

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 3.8m

Date: September 28, 2017.

Selected reactions:
"lAra"

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase: 699

Aqueous phase: 89

All species: 788

Number of reactions in selected mechanism:

Gas phase (Gnn): 1789

Aqueous phase (Annn): 145

Henry (Hnn): 93

Photolysis (Jnn): 384

Aqueous phase photolysis (PHnn): 2

Heterogeneous (HETnn): 21

Equilibria (EQnn): 68

Isotope exchange (IEXnn): 0

Tagging equations (TAGnn): 0

Dummy (Dnn): 1

All equations: 2503

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	$O_2 + O(^3P) \rightarrow O_3$	$6.0E-34*((temp/300.)**(-2.4))$ *cair	Burkholder et al. (2015)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2 O_2$	$1.2E-10$	Burkholder et al. (2015)*
G1002b	UpG	$O_3 + O(^1D) \rightarrow O_2 + 2 O(^3P)$	$1.2E-10$	Burkholder et al. (2015)
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2 O_2$	$8.0E-12*EXP(-2060./temp)$	Burkholder et al. (2015)
G1004	UpG	$O_2 + O^+ \rightarrow O_2^+ + O(^3P)$	$k_{0p_02}(temp,temp_ion)$	Fuller-Rowell (1993)
G1101	UpG	$O_2^+ + e^- \rightarrow 2 O(^3P)$	$2.7E-7*(300./temp_elec)**.7$	Fuller-Rowell (1993)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	$k_{3rd}(temp,cair,4.4E-32,1.3,$ $7.5E-11,-0.2,0.6)$	Burkholder et al. (2015)
G2101	UpStG	$H + O_3 \rightarrow OH + O_2$	$1.4E-10*EXP(-470./temp)$	Burkholder et al. (2015)
G2102	UpStG	$H_2 + O(^1D) \rightarrow H + OH$	$1.2E-10$	Burkholder et al. (2015)
G2103	UpStG	$OH + O(^3P) \rightarrow H + O_2$	$1.8E-11*EXP(180./temp)$	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)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow OH + O_2$	$3.E-11*EXP(200./temp)$	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)
G2108a	UpStG	$HO_2 + H \rightarrow 2 OH$	$7.2E-11$	Burkholder et al. (2015)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	$6.9E-12$	Burkholder et al. (2015)
G2108c	UpStG	$HO_2 + H \rightarrow O(^3P) + H_2O$	$1.6E-12$	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)
G2113	UpG	$H_2 + O(^3P) \rightarrow H + OH$	$1.60E-11*EXP(-4570./temp)$	Roble (1995)
G2114a	UpG	$OH + OH \rightarrow H_2O + O(^3P)$	$4.20E-12*EXP(-240./temp)$	Sander et al. (2003)
G2114b	UpG	$OH + OH \rightarrow H_2O_2$	$k_{3rd}(temp,cair,6.9E-31,1.0,$ $2.6E-11,0.,0.6)$	Burkholder et al. (2015)
G2115	UpG	$H + H \rightarrow H_2$	$5.7E-32*(300./temp)**1.6*cair$	Roble (1995)
G2116	UpG	$H_2O_2 + O(^3P) \rightarrow OH + HO_2$	$1.40E-12*EXP(-2000./temp)$	Sander et al. (2003)
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*
G3001	UpGN	$NO^+ + e^- \rightarrow .15 N + .85 N(^2D) + O(^3P)$	$4.2E-7*(300./temp_elec)**0.85$	Bailey et al. (2002)

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

#	labels	reaction	rate coefficient	reference
G3002	UpGN	$N_2^+ + e^- \rightarrow .88 N + 1.12 N(^2D)$	$1.8E-7*(temp_elec/300.)**(-0.39)$	Swaminathan et al. (1998)
G3003	UpGN	$N(^2D) + e^- \rightarrow N + e^-$	$3.8E-12*(temp_elec)**.81$	Swaminathan et al. (1998)
G3100	UpStGN	$N + O_2 \rightarrow NO + O(^3P)$	$1.5E-11*EXP(-3600./temp)$	Burkholder et al. (2015)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Burkholder et al. (2015)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow 2 NO$	$7.259E-11*EXP(20./temp)$	Burkholder et al. (2015)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	$4.641E-11*EXP(20./temp)$	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.0E-12*EXP(-1500./temp)$	Burkholder et al. (2015)
G3104	UpStGN	$NO + N \rightarrow O(^3P) + N_2$	$2.1E-11*EXP(100./temp)$	Burkholder et al. (2015)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.1E-12*EXP(210./temp)$	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)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	$5.8E-12*EXP(220./temp)$	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)*
G3111	UpGN	$N(^2D) + NO \rightarrow N_2 + O(^3P)$	6.70E-11	Fuller-Rowell (1993)
G3112	UpGN	$N(^2D) + O_2 \rightarrow NO + O(^3P)$	$6.20E-12*(temp/300.)$	Duff et al. (2003)
G3113	UpGN	$N(^2D) + O(^3P) \rightarrow N + O(^3P)$	6.90E-13	Fell et al. (1990)
G3114	UpGN	$N(^2D) + O_3 \rightarrow NO + O_2$	0.80E-16	Sander et al. (2003)
G3115	UpGN	$NO + O(^3P) \rightarrow NO_2$	$k_3rd(temp, cair, 9.0E-32, 1.5, 3.0E-11, 0.0, 0.6)$	Burkholder et al. (2015)
G3116	UpGN	$NO_2 + O(^3P) \rightarrow NO_3$	$k_3rd(temp, cair, 2.5E-31, 1.8, 2.2E-11, 0.7, 0.6)$	Burkholder et al. (2015)
G3117	UpGN	$N(^2D) \rightarrow N$	10.6	Fuller-Rowell (1993)
G3118	UpGN	$N^+ + O_2 \rightarrow NO + O^+$	3.66E-11	Barth (1992)
G3119	UpGN	$N_2^+ + O(^3P) \rightarrow NO^+ + N(^2D)$	$k_N2_0(temp, temp_ion)$	Fuller-Rowell (1993)
G3120a	UpGN	$N^+ + O_2 \rightarrow NO^+ + O(^3P)$	2.60E-10	Fuller-Rowell (1993)
G3120b	UpGN	$N^+ + O_2 \rightarrow O_2^+ + N$	3.10E-10	Swaminathan et al. (1998)
G3121	UpGN	$N^+ + O(^3P) \rightarrow O^+ + N$	1.00E-12	Fuller-Rowell (1993)
G3122	UpGN	$O_2^+ + N \rightarrow NO^+ + O(^3P)$	1.20E-10	Fuller-Rowell (1993)
G3123	UpGN	$O_2^+ + NO \rightarrow NO^+ + O_2$	4.40E-10	Fuller-Rowell (1993)
G3124	UpGN	$O^+ + N_2 \rightarrow NO^+ + N$	$k_Op_N2(temp, temp_ion)$	Fuller-Rowell (1993)
G3125	UpGN	$N_2^+ + O_2 \rightarrow N_2 + O_2^+$	$5.10E-11*(temp/300.)**(-0.8)$	Fuller-Rowell (1993)
G3200	TrGN	$NO + OH \rightarrow HONO$	$k_3rd(temp, cair, 7.0E-31, 2.6, 3.6E-11, 0.1, 0.6)$	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.3\text{E}-12 \cdot \text{EXP}(270./\text{temp})$	Burkholder et al. (2015)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 1.8\text{E}-30, 3.0, 2.8\text{E}-11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$k_{\text{NO2_HO2}}$	Burkholder et al. (2015)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E}-12$	Burkholder et al. (2015)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E}-11 \cdot \text{EXP}(-390./\text{temp})$	Burkholder et al. (2015)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$k_{\text{HNO3_OH}}$	Burkholder et al. (2015)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$k_{\text{NO2_HO2}} / (2.1\text{E}-27 \cdot \text{EXP}(10900./\text{temp}))$	Burkholder et al. (2015)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E}-12 \cdot \text{EXP}(380./\text{temp})$	Burkholder et al. (2015)
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E}-12 \cdot \text{EXP}(-710./\text{temp})$	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	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E}-07 \cdot \text{EXP}(-628./\text{temp})$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$\text{temp}^{**}(-1.32)$ $9.4\text{E}-09 \cdot \text{EXP}(-356./\text{temp})$ $\text{temp}^{**}(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E}-12 \cdot ((\text{temp}/298.)^{**}(-1.5))$	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)
G3225	UpGN	$\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$	$5.00\text{E}-11$	Roble (1995)
G3226	UpGN	$\text{NO}_2 + \text{H} \rightarrow \text{NO} + \text{OH}$	$4.00\text{E}-10 \cdot \text{EXP}(-340./\text{temp})$	Sander et al. (2003)
G4100	UpStG	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow .75 \text{CH}_3 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	$1.75\text{E}-10$	Burkholder et al. (2015)
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)

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

#	labels	reaction	rate coefficient	reference
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{ HCHO} + .85 \text{ HO}_2 + .15 \text{ CH}_3\text{O} + \text{H}_2\text{O}$	$6.38\text{E-}18 * (\text{temp}^{**2}) * \text{EXP}(144./\text{temp})$	Atkinson et al. (2006)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$3.8\text{E-}13 * \text{EXP}(780./\text{temp}) / (1.+1./498.*\text{EXP}(1160./\text{temp}))$	Atkinson et al. (2006)
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$3.8\text{E-}13 * \text{EXP}(780./\text{temp}) / (1.+498.*\text{EXP}(-1160./\text{temp}))$	Atkinson et al. (2006)
G4104a	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	$2.3\text{E-}12 * \text{EXP}(360./\text{temp}) * (1.-\text{beta_CH3NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$	$2.3\text{E-}12 * \text{EXP}(360./\text{temp}) * \text{beta_CH3NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$	1.2E-12	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{ O}_2$	$7.4\text{E-}13 * \text{EXP}(-520./\text{temp}) * \text{R02} * 2.$	Atkinson et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{ HCHO} + .5 \text{ CH}_3\text{OH} + .5 \text{ O}_2$	$(\text{k_CH3O2} - 7.4\text{E-}13 * \text{EXP}(-520./\text{temp})) * \text{R02} * 2.$	Atkinson et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{ CH}_3\text{O}_2 + .4 \text{ HCHO} + .4 \text{ OH} + \text{H}_2\text{O}$	k_CH3OOH_OH	Wallington et al. (2017)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 * \text{EXP}(2.03 * \text{LOG}(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E-}13 * \text{EXP}(-1900./\text{temp})$	Burkholder et al. (2015)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E-}13 + \text{cair} * 3.54\text{E-}33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$2.94\text{E-}14 * \text{exp}(786./\text{temp}) + 9.85\text{E-}13 * \text{EXP}(-1036./\text{temp})$	Paulot et al. (2011)
G4112	UpStG	$\text{CO} + \text{O}(^3\text{P}) \rightarrow \text{CO}_2$	$6.60\text{E-}33 * \text{EXP}(-1103./\text{temp})$	Roble (1995)
G4113	UpStG	$\text{CH}_4 + \text{O}(^3\text{P}) \rightarrow .51 \text{ CH}_3 + .51 \text{ OH} + .49 \text{ CH}_3\text{O} + .49 \text{ H}$	$6.03\text{E-}18 * \text{temp}^{**}(2.17) * \text{EXP}(-3619./\text{temp})$	Roble (1995), Garton et al. (2003), Espinosa-Garcia and Garcia-Bernáldez (2000)
G4114	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	k_NO2_CH3O2	Burkholder et al. (2015)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$\text{k_NO2_CH3O2} / (9.5\text{E-}29 * \text{EXP}(11234./\text{temp}))$	Burkholder et al. (2015)*
G4116	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$	3.00E-14	see note*
G4117	StTrGN	$\text{CH}_3\text{ONO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}_2$	$4.0\text{E-}13 * \text{EXP}(-845./\text{temp})$	Atkinson et al. (2006)
G4118	StTrG	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E-}14 * \text{exp}(-663./\text{temp}) * \text{c}(\text{ind_02})$	Chai et al. (2014)
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.1\text{E-}29, 4.5, 2.1\text{E-}11, 0., 0.44)$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4119b	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$	$9.6\text{E}-12 \cdot \text{EXP}(-1150./\text{temp})$	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	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$	$2.3\text{E}-12 \cdot (\text{temp}/300.)^{**0.7}$	Atkinson et al. (2006)
G4121	StTrG	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E}-16 \cdot \exp(-1000./\text{temp})$	Burkholder et al. (2015)
G4122	StTrGN	$\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$	$1.\text{E}-10 \cdot \exp(-1764./\text{temp})$	Nielsen et al. (1991)
G4123	StTrG	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$9.7\text{E}-15 \cdot \text{EXP}(625./\text{temp})$	Atkinson et al. (2006)
G4124	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.4\text{E}12 \cdot \text{EXP}(-7000./\text{temp})$	Atkinson et al. (2006)
G4125	StTrG	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2 \text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$	$5.6\text{E}-15 \cdot \text{EXP}(2300./\text{temp})$	Atkinson et al. (2006)
G4126	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$0.7275 \cdot 2.3\text{E}-12 \cdot \text{EXP}(360./\text{temp})$	Atkinson et al. (2006)*
G4127	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	1.2E-12	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(k_{\text{CH302}} \cdot 5.5\text{E}-12) \cdot **0.5 \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(k_{\text{CH302}} \cdot 5.7\text{E}-14 \cdot \text{EXP}(750./\text{temp})) \cdot **0.5 \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H_OH}}$	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)*
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$k_{\text{rohro}} + 2 \cdot k_{\text{s*f_soh*f_soh}}$	Taraborrelli (2010)*
G4133	StTrG	$\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$	1.4E-10	Bossolasco et al. (2014)*
G4134	StTrG	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E}+14 \cdot \text{EXP}(-10000/\text{temp})$	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	$\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$	5.2E-12	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$	6.E-14	Welz et al. (2012)*
G4138	StTrGN	$\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$	$k_{\text{CH200_N02}}$	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$	3.6E-14	Vereecken et al. (2012)
G4141	StTrG	$\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$	1.E-10	Welz et al. (2014)*
G4142	StTrG	$\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$	1.7E-12	Stone et al. (2014)*
G4143	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4144	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4145	StTrG	$\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$	5.E-12	Vereecken et al. (2012)
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	1.E-12	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	6.E-11	Buras et al. (2014)

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

#	labels	reaction	rate coefficient	reference
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	k_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_N02_CH302/(9.5E-29*EXP(11234./temp))	Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	9.50E-13*EXP(-650./temp)*f_soh	see note*
G4151	StTrG	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	k_3rd_iupac(temp, cair, 7.0E-31, 3., 1.8E-12, -1.1, 0.33)	Atkinson et al. (2006)
G4152	StTrG	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{ HCHO} + .956 \text{ H} + .044 \text{ CH}_3\text{O} + \text{O}_2$	5.1E-12*exp(-210./temp)	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{ HCHO} + .83 \text{ H} + .17 \text{ CO} + .17 \text{ H}_2 + .17 \text{ H}$	1.3E-10	Atkinson et al. (2006)
G4154	StTrG	$\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$	2.53E-14	Albaladejo et al. (2002)*
G4155	StTrG	$\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{ CH}_3 + .75 \text{ O}_2 + .25 \text{ HCHO} + .25 \text{ OH}$	2.5E-11	Baulch et al. (2005)
G4156	StTrG	$\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$	4.3E-11	Zellner et al. (1988)
G4157	StTrG	$\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{ OH} + .7 \text{ CO} + .3 \text{ H} + .3 \text{ CO}_2 + \text{HO}_2$	3.4E-11*EXP(-1600./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)
G4159	TrGN	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	k_3rd(temp, cair, 4.28E-33, 1.0, REAL(4.25E-13*EXP(-1150./temp), SP), 1.0, 0.8)	Kleinböhl et al. (2006)
G4160a	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{HCN}$	1.08E-10*EXP(105./temp)*0.15*EXP(200/temp)	Strekowski et al. (2010)
G4160b	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{NCO}$	1.08E-10*EXP(105./temp)*0.68/2.	Strekowski et al. (2010)*
G4160c	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{CN}$	1.08E-10*EXP(105./temp)*(1.-(0.68/2.+0.15*EXP(200/temp)))	Strekowski et al. (2010)*
G4161	TrGN	$\text{HCN} + \text{O}(^3\text{P}) \rightarrow \text{H} + \text{NCO}$	1.0E-11*EXP(-4000./temp)	Burkholder et al. (2015)*
G4162	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}(^3\text{P})$	1.2E-11*EXP(210./temp)*0.75	Baulch et al. (2005)
G4163	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{CO} + \text{NO}$	1.2E-11*EXP(210./temp)*0.25	Baulch et al. (2005)
G4164	TrGN	$\text{NCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{NO}$	7.E-15	Becker et al. (2000)*
G42000	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	1.49E-17*temp*temp*EXP(-499./temp)	Atkinson et al. (2006)
G42001	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{OO}^*$	9.1E-15*EXP(-2580./temp)	Atkinson et al. (2006)*
G42002	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	k_3rd_iupac(temp, cair, 8.6E-29, 3.1, 9.E-12, 0.85, 0.48)	Atkinson et al. (2006), Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G42003	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E}-13 \cdot \text{EXP}(700./\text{temp})$	Burkholder et al. (2015)
G42004a	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.55\text{E}-12 \cdot \text{EXP}(380./\text{temp}) \cdot (1.-\text{beta_C2H5N03})$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$2.55\text{E}-12 \cdot \text{EXP}(380./\text{temp}) \cdot \text{beta_C2H5N03}$	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. (2017)
G42006	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .8 \text{ CH}_3\text{CHO} + .6 \text{ HO}_2 + .2 \text{ C}_2\text{H}_5\text{OH}$	$2 \cdot (7.6\text{E}-14 \cdot k_{\text{CH3O2}}) \cdot (.5) \cdot R02$	Taraborrelli (2016), Atkinson et al. (2006)
G42007a	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G42007b	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{OH}$	$k_{\text{s} \cdot \text{f_sooh}}$	Taraborrelli (2016)
G42008a	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O}$	$4.4\text{E}-12 \cdot \text{EXP}(365./\text{temp}) \cdot 0.95$	Atkinson et al. (2006)
G42008b	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$4.4\text{E}-12 \cdot \text{EXP}(365./\text{temp}) \cdot 0.05$	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	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$	$4.0\text{E}-14 \cdot \text{EXP}(850./\text{temp})$	Atkinson et al. (2006)*
G42011a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$	$5.20\text{E}-13 \cdot \text{EXP}(980./\text{temp}) \cdot 1.507 \cdot 0.61$	Groß et al. (2014)
G42011b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$5.20\text{E}-13 \cdot \text{EXP}(980./\text{temp}) \cdot 1.507 \cdot 0.23$	Groß et al. (2014)
G42011c	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$5.20\text{E}-13 \cdot \text{EXP}(980./\text{temp}) \cdot 1.507 \cdot 0.16$	Groß et al. (2014)
G42012	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E}-12 \cdot \text{EXP}(270./\text{temp})$	Tyndall et al. (2001a)
G42013	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	$k_{\text{CH3C03_N02}}$	Burkholder et al. (2015)*
G42014	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$	$4\text{E}-12$	Canosa-Mas et al. (1996)
G42017a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3 + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Taraborrelli (2016)
G42017b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOH}$	$k1_{\text{R02RC03}} \cdot 0.1$	Taraborrelli (2016)
G42018	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)*
G42020	TrGCN	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$3.00\text{E}-14$	Rickard and Pascoe (2009)
G42021	TrGCN	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	$k_{\text{PAN_M}}$	Burkholder et al. (2015)*
G42022a	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 5.5\text{e}-30, 0.0, 8.3\text{e}-13, -2., 0.6) \cdot 0.71$	Burkholder et al. (2015)*
G42022b	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 5.5\text{e}-30, 0.0, 8.3\text{e}-13, -2., 0.6) \cdot 0.29$	Burkholder et al. (2015)*
G42023a	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$	$8.00\text{E}-12 \cdot 0.80$	Atkinson et al. (2006)
G42023b	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$	$8.00\text{E}-12 \cdot 0.20$	Atkinson et al. (2006)
G42024a	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$	$5.1\text{E}-12 \cdot (1.-1./((1+1.85\text{E}-18 \cdot \text{cair})))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42024b	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	$5.1\text{E}-12 \cdot 1./((1+1.85\text{E}-18 \cdot \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*

