocean, *Eos, Trans. AGU
(Abstract Supplement)*, 80, F149–F150, 1999.
- Wollesen de Jonge, R., Elm, J., Rosati, B., Chris-
tiansen, S., Hyttinen, N., Lüdemann, Bilde, M.,
and Roldin, P.: Secondary aerosol formation from
dimethyl sulfide - improved mechanistic understand-
ing based on smog chamber experiments and mod-
elling, *Atmos. Chem. Phys.*, 21, 9955–9976, doi:
10.5194/acp-21-9955-2021, 2021.
- Wu, D., Wong, D., and Di Bartolo, B.: Evolution of
 Cl_2^- in aqueous NaCl solutions, *J. Photochem.*, 14,
303–310, doi:10.1016/0047-2670(80)85102-1, 1980.
- Wu, R., Wang, S., and Wang, L.: New Mechanism
for the Atmospheric Oxidation of Dimethyl Sulfide.
The Importance of Intramolecular Hydrogen Shift in
a $\text{CH}_3\text{SCH}_2\text{OO}$ Radical, *J. Phys. Chem. A*, 119, 112–
117, doi:10.1021/jp511616j, 2015.
- Yiin, B. S. and Margerum, D. W.: Nonmetal redox
kinetics: reactions of iodine and triiodide with sul-
fite and hydrogen sulfite and the hydrolysis of io-
dosulfate, *Inorg. Chem.*, 29, 1559–1564, doi:10.1021/
IC00333A023, 1990.
- Yoon, M.-C., Choi, Y. S., and Kim, S. K.: The OH
production from the $\pi - \pi^*$ transition of acetylac-
etone, *Chem. Phys. Lett.*, 300, 207–212, doi:10.1016/
S0009-2614(98)01373-6, 1999.
- Yu, X.-Y.: Critical evaluation of rate constants and
equilibrium constants of hydrogen peroxide photol-
ysis in acidic aqueous solutions containing chloride
ions, *J. Phys. Chem. Ref. Data*, 33, 747–763, doi:
10.1063/1.1695414, 2004.
- Zellner, R., Hartmann, D., Karthäuser, J., Rhäsa, D.,
and Weibring, G.: A laser photolysis/LIF study of
the reactions of $\text{O}(^3\text{P})$ atoms with CH_3 and CH_3O_2
radicals, *J. Chem. Soc. Faraday Trans. 2*, 84, 549–
568, doi:10.1039/f29888400549, 1988.
- Ziajka, J., Beer, F., and Warneck, P.: Iron-catalysed
oxidation of bisulphite aqueous solution: evidence for
free radical chain mechanism, *Atmos. Environ.*, 28,
2549–2552, doi:10.1016/1352-2310(94)90405-7, 1994.