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

#	labels	reaction	rate coefficient	reference
G42025	TrGC	$\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Taraborrelli (2016)
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	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	$k1_R02RC03*0.9$	Taraborrelli (2016)
G42027b	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$k1_R02RC03*0.1$	Taraborrelli (2016)
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	Taraborrelli (2016), 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	Taraborrelli (2016), 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	Taraborrelli (2016), 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	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	$KR02N03*1.60$	Rickard and Pascoe (2009)
G42032	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{HCHO} + .09 \text{CO}_2 + .91 \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	$k_co2h+k_s*f_soh*f_co2h$	Taraborrelli (2016)
G42033a	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Taraborrelli (2016)
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	$k_s*f_soh*f_co2h$	Taraborrelli (2016)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42035	TrGCN	$\text{PHAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_s*f_soh*f_cpan+k_rohro$	Taraborrelli (2016)
G42036	TrGC	$\text{GLYOX} + \text{OH} \rightarrow \text{HCOCO} + \text{H}_2\text{O}$	$3.1E-12*EXP(340./temp)$	Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013)
G42037	TrGCN	$\text{GLYOX} + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42038a	TrGC	$\text{HCOCO} \rightarrow \text{CO} + \text{CO} + \text{HO}_2$	$7.E11*EXP(-3160./temp) + 5.E-12*c(ind_02)$	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	$\text{HCOCO} \rightarrow \text{HCOCO}_3$	$5.E-12*c(ind_02)*3.2*exp(-550./temp)$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	$\text{HCOCO} \rightarrow \text{OH} + \text{CO} + \text{CO}_2$	$5.E-12*c(ind_02) * (1.-3.2*exp(-550./temp))$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	$\text{HCOCO}_3 \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2$	$k1_R02RC03*0.9$	Taraborrelli (2016)
G42039b	TrGC	$\text{HCOCO}_3 \rightarrow \text{HCOCO}_2\text{H}$	$k1_R02RC03*0.1$	Taraborrelli (2016)
G42040	TrGC	$\text{HCOCO}_3 + \text{HO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02	Feierabend et al. (2008), Taraborrelli (2016)
G42041	TrGCN	$\text{HCOCO}_3 + \text{NO} \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G42042	TrGCN	$\text{HCOCO}_3 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	$\text{KR02N03} \times 1.60$	Rickard and Pascoe (2009)
G42043	TrGCN	$\text{HCOCO}_3 + \text{NO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_3 + \text{CO}_2$	k_CH3C03_N02	Orlando and Tyndall (2001), Taraborrelli (2016)
G42044	TrGC	$\text{HCOCO}_2\text{H} + \text{OH} \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{k_co2h} + \text{k_t*f_o*f_co2h}$	Taraborrelli (2016)
G42045a	TrGC	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3 + \text{H}_2\text{O}$	$0.6 \times \text{k_CH300H_OH}$	Taraborrelli (2016)
G42045b	TrGC	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{CO} + \text{CO}_2 + \text{H}_2\text{O} + \text{OH}$	k_t*f_o*f_co2h	Taraborrelli (2016)
G42046	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 \rightarrow .6 \text{HOCH}_2\text{CH}_2\text{O} + .2 \text{HOCH}_2\text{CHO} + .2 \text{ETHGLY}$	$2 \times (7.8\text{E}-14 \times \text{EXP}(1000./\text{temp})) \times \text{k_CH302} \times (.5) \times \text{R02}$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow .25 \text{HO}_2 + .5 \text{HCHO} + .75 \text{HOCH}_2\text{CH}_2\text{O} + \text{NO}_2$	$\text{KR02N0} \times (1 - \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G42048	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{ETHOHNO}_3$	$\text{KR02N0} \times \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair})$	Taraborrelli (2016)
G42049a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HYETHO2H}$	$1.53\text{E}-13 \times \text{EXP}(1300./\text{temp}) \times (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G42049b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$1.53\text{E}-13 \times \text{EXP}(1300./\text{temp}) \times \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)
G42050	TrGCN	$\text{ETHOHNO}_3 + \text{OH} \rightarrow .93 \text{NO}_3\text{CH}_2\text{CHO} + .93 \text{HO}_2 + .07 \text{HOCH}_2\text{CHO} + .07 \text{NO}_2 + \text{H}_2\text{O}$	$\text{k_s} \times (\text{f_soh} \times \text{f_ch2ono2} + \text{f_ono2} \times \text{f_pch2oh}) + \text{k_rohro}$	Taraborrelli (2016)
G42051a	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \times \text{k_CH300H_OH}$	Rickard and Pascoe (2009)*
G42051b	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$	$\text{k_s} \times \text{f_soh} \times \text{f_pch2oh}$	Taraborrelli (2016)
G42051c	TrGC	$\text{HYETHO2H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$\text{k_s} \times \text{f_soh} \times \text{f_pch2oh} + \text{k_rohro}$	Taraborrelli (2016)
G42052a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HOCH}_2\text{CHO}$	$6.00\text{E}-14 \times \text{EXP}(-550./\text{temp}) \times \text{C}(\text{ind_02})$	Rickard and Pascoe (2009)
G42052b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HCHO} + \text{HCHO}$	$9.50\text{E}13 \times \text{EXP}(-5988./\text{temp})$	Rickard and Pascoe (2009)
G42053	TrGC	$\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$2 \times \text{k_s} \times \text{f_soh} \times \text{f_pch2oh} + 2 \times \text{k_rohro}$	Taraborrelli (2016)
G42054	TrGC	$\text{HCOCH}_2\text{O}_2 \rightarrow .6 \text{HCHO} + .6 \text{CO} + .6 \text{HO}_2 + .2 \text{GLYOX} + .2 \text{HOCH}_2\text{CHO}$	k1_R02pOR02	Taraborrelli (2016)
G42055a	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CHO}$	$\text{KR02H02}(2) \times \text{rcoch2o2_ooh}$	Taraborrelli (2016)
G42055b	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(2) \times \text{rcoch2o2_oh}$	Taraborrelli (2016)
G42056a	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{KR02N0} \times (1 - \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair}))$	Taraborrelli (2016)
G42056b	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	$\text{KR02N0} \times \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair})$	Taraborrelli (2016)
G42057	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G42058a	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2$	$0.6 \times \text{k_CH300H_OH}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G42058b	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH}$	$.8*8.\text{E}-12$	Taraborrelli (2016)*
G42058c	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	$k_s*f_sooh*f_cho$	Taraborrelli (2016)
G42059	TrGCN	$\text{HOOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42060	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	KAPN0	Taraborrelli (2016)
G42061	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	KR02N03*1.60	Taraborrelli (2016)
G42062a	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 2 \text{OH} + \text{HCHO} + \text{CO}_2$	KAPH02*rco3_oh	Taraborrelli (2016)
G42062b	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	KAPH02*rco3_ooH	Taraborrelli (2016)
G42062c	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rco3_o3	Taraborrelli (2016)
G42063a	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	$k1_R02RC03*0.9$	Taraborrelli (2016)
G42063b	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$	$k1_R02RC03*0.1$	Taraborrelli (2016)
G42064a	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$2.*0.6*k_CH300H_OH$	Taraborrelli (2016)
G42064b	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_s*f_sooh*f_co2h$	Taraborrelli (2016)
G42065	TrGC	$\text{HOOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCO}_2\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_s*f_sooh*f_co2h+k_co2h$	Taraborrelli (2016)
G42066	TrGC	$\text{CH}_2\text{CO} + \text{OH} \rightarrow .6 \text{HCHO} + .6 \text{HO}_2 + .6 \text{CO} + .4 \text{HOOCH}_2\text{CO}_2\text{H}$	$2.8\text{E}-12*\exp(510./\text{temp})$	Baulch et al. (2005), Taraborrelli (2016)
G42067a	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{OH}$	$(k_t*f_tooh*f_toh + k_rohro)$	Taraborrelli (2016)
G42067b	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$	$0.6*k_CH300H_OH$	Taraborrelli (2016)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{CH}_3\text{CHOHOOH} + .3 \text{CH}_3\text{COOH} + .2 \text{CH}_3 + .2 \text{HCOOH} + .2 \text{OH}$	$5.6\text{E}-15*\text{EXP}(2300./\text{temp})$	Taraborrelli (2016)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	$k1_R02s0R02$	Taraborrelli (2016)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KR02N0	Taraborrelli (2016)
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), Taraborrelli (2016)*
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), Taraborrelli (2016)*
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)*

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

#	labels	reaction	rate coefficient	reference
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	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	9.50E-13*EXP(-650./temp)	Taraborrelli (2016)*
G42083a	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	5.1E-12*(1. - 1./(1.+ 9.4E-18*cair))	Atkinson et al. (2006), Beyers- dorf et al. (2010)*
G42083b	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$	5.1E-12*1./(1.+9.4E-18*cair)	Atkinson et al. (2006), Beyers- dorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{ C}_2\text{H}_5\text{O}_2 + .95 \text{ HO}_2 + .05$ $\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	3.0E-12*EXP(20./temp)	Taraborrelli (2016), Atkinson et al. (2006)
G42085a	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$	8.1E-13*EXP(-1080./temp)*0.40	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42085b	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$	8.1E-13*EXP(-1080./temp)*(1.-0.40)	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$	2.54E-10*EXP(-24./temp) *0.0269*EXP(137./temp)	Strekowski et al. (2010)
G42086b	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{ H} + \text{CO} + \text{HCN}$	2.54E-10*EXP(-24./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 OH	2.54E-10*EXP(-24./temp)*(1.-(0.16+ 0.0269*EXP(137./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	Taraborrelli (2016), 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	Taraborrelli (2016), So et al. (2014)
G42090	TrGC	$\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G42091	TrGC	$\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (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	Taraborrelli (2016)
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	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43001a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{CHOHOOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	$5.5\text{E}-15*\text{EXP}(-1880./\text{temp})*.57$	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	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO2}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.6\text{E}-27, 3.5, 3.\text{E}-11, 1., 0.5)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO3BO2}$	$4.6\text{E}-13*\text{EXP}(-1155./\text{temp})$	Wallington et al. (2017)
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. (2017)
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. (2017)
G43006	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{CH}_3\text{COCH}_3 + .2 \text{IPROPOL} + .6 \text{HO}_2$	$2.*(1.6\text{E}-12*\text{EXP}(-2200./\text{temp})*\text{k_CH302})*(.5)*\text{R02}$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	$0.6*\text{k_CH300H_OH}$	Taraborrelli (2016)
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	Taraborrelli (2016)
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	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.7\text{E}-12*\text{EXP}(360./\text{temp})*(1.-\alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Wallington et al. (2017)
G43009b	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_3\text{H}_7\text{ONO}_2$	$2.7\text{E}-12*\text{EXP}(360./\text{temp})*\alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair})$	Wallington et al. (2017)
G43010	TrGC	$\text{C}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{CH}_3\text{COCH}_3 + .2 \text{NPROPOL} + .6 \text{HO}_2$	$2.*(\text{k_CH302}*3.\text{E}-13)*(.5)*\text{R02}$	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), Taraborrelli (2016)
G43012b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{HCHO}$	$8.6\text{E}-13*\text{EXP}(700./\text{temp})*\text{rcoch2o2_oh}$	Tyndall et al. (2001a), Taraborrelli (2016)
G43013a	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12*\text{EXP}(300./\text{temp})*(1.-\alpha_{\text{AN}}(4, 1, 1, 0, 0, \text{temp}, \text{cair}))$	Burkholder et al. (2015)
G43013b	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NOA}$	$2.9\text{E}-12*\text{EXP}(300./\text{temp})*\alpha_{\text{AN}}(4, 1, 1, 0, 0, \text{temp}, \text{cair})$	Burkholder et al. (2015)
G43014	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .3 \text{CH}_3\text{C}(\text{O}) + .3 \text{HCHO} + .5 \text{MGLYOX} + .2 \text{CH}_3\text{COCH}_2\text{OH}$	k1_R02pOR02	Orlando and Tyndall (2012)

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

#	labels	reaction	rate coefficient	reference
G43015a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H_OH}}$	see note*
G43015b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f_sooh*f_co}}$	Taraborrelli (2016)
G43016	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$1.6\text{E-}12 \cdot \text{EXP}(305./\text{temp})$	Atkinson et al. (2006)
G43017	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{ CH}_3 + .6 \text{ CH}_3\text{C}(\text{O}) + 1.4 \text{ CO} + \text{H}_2\text{O}$	$1.9\text{E-}12 \cdot \text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13 \cdot \text{EXP}(-230./\text{temp})$	Wallington et al. (2017)
G43021	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43022	TrGC	$\text{HYPROPO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	k1_R02sOR02	Rickard and Pascoe (2009)
G43023a	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{HYPROPO}_2\text{H}$	$\text{KR02H02}(3) \cdot (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G43023b	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(3) \cdot \text{rchohch2o2_oh}$	Rickard and Pascoe (2009)
G43024a	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G43024b	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{PROPOLNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G43025	TrGCN	$\text{HYPROPO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43026a	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{HYPROPO}_2$	$0.6 \cdot k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G43026b	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{\text{s*f_soh*f_pch2oh}} + k_{\text{t*f_tooh*f_pch2oh}})$	Taraborrelli (2016)
G43027	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{HO}_2 \rightarrow \text{PR}_2\text{O}_2\text{HNO}_3$	KR02H02(3)	Rickard and Pascoe (2009)
G43028	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43029	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G43030a	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{PRONO}_3\text{BO}_2$	$0.6 \cdot k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G43030b	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{\text{t*f_tooh*f_ch2ono2}}$	Taraborrelli (2016)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HNO}_3$	$\text{KN03AL} \cdot 2.4$	Rickard and Pascoe (2009)
G43032	TrGCN	$\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$	$(k_{\text{s*f_co*f_ono2}} + k_{\text{p*f_co}})$	Taraborrelli (2016)
G43033	TrGC	$\text{HOCH}_2\text{COCHO} + \text{OH} \rightarrow .8609 \text{ HOCH}_2\text{CO} + .8609 \text{ CO} + .1391 \text{ HCOCOCHO} + .1391 \text{ HO}_2$	$(1.9\text{E-}12 \cdot \text{EXP}(575./\text{temp}) + k_{\text{s*f_soh*f_co}})$	Taraborrelli (2016)
G43034	TrGCN	$\text{HOCH}_2\text{COCHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL} \cdot 2.4$	Taraborrelli (2016)
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E-}14 \cdot \text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Taraborrelli (2016)
G43036	TrGC	$\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{ HCOCO} + .6 \text{ HCHO} + .2 \text{ HCOCOCHO} + .2 \text{ HOCH}_2\text{COCHO}$	k1_R02pOR02	Taraborrelli (2016)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$\text{KR02H02}(3) \cdot \text{rcoch2o2_ooh}$	Taraborrelli (2016)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{KR02H02}(3) \cdot \text{rcoch2o2_oh}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{\text{t}*\text{f}_{\text{co}}*\text{f}_{\text{o}}}$	Taraborrelli (2016)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}*\text{f}_{\text{sooh}}*\text{f}_{\text{co}}}$	Taraborrelli (2016)*
G43040c	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H}_{\text{OH}}}$	Taraborrelli (2016)
G43041	TrGCN	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	KN03AL*2.4	Taraborrelli (2016)
G43042	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO}$	k1_R02p0R02	Taraborrelli (2016)
G43043a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$\text{KR02H02(3)*rcoch2o2}_{\text{ooH}}$	Taraborrelli (2016)
G43043b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{OH}$	$\text{KR02H02(3)*rcoch2o2}_{\text{oh}}$	Taraborrelli (2016)
G43044	TrGCN	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G43045a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCHO} + \text{OH}$	$k_{\text{s}*\text{f}_{\text{sooh}}*\text{f}_{\text{co}}}$	Taraborrelli (2016)
G43045b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{O}_2$	$.6*k_{\text{CH300H}_{\text{OH}}}$	Taraborrelli (2016)
G43045c	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E}-12*\text{EXP}(305./\text{temp})$	Taraborrelli (2016)*
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), Taraborrelli (2016)
G43047	TrGCN	$\text{PROPOLNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{\text{t}*\text{f}_{\text{ono2}}*\text{f}_{\text{pch2oh}}+k_{\text{s}*\text{f}_{\text{soh}}*\text{f}_{\text{ch2ono2}}}}$	Taraborrelli (2016)
G43048	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$2.3\text{E}-12*\text{EXP}(300./\text{temp})$	Tyndall et al. (2001a)*
G43049	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2$	$1.9\text{E}16*\text{EXP}(-10830./\text{temp})$	Sehested et al. (1998)*
G43050	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13*\text{EXP}(-650./\text{temp})*\text{f}_{\text{co}}$	Taraborrelli (2016)*
G43051a	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H}_{\text{OH}}}$	Taraborrelli (2016)
G43051b	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}*\text{f}_{\text{sooh}}}$	Taraborrelli (2016)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{s}*\text{f}_{\text{pch2oh}}}$	Taraborrelli (2016)*
G43052	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$4.9\text{E}-12*\text{EXP}(405./\text{temp})$	Atkinson et al. (2006)*
G43053	TrGCN	$\text{C}_2\text{H}_5\text{CHO} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HNO}_3$	$6.3\text{E}-15$	Atkinson et al. (2006)
G43054a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}}*0.9$	Taraborrelli (2016)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	$k1_{\text{R02RC03}}*0.1$	Taraborrelli (2016)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02*rco3}_{\text{oh}}$	Taraborrelli (2016), Groß et al. (2014)
G43055b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$	$\text{KAPH02*rco3}_{\text{ooH}}$	Taraborrelli (2016), Groß et al. (2014)
G43055c	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02*rco3}_{\text{o3}}$	Taraborrelli (2016), 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	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	$k_{\text{CH3C03}_{\text{N02}}}$	Rickard and Pascoe (2009)
G43058	TrGCN	$\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN}_{\text{M}}}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43059	TrGC	$\text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$k_{\text{co2h}+\text{k}_\text{p}+\text{k}_\text{s}*\text{f}_{\text{co2h}}}$	Taraborrelli (2016)*
G43060a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G43060b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$k_{\text{s}*\text{f}_{\text{co2h}}+\text{k}_\text{p}}$	Taraborrelli (2016)*
G43061	TrGCN	$\text{PPN} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}*\text{f}_{\text{cpan}}+\text{k}_\text{p}}$	Taraborrelli (2016)*
G43062	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_3 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G43063a	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{co3_oh}}$	Taraborrelli (2016)
G43063b	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	$\text{KAPH02}*(r_{\text{co3_ooh}}+r_{\text{co3_o3}})$	Taraborrelli (2016)
G43064	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_2$	KAPNO	Taraborrelli (2016)
G43065	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_3$	$k_{\text{CH3CO3_NO2}}$	Taraborrelli (2016)*
G43066	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2 + \text{NO}_2$	$\text{KR02NO3}*1.74$	Taraborrelli (2016)
G43067	TrGC	$\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2$	$k_{1_R02RC03}$	Taraborrelli (2016)
G43068	TrGC	$\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{CO} + \text{HO}_2$	$2.*k_{\text{t}*\text{f}_{\text{co}*\text{f}_{\text{o}}}}$	Taraborrelli (2016)
G43069	TrGC	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$	$2.6\text{E}-12*\text{EXP}(200./\text{temp})$	Atkinson et al. (2006)
G43070a	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$4.6\text{E}-12*\text{EXP}(70./\text{temp})*(k_{\text{s}*\text{f}_{\text{soh}}}/(k_{\text{p}}+k_{\text{s}*\text{f}_{\text{pch2oh}}+k_{\text{s}*\text{f}_{\text{soh}}}}))$	Atkinson et al. (2006), Taraborrelli (2016)*
G43070b	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO2} + \text{H}_2\text{O}$	$4.6\text{E}-12*\text{EXP}(70./\text{temp})*((k_{\text{p}}+k_{\text{s}*\text{f}_{\text{pch2oh}}})/(k_{\text{p}}+k_{\text{s}*\text{f}_{\text{pch2oh}}+k_{\text{s}*\text{f}_{\text{soh}}}}))$	Atkinson et al. (2006), Taraborrelli (2016)*
G43071a	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$	$k_{\text{CH2CHOH_OH_HCOOH}}$	Taraborrelli (2016), So et al. (2014)*
G43072	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCOOH}$	$k_{\text{CH2CHOH_HCOOH}}$	Taraborrelli (2016), daSilva (2010)*
G43073	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH}$	$k_{\text{ALD_HCOOH}}$	Taraborrelli (2016), daSilva (2010)*
G43074	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{s}*\text{f}_{\text{sooh}}*\text{f}_{\text{co}}+0.6*k_{\text{CH300H_OH}}}$	Taraborrelli (2016)*
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	$\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$	$2.*\text{KN03AL}*2.4$	Rickard and Pascoe (2009)
G43204a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$k_{1_R02RC03}*0.9$	Taraborrelli (2016)
G43204b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$k_{1_R02RC03}*0.1$	Taraborrelli (2016)
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	$\text{HCOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN2}$	$k_{\text{CH3CO3_NO2}}$	Rickard and Pascoe (2009)
G43207a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02}*r_{\text{co3_ooh}}$	Rickard and Pascoe (2009)
G43207b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02}*r_{\text{co3_o3}}$	Rickard and Pascoe (2009)
G43207c	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{co3_oh}}$	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)

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

#	labels	reaction	rate coefficient	reference
G43211	TrGTerCN	$\text{C}_3\text{PAN2} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	2.10E-11	Rickard and Pascoe (2009)
G43212	TrGTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	2.14E-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_R02RC03*0.9	Taraborrelli (2016)
G43213b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	k1_R02RC03*0.1	Taraborrelli (2016)
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	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G43215b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G43215c	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{O}_3$	KAPH02*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_CH3C03_N02	Rickard and Pascoe (2009)
G43219	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	1.39E-11	Rickard and Pascoe (2009)
G43220	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3$	1.73E-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_PAN_M	Rickard and Pascoe (2009)
G43222	TrGTerCN	$\text{C}_3\text{PAN1} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{CO} + \text{NO}_2$	4.51E-12	Rickard and Pascoe (2009)
G43223	TrGTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	2.49E-11	Rickard and Pascoe (2009)*
G43415	TrGAroC	$\text{C3DIALOOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{OH}$	1.44E-10	Rickard and Pascoe (2009)
G43418a	TrGAroC	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{C3DIALOOH}$	KR02H02(3)*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G43418b	TrGAroC	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	KR02H02(3)*rco3_oh	Rickard and Pascoe (2009)
G43419	TrGAroCN	$\text{C3DIALO}_2 + \text{NO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43420	TrGAroCN	$\text{C3DIALO}_2 + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G43421	TrGAroC	$\text{C3DIALO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G43422a	TrGAroC	$\text{HCOCOHO}_3 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G43422b	TrGAroC	$\text{HCOCOHO}_3 + \text{HO}_2 \rightarrow \text{HCOCOHO}_3\text{H}$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G43424	TrGAroCN	$\text{HCOCOHO}_3 + \text{NO} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43425	TrGAroCN	$\text{HCOCOHO}_3 + \text{NO}_2 \rightarrow \text{HCOCOHPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G43426	TrGAroCN	$\text{HCOCOHO}_3 + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	$\text{HCOCOHO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G43428	TrGAroC	$\text{METACETHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2$	9.82E-11	Rickard and Pascoe (2009)
G43442	TrGAroCN	$\text{HCOCOHPAN} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	6.97E-11	Rickard and Pascoe (2009)
G43443	TrGAroCN	$\text{HCOCOHPAN} \rightarrow \text{HCOCOHO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	$\text{C32OH13CO} + \text{OH} \rightarrow \text{HCOCOHO}_3$	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	$\text{HCOCOHO}_3\text{H} + \text{OH} \rightarrow \text{HCOCOHO}_3$	7.33E-11	Rickard and Pascoe (2009)
G44000	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	2.03E-17*temp*temp*EXP(78./temp)	Atkinson et al. (2006)*
G44001a	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	(k1_R02pR02*0.1273+k1_R02sR02*0.8727)*0.1273	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44001b	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$(k1_R02pR02*0.1273+k1_R02sR02*0.8727)*0.8727$	Rickard and Pascoe (2009), Taraborrelli (2016)*
G44002	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	$\text{KR02H02}(4)$	Rickard and Pascoe (2009)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N0}*(1-(0.1273*\alpha_AN(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_AN(4,2,0,0,0,\text{temp},\text{cair}))) * 0.1273$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N0}*(1-(0.1273*\alpha_AN(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_AN(4,2,0,0,0,\text{temp},\text{cair}))) * 0.8727$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*(0.1273*\alpha_AN(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_AN(4,2,0,0,0,\text{temp},\text{cair}))$	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), Taraborrelli (2016)
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), Taraborrelli (2016)
G44005a	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Taraborrelli (2016)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_s*f_tooh*f_alk*(k_p/(k_p+k_s))$	Taraborrelli (2016)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_t*f_tooh*f_alk*(k_s/(k_p+k_s))$	Taraborrelli (2016)
G44006a	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp})*k_t/(3.*k_p+k_t)$	Atkinson (2003)
G44006b	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp})*3.*k_p/(3.*k_p+k_t)$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$k1_R02tR02$	Rickard and Pascoe (2009), Taraborrelli (2016)
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	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02N0}*(1-\alpha_AN(4,3,0,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0}*\alpha_AN(4,3,0,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G44010a	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_CH300H_OH$	Taraborrelli (2016)
G44010b	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$3.*k_p*f_tch2oh$	Taraborrelli (2016)*
G44011	TrGCN	$\text{TC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$3.*k_p*f_ch2ono2$	Taraborrelli (2016)*
G44012	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k1_R02sR02$	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44013	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$	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), Taraborrelli (2016)
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	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{sooh}}+2.*k_{\text{s}}+k_{\text{t}}*f_{\text{pch2oh}}$	Taraborrelli (2016)*
G44016	TrGCN	$\text{IC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{ono2}}+2.*k_{\text{p}}+k_{\text{t}}*f_{\text{ch2ono2}}$	Taraborrelli (2016)*
G44017	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .87 \text{ MGLYOX} + .5481 \text{ CO} + .1392 \text{ HO}_2 + .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .13 \text{ HCHO} + .04680 \text{ OH} + .04680 \text{ CO} + .07280 \text{ CH}_3\text{C}(\text{O}) + .026 \text{ CH}_3\text{CHO} + .026 \text{ CO}_2 + .026 \text{ HCHO} + .026 \text{ HO}_2 + .02402 \text{ MGLYOX} + .02402 \text{ H}_2\text{O}_2 + .00718 \text{ CH}_3\text{COCO}_2\text{H}$	$8.5\text{E}-16*\text{EXP}(-1520./\text{temp})$	Taraborrelli (2016)
G44018	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{LHMVKABO}_2$	$2.6\text{E}-12*\text{EXP}(610./\text{temp})$	Taraborrelli (2016), Atkinson et al. (2006)*
G44019	TrGC	$\text{MEK} + \text{OH} \rightarrow \text{LMEKO}_2 + \text{H}_2\text{O}$	$1.5\text{E}-12*\text{EXP}(-90./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)*
G44020	TrGC	$\text{LMEKO}_2 + \text{HO}_2 \rightarrow \text{LMEKOOH}$	KR02H02(4)	Taraborrelli (2016)
G44021a	TrGCN	$\text{LMEKO}_2 + \text{NO} \rightarrow .62 \text{ CH}_3\text{CHO} + .62 \text{ CH}_3\text{C}(\text{O}) + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-(.62*\alpha_{\text{AN}}(4,2,1,0,0,\text{temp},\text{cair})+.38*\alpha_{\text{AN}}(4,1,0,1,0,\text{temp},\text{cair})))$	Taraborrelli (2016)*
G44021b	TrGCN	$\text{LMEKO}_2 + \text{NO} \rightarrow \text{LMEKNO}_3$	$\text{KR02N0}*(.62*\alpha_{\text{AN}}(4,2,1,0,0,\text{temp},\text{cair})+.38*\alpha_{\text{AN}}(4,1,0,1,0,\text{temp},\text{cair}))$	Taraborrelli (2016)
G44022a	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow \text{LMEKO}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G44022b	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow .62 \text{ BIACET} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O} + \text{OH}$	$(.62*k_{\text{t}}*f_{\text{tooh}}*f_{\text{co}}+.38*k_{\text{s}}*f_{\text{sooh}})$	Taraborrelli (2016)
G44023a	TrGCN	$\text{LC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{t}}*f_{\text{ono2}}*f_{\text{alk}}+k_{\text{p}}*f_{\text{alk}}+k_{\text{s}}*f_{\text{ch2ono2}}+k_{\text{p}})*(k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}))$	Taraborrelli (2016)*
G44023b	TrGCN	$\text{LC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{p}}+k_{\text{s}}*(1+f_{\text{ch2ono2}}+f_{\text{ono2}})*f_{\text{alk}})*(k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}))$	Taraborrelli (2016)*
G44024	TrGCN	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{NO}_2$	$3.2\text{E}-11$	Orlando et al. (2002)
G44025	TrGCN	$\text{MPAN} \rightarrow \text{MACO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	see note*

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

#	labels	reaction	rate coefficient	reference
G44026	TrGC	$\text{LMEKO2} \rightarrow .538 \text{ HCHO} + .538 \text{ CO}_2 + .459 \text{ HOCH}_2\text{CH}_2\text{O}_2 + .079 \text{ C}_2\text{H}_5\text{O}_2 + .462 \text{ CH}_3\text{C(O)} + .462 \text{ CH}_3\text{CHO}$	$(.62 * k1_R02s0R02 + .38 * k1_R02p0R02)$	Rickard and Pascoe (2009)*
G44027	TrGC	$\text{MACR} + \text{OH} \rightarrow .45 \text{ MACO3} + .55 \text{ MACRO2}$	$8.E-12 * \text{EXP}(380./\text{temp})$	Orlando et al. (1999b), Taraborrelli (2016)
G44028	TrGC	$\text{MACR} + \text{O}_3 \rightarrow .5481 \text{ CO} + .1392 \text{ HO}_2 + .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .87 \text{ MGLYOX} + .13 \text{ HCHO} + .13 \text{ OH} + .065 \text{ HCOCOCH}_2\text{O}_2 + .065 \text{ CO} + .065 \text{ CH}_3\text{C(O)}$	$1.36E-15 * \text{EXP}(-2112./\text{temp})$	Taraborrelli (2016)
G44029	TrGCN	$\text{MACR} + \text{NO}_3 \rightarrow \text{MACO3} + \text{HNO}_3$	$\text{KN03AL} * 2.0$	Rickard and Pascoe (2009)
G44030a	TrGC	$\text{MACO3} \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{CO}_2$	$k1_R02RC03 * 0.9$	Taraborrelli (2016)
G44030b	TrGC	$\text{MACO3} \rightarrow \text{MACO2H}$	$k1_R02RC03 * 0.1$	Taraborrelli (2016)
G44031a	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO2} + \text{OH}$	$\text{KAPH02} * rco3_oh$	Taraborrelli (2016)
G44031b	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO3H}$	$\text{KAPH02} * rco3_ooh$	Taraborrelli (2016)
G44031c	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO2H} + \text{O}_3$	$\text{KAPH02} * rco3_o3$	Taraborrelli (2016)
G44032	TrGCN	$\text{MACO3} + \text{NO} \rightarrow \text{MACO2} + \text{NO}_2$	$8.70E-12 * \text{EXP}(290./\text{temp})$	Taraborrelli (2016)
G44033	TrGCN	$\text{MACO3} + \text{NO}_2 \rightarrow \text{MPAN}$	k_CH3CO3_N02	Rickard and Pascoe (2009)
G44034	TrGCN	$\text{MACO3} + \text{NO}_3 \rightarrow \text{MACO2} + \text{NO}_2$	$\text{KR02N03} * 1.60$	Taraborrelli (2016)
G44035	TrGC	$\text{MACRO2} \rightarrow .7 \text{ CH}_3\text{COCH}_2\text{OH} + .7 \text{ HCHO} + .7 \text{ HO}_2 + .3 \text{ MACROH}$	$k1_R02t0R02$	Rickard and Pascoe (2009)*
G44036a	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACRO} + \text{OH}$	$\text{KR02H02}(4) * rcoch2o2_oh$	Taraborrelli (2016)
G44036b	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACROOH}$	$\text{KR02H02}(4) * rcoch2o2_ooh$	Taraborrelli (2016)
G44037a	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRO} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_AN(6, 3, 1, 0, 0, \text{temp}, \text{cair}))$	Taraborrelli (2016)
G44037b	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRN}$	$\text{KR02N0} * \alpha_AN(6, 3, 1, 0, 0, \text{temp}, \text{cair})$	Taraborrelli (2016)
G44038	TrGCN	$\text{MACRO2} + \text{NO}_3 \rightarrow \text{MACRO} + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G44039a	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{MACRO2}$	$0.6 * k_CH300H_OH$	Taraborrelli (2016)
G44039b	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$k_tf_o * f_tch2oh * f_alk$	Taraborrelli (2016)
G44039c	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$(k_s * f_soh * f_pch2oh + k_rohro)$	Taraborrelli (2016)
G44040	TrGC	$\text{MACROH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2$	$k_tf_o * f_tch2oh * f_alk$	Taraborrelli (2016)
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	Taraborrelli (2016)
G44042	TrGC	$\text{MACO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2 + \text{CO}_2$	$((k_adt + k_adp) * a_co2h + k_co2h)$	Taraborrelli (2016)
G44043a	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{OH}$	$(k_adt + k_adp) * a_co2h$	Taraborrelli (2016)
G44043b	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{MACO3}$	$0.6 * k_CH300H_OH$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44044	TrGC	LHMKABO2 \rightarrow .024 CO2H3CHO + .072 MGLYOX + .072 HO ₂ + .072 HCHO + .5280 CH ₃ C(O) + .5280 HOCH ₂ CHO + .176 BIACETOH + .2 HO12CO3C4	(.12*k1_R02p0R02+.88*k1_R02s0R02)	Taraborrelli (2016)
G44045a	TrGC	LHMKABO2 + HO ₂ \rightarrow OH + HOCH ₂ CHO + CH ₃ C(O)	KR02H02(4)*.88*rcoch2o2_oh	Taraborrelli (2016)
G44045b	TrGC	LHMKABO2 + HO ₂ \rightarrow LHMKABOOH	KR02H02(4)*(.12+.88*rcoch2o2_oh)	Taraborrelli (2016)
G44046a	TrGCN	LHMKABO2 + NO \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + NO ₂	KR02N0*(1-(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)))	Taraborrelli (2016)
G44046b	TrGCN	LHMKABO2 + NO \rightarrow MVKNO3	KR02N0*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair))	Taraborrelli (2016)*
G44047	TrGCN	LHMKABO2 + NO ₃ \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + .12 HO ₂ + NO ₂	KR02N03	Taraborrelli (2016)
G44048a	TrGC	LHMKABOOH + OH \rightarrow LHMKABO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G44048b	TrGC	LHMKABOOH + OH \rightarrow .12 CO2H3CHO + .88 BIACETOH + OH	(.12*k_sf_soh*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co)	Taraborrelli (2016)
G44049a	TrGC	CO2H3CHO + OH \rightarrow CO2H3CO3	k_t*f_o*f_alk	Taraborrelli (2016)
G44049b	TrGC	CO2H3CHO + OH \rightarrow CH ₃ COCOCHO + HO ₂ + H ₂ O	k_t*f_co*f_toh*f_cho	Taraborrelli (2016)
G44050	TrGCN	CO2H3CHO + NO ₃ \rightarrow CO2H3CO3 + HNO ₃	KN03AL*4.0	Rickard and Pascoe (2009)
G44051	TrGC	CO2H3CO3 \rightarrow MGLYOX + HO ₂ + CO ₂	k1_R02RC03	Taraborrelli (2016)
G44052a	TrGC	CO2H3CO3 + HO ₂ \rightarrow OH + MGLYOX + HO ₂ + CO ₂	KAPH02*rco3_oh	Taraborrelli (2016)
G44052b	TrGC	CO2H3CO3 + HO ₂ \rightarrow CO2H3CO2H + O ₃	KAPH02*rco3_o3	Taraborrelli (2016)
G44052c	TrGC	CO2H3CO3 + HO ₂ \rightarrow CO2H3CO3H	KAPH02*rco3_oh	Taraborrelli (2016)
G44053	TrGCN	CO2H3CO3 + NO \rightarrow MGLYOX + HO ₂ + NO ₂ + CO ₂	KAPN0	Taraborrelli (2016)
G44054	TrGCN	CO2H3CO3 + NO ₃ \rightarrow MGLYOX + HO ₂ + NO ₂ + CO ₂	KR02N03*1.60	Taraborrelli (2016)
G44055a	TrGC	CO2H3CO3H + OH \rightarrow CO2H3CO3	0.6*k_CH300H_OH	Taraborrelli (2016)
G44055b	TrGC	CO2H3CO3H + OH \rightarrow CH ₃ C(O) + CO + CO ₂ + OH	(k_t*f_co2h*f_co*f_toh)	Taraborrelli (2016)
G44056	TrGC	CO2H3CO2H + OH \rightarrow CH ₃ COCOCHO + HO ₂	k_t*f_co2h*f_co*f_toh+k_co2h	Taraborrelli (2016)
G44057a	TrGC	HO12CO3C4 + OH \rightarrow BIACETOH + HO ₂	k_t*f_toh*f_alk*f_co	Taraborrelli (2016)
G44057b	TrGC	HO12CO3C4 + OH \rightarrow CO2H3CHO + HO ₂	k_sf_soh*f_alk	Taraborrelli (2016)
G44058	TrGC	MACO2 \rightarrow .65 CH ₃ + .65 CO + .65 HCHO + .35 OH + .35 CH ₃ COCH ₂ O ₂ + CO ₂	KDEC	Taraborrelli (2016)
G44059	TrGC	LHMKABO2 \rightarrow .88 MGLYOX + .88 HCHO + .12 HOOCH ₂ CHO + .12 CH ₃ C(O) + OH	KHSD	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44060	TrGC	MACRO2 \rightarrow MGLYOX + HCHO + OH	KHSB	Taraborrelli (2016)
G44061a	TrGCN	MVKNO3 + OH \rightarrow MGLYOX + CO ₂ + HO ₂ + NO ₂ + H ₂ O	k_s*f_sooh*f_ch2ono2+k_rohro	Taraborrelli (2016)*
G44061b	TrGCN	MVKNO3 + OH \rightarrow BIACETOH + NO ₂ + H ₂ O	k_t*f_ono2*f_co*f_pch2oh	Taraborrelli (2016)*
G44062a	TrGCN	MACRN + OH \rightarrow CH ₃ COCH ₂ OH + CO ₂ + NO ₂ + H ₂ O	k_t*f_o*f_ch2ono2	Taraborrelli (2016)*
G44062b	TrGCN	MACRN + OH \rightarrow MGLYOX + CO + NO ₂ + H ₂ O	k_rohro+k_s*f_sooh*f_ch2ono2	Taraborrelli (2016)*
G44063	TrGC	MACRO2 \rightarrow CH ₃ COCH ₂ OH + OH + CO	K14HSAL	Taraborrelli (2016)
G44064	TrGC	EZCH3CO2CHCHO \rightarrow .9 CH ₃ COCHCO + .1 CH ₃ C(O) + .01 GLYOX + .18 CO + .09 HO ₂ + OH	K15HS24VYNAL	Taraborrelli (2016)
G44065	TrGC	EZCH3CO2CHCHO + HO ₂ \rightarrow CH ₃ COOHCHCHO	KR02H02(4)	Taraborrelli (2016)
G44066	TrGCN	EZCH3CO2CHCHO + NO \rightarrow CH ₃ COCHO ₂ CHO + NO ₂	KR02N0	Taraborrelli (2016)*
G44067	TrGCN	EZCH3CO2CHCHO + NO ₃ \rightarrow CH ₃ COCHO ₂ CHO + NO ₂	kR02N03	Taraborrelli (2016)
G44068	TrGC	EZCH3CO2CHCHO \rightarrow CH ₃ COCHO ₂ CHO	k1_R02sOR02	Taraborrelli (2016)
G44069	TrGC	EZCHOCCH3CHO2 \rightarrow HCOCCH ₃ CO + OH	K15HS24VYNAL	Taraborrelli (2016)
G44070	TrGCN	EZCHOCCH3CHO2 + NO \rightarrow HCOCO ₂ CH ₃ CHO + NO ₂	KR02N0	Taraborrelli (2016)*
G44071	TrGC	EZCHOCCH3CHO2 + HO ₂ \rightarrow HCOCCH ₃ CHOOH	KR02H02(4)	Taraborrelli (2016)
G44072	TrGCN	EZCHOCCH3CHO2 + NO ₃ \rightarrow HCOCO ₂ CH ₃ CHO + NO ₂	KR02N03	Taraborrelli (2016)
G44073	TrGC	EZCHOCCH3CHO2 \rightarrow HCOCO ₂ CH ₃ CHO	k1_R02pOR02	Taraborrelli (2016)
G44074	TrGC	CH ₃ COOHCHCHO \rightarrow CH ₃ COCHO ₂ CHO + OH	KHYDEC	Taraborrelli (2016)
G44075	TrGC	HCOCCH ₃ CHOOH \rightarrow HCOCO ₂ CH ₃ CHO + OH	KHYDEC	Taraborrelli (2016)
G44076	TrGCN	CH ₃ COCHO ₂ CHO + NO \rightarrow CH ₃ C(O) + GLYOX + NO ₂	KR02N0	Taraborrelli (2016)*
G44077	TrGCN	CH ₃ COCHO ₂ CHO + NO ₃ \rightarrow CH ₃ C(O) + GLYOX + NO ₂	KR02N03	Taraborrelli (2016)
G44078	TrGC	CH ₃ COCHO ₂ CHO + HO ₂ \rightarrow CH ₃ C(O) + GLYOX + OH	KR02H02(4)	Taraborrelli (2016)*
G44079	TrGC	CH ₃ COCHO ₂ CHO \rightarrow CH ₃ C(O) + GLYOX	k1_R02sOR02	Taraborrelli (2016)
G44080	TrGC	HCOCO ₂ CH ₃ CHO \rightarrow MGLYOX + CO + HO ₂	k1_R02tOR02	Taraborrelli (2016)
G44081	TrGCN	HCOCO ₂ CH ₃ CHO + NO \rightarrow MGLYOX + CO + HO ₂ + NO ₂	KR02N0	Taraborrelli (2016)*
G44082	TrGC	HCOCO ₂ CH ₃ CHO + HO ₂ \rightarrow MGLYOX + CO + HO ₂ + OH	KR02H02(4)	Taraborrelli (2016)*
G44083	TrGCN	HCOCO ₂ CH ₃ CHO + NO ₃ \rightarrow MGLYOX + CO + HO ₂ + NO ₂	KR02N03	Taraborrelli (2016)
G44084	TrGC	HCOCCH ₃ CO + OH \rightarrow CO + MGLYOX + HO ₂	1E-10*a_cho	Hatakeyama et al. (1985), Taraborrelli (2016)
G44085	TrGC	CH ₃ COCHCO + OH \rightarrow CO + MGLYOX + HO ₂	7.6E-11*a_coch3	Hatakeyama et al. (1985), Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
G44086	TrGCN	LMEKNO3 + OH \rightarrow .62 MGLYOX + .62 HCHO + .62 HO ₂ + .62 NO ₂ + .38 CH ₃ C(O) + .38 NO ₃ CH ₂ CHO	.62*(k_p*(f_co+f_ch2ono2)) +.38*(k_s*f_ch2ono2*f_co)	Taraborrelli (2016)*
G44087	TrGC	MEPROPENE + OH \rightarrow IBUTOLBO2	9.4E-12*EXP(505./temp)	Atkinson et al. (2006)
G44088a	TrGC	MEPROPENE + O ₃ \rightarrow CH ₃ COCH ₃ + CH ₂ OO*	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Taraborrelli (2016)
G44088b	TrGC	MEPROPENE + O ₃ \rightarrow CH ₃ COCH ₂ O ₂ + OH + HCHO	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Taraborrelli (2016)
G44089	TrGCN	MEPROPENE + NO ₃ \rightarrow CH ₃ COCH ₃ + HCHO + NO ₂	3.4E-13	Atkinson et al. (2006), Taraborrelli (2016)*
G44090	TrGC	IBUTOLBO2 \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂	k1_R02t0R02	Taraborrelli (2016)
G44091a	TrGC	IBUTOLBO2 + HO ₂ \rightarrow IBUTOLBOOH	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44091b	TrGC	IBUTOLBO2 + HO ₂ \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)
G44092a	TrGCN	IBUTOLBO2 + NO \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(5,3,0,0,0, temp, cair))	Taraborrelli (2016)
G44092b	TrGCN	IBUTOLBO2 + NO \rightarrow IBUTOLBNO3	KR02N0*alpha_AN(5,3,0,0,0,temp, cair)	Taraborrelli (2016)
G44093	TrGCN	IBUTOLBO2 + NO ₃ \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02N03	Taraborrelli (2016)
G44094a	TrGC	IBUTOLBOOH + OH \rightarrow IBUTOLBO2	.6*k_CH300H_OH	Taraborrelli (2016)
G44094b	TrGC	IBUTOLBOOH + OH \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂	k_s*f_s0oh*f_pch2oh	Taraborrelli (2016)
G44095	TrGCN	IBUTOLBNO3 + OH \rightarrow CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	3.*k_p	Taraborrelli (2016)
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), Taraborrelli (2016)*
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), Taraborrelli (2016)*
G44098	TrGCN	BUT1ENE + NO ₃ \rightarrow C ₂ H ₅ CHO + HCHO + NO ₂	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44099	TrGC	LBUT1ENO2 \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02s0R02	Taraborrelli (2016)
G44100a	TrGC	LBUT1ENO2 + HO ₂ \rightarrow LBUT1ENOOH	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44100b	TrGC	LBUT1ENO2 + HO ₂ \rightarrow C ₂ H ₅ CHO + HCHO + HO ₂ + OH	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44101a	TrGCN	$\text{LBUT1ENO2} + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1-\alpha_{\text{AN}}(5,2,0,0,0,\text{temp},\text{cair}))$	Taraborrelli (2016)
G44101b	TrGCN	$\text{LBUT1ENO2} + \text{NO} \rightarrow \text{LBUT1ENNO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(5,2,0,0,0,\text{temp},\text{cair})$	Taraborrelli (2016)
G44102	TrGCN	$\text{LBUT1ENO2} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G44103a	TrGC	$\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{LBUT1ENO2}$	$.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G44103b	TrGC	$\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HCHO} + \text{HO}_2$	$k_{\text{t*f_tooh*f_pch2oh}}$	Taraborrelli (2016)*
G44104	TrGCN	$\text{LBUT1ENNO3} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$k_{\text{s*f_soh*f_ch2ono2}}$	Taraborrelli (2016)*
G44105	TrGC	$\text{CBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$	$1.1\text{E}-11*\text{EXP}(485./\text{temp})$	Atkinson et al. (2006)
G44106	TrGC	$\text{CBUT2ENE} + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + .16 \text{ CH}_3\text{CHOHOOH} + .50 \text{ OH} + .50 \text{ HCOCH}_2\text{O}_2 + .05 \text{ CH}_2\text{CO} + .09 \text{ CH}_3\text{OH} + .09 \text{ CO} + .2 \text{ CH}_4 + .2 \text{ CO}_2$	$3.2\text{E}-15*\text{EXP}(-965./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)*
G44107	TrGCN	$\text{CBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{NO}_2$	$3.5\text{E}-13$	Atkinson et al. (2006), Taraborrelli (2016)*
G44108	TrGC	$\text{TBUT2ENE} + \text{OH} \rightarrow \text{BUT2OLO2}$	$1.0\text{E}-11*\text{EXP}(553./\text{temp})$	Atkinson et al. (2006)
G44109	TrGC	$\text{TBUT2ENE} + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + .16 \text{ CH}_3\text{CHOHOOH} + .50 \text{ OH} + .50 \text{ HCOCH}_2\text{O}_2 + .05 \text{ CH}_2\text{CO} + .09 \text{ CH}_3\text{OH} + .09 \text{ CO} + .2 \text{ CH}_4 + .2 \text{ CO}_2$	$6.6\text{E}-15*\text{EXP}(-1060./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)
G44110	TrGCN	$\text{TBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{NO}_2$	$1.78\text{E}-12*\text{EXP}(-530./\text{temp}) + 1.28\text{E}-14*\text{EXP}(570./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)*
G44111	TrGC	$\text{BUT2OLO2} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2$	$k1_{\text{R02sOR02}}$	Taraborrelli (2016)
G44112a	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow \text{BUT2OLOOH}$	$\text{KR02H02}(4)*\text{rcoch2o2_ooh}$	Taraborrelli (2016)
G44112b	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(4)*\text{rcoch2o2_oh}$	Taraborrelli (2016)
G44113a	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1-\alpha_{\text{AN}}(5,2,0,0,0,\text{temp},\text{cair}))$	Taraborrelli (2016)
G44113b	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow \text{BUT2OLNO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(5,2,0,0,0,\text{temp},\text{cair})$	Taraborrelli (2016)
G44114	TrGCN	$\text{BUT2OLO2} + \text{NO}_3 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G44115a	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO2}$	$.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G44115b	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{LMEKOOH} + \text{HO}_2$	$k_{\text{t*f_toh*f_pch2oh}}$	Taraborrelli (2016)
G44115c	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO} + \text{OH}$	$k_{\text{t*f_tooh*f_pch2oh}}$	Taraborrelli (2016)
G44116	TrGCN	$\text{BUT2OLNO3} + \text{OH} \rightarrow \text{LMEKNO3} + \text{HO}_2$	$k_{\text{t*f_toh*f_ch2ono2}}$	Taraborrelli (2016)
G44117	TrGC	$\text{BUT2OLO} + \text{OH} \rightarrow \text{BIACET} + \text{HO}_2$	$k_{\text{t*f_toh*f_co}}$	Taraborrelli (2016)
G44118	TrGC	$\text{IPRCHO} + \text{OH} \rightarrow \text{IPRCO3} + \text{H}_2\text{O}$	$6.8\text{E}-12*\text{EXP}(410./\text{temp})$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G44119	TrGCN	$\text{IPRCHO} + \text{NO}_3 \rightarrow \text{IPRCO}_3 + \text{HNO}_3$	$1.67\text{E}-12 \cdot \text{EXP}(-1460./\text{temp})$	Atkinson et al. (2006)
G44120	TrGC	$\text{IPRCO}_3 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)
G44121a	TrGC	$\text{IPRCO}_3 + \text{HO}_2 \rightarrow \text{PERIBUACID}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44121b	TrGC	$\text{IPRCO}_3 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*(1-rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44122	TrGCN	$\text{IPRCO}_3 + \text{NO}_2 \rightarrow \text{PIPN}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44123	TrGCN	$\text{IPRCO}_3 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G44124a	TrGC	$\text{PERIBUACID} + \text{OH} \rightarrow \text{IPRCO}_3 + \text{H}_2\text{O}$.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44124b	TrGC	$\text{PERIBUACID} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{CO}_2$	k_s*f_co2h	Taraborrelli (2016)*
G44125	TrGCN	$\text{PIPN} \rightarrow \text{IPRCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	$\text{PIPN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{NO}_2$	k_s*f_cpan	Taraborrelli (2016)*
G44127	TrGC	$\text{MPROPENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{COCH}_3$	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44128	TrGC	$\text{MPROPENOL} + \text{HCOOH} \rightarrow \text{IPRCHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44129	TrGC	$\text{IPRCHO} + \text{HCOOH} \rightarrow \text{MPROPENOL} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44130	TrGC	$\text{BUTENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C}_2\text{H}_5\text{CHO}$	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44131	TrGC	$\text{BUTENOL} + \text{HCOOH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44132	TrGC	$\text{C}_3\text{H}_7\text{CHO} + \text{HCOOH} \rightarrow \text{BUTENOL} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44133	TrGC	$\text{HVMK} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	$\text{HVMK} + \text{HCOOH} \rightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44135	TrGC	$\text{CO}_2\text{C}_3\text{CHO} + \text{HCOOH} \rightarrow \text{HVMK} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44136	TrGC	$\text{HMAC} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	$\text{HMAC} + \text{HCOOH} \rightarrow \text{IBUTDIAL} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*

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

#	labels	reaction	rate coefficient	reference
G44138	TrGC	IBUTDIAL + HCOOH \rightarrow HMAc + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (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	Taraborrelli (2016)*
G44140	TrGCN	CO ₂ C ₃ CHO + NO ₃ \rightarrow CH ₃ COCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*4.0	Taraborrelli (2016)*
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	Taraborrelli (2016)*
G44142	TrGCN	IBUTDIAL + NO ₃ \rightarrow CH ₃ CHO + CO + HO ₂ + CO ₂ + HNO ₃	2.*KN03AL*4.0	Taraborrelli (2016)*
G44200	TrGTerC	CH ₃ COCOCH ₂ O ₂ \rightarrow CH ₃ C(O) + HCHO + CO	k1_R02pOR02	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	KR02NO	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	.6*k_CH300H_OH	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	KR02NO	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O ₂ \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)
G44207	TrGTerC	C44OOH + OH \rightarrow C44O ₂	7.46E-11	Rickard and Pascoe (2009)
G44208	TrGTerC	CHOC ₃ COO ₂ \rightarrow HCOCH ₂ CO ₃ + HCHO	k1_R02pOR02	Rickard and Pascoe (2009)
G44209	TrGTerC	CHOC ₃ COO ₂ + HO ₂ \rightarrow C413COOOH	KR02H02(4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	CHOC ₃ COO ₂ + NO \rightarrow HCOCH ₂ CO ₃ + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44211	TrGTerC	C413COOOH + OH \rightarrow CHOC ₃ COO ₂	8.33E-11	Rickard and Pascoe (2009)
G44212	TrGTerC	C4CODIAL + OH \rightarrow C312COCO ₃	3.39E-11	Rickard and Pascoe (2009)
G44213	TrGTerCN	C4CODIAL + NO ₃ \rightarrow C312COCO ₃ + HNO ₃	2.*KN03AL*4.0	Rickard and Pascoe (2009)
G44214	TrGTerC	C312COCO ₃ \rightarrow HCOCOCH ₂ O ₂ + CO ₂	k1_R02RCO3	Rickard and Pascoe (2009)
G44215a	TrGTerC	C312COCO ₃ + HO ₂ \rightarrow C312COCO ₃ H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44215b	TrGTerC	C312COCO ₃ + HO ₂ \rightarrow HCOCOCH ₂ O ₂ + CO ₂ + OH	KAPH02*(1-rco3_ooh)	Rickard and Pascoe (2009)
G44216	TrGTerCN	C312COCO ₃ + NO ₂ \rightarrow C312COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44217	TrGTerCN	C312COCO ₃ + NO \rightarrow HCOCOCH ₂ O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44218	TrGTerC	C312COCO ₃ H + OH \rightarrow C312COCO ₃	1.63E-11	Rickard and Pascoe (2009)
G44219	TrGTerCN	C312COPAN \rightarrow C312COCO ₃ + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44220	TrGTerCN	C312COPAN + OH \rightarrow HCOCOCHO + CO + NO ₂	1.27E-11	Rickard and Pascoe (2009)
G44221	TrGTerC	CH ₃ COCOCHO + OH \rightarrow CH ₃ C(O) + 2 CO	8.4E-13*EXP(830./temp)	Taraborrelli (2016)*
G44222	TrGTerCN	CH ₃ COCOCHO + NO ₃ \rightarrow CH ₃ C(O) + 2 CO + HNO ₃	KN03AL*4.0	Rickard and Pascoe (2009)
G44223	TrGTerC	IBUTALOH + OH \rightarrow IPRHOCO ₃	1.4E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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), Taraborrelli (2016)
G44224b	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2016)
G44224c	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44225	TrGTerCN	$\text{IPRHOCO3} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G44226	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_2 \rightarrow \text{C4PAN5}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44227	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02NO3*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	$\text{IPRHOCO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	1.72E-12	Rickard and Pascoe (2009)
G44230	TrGTerC	$\text{OH} + \text{IPRHOCO3H} \rightarrow \text{IPRHOCO3}$	4.80E-12	Rickard and Pascoe (2009)
G44231	TrGTerCN	$\text{C4PAN5} \rightarrow \text{IPRHOCO3} + \text{NO}_2$	K_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	$\text{C4PAN5} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO} + \text{NO}_2$	4.75E-13	Rickard and Pascoe (2009)
G44233a	TrGTerC	$\text{MBOOO} \rightarrow \text{IPRHOCO2H}$	$1.60\text{E-}17 * \text{C}(\text{ind_H2O}) * (0.08 + 0.15)$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44233b	TrGTerC	$\text{MBOOO} \rightarrow \text{IBUTALOH} + \text{H}_2\text{O}_2$	$1.60\text{E-}17 * \text{C}(\text{ind_H2O}) * 0.77$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44234	TrGTerC	$\text{MBOOO} + \text{CO} \rightarrow \text{IBUTALOH} + \text{CO}_2$	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	$\text{MBOOO} + \text{NO} \rightarrow \text{IBUTALOH} + \text{NO}_2$	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	$\text{MBOOO} + \text{NO}_2 \rightarrow \text{IBUTALOH} + \text{NO}_3$	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	$\text{MALANHY} + \text{OH} \rightarrow \text{MALANHYO2}$	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{HOCOC4DIAL} + \text{OH}$	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{MALDIALO2}$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G44402	TrGAroCN	$\text{NC4DCO2H} + \text{OH} \rightarrow \text{MALANHY} + \text{NO}_2$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)*
G44403	TrGAroC	$\text{CO14O3CO2H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + 2 \text{CO}_2$	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	$\text{BZFUOOH} + \text{OH} \rightarrow \text{BZFUO2}$	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	$\text{HOCOC4DIAL} + \text{OH} \rightarrow \text{CO2C4DIAL} + \text{HO}_2$	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow \text{MALDALCO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44406b	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow \text{MALDALCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44406c	TrGAroC	$\text{MALDIALCO3} + \text{HO}_2 \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)*
G44407	TrGAroCN	$\text{MALDIALCO3} + \text{NO} \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44408	TrGAroCN	MALDIALCO ₃ + NO ₂ → MALDIALPAN	k_CH3CO3_N02	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO ₃ + NO ₃ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)*
G44410	TrGAroC	MALDIALCO ₃ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO ₃ → NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O ₃ → .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 → BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH → NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH → MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH → C3DIALO2 + CO ₂	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO ₂ → C3DIALO2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO ₂ → EPXDLCO2H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO ₂ → EPXDLCO3H	KAPH02*rco3_ooH	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO → C3DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44419	TrGAroCN	EPXDLCO3 + NO ₂ → EPXDLPAN	k_CH3CO3_N02	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_R02RC03	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), Taraborrelli (2016)
G44429b	TrGAroC	MALANHYO2 + HO ₂ → HCOCOHCOC3 + CO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCOHCOC3 + CO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44431	TrGAroCN	$\text{MALANHYO}_2 + \text{NO}_3 \rightarrow \text{HCOCOHC}_3 + \text{CO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44432	TrGAroC	$\text{MALANHYO}_2 \rightarrow \text{HCOCOHC}_3 + \text{CO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G44433	TrGAroC	$\text{EPXDLC}_3\text{H} + \text{OH} \rightarrow \text{EPXDLC}_3$	2.62E-11	Rickard and Pascoe (2009)
G44434	TrGAroC	$\text{CO}_2\text{C}_4\text{DIAL} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CO} + \text{CO} + \text{HO}_2$	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	$\text{NBZFUO}_2 + \text{HO}_2 \rightarrow \text{NBZFUOOH}$	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44435b	TrGAroCN	$\text{NBZFUO}_2 + \text{HO}_2 \rightarrow .5 \text{CO}_{14}\text{O}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2 + \text{OH}$	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44436	TrGAroCN	$\text{NBZFUO}_2 + \text{NO} \rightarrow .5 \text{CO}_{14}\text{O}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44437	TrGAroCN	$\text{NBZFUO}_2 + \text{NO}_3 \rightarrow .5 \text{CO}_{14}\text{O}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44438	TrGAroCN	$\text{NBZFUO}_2 \rightarrow .5 \text{CO}_{14}\text{O}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G44439	TrGAroC	$\text{MALDALCO}_2\text{H} + \text{OH} \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO} + .4 \text{CO}_2$	3.70E-11	Rickard and Pascoe (2009)*
G44440	TrGAroCN	$\text{EPXC}_4\text{DIAL} + \text{NO}_3 \rightarrow \text{EPXDLC}_3 + \text{HNO}_3$	2*KN03AL*4.0	Rickard and Pascoe (2009)
G44441	TrGAroC	$\text{EPXC}_4\text{DIAL} + \text{OH} \rightarrow \text{EPXDLC}_3$	4.32E-11	Rickard and Pascoe (2009)
G44442a	TrGAroC	$\text{MECOACETO}_2 + \text{HO}_2 \rightarrow \text{MECOACEOOH}$	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44442b	TrGAroC	$\text{MECOACETO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO}_2 + \text{OH}$	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44443	TrGAroCN	$\text{MECOACETO}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44444	TrGAroCN	$\text{MECOACETO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44445	TrGAroC	$\text{MECOACETO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} + \text{CO}_2$	k1_R02p0R02	Rickard and Pascoe (2009)*
G44446	TrGAroCN	$\text{CO}_{14}\text{O}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{HNO}_3$	KN03AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	$\text{CO}_{14}\text{O}_3\text{CHO} + \text{OH} \rightarrow \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	3.44E-11	Rickard and Pascoe (2009)
G44448	TrGAroCN	$\text{NBZFUONE} + \text{OH} \rightarrow \text{BZFUCO} + \text{NO}_2$	1.16E-12	Rickard and Pascoe (2009)
G44449a	TrGAroC	$\text{BZFUO}_2 + \text{HO}_2 \rightarrow \text{BZFUOOH}$	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44449b	TrGAroC	$\text{BZFUO}_2 + \text{HO}_2 \rightarrow \text{CO}_{14}\text{O}_3\text{CHO} + \text{HO}_2 + \text{OH}$	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44450	TrGAroCN	BZFUO2 + NO → CO14O3CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44451	TrGAroCN	BZFUO2 + NO ₃ → CO14O3CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44452	TrGAroC	BZFUO2 → CO14O3CHO + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44453	TrGAroC	BZFUCO + OH → CO14O3CHO + HO ₂	1.78E-11	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO ₂ → MALDIALOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO ₂ → GLYOX + GLYOX + HO ₂ + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)
G44457	TrGAroCN	MALDIALO2 + NO → GLYOX + GLYOX + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44458	TrGAroCN	MALDIALO2 + NO ₃ → GLYOX + GLYOX + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44459	TrGAroC	MALDIALO2 → GLYOX + GLYOX + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH → HCOCOCHO + CO + NO ₂	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN → EPXDLCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH → MECOACETO2	3.59E-12	Rickard and Pascoe (2009)
G45000	TrGC	C ₅ H ₈ + O ₃ → .3508 MACR + .01518 MACO2H + .2440 MVK + .7085 HCHO + .11 CH ₂ OO + .1275 C ₃ H ₆ + .1575 CH ₃ C(O) + .0510 CH ₃ + .2625 HO ₂ + .27 OH + .09482 H ₂ O ₂ + .255 CO ₂ + .522 CO + .07182 HCHO + .03618 HCOCH ₂ O ₂ + .01782 CO + 0.05408 LCARBON	1.03E-14*EXP(-1995./temp)	Atkinson et al. (2006), Taraborrelli (2016)
G45001	TrGC	C ₅ H ₈ + OH → .63 ISOPAB + .30 ISOPCD + .07 LISOPEFO2	2.7E-11*EXP(390./temp)	Atkinson et al. (2006), Taraborrelli (2016)
G45002	TrGCN	C ₅ H ₈ + NO ₃ → NISOPO2	3.0E-12*EXP(-450./temp)	Atkinson et al. (2006)
G45003a	TrGC	ISOPAB + O ₂ → LISOPACO2	5.530E-13	Taraborrelli (2016)
G45003b	TrGC	ISOPAB + O ₂ → ISOPBO2	3.E-12	Taraborrelli (2016)
G45004a	TrGC	ISOPCD + O ₂ → LDISOPACO2	6.780E-13	Taraborrelli (2016)
G45004b	TrGC	ISOPCD + O ₂ → ISOPDO2	3.E-12	Taraborrelli (2016)
G45005	TrGC	LISOPACO2 → ISOPAB + O ₂	3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4	Taraborrelli (2016)
G45006	TrGC	ISOPBO2 → ISOPAB + O ₂	3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp)	Taraborrelli (2016)
G45007	TrGC	LDISOPACO2 → ISOPCD + O ₂	5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58	Taraborrelli (2016)
G45008	TrGC	ISOPDO2 → ISOPCD + O ₂	5.0E14*exp(-10120./temp)+8.25E14*exp(-10220./temp)	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45009a	TrGC	LISOPACO2 \rightarrow C1ODC2O2C4OOH	K16HSZ14 * 2./3.*(1-fhpal)	Taraborrelli (2016)
G45009b	TrGC	LISOPACO2 \rightarrow ZCODC23DBCOOH + HO ₂	K16HSZ14 * (2./3.*fhpal + 1./3.)	Taraborrelli (2016)
G45010a	TrGC	LDISOPACO2 \rightarrow C1OOHC3O2C4OD	k16HSZ41 * 2./3.*(1-fhpal)	Taraborrelli (2016)
G45010b	TrGC	LDISOPACO2 \rightarrow ZCODC23DBCOOH + HO ₂	k16HSZ41 * (2./3.*fhpal + 1./3.)	Taraborrelli (2016)
G45011	TrGC	LISOPACO2 \rightarrow .9 LISOPACO + .1 ISOPAOH	k1_R02LISOPACO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G45012	TrGC	LISOPACO2 + HO ₂ \rightarrow LISOPACOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45013a	TrGCN	LISOPACO2 + NO \rightarrow LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45013b	TrGCN	LISOPACO2 + NO \rightarrow LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45014	TrGCN	LISOPACO2 + NO ₃ \rightarrow LISOPACO + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45015	TrGC	LDISOPACO2 \rightarrow .9 LISOPACO + .1 ISOPAOH	k1_R02LISOPACO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G45016	TrGC	LDISOPACO2 + HO ₂ \rightarrow LISOPACOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO \rightarrow LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45017b	TrGCN	LDISOPACO2 + NO \rightarrow LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45018	TrGCN	LDISOPACO2 + NO ₃ \rightarrow LISOPACO + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH \rightarrow LISOPACO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G45019b	TrGC	LISOPACOOH + OH \rightarrow ZCODC23DBCOOH + HO ₂	k_s*f_allyl*f_soh	Taraborrelli (2016)
G45019c	TrGC	LISOPACOOH + OH \rightarrow LHC4ACCHO + OH	(k_s*f_soh*f_allyl+ k_rohro)	Taraborrelli (2016)
G45019d	TrGC	LISOPACOOH + OH \rightarrow LIEPOX + OH	(k_adt+k_ads)*a_ch2oh*a_ch2ooh	Taraborrelli (2016)*
G45020	TrGC	ISOPAOH + OH \rightarrow LHC4ACCHO + HO ₂	(k_adt+k_ads)*a_ch2oh*a_ch2oh+k_ s*f_soh*f_allyl+k_rohro	Taraborrelli (2016)
G45021	TrGCN	LISOPACNO3 + OH \rightarrow LISOPACNO3O2	(k_adt+k_ads)*a_ch2ono2*a_ch2oh	Taraborrelli (2016)*
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)	Taraborrelli (2016)
G45023b	TrGC	ISOPBO2 + HO ₂ \rightarrow MVK + HCHO + HO ₂ + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45024a	TrGCN	$\text{ISOPBO2} + \text{NO} \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(6,3,0,0,0,\text{temp},\text{cair}))$	Lockwood et al. (2010), Taraborrelli (2016)
G45024b	TrGCN	$\text{ISOPBO2} + \text{NO} \rightarrow \text{ISOPBNO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(6,3,0,0,0,\text{temp},\text{cair})$	Lockwood et al. (2010), Taraborrelli (2016)
G45025	TrGCN	$\text{ISOPBO2} + \text{NO}_3 \rightarrow \text{MVK} + .75 \text{HCHO} + .75 \text{HO}_2 + .25 \text{CH}_3 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45026a	TrGC	$\text{ISOPBOOH} + \text{OH} \rightarrow \text{LIEPOX} + \text{OH}$	$(k_{\text{ads}}+k_{\text{adp}})*a_{\text{ch2ooh}}$	Paulot et al. (2009b), Taraborrelli (2016)
G45026b	TrGC	$\text{ISOPBOOH} + \text{OH} \rightarrow \text{ISOPBO2}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G45026c	TrGC	$\text{ISOPBOOH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO}$	$k_{\text{rohro}}+k_{\text{s}}*f_{\text{alk}}*f_{\text{soh}}$	Taraborrelli (2016)
G45027	TrGC	$\text{ISOPBOOH} + \text{O}_3 \rightarrow .1368 \text{MACROOH} + .1368 \text{H}_2\text{O}_2 + .2280 \text{HO}_2 + .4332 \text{CH}_3\text{COCH}_2\text{OH} + .2280 \text{CO}_2 + .6384 \text{OH} + .2052 \text{CO} + .57 \text{HCHO} + .43 \text{MACROOH} + .06880 \text{HO}_2 + .06880 \text{OH} + .2709 \text{CO} + .1591 \text{CH}_2\text{OO}$	1.E-17	Taraborrelli (2016)
G45028	TrGC	$\text{ISOPBOH} + \text{OH} \rightarrow \text{MVK} + .75 \text{HCHO} + .75 \text{HO}_2 + .25 \text{CH}_3$	$k_{\text{s}}*f_{\text{alk}}*f_{\text{soh}}+(k_{\text{adp}}+k_{\text{ads}})*a_{\text{ch2oh}}$	Taraborrelli (2016)
G45029	TrGCN	$\text{ISOPBNO3} + \text{OH} \rightarrow \text{ISOPBDNO3O2}$	$(k_{\text{adt}}+k_{\text{adp}})*f_{\text{ch2ono2}}$	Taraborrelli (2016)
G45030	TrGC	$\text{ISOPDO2} \rightarrow .8 \text{MACR} + .8 \text{HCHO} + .8 \text{HO}_2 + .1 \text{HCOC5} + .1 \text{ISOPDOH}$	k1_R02ISOPD02	Rickard and Pascoe (2009)
G45031a	TrGC	$\text{ISOPDO2} + \text{HO}_2 \rightarrow \text{ISOPDOOH}$	$\text{KR02H02}(5)*(1.-r_{\text{chohch2o2_oh}})$	Taraborrelli (2016)
G45031b	TrGC	$\text{ISOPDO2} + \text{HO}_2 \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(5)*r_{\text{chohch2o2_oh}}$	Taraborrelli (2016)
G45032a	TrGCN	$\text{ISOPDO2} + \text{NO} \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(6,2,0,0,0,\text{temp},\text{cair}))$	Lockwood et al. (2010), Taraborrelli (2016)
G45032b	TrGCN	$\text{ISOPDO2} + \text{NO} \rightarrow \text{ISOPDNO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(6,2,0,0,0,\text{temp},\text{cair})$	Lockwood et al. (2010), Taraborrelli (2016)
G45033	TrGCN	$\text{ISOPDO2} + \text{NO}_3 \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45034a	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{LIEPOX} + \text{OH}$	$(k_{\text{adt}}+k_{\text{adp}})*a_{\text{ch2ooh}}$	Paulot et al. (2009b), Taraborrelli (2016)
G45034b	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{ISOPDO2}$	$0.6*k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G45034c	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{HCOC5} + \text{OH}$	$k_{\text{t}}*f_{\text{tooh}}*f_{\text{allyl}}*f_{\text{pch2oh}}$	Taraborrelli (2016)
G45034d	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{GLYOX} + \text{OH}$	$k_{\text{s}}*f_{\text{pch2oh}}*f_{\text{soh}}$	Taraborrelli (2016)
G45035	TrGC	$\text{ISOPDOOH} + \text{O}_3 \rightarrow 1.393 \text{OH} + \text{BIACETOH} + .67 \text{HCHO} + .05280 \text{HO}_2 + .2079 \text{CO} + .1221 \text{CH}_2\text{OO}$	1.E-17	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45036	TrGC	ISOPDOH + OH \rightarrow HCOC5 + HO ₂	$2.*k_{rohro}+(k_t*f_{toh}*f_{allyl}+k_s*f_{soh})*f_{pch2oh}+(k_{adt}+k_{adp})*a_{ch2oh}$	Taraborrelli (2016)
G45037	TrGCN	ISOPDNO3 + OH \rightarrow ISOPBDNO3O2	$(k_{adp}+k_{ads})*a_{ch2ono2}$	Taraborrelli (2016)*
G45038	TrGCN	NISOP02 \rightarrow .8 NC4CHO + .6 HO ₂ + .2 LISOPACNO3	k1_R02LISOPAC02	Rickard and Pascoe (2009)
G45039	TrGCN	NISOP02 + HO ₂ \rightarrow NISOP0OH	KR02H02(5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOP02 + NO \rightarrow NC4CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOP02 + NO ₃ \rightarrow NC4CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45042	TrGCN	NISOP0OH + OH \rightarrow NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC4CHO + OH \rightarrow LNISO3	$(k_{adt}+k_{ads})*a_{cho}*a_{ch2ono2}$	Taraborrelli (2016)*
G45044	TrGCN	NC4CHO + O ₃ \rightarrow .27 NOA + .027 HCOCO ₂ H + .0162 GLYOX + .0162 H ₂ O ₂ + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO ₂ + 0.7705 HCHO + .4055 CO ₂ + .73 GLYOX	2.40E-17	Taraborrelli (2016)
G45045	TrGCN	NC4CHO + NO ₃ \rightarrow LNISO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO3 + HO ₂ \rightarrow LNISOOH	$.5*KR02H02(5) + .5*KAPH02$	Rickard and Pascoe (2009)
G45047	TrGCN	LNISO3 + NO \rightarrow NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	$.5*KAPN0 + .5*KR02N0$	Rickard and Pascoe (2009)*
G45048	TrGCN	LNISO3 + NO ₃ \rightarrow NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	1.3*KR02N03	Rickard and Pascoe (2009)
G45049	TrGCN	LNISOOH + OH \rightarrow LNISO3	2.65E-11	Rickard and Pascoe (2009)
G45050a	TrGC	LHC4ACCHO + OH \rightarrow LC578O2	$(k_{adtertprim}+k_{ads})*a_{cho}*a_{ch2oh}$	Taraborrelli (2016)
G45050b	TrGC	LHC4ACCHO + OH \rightarrow LHC4ACCO3	k_t*f_o	Taraborrelli (2016)
G45050c	TrGC	LHC4ACCHO + OH \rightarrow ZCODC23DBCOD + HO ₂	k_s*f_soh*f_allyl	Taraborrelli (2016)
G45051	TrGC	LHC4ACCHO + O ₃ \rightarrow .2225 CH ₃ C(O) + .89 CO + .0171875 HOCH ₂ CO ₂ H + .075625 H ₂ O ₂ + .0171875 HCOCO ₂ H + .2775 CH ₃ COCH ₂ OH + .6675 HO ₂ + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 HOCH ₂ CHO + .5 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
G45052	TrGCN	LHC4ACCHO + NO ₃ \rightarrow LHC4ACCO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G45053	TrGC	LC578O2 \rightarrow .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂	k1_R02t0R02	Rickard and Pascoe (2009)
G45054a	TrGC	LC578O2 + HO ₂ \rightarrow MGLYOX + HOCH ₂ CHO + OH	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45054b	TrGC	LC578O2 + HO ₂ \rightarrow LC578OOH	KR02H02(5)*rcoch2o2_ooH	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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	Taraborrelli (2016)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	$0.6 * k_{\text{CH300H_OH}}$	Taraborrelli (2016)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C10DC2OOHC4OD} + \text{HO}_2$	$k_{\text{t*f_o*f_tch2oh*f_alk}} + k_{\text{t*f_toh*f_pch2oh*f_pch2oh}} + k_{\text{s*f_soh*f_pch2oh}}$	Taraborrelli (2016)
G45059a	TrGC	$\text{LHC4ACCO3} \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{CO}_2$	$k1_{\text{R02RC03}} * 0.9$	Taraborrelli (2016)
G45059b	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LHC4ACCO2H}$	$k1_{\text{R02RC03}} * 0.1$	Taraborrelli (2016)
G45060a	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 2 \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{CO}_2$	$\text{KAPH02} * r_{\text{co3_oh}}$	Taraborrelli (2016)
G45060b	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO3H}$	$\text{KAPH02} * r_{\text{co3_ooh}}$	Taraborrelli (2016)
G45060c	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$	$\text{KAPH02} * r_{\text{co3_o3}}$	Taraborrelli (2016)
G45061	TrGCN	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{NO}_2 + \text{CO}_2$	KAPN0	Taraborrelli (2016)
G45062	TrGCN	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G45063	TrGCN	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{NO}_2 + \text{CO}_2$	$1.6 * \text{KR02N03}$	Taraborrelli (2016)
G45064a	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{CO}_2$	$2.52\text{E-}11$	Taraborrelli (2016)
G45064b	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$2.88\text{E-}11$	Rickard and Pascoe (2009)
G45065	TrGCN	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	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	$\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{H}_2\text{O}_2 + .67 \text{HCHO} + .2079 \text{CO} + .1221 \text{CH}_2\text{OO} + .05280 \text{OH}$	$7.51\text{E-}16 * \text{EXP}(-1521./\text{temp})$	Taraborrelli (2016)
G45069	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$k1_{\text{R02t0R02}}$	Taraborrelli (2016)
G45070a	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$\text{KR02H02(5)} * r_{\text{coch2o2_oh}}$	Taraborrelli (2016)
G45070b	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	$\text{KR02H02(5)} * r_{\text{coch2o2_ooh}}$	Taraborrelli (2016)
G45071	TrGCN	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N0	Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
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	Taraborrelli (2016)
G45073	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	9.7E-12	Rickard and Pascoe (2009)
G45074	TrGC	$\text{LIEPOX} + \text{OH} \rightarrow \text{DB1O2} + \text{H}_2\text{O}$	$5.78\text{E-}11 \cdot \text{EXP}(-400./\text{temp})$ $\cdot (1.52/3.+0.98 \cdot 2./3.)/1.51$	Paulot et al. (2009b), Bates et al. (2014), Taraborrelli (2016)*
G45075	TrGC	$\text{ISOPBO2} \rightarrow \text{MVK} + \text{HCHO} + \text{OH}$	KHSB	Taraborrelli (2016)
G45076	TrGC	$\text{ISOPDO2} \rightarrow \text{MACR} + \text{HCHO} + \text{OH}$	KHSD	Taraborrelli (2016)
G45077a	TrGC	$\text{ZCODC23DBC0OH} + \text{OH} \rightarrow .6 \text{ C1ODC2O2C4OOH} + .4 \text{ C1OOHC2O2C4OD}$	$k_{\text{adt}} \cdot a_{\text{cho}} \cdot a_{\text{ch2ooh}}$	Taraborrelli (2016)
G45077b	TrGC	$\text{ZCODC23DBC0OH} + \text{OH} \rightarrow .6 \text{ C1ODC3O2C4OOH} + .4 \text{ C1OOHC3O2C4OD}$	$k_{\text{ads}} \cdot a_{\text{cho}} \cdot a_{\text{ch2ooh}}$	Taraborrelli (2016)
G45077c	TrGC	$\text{ZCODC23DBC0OH} + \text{OH} \rightarrow \text{ZCO3HC23DBCOD}$	$k_{\text{t}} \cdot f_{\text{o}} \cdot f_{\text{alk}} + 0.6 \cdot k_{\text{CH30OH_OH}}$	Taraborrelli (2016)
G45077d	TrGC	$\text{ZCODC23DBC0OH} + \text{OH} \rightarrow \text{ZCODC23DBCOD} + \text{OH}$	$k_{\text{s}} \cdot f_{\text{sooh}} \cdot f_{\text{allyl}}$	Taraborrelli (2016)
G45078	TrGC	$\text{ZCODC23DBC0OH} + \text{O}_3 \rightarrow .4672 \text{ OH} + .2336 \text{ HCOCOCH}_2\text{O}_2 + .2336 \text{ CO} + .2336 \text{ CH}_3\text{C(O)} + .4672 \text{ HOOCH}_2\text{CHO} + .1728 \text{ MGLYOX} + .1901 \text{ OH} + .0864 \text{ GLYOX} + .02765 \text{ HOOCH}_2\text{CHO} + .02765 \text{ H}_2\text{O}_2 + .02592 \text{ CH}_3\text{OOH} + .02592 \text{ CO}_2 + .01037 \text{ HCOCO} + .01555 \text{ CH}_2\text{OO} + .01555 \text{ CO} + .006908 \text{ HOOCH}_2\text{CO}_3 + .2628 \text{ OH} + .1314 \text{ MGLYOX} + .1314 \text{ OH} + .1314 \text{ HCOCOCH}_2\text{OOH} + .2628 \text{ GLYOX} + .0972 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .00972 \text{ HCOCO}_2\text{H} + .005832 \text{ GLYOX} + .005832 \text{ H}_2\text{O}_2 + .05249 \text{ OH} + .05249 \text{ HCOCO} + .01458 \text{ HCHO} + .01458 \text{ CO}_2 + .01458 \text{ HCOOH} + .01458 \text{ CO}$	2.4E-17	Taraborrelli (2016)
G45079	TrGC	$\text{C1OOHC2O2C4OD} \rightarrow .78 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .78 \text{ HOCHCHO} + .22 \text{ CO}_2\text{H}_3\text{CHO} + .22 \text{ HCHO} + .22 \text{ OH}$	$k1_{\text{R02t0R02}}$	Taraborrelli (2016)
G45080	TrGCN	$\text{C1OOHC2O2C4OD} + \text{NO} \rightarrow .78 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .78 \text{ HOCHCHO} + .22 \text{ CO}_2\text{H}_3\text{CHO} + .22 \text{ HCHO} + .22 \text{ OH} + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G45081a	TrGC	$\text{C1OOHC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1OOHC2OOHC4OD}$	$\text{KR02H02(5)} \cdot r_{\text{coch2o2_ooh}}$	Taraborrelli (2016)
G45081b	TrGC	$\text{C1OOHC2O2C4OD} + \text{HO}_2 \rightarrow .78 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .78 \text{ HOCHCHO} + .22 \text{ CO}_2\text{H}_3\text{CHO} + .22 \text{ HCHO} + 1.22 \text{ OH}$	$\text{KR02H02(5)} \cdot r_{\text{coch2o2_oh}}$	Taraborrelli (2016)
G45082	TrGC	$\text{C1OOHC2O2C4OD} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{GLYOX} + \text{OH}$	KHSB	Taraborrelli (2016)
G45083	TrGC	$\text{C1ODC2O2C4OOH} \rightarrow \text{OH} + \text{C1ODC2OOHC4OD}$	K15HSDHB	Taraborrelli (2016)
G45084a	TrGC	$\text{C1OOHC2OOHC4OD} + \text{OH} \rightarrow \text{C1ODC2OOHC4OD} + \text{OH}$	$2 \cdot k_{\text{s}} \cdot f_{\text{sooh}} \cdot f_{\text{tch2oh}}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45084b	TrGC	$\text{C10OHC2OOHC4OD} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + 2 \text{CO} + 2 \text{HO}_2 + \text{OH}$	$k_{\text{t}*\text{f}_{\text{toh}}*\text{f}_{\text{pch2oh}}*\text{f}_{\text{pch2oh}}}$	Taraborrelli (2016)
G45084c	TrGC	$\text{C10OHC2OOHC4OD} + \text{OH} \rightarrow \text{C10OHC2O2C4OD}$	$0.6*k_{\text{CH300H}_{\text{OH}}}$	Taraborrelli (2016)
G45085	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{CO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t}*\text{f}_{\text{o}}*\text{f}_{\text{tch2oh}}+k_{\text{t}*\text{f}_{\text{toh}}*\text{f}_{\text{toh}}*\text{f}_{\text{cho}}}}$	Taraborrelli (2016)
G45086	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{HOOCH}_2\text{CHO} + \text{HO}_2$	$k1_{\text{R02s0R02}}$	Taraborrelli (2016)
G45087	TrGCN	$\text{C1ODC3O2C4OOH} + \text{NO} \rightarrow \text{MGLYOX} + \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Taraborrelli (2016)
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)	Taraborrelli (2016)
G45089	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{OH} + \text{HOOCH}_2\text{CHO}$	KHSD	Taraborrelli (2016)
G45090	TrGC	$\text{C10OHC3O2C4OD} \rightarrow .625 \text{MGLYOX} + 2 \text{CO} + 1.625 \text{HO}_2 + .375 \text{CH}_3\text{C(O)} + .375 \text{CO}_2 + \text{OH}$	K15HSDHB	Taraborrelli (2016)
G45091	TrGC	$\text{LHC4ACCO}_3 \rightarrow \text{ZCO}_3\text{HC23DBCOD} + \text{HO}_2$	K16HS	Taraborrelli (2016)
G45092a	TrGC	$\text{ZCODC23DBCOD} + \text{OH} \rightarrow \text{C1ODC2O2C4OD}$	$(k_{\text{adt}}+k_{\text{ads}})*a_{\text{cho}}*a_{\text{cho}}$	Taraborrelli (2016)*
G45092b	TrGC	$\text{ZCODC23DBCOD} + \text{OH} \rightarrow \text{ZCO}_3\text{C23DBCOD}$	$2*k_{\text{t}*\text{f}_{\text{o}}*\text{f}_{\text{alk}}}$	Taraborrelli (2016)*
G45093	TrGCN	$\text{ZCODC23DBCOD} + \text{NO}_3 \rightarrow \text{ZCO}_3\text{C23DBCOD} + \text{HNO}_3$	KN03AL*4.25*2.	Taraborrelli (2016)*
G45094a	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$	$\text{KR02H02(5)*rcoch2o2_{oh}}$	Taraborrelli (2016)
G45094b	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1ODC2OOHC4OD}$	$\text{KR02H02(5)*rcoch2o2_{ooh}}$	Taraborrelli (2016)
G45095	TrGCN	$\text{C1ODC2O2C4OD} + \text{NO} \rightarrow \text{NO}_2 + \text{MGLYOX} + \text{HOCHCHO}$	KR02N0	Taraborrelli (2016)*
G45096	TrGC	$\text{C1ODC2O2C4OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$	$k1_{\text{R02t0R02}}$	Taraborrelli (2016)
G45097a	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{CO}$	$(2*k_{\text{t}*\text{f}_{\text{o}}*\text{f}_{\text{tch2oh}}*\text{f}_{\text{alk}}+k_{\text{t}*\text{f}_{\text{toh}}*\text{f}_{\text{cho}}*\text{f}_{\text{pch2oh}}})*.5$	Taraborrelli (2016)
G45097b	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{CO} + \text{OH}$	$(2*k_{\text{t}*\text{f}_{\text{o}}*\text{f}_{\text{tch2oh}}*\text{f}_{\text{alk}}+k_{\text{t}*\text{f}_{\text{toh}}*\text{f}_{\text{cho}}*\text{f}_{\text{pch2oh}}})*.5$	Taraborrelli (2016)
G45098	TrGCN	$\text{LISOPACNO}_3\text{O}_2 + \text{NO} \rightarrow .21 \text{NOA} + .21 \text{HOCH}_2\text{CHO} + .21 \text{HO}_2 + .49 \text{HO}_2\text{CO}_3\text{C}_4 + .49 \text{HCHO} + .49 \text{NO}_2 + .045 \text{MVKNO}_3 + .045 \text{HCHO} + .255 \text{CH}_3\text{COCH}_2\text{OH} + .255 \text{NO}_3\text{CH}_2\text{CHO} + .225 \text{H}_2\text{O}_2 + \text{NO}_2$	KR02N0	Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
G45099	TrGCN	LISOPACNO3O2 \rightarrow .21 NOA + .21 HOCH ₂ CHO + .21 HO ₂ + .49 HO12CO3C4 + .49 HCHO + .49 NO ₂ + .045 MVKNO3 + .045 HCHO + .255 CH ₃ COCH ₂ OH + .255 NO ₃ CH ₂ CHO + .225 H ₂ O ₂	k1_R02t0R02+KR02H02(5)*c(ind_H02)	Taraborrelli (2016)
G45100	TrGCN	ISOPBDNO3O2 + NO \rightarrow .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO ₂ + 1.6 NO ₂	KR02N0	Taraborrelli (2016)*
G45101	TrGCN	ISOPBDNO3O2 \rightarrow .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO ₂ + .6 NO ₂	k1_R02s0R02+KR02H02(5)*c(ind_H02)	Taraborrelli (2016)
G45102	TrGCN	LISOPACNO3 + O ₃ \rightarrow .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), Taraborrelli (2016)
G45103	TrGC	DB1O2 \rightarrow DB1O2	k1_R02s0R02	Taraborrelli (2016)
G45104a	TrGC	DB1O2 + HO ₂ \rightarrow DB1OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)*
G45104b	TrGC	DB1O2 + HO ₂ \rightarrow DB1O2 + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45105a	TrGCN	DB1O2 + NO \rightarrow DB1O2 + NO ₂	KR02N0*(1.-alpha_AN(7,2,0,0,0,temp,cair))	Taraborrelli (2016)
G45105b	TrGCN	DB1O2 + NO \rightarrow DB1NO3	KR02N0*alpha_AN(7,2,0,0,0,temp,cair)	Taraborrelli (2016)
G45106	TrGCN	DB1O2 + NO ₃ \rightarrow DB1O2 + NO ₂	KR02N03	Taraborrelli (2016)
G45107	TrGC	DB1O2 \rightarrow DB1O2 + OH	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 \rightarrow DB1O2	KDEC*0.72	see note*
G45108b	TrGC	DB1O2 \rightarrow .5 HVMK + .5 HMAc + HCHO + HO ₂	KDEC*0.28	see note*
G45109	TrGC	DB1O2 \rightarrow .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂	k1_R02s0R02	Taraborrelli (2016)
G45110a	TrGC	DB1O2 + HO ₂ \rightarrow DB2OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45110b	TrGC	DB1O2 + HO ₂ \rightarrow .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45111	TrGCN	DB1O2 + NO \rightarrow .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 \rightarrow .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02N03	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45113	TrGC	DB1O2 \rightarrow .48 MACROOH + .52 LHMVKABOOH + CO + OH	K14HSAL	Taraborrelli (2016)
G45114a	TrGC	DB1OOH + OH \rightarrow DB1O2	.6*k_CH300H_OH	Taraborrelli (2016)
G45114b	TrGC	DB1OOH + OH \rightarrow HCOOH + HO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Taraborrelli (2016)*
G45115	TrGC	DB1OOH + HCOOH \rightarrow C1ODC2OOHC4OD + HCOOH	4.67E-26*temp**3.286*EXP(4509./ (1.987*temp))	Taraborrelli (2016), daSilva (2010)*
G45116	TrGCN	DB1NO3 + OH \rightarrow HCOOH + NO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Taraborrelli (2016)*
G45117	TrGC	DB2OOH + OH \rightarrow DB1O2	.6*k_CH300H_OH	Taraborrelli (2016)*
G45118	TrGC	LISOPACOOH + O ₃ \rightarrow 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	Taraborrelli (2016)
G45119a	TrGC	ZCO3HC23DBCOD + OH \rightarrow .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	Taraborrelli (2016)
G45119b	TrGC	ZCO3HC23DBCOD + OH \rightarrow .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	Taraborrelli (2016)
G45120	TrGC	LISOPEFO2 \rightarrow LISOPEFO	k1_R02pOR02	Taraborrelli (2016)
G45121a	TrGCN	LISOPEFO2 + NO \rightarrow LISOPEFO + NO ₂	KR02NO*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Taraborrelli (2016)
G45121b	TrGCN	LISOPEFO2 + NO \rightarrow ISOPDNO3	KR02NO*alpha_AN(6,1,0,0,0,temp, cair)	Taraborrelli (2016)*
G45122a	TrGC	LISOPEFO2 + HO ₂ \rightarrow .7143 ISOPDOOH + .2857 ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45122b	TrGC	LISOPEFO2 + HO ₂ \rightarrow LISOPEFO + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45123	TrGCN	LISOPEFO2 + NO ₃ \rightarrow LISOPEFO + NO ₂	KR02NO3	Taraborrelli (2016)
G45124	TrGC	LISOPEFO2 \rightarrow .7143 MACR + .2857 MVK + HCHO + OH	.7143*KHSD+.2857*KHSB	Taraborrelli (2016)
G45125	TrGC	LISOPEFO \rightarrow .7143 MACR + .2857 MVK + HCHO + HO ₂	KDEC	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45126a	TrGC	LISOPACO \rightarrow 3METHYLFURAN + HO ₂	KDEC*0.37	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	LISOPACO \rightarrow .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO \rightarrow 3METHYLFURAN + HO ₂	KDEC*0.37	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	LISOPACO \rightarrow .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	3METHYLFURAN + OH \rightarrow L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Taraborrelli (2016)*
G45129	TrGCN	3METHYLFURAN + NO ₃ \rightarrow L3METHYLFURANO2 + NO ₂	1.9E-11	Taraborrelli (2016), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 \rightarrow ZCODC23DBCOD + HO ₂	k1_R02s0R02	Taraborrelli (2016)
G45131	TrGCN	L3METHYLFURANO2 + NO \rightarrow ZCODC23DBCOD + HO ₂ + NO ₂	KR02NO	Taraborrelli (2016)*
G45132	TrGC	L3METHYLFURANO2 + HO ₂ \rightarrow ZCODC23DBCOD + HO ₂	KR02H02(5)	Taraborrelli (2016)*
G45133	TrGC	ZCO3C23DBCOD \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂	k1_R02RC03	Taraborrelli (2016)
G45134a	TrGC	ZCO3C23DBCOD + HO ₂ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH	KAPH02*rco3_oh	Taraborrelli (2016)
G45134b	TrGC	ZCO3C23DBCOD + HO ₂ \rightarrow ZCO3HC23DBCOD	KAPH02*(rco3_ooh+rco3_o3)	Taraborrelli (2016)*
G45135	TrGCN	ZCO3C23DBCOD + NO \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KAPNO	Taraborrelli (2016)
G45136	TrGCN	ZCO3C23DBCOD + NO ₂ \rightarrow ZCPANC23DBCOD	k_CH3C03_N02	Rickard and Pascoe (2009)
G45137	TrGCN	ZCO3C23DBCOD + NO ₃ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	1.6*KR02N03	Taraborrelli (2016)
G45138	TrGCN	ZCPANC23DBCOD \rightarrow ZCO3C23DBCOD + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	ZCPANC23DBCOD + OH \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	2.52E-11	Taraborrelli (2016)*
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	KR02NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45202a	TrGTerC	$\text{C511O2} + \text{HO}_2 \rightarrow \text{C511OOH}$	$\text{KR02H02(5)*rcoch2o2_ooh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45202b	TrGTerC	$\text{C511O2} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCH}_2\text{CHO} + \text{OH}$	$\text{KR02H02(5)*rcoch2o2_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45203	TrGTerC	$\text{C511OOH} + \text{OH} \rightarrow \text{C511O2}$	7.49E-11	Rickard and Pascoe (2009)
G45204	TrGTerC	$\text{CO23C4CHO} + \text{OH} \rightarrow \text{CO23C4CO3}$	6.65E-11	Rickard and Pascoe (2009)
G45205	TrGTerCN	$\text{CO23C4CHO} + \text{NO}_3 \rightarrow \text{CO23C4CO3} + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45206	TrGTerC	$\text{CO23C4CO3} \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)
G45207	TrGTerCN	$\text{CO23C4CO3} + \text{NO} \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*
G45208	TrGTerCN	$\text{CO23C4CO3} + \text{NO}_2 \rightarrow \text{C5PAN9}$	k_CH3CO3_N02	Rickard and Pascoe (2009)
G45209a	TrGTerC	$\text{CO23C4CO3} + \text{HO}_2 \rightarrow \text{CO23C4CO3H}$	$\text{KAPH02*(rco3_ooh+rco3_o3)}$	Rickard and Pascoe (2009)
G45209b	TrGTerC	$\text{CO23C4CO3} + \text{HO}_2 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45210	TrGTerCN	$\text{C5PAN9} \rightarrow \text{CO23C4CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45211	TrGTerCN	$\text{C5PAN9} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{CO} + \text{NO}_2$	3.12E-13	Rickard and Pascoe (2009)
G45212	TrGTerC	$\text{C512O2} \rightarrow \text{C513O2}$	k1_R02pR02	Rickard and Pascoe (2009)
G45213	TrGTerC	$\text{C512O2} + \text{HO}_2 \rightarrow \text{C512OOH}$	KR02H02(5)	Rickard and Pascoe (2009)
G45214	TrGTerCN	$\text{C512O2} + \text{NO} \rightarrow \text{C513O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45215	TrGTerC	$\text{C512OOH} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{OH}$	1.01E-10	Rickard and Pascoe (2009)
G45216	TrGTerC	$\text{C513O2} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3$	k1_R02sOR02	Rickard and Pascoe (2009)
G45217	TrGTerCN	$\text{C513O2} + \text{NO} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45218a	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{C513OOH}$	$\text{KR02H02(5)*rcoch2o2_ooh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45218b	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$\text{KR02H02(5)*rcoch2o2_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45219	TrGTerC	$\text{CO13C4CHO} + \text{OH} \rightarrow \text{CHOC3COCO3}$	1.33E-10	Rickard and Pascoe (2009)
G45220	TrGTerCN	$\text{CO13C4CHO} + \text{NO}_3 \rightarrow \text{CHOC3COCO3} + \text{HNO}_3$	$2.*\text{KN03AL*5.5}$	Rickard and Pascoe (2009)
G45221	TrGTerC	$\text{C513OOH} + \text{OH} \rightarrow \text{C513CO} + \text{OH}$	9.23E-11	Rickard and Pascoe (2009)
G45222	TrGTerC	$\text{CHOC3COCO3} \rightarrow \text{CHOC3COO2} + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)
G45223	TrGTerC	$\text{CHOC3COCO3} + \text{HO}_2 \rightarrow \text{CHOC3COOOH}$	KAPH02	Rickard and Pascoe (2009)
G45224	TrGTerCN	$\text{CHOC3COCO3} + \text{NO}_2 \rightarrow \text{CHOC3COPAN}$	k_CH3CO3_N02	Rickard and Pascoe (2009)
G45225	TrGTerCN	$\text{CHOC3COCO3} + \text{NO} \rightarrow \text{CHOC3COO2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*
G45226	TrGTerC	$\text{C513CO} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{CO} + \text{CO}$	2.64E-11	Rickard and Pascoe (2009)
G45227	TrGTerC	$\text{C514O2} + \text{HO}_2 \rightarrow \text{C514OOH}$	KR02H02(5)	Rickard and Pascoe (2009)
G45228a	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0*(1.-alpha_AN(7,2,0,1,0, temp, cair))}$	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45228b	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{C514NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(7, 2, 0, 1, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45229	TrGTerCN	$\text{C514O2} + \text{NO}_3 \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45230	TrGTerC	$\text{C514O2} \rightarrow \text{CO13C4CHO} + \text{HO}_2$	k1_R02sR02	Rickard and Pascoe (2009)
G45231	TrGTerC	$\text{C514OOH} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{OH}$	1.10E-10	Rickard and Pascoe (2009)
G45232	TrGTerCN	$\text{C514NO3} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{NO}_2$	4.33E-11	Rickard and Pascoe (2009)
G45233	TrGTerC	$\text{CHOC3COOOH} + \text{OH} \rightarrow \text{CHOC3COCO3}$	7.55E-11	Rickard and Pascoe (2009)
G45234	TrGTerCN	$\text{CHOC3COPAN} \rightarrow \text{CHOC3COCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45235	TrGTerCN	$\text{CHOC3COPAN} + \text{OH} \rightarrow \text{C4CODIAL} + \text{CO} + \text{NO}_2$	7.19E-11	Rickard and Pascoe (2009)
G45236	TrGTerC	$\text{MBO} + \text{OH} \rightarrow \text{LMBOABO2}$	$8.1\text{E-12} * \text{EXP}(610./\text{TEMP})$	Rickard and Pascoe (2009), Taraborrelli (2016)*
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G45238	TrGTerCN	$\text{MBO} + \text{NO}_3 \rightarrow \text{LNMBOABO2}$	$4.6\text{E-14} * \text{EXP}(-400./\text{TEMP})$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45239	TrGTerC	$\text{LMBOABO2} + \text{HO}_2 \rightarrow \text{LMBOABOOH}$	KR02H02(5)	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G45241a	TrGTerC	$\text{LMBOABO2} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2$	k1_R02sOR02*.67	Rickard and Pascoe (2009), Taraborrelli (2016)
G45241b	TrGTerC	$\text{LMBOABO2} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2$	k1_R02pOR02*.33	Rickard and Pascoe (2009), Taraborrelli (2016)
G45242a	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{MBOACO}$	$.67 * 2.93\text{E-11} + .33 * 2.05\text{E-12}$	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45242b	TrGTerC	LMBOABOOH + OH \rightarrow LMBOABO2	.6*k_CH300H_OH	Rickard and Pascoe (2009), Taraborrelli (2016)
G45243	TrGTerCN	LMBOABNO3 + OH \rightarrow MBOACO + NO ₂	.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45244	TrGTerC	MBOACO + OH \rightarrow MBOCOCO + HO ₂	3.79E-12	Rickard and Pascoe (2009)
G45245	TrGTerC	MBOCOCO + OH \rightarrow CO + IPRHOCO3	1.38E-11	Rickard and Pascoe (2009)
G45246	TrGTerCN	LNMBOABO2 + HO ₂ \rightarrow LNMBOABOOH	KR02H02(5)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45247	TrGTerCN	LNMBOABO2 + NO \rightarrow .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2016)*
G45248	TrGTerCN	LNMBOABO2 + NO ₃ \rightarrow .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009), Taraborrelli (2016)
G45249	TrGTerCN	LNMBOABO2 \rightarrow .65 NO ₃ CH ₂ CHO + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 IBUTALOH + .35 HCHO + .35 NO ₂	k1_R02sOR02	Rickard and Pascoe (2009), Taraborrelli (2016)
G45250a	TrGTerCN	LNMBOABOOH + OH \rightarrow .65 C4MCONO3OH + .35 NMBOBCO	.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45250b	TrGTerCN	LNMBOABOOH + OH \rightarrow LNMBOABO2	.6*k_CH300H_OH	Rickard and Pascoe (2009), Taraborrelli (2016)
G45251	TrGTerCN	NMBOBCO + OH \rightarrow NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45252a	TrGTerCN	NC4OHCO3 + HO ₂ \rightarrow IBUTALOH + CO ₂ + NO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45252b	TrGTerCN	NC4OHCO3 + HO ₂ \rightarrow NC4OHCO3H	KAPH02*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45253	TrGTerCN	NC4OHCO3 + NO \rightarrow IBUTALOH + CO ₂ + NO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G45254	TrGTerCN	NC4OHCO3 + NO ₂ \rightarrow NC4OHCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G45255	TrGTerCN	NC4OHCO3 + NO ₃ \rightarrow IBUTALOH + CO ₂ + NO ₂ + NO ₂	KR02NO3*1.74	Rickard and Pascoe (2009)
G45256	TrGTerCN	NC4OHCO3 \rightarrow IBUTALOH + CO ₂ + NO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G45257	TrGTerCN	NC4OHCO3H + OH \rightarrow NC4OHCO3	4.50E-12	Rickard and Pascoe (2009)
G45258	TrGTerCN	NC4OHCPAN + OH \rightarrow IBUTALOH + CO + NO ₂ + NO ₂	1.27E-12	Rickard and Pascoe (2009)
G45259	TrGTerCN	NC4OHCPAN \rightarrow NC4OHCO3 + NO ₂	K_PAN_M	Rickard and Pascoe (2009)
G45260	TrGTerCN	C4MCONO3OH + OH \rightarrow CH ₃ COCH ₃ + HCHO + CO ₂ + NO ₂	1.23E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45400	TrGAroCN	NC4MDCO2HN + OH \rightarrow MMALANHY + NO ₂	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45401	TrGAroCN	$C54CO + NO_3 \rightarrow 3 CO + CH_3C(O)OO + HNO_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	$C54CO + OH \rightarrow 3 CO + CH_3C(O)OO$	1.72E-11	Rickard and Pascoe (2009)
G45403a	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow NTLFUOOH$	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow ACCOMECHO + NO_2 + OH$	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45404	TrGAroCN	$NTLFUO2 + NO \rightarrow ACCOMECHO + NO_2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G45405	TrGAroCN	$NTLFUO2 + NO_3 \rightarrow ACCOMECHO + NO_2 + NO_2$	KR02NO3	Rickard and Pascoe (2009)*
G45406	TrGAroCN	$NTLFUO2 \rightarrow ACCOMECHO + NO_2$	k1_R02tOR02	Rickard and Pascoe (2009)*
G45407	TrGAroC	$C5134CO2OH + OH \rightarrow C54CO + HO_2$	7.48E-11	Rickard and Pascoe (2009)
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), Taraborrelli (2016)
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_CH3CO3_N02	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$C4CO2DBC03 + NO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	KR02NO3*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), Taraborrelli (2016)
G45421b	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow CO2H3CO3 + CO_2 + OH$	KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45422	TrGAroCN	$MMALANHYO2 + NO \rightarrow CO2H3CO3 + CO_2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$MMALANHYO2 + NO_3 \rightarrow CO2H3CO3 + CO_2 + NO_2$	KR02NO3	Rickard and Pascoe (2009)*
G45424	TrGAroC	$MMALANHYO2 \rightarrow CO2H3CO3 + CO_2$	k1_R02tOR02	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)

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

#	labels	reaction	rate coefficient	reference
G45431	TrGAroCN	$C_5CO_{14}O_2 + NO \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)*
G45432	TrGAroCN	$C_5CO_{14}O_2 + NO_2 \rightarrow C_5COO_2NO_2$	k_CH3CO3_N02	Rickard and Pascoe (2009)*
G45433	TrGAroCN	$C_5CO_{14}O_2 + NO_3 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	$C_5CO_{14}O_2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G45436	TrGAroC	$C_5CO_{14}OH + OH \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	$C_5DICARB + NO_3 \rightarrow C_5CO_{14}O_2 + HNO_3$	KN03AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	$C_5DICARB + O_3 \rightarrow .5338 \text{ GLYOX} + .063 \text{ CH}_3\text{CHO} + .348 \text{ CH}_3\text{C(O)OO} + .918 \text{ CO} + .57 \text{ OH} + .473 \text{ HO}_2 + .0563 \text{ CH}_3\text{COCO}_2\text{H} + .5338 \text{ MGLYOX} + .676 \text{ H}_2\text{O}_2 + .063 \text{ HCHO} + .0563 \text{ HCOCO}_2\text{H} + .2465 \text{ CO}_2$	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	$C_5DICARB + OH \rightarrow .48 \text{ C}_5\text{CO}_{14}O_2 + .52 \text{ C}_5\text{DICARBO}_2$	6.2E-11	Rickard and Pascoe (2009)
G45444	TrGAroC	$MC_3ODBCO_2H + OH \rightarrow .35 \text{ GLYOX} + .35 \text{ CH}_3 + .35 \text{ CO} + .35 \text{ CO}_2 + .65 \text{ MMALANHY} + .65 \text{ HO}_2$	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	$TLFUONE + NO_3 \rightarrow NTLFUO_2$	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	$TLFUONE + O_3 \rightarrow .5 \text{ CO} + .5 \text{ OH} + .5 \text{ MECOACETO}_2 + .3125 \text{ C}_{24}O_3CCO_2H + .1875 \text{ ACCOMECHO} + .1875 \text{ H}_2O_2$	8.00E-19	see note*
G45453	TrGAroC	$TLFUONE + OH \rightarrow TLFUO_2$	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	$ACCOMECO_3 + HO_2 \rightarrow ACCOMECHO_3$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	$ACCOMECO_3 + HO_2 \rightarrow MECOACETO_2 + CO_2 + OH$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45455	TrGAroCN	$ACCOMECO_3 + NO \rightarrow MECOACETO_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	$ACCOMECO_3 + NO_2 \rightarrow ACCOMECHAN$	k_CH3CO3_N02	Rickard and Pascoe (2009)*
G45457	TrGAroCN	$ACCOMECO_3 + NO_3 \rightarrow MECOACETO_2 + CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	$ACCOMECO_3 \rightarrow MECOACETO_2 + CO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45459	TrGAroC	$C_4CO_2DCO_3H + OH \rightarrow C_4CO_2DBCO_3$	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	$ACCOMECO_3 + NO_3 \rightarrow ACCOMECHO_3 + HNO_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	$ACCOMECO_3 + OH \rightarrow ACCOMECHO_3$	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	$MMALNHYOOH + OH \rightarrow MMALANHYO_2$	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	$C_5DICAROOH + OH \rightarrow C_5I_3CO_2OH + OH$	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	$C_5DICAROOH + OH \rightarrow C_5DICARBO_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G45468	TrGAroC	$C_{24}O_3CCO_2H + OH \rightarrow MECOACETO_2 + CO_2$	8.76E-13	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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 ACCOMECO3 + 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)
G45476b	TrGAroC	TLFUO2 + HO ₂ \rightarrow ACCOMECHO + HO ₂ + OH	KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
G45477	TrGAroCN	TLFUO2 + NO \rightarrow ACCOMECHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45478	TrGAroCN	TLFUO2 + NO ₃ \rightarrow ACCOMECHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G45479	TrGAroC	TLFUO2 \rightarrow ACCOMECHO + HO ₂	k1_R02tOR02	Rickard and Pascoe (2009)*
G45480	TrGAroC	C5CO14OOH + OH \rightarrow C5CO14O2	3.59E-12	Rickard and Pascoe (2009)
G45483	TrGAroC	TLFUOOH + OH \rightarrow TLFUO2	2.53E-11	Rickard and Pascoe (2009)
G45485	TrGAroC	ACCOMECO3H + OH \rightarrow ACCOMECO3	3.59E-12	Rickard and Pascoe (2009)
G45486a	TrGAroC	C5DIALO2 + HO ₂ \rightarrow C5DIALOOH	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45486b	TrGAroC	C5DIALO2 + HO ₂ \rightarrow MALDIAL + CO + HO ₂ + OH	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G45487	TrGAroCN	C5DIALO2 + NO \rightarrow MALDIAL + CO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45488	TrGAroCN	C5DIALO2 + NO ₃ \rightarrow MALDIAL + CO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G45489	TrGAroC	C5DIALO2 \rightarrow MALDIAL + CO + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G45490a	TrGAroC	C5DICARBO2 + HO ₂ \rightarrow C5DICAROOH	KR02H02(5)*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45491b	TrGAroC	C5DICARBO2 + HO ₂ \rightarrow MGLYOX + GLYOX + HO ₂ + OH	KR02H02(5)*rco3_oh	Rickard and Pascoe (2009)*
G45492	TrGAroCN	C5DICARBO2 + NO \rightarrow MGLYOX + GLYOX + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45493	TrGAroCN	C5DICARBO2 + NO ₃ \rightarrow MGLYOX + GLYOX + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G45494	TrGAroC	C5DICARBO2 \rightarrow MGLYOX + GLYOX + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G46200a	TrGTerC	CO235C6O2 + HO ₂ \rightarrow CO235C6OOH	KR02H02(6)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G46200b	TrGTerC	CO235C6O2 + HO ₂ \rightarrow CO23C4CO3 + HCHO + OH	KR02H02(6)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G46201	TrGTerCN	CO235C6O2 + NO \rightarrow CO23C4CO3 + HCHO + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46202	TrGTerC	CO235C6O2 \rightarrow CO23C4CO3 + HCHO	k1_R02pOR02	Rickard and Pascoe (2009)
G46203	TrGTerC	CO235C6OOH + OH \rightarrow CO235C6O2	1.01E-11	Rickard and Pascoe (2009)
G46204	TrGTerC	C614O2 \rightarrow CO23C4CHO + HCHO + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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), Taraborrelli (2016)
G46206b	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(6) * \text{rchohch2o2_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
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	$\text{CO235C5CHO} + \text{NO}_3 \rightarrow \text{CO23C4CO3} + \text{CO} + \text{HNO}_3$	$\text{KN03AL} * 5.5$	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	$\text{NDNPHENOOH} + \text{OH} \rightarrow \text{NDNPHENO2}$	$0.6 * k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G46404a	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C615CO2OOH}$	$\text{KR02H02}(6) * (1 - \text{rcoch2o2_oh})$	Rickard and Pascoe (2009)
G46404b	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(6) * \text{rcoch2o2_oh}$	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	$\text{C615CO2O2} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2$	$k1_R02sOR02$	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	$\text{BZEMUCPAN} \rightarrow \text{BZEMUCCO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	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	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NDNPHENOOH}$	$\text{KR02H02}(6) * (1 - \text{rchohch2o2_oh})$	Rickard and Pascoe (2009)
G46413b	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	$\text{KR02H02}(6) * \text{rchohch2o2_oh}$	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)*

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

#	labels	reaction	rate coefficient	reference
G46416	TrGAroCN	NDNPHEO2 \rightarrow NC4DCO2H + HNO ₃ + CO + CO + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46417	TrGAroC	PBZQCO + OH \rightarrow C5CO2OHCO3	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	CATECHOL + NO ₃ \rightarrow CATEC1O + HNO ₃	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	CATECHOL + O ₃ \rightarrow MALDALCO2H + HCOCO ₂ H + HO ₂ + OH	9.2E-18	Rickard and Pascoe (2009)
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_CH3CO3_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_R02ISOPD02	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)

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

#	labels	reaction	rate coefficient	reference
G46437b	TrGAroCN	$\text{NPHENO}_2 + \text{HO}_2 \rightarrow \text{MALDALCO}_2\text{H} + \text{GLYOX} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G46438	TrGAroCN	$\text{NPHENO}_2 + \text{NO} \rightarrow \text{MALDALCO}_2\text{H} + \text{GLYOX} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46439	TrGAroCN	$\text{NPHENO}_2 + \text{NO}_3 \rightarrow \text{MALDALCO}_2\text{H} + \text{GLYOX} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46440	TrGAroCN	$\text{NPHENO}_2 \rightarrow \text{MALDALCO}_2\text{H} + \text{GLYOX} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46441	TrGAroC	$\text{BENZENE} + \text{OH} \rightarrow .352 \text{ BZBIPERO}_2 + .118 \text{ BZEPOXMUC} + .118 \text{ HO}_2 + .53 \text{ PHENOL} + .53 \text{ HO}_2$	$2.3\text{E}-12*\text{EXP}(-190/\text{TEMP})$	Rickard and Pascoe (2009)*
G46442	TrGAroCN	$\text{C5CO}_2\text{OHPAN} + \text{OH} \rightarrow \text{HOCOC4DIAL} + \text{CO} + \text{CO} + \text{NO}_2$	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	$\text{C5CO}_2\text{OHPAN} \rightarrow \text{C5CO}_2\text{OHCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46444	TrGAroCN	$\text{CATEC1O} + \text{NO}_2 \rightarrow \text{NCATECHOL}$	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46445	TrGAroC	$\text{CATEC1O} + \text{O}_3 \rightarrow \text{CATEC1O}_2$	k_C6H50_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46446	TrGAroC	$\text{BZEMUCCO} + \text{OH} \rightarrow \text{EPXDLCO}_3 + \text{GLYOX}$	9.20E-11	Rickard and Pascoe (2009)
G46447a	TrGAroCN	$\text{NNCATECO}_2 + \text{HO}_2 \rightarrow \text{NNCATECOOH}$	$\text{KR02H02(6)*(1-rchohch2o2_oh)}$	Rickard and Pascoe (2009)
G46447b	TrGAroCN	$\text{NNCATECO}_2 + \text{HO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G46448	TrGAroCN	$\text{NNCATECO}_2 + \text{NO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46449	TrGAroCN	$\text{NNCATECO}_2 + \text{NO}_3 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46450	TrGAroCN	$\text{NNCATECO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46451	TrGAroC	$\text{BZEMUCCO}_2\text{H} + \text{OH} \rightarrow \text{C5DIALO}_2 + \text{CO}_2$	4.06E-11	Rickard and Pascoe (2009)
G46452	TrGAroCN	$\text{NNCATECOOH} + \text{OH} \rightarrow \text{NNCATECO}_2$	$0.6*k_{\text{CH300H_OH}}$	Rickard and Pascoe (2009)
G46453	TrGAroCN	$\text{NPHEN1O} + \text{NO}_2 \rightarrow \text{DNPHEN}$	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46454	TrGAroCN	$\text{NPHEN1O} + \text{O}_3 \rightarrow \text{NPHEN1O}_2$	k_C6H50_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46455	TrGAroCN	$\text{DNPHEN} + \text{NO}_3 \rightarrow \text{NDNPHENO}_2$	2.25E-15	Rickard and Pascoe (2009)
G46456	TrGAroCN	$\text{DNPHEN} + \text{OH} \rightarrow \text{DNPHENO}_2$	3.00E-14	Rickard and Pascoe (2009)
G46457	TrGAroCN	$\text{PHENOL} + \text{NO}_3 \rightarrow .742 \text{ C6H5O} + .742 \text{ HNO}_3 + .258 \text{ NPHENO}_2$	3.8E-12	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
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 PHENOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46461b	TrGAroC	PHENO2 + HO ₂ \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46462	TrGAroCN	PHENO2 + NO \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46463	TrGAroCN	PHENO2 + NO ₃ \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46464	TrGAroC	PHENO2 \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46465	TrGAroC	C615CO2OOH + OH \rightarrow C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
G46466a	TrGAroC	C5CO2DBC03 + HO ₂ \rightarrow C5CO2DCO3H	KAPH02*(rco3_ooH+rco3_o3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBC03 + HO ₂ \rightarrow CH ₃ C(O) + HCOCOCHO + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBC03 + NO \rightarrow CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBC03 + NO ₂ \rightarrow C5CO2DBPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBC03 + NO ₃ \rightarrow CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBC03 \rightarrow CH ₃ C(O) + HCOCOCHO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46471	TrGAroCN	NPHEN1O2 + HO ₂ \rightarrow NPHEN1OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46472a	TrGAroCN	NPHEN1O2 + NO \rightarrow NPHEN1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G46472b	TrGAroCN	NPHEN1O2 + NO ₂ \rightarrow NPHEN1O + NO ₃	k_C6H502_N02	Jagiella and Zabel (2007)*
G46473	TrGAroCN	NPHEN1O2 + NO ₃ \rightarrow NPHEN1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G46474	TrGAroCN	NPHEN1O2 \rightarrow NPHEN1O	k1_R02sR02	Rickard and Pascoe (2009)
G46475	TrGAroCN	NPHENOOH + OH \rightarrow NPHENO2	1.07E-10	Rickard and Pascoe (2009)
G46476	TrGAroCN	C6H5O + NO ₂ \rightarrow HOC6H4NO2	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O ₃ \rightarrow C6H5O2	k_C6H50_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46478	TrGAroCN	NCATECOOH + OH \rightarrow NCATECO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH \rightarrow PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46480a	TrGAroC	$\text{PBZQO}_2 + \text{HO}_2 \rightarrow \text{PBZQOOH}$	$\text{KR02H02(6)*(1-rchohch2o2_oh-rcoch2o2_oh)}$	Rickard and Pascoe (2009)
G46480b	TrGAroC	$\text{PBZQO}_2 + \text{HO}_2 \rightarrow \text{C5CO2OHCO3} + \text{OH}$	$\text{KR02H02(6)*(rchohch2o2_oh+rcoch2o2_oh)}$	Rickard and Pascoe (2009)*
G46481	TrGAroCN	$\text{PBZQO}_2 + \text{NO} \rightarrow \text{C5CO2OHCO3} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46482	TrGAroCN	$\text{PBZQO}_2 + \text{NO}_3 \rightarrow \text{C5CO2OHCO3} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46483	TrGAroC	$\text{PBZQO}_2 \rightarrow \text{C5CO2OHCO3}$	k1_R02sOR02	Rickard and Pascoe (2009)*
G46484	TrGAroC	$\text{BZOBIPEROH} + \text{OH} \rightarrow \text{MALDIALCO3} + \text{GLYOX}$	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	$\text{DNPHENO}_2 + \text{HO}_2 \rightarrow \text{DNPHENOOH}$	$\text{KR02H02(6)*(1-rchohch2o2_oh)}$	Rickard and Pascoe (2009)
G46485b	TrGAroCN	$\text{DNPHENO}_2 + \text{HO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G46486	TrGAroCN	$\text{DNPHENO}_2 + \text{NO} \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46487	TrGAroCN	$\text{DNPHENO}_2 + \text{NO}_3 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46488	TrGAroCN	$\text{DNPHENO}_2 \rightarrow \text{NC4DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46489	TrGAroC	$\text{BZBIPEROOH} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{OH}$	9.77E-11	Rickard and Pascoe (2009)
G46490a	TrGAroC	$\text{BZEMUCO}_2 + \text{HO}_2 \rightarrow \text{BZEMUCOOH}$	KR02H02(6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	$\text{BZEMUCO}_2 + \text{HO}_2 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{OH}$	KR02H02(6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO} \rightarrow \text{BZEMUCNO}_3$	$\text{KR02N0*alpha_AN(10,2,0,1,0,temp,cair)}$	Rickard and Pascoe (2009)
G46491b	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO} \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{NO}_2$	$\text{KR02N0*(1-alpha_AN(10,2,0,1,0,temp,cair))}$	Rickard and Pascoe (2009)*
G46492	TrGAroCN	$\text{BZEMUCO}_2 + \text{NO}_3 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46493	TrGAroC	$\text{BZEMUCO}_2 \rightarrow .5 \text{EPXC4DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C3DIALO}_2 + .5 \text{C32OH13CO}$	k1_R02sOR02	Rickard and Pascoe (2009)*
G46494	TrGAroCN	$\text{C5CO2DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2$	3.28E-11	Rickard and Pascoe (2009)
G46495	TrGAroCN	$\text{C5CO2DBPAN} \rightarrow \text{C5CO2DBC03} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	$\text{NBZQOOH} + \text{OH} \rightarrow \text{NBZQO}_2$	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	$\text{CATEC1OOH} + \text{OH} \rightarrow \text{CATEC1O}_2$.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46498	TrGAroC	$\text{C6125CO} + \text{OH} \rightarrow \text{C5CO14O}_2 + \text{CO}$	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	$\text{NBZQO}_2 + \text{HO}_2 \rightarrow \text{NBZQOOH}$	$\text{KR02H02(6)*(1-rcoch2o2_oh)}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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_R02sOR02	Rickard and Pascoe (2009)*
G46503	TrGAroCN	DNPHENO0H + OH → DNPHENO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
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_R02sOR02	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_oh	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)*

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

#	labels	reaction	rate coefficient	reference
G46525	TrGAroC	BZBIPERO2 \rightarrow GLYOX + HO ₂ + BZFUONE	k1_R02sOR02	Rickard and Pascoe (2009)*
G47200	TrGTerCN	CO235C6CHO + NO ₃ \rightarrow CO235C6CO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	CO235C6CHO + OH \rightarrow CO235C6CO3	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	CO235C6CO3 + HO ₂ \rightarrow C235C6CO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO ₂ \rightarrow CO235C6O2 + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47203	TrGTerCN	CO235C6CO3 + NO \rightarrow CO235C6O2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G47204	TrGTerCN	CO235C6CO3 + NO ₂ \rightarrow C7PAN3	k_CH3C03_N02	Rickard and Pascoe (2009)
G47205	TrGTerC	CO235C6CO3 \rightarrow CO235C6O2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G47206	TrGTerC	C235C6CO3H + OH \rightarrow CO235C6CO3	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	C7PAN3 + OH \rightarrow CO235C5CHO + CO + NO ₂	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	C7PAN3 \rightarrow CO235C6CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G47209a	TrGTerC	C716O2 + HO ₂ \rightarrow C716OOH	KR02H02(7)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G47209b	TrGTerC	C716O2 + HO ₂ \rightarrow CO13C4CHO + CH ₃ C(O) + OH	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G47210	TrGTerCN	C716O2 + NO \rightarrow CO13C4CHO + CH ₃ C(O) + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47211	TrGTerC	C716O2 \rightarrow CO13C4CHO + CH ₃ C(O)	k1_R02sOR02	Rickard and Pascoe (2009)
G47212	TrGTerC	C716OOH + OH \rightarrow CO235C6CHO + OH	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	C721O2 + HO ₂ \rightarrow C721OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	C721O2 + NO \rightarrow C722O2 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47215	TrGTerC	C721O2 \rightarrow C722O2	k1_R02pR02	Rickard and Pascoe (2009)
G47216	TrGTerC	C721OOH + OH \rightarrow C721O2	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	C722O2 + HO ₂ \rightarrow C722OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	C722O2 + NO \rightarrow CH ₃ COCH ₃ + C44O2 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G47219	TrGTerC	C722O2 \rightarrow CH ₃ COCH ₃ + C44O2	k1_R02tR02	Rickard and Pascoe (2009)
G47220	TrGTerC	C722OOH + OH \rightarrow C722O2	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	ROO6R3O2 \rightarrow ROO6R5O2	5.68E10*EXP(-8745./TEMP)	Vereecken and Peeters (2012)
G47222	TrGTerCN	ROO6R3O2 + NO \rightarrow ROO6R3O + NO ₂	KR02NO	Vereecken and Peeters (2012)*
G47223	TrGTerC	ROO6R3O2 + HO ₂ \rightarrow 7 LCARBON	KR02H02(7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	ROO6R3O2 \rightarrow ROO6R3O	k1_R02sR02	Vereecken and Peeters (2012)
G47225	TrGTerC	ROO6R3O \rightarrow 7 LCARBON + HO ₂	5.7E10*EXP(-2949./TEMP)	Vereecken and Peeters (2012)*
G47226	TrGTerC	ROO6R5O2 \rightarrow 7 LCARBON + OH	9.17E10*EXP(-8706./TEMP)	Vereecken and Peeters (2012)*
G47400	TrGAroC	TOLUENE + OH \rightarrow .07 C6H5CH2O2 + .18 CRESOL + .18 HO ₂ + .65 TLBIPERO2 + .10 TLEPOXMUC + .10 HO ₂	1.8E-12*EXP(340/TEMP)	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47401	TrGAroC	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{OOH}$	$1.5\text{E}-13 \cdot \text{EXP}(1310/\text{TEMP})$	Rickard and Pascoe (2009)
G47402a	TrGAroCN	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{NO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{BENZAL} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
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	$\text{C}_6\text{H}_5\text{CH}_2\text{O}_2 \rightarrow \text{BENZAL} + \text{HO}_2$	$2 \cdot (\text{k}_{\text{CH302}} \cdot 2.4\text{E}-14 \cdot \text{EXP}(1620./\text{TEMP})) \cdot 0.5 \cdot \text{R02}$	Rickard and Pascoe (2009)*
G47405	TrGAroCN	$\text{CRESOL} + \text{NO}_3 \rightarrow .103 \text{ CRESO}_2 + .103 \text{ HNO}_3 + .506 \text{ NCRESO}_2 + .391 \text{ TOL1O} + .391 \text{ HNO}_3$	$1.4\text{E}-11$	Rickard and Pascoe (2009)*
G47406	TrGAroC	$\text{CRESOL} + \text{OH} \rightarrow .2 \text{ CRESO}_2 + .727 \text{ MCATECHOL} + .727 \text{ HO}_2 + .073 \text{ TOL1O}$	$4.65\text{E}-11$	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	$\text{TLBIPERO}_2 + \text{HO}_2 \rightarrow \text{OH} + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	$\text{KR02H02}(7) \cdot \text{rbipero2_oh}$	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G47408a	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO} \rightarrow \text{NO}_2 + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(11, 2, 0, 0, 1, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO} \rightarrow \text{TLBIPERNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(11, 2, 0, 0, 1, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)*
G47409	TrGAroCN	$\text{TLBIPERO}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	KR02N03	Rickard and Pascoe (2009)*
G47410	TrGAroC	$\text{TLBIPERO}_2 \rightarrow .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	k1_R02sOR02	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)

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

#	labels	reaction	rate coefficient	reference
G47416	TrGAroCN	BENZAL + NO ₃ → C ₆ H ₅ CO ₃ + HNO ₃	2.40E-15	Rickard and Pascoe (2009)
G47417	TrGAroC	BENZAL + OH → C ₆ H ₅ CO ₃	5.9E-12*EXP(225/TEMP)	Rickard and Pascoe (2009)
G47418a	TrGAroC	CRESO ₂ + HO ₂ → CRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO ₂ + HO ₂ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO ₂ + NO → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO ₂ + NO ₃ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47421	TrGAroC	CRESO ₂ → .68 C ₅ CO ₁₄ OH + .68 GLYOX + HO ₂ + .32 PTLQONE	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO ₂ + HO ₂ → NCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO ₂ + HO ₂ → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO ₂ + NO → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO ₂ + NO ₃ → C ₅ CO ₁₄ OH + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO ₂ → C ₅ CO ₁₄ OH + GLYOX + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47426	TrGAroCN	TOL1O + NO ₂ → TOL1OHNO ₂	k_C6H5O_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O ₃ → OXYL1O ₂	k_C6H5O_O3	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 → MC3ODBCO ₂ H + 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	TLBIPERNO ₃ + OH → TLOBIPEROH + NO ₂	7.16E-11	Rickard and Pascoe (2009)
G47433	TrGAroC	TLOBIPEROH + OH → C ₅ CO ₁₄ O ₂ + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO ₃ + HO ₂ → C ₆ 15CO ₂ O ₂ + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₂ H + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₃ H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO ₃ + NO → C ₆ 15CO ₂ O ₂ + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO ₃ + NO ₂ → TLEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO ₃ + NO ₃ → C ₆ 15CO ₂ O ₂ + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47438	TrGAroC	$\text{TLEMUCCO}_3 \rightarrow \text{C}_6\text{H}_5\text{CO}_2\text{O}_2 + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)*
G47439a	TrGAroC	$\text{TLEMUCO}_2 + \text{HO}_2 \rightarrow \text{TLEMUCOOH}$	KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47439b	TrGAroC	$\text{TLEMUCO}_2 + \text{HO}_2 \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{OH}$	KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G47440a	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO} \rightarrow \text{TLEMUCNO}_3$	KR02N0*alpha_AN(11,2,1,0,0,temp,cair)	Rickard and Pascoe (2009)
G47440b	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO} \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-alpha_AN(11,2,1,0,0,temp,cair))	Rickard and Pascoe (2009)*
G47441	TrGAroCN	$\text{TLEMUCO}_2 + \text{NO}_3 \rightarrow .5 \text{C}_3\text{DIALO}_2 + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{EPXC}_4\text{DIAL} + .5 \text{MGLYOX} + .5 \text{HO}_2 + \text{NO}_2$	KR02N03	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_R02sOR02	Rickard and Pascoe (2009)*
G47443a	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{CO}_3\text{H}$	1.1E-11*EXP(364./temp)*0.65	Roth et al. (2010)
G47443b	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	1.1E-11*EXP(364./temp)*0.20	Roth et al. (2010)
G47443c	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{PHCOOH} + \text{O}_3$	1.1E-11*EXP(364./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_CH3CO3_N02	Rickard and Pascoe (2009)*
G47446	TrGAroCN	$\text{C}_6\text{H}_5\text{CO}_3 + \text{NO}_3 \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KR02N03*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_R02RCO3	Rickard and Pascoe (2009)*
G47448	TrGAroC	$\text{CRESOOH} + \text{OH} \rightarrow \text{CRESO}_2$	1.15E-10	Rickard and Pascoe (2009)
G47449	TrGAroCN	$\text{NCRESOOH} + \text{OH} \rightarrow \text{NCRESO}_2$	1.07E-10	Rickard and Pascoe (2009)
G47450	TrGAroCN	$\text{TOL1OHNO}_2 + \text{NO}_3 \rightarrow \text{NCRES1O} + \text{HNO}_3$	3.13E-13*1.0	Rickard and Pascoe (2009)
G47451	TrGAroCN	$\text{TOL1OHNO}_2 + \text{OH} \rightarrow \text{NCRES1O}$	2.8E-12	Rickard and Pascoe (2009)
G47452	TrGAroC	$\text{OXYL1O}_2 + \text{HO}_2 \rightarrow \text{OXYL1OOH}$	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	$\text{OXYL1O}_2 + \text{NO}_3 \rightarrow \text{TOL1O} + \text{NO}_2$	KR02N03	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	$\text{TLEMUCCO}_2\text{H} + \text{OH} \rightarrow \text{C}_6\text{H}_5\text{CO}_2\text{O}_2 + \text{CO}_2$	5.98E-11	Rickard and Pascoe (2009)
G47460	TrGAroC	$\text{TLEMUCCO}_3\text{H} + \text{OH} \rightarrow \text{TLEMUCCO}_3$	6.29E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47461	TrGAroCN	TLEMUCPAN + OH \rightarrow C5DICARB + CO + CO ₂ + NO ₂	5.96E-11	Rickard and Pascoe (2009)
G47462	TrGAroCN	TLEMUCPAN \rightarrow TLEMUCCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G47463	TrGAroC	TLEMUCOOH + OH \rightarrow TLEMUCCO + OH	7.04E-11	Rickard and Pascoe (2009)
G47464	TrGAroCN	TLEMUCNO3 + OH \rightarrow TLEMUCCO + NO ₂	3.06E-11	Rickard and Pascoe (2009)
G47465	TrGAroC	TLEMUCCO + OH \rightarrow CH ₃ C(O) + EPXC4DIAL + CO	4.06E-11	Rickard and Pascoe (2009)
G47466	TrGAroC	C6H5CO3H + OH \rightarrow C6H5CO3	4.66E-12	Rickard and Pascoe (2009)
G47467	TrGAroC	PHCOOH + OH \rightarrow C6H5O2 + CO ₂	1.10E-12	Rickard and Pascoe (2009)
G47468	TrGAroCN	PBZN + OH \rightarrow C6H5OOH + CO + NO ₂	1.06E-12	Rickard and Pascoe (2009)
G47469	TrGAroCN	PBZN \rightarrow C6H5CO3 + NO ₂	k_PAN_M*0.67	Rickard and Pascoe (2009)
G47470	TrGAroCN	PTLQONE + NO ₃ \rightarrow NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
G47471	TrGAroC	PTLQONE + OH \rightarrow PTLQO2	2.3E-11	Rickard and Pascoe (2009)
G47472	TrGAroCN	NCRES1O + NO ₂ \rightarrow DNCRES	k_C6H5O_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O ₃ \rightarrow NCRES1O2	k_C6H5O_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47474	TrGAroC	OXYL1OOH + OH \rightarrow OXYL1O2	4.65E-11	Rickard and Pascoe (2009)
G47475	TrGAroCN	MNCATECH + NO ₃ \rightarrow MNNCATECO2	5.03E-12	Rickard and Pascoe (2009)
G47476	TrGAroCN	MNCATECH + OH \rightarrow MNCATECO2	6.83E-12	Rickard and Pascoe (2009)
G47477	TrGAroC	MCATEC1O2 + HO ₂ \rightarrow MCATEC1OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47478	TrGAroCN	MCATEC1O2 + NO \rightarrow MCATEC1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G47479	TrGAroCN	MCATEC1O2 + NO ₂ \rightarrow MCATEC1O + NO ₃	K_C6H5O2_N02	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO ₃ \rightarrow MCATEC1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G47481	TrGAroC	MCATEC1O2 \rightarrow MCATEC1O	k1_R02sOR02	Rickard and Pascoe (2009)
G47482a	TrGAroCN	NPTLQO2 + HO ₂ \rightarrow NPTLQOOH	KR02H02(7)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO ₂ \rightarrow C7CO4DB + NO ₂ + OH	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G47483	TrGAroCN	NPTLQO2 + NO \rightarrow C7CO4DB + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47484	TrGAroCN	NPTLQO2 + NO ₃ \rightarrow C7CO4DB + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47485	TrGAroCN	NPTLQO2 \rightarrow C7CO4DB + NO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G47486a	TrGAroC	PTLQO2 + HO ₂ \rightarrow PTLQOOH	KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO ₂ \rightarrow C6CO2OHCO3 + OH	KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G47487	TrGAroCN	PTLQO2 + NO \rightarrow C6CO2OHCO3 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47488	TrGAroCN	PTLQO2 + NO ₃ \rightarrow C6CO2OHCO3 + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47489	TrGAroC	PTLQO2 \rightarrow C6CO2OHCO3	k1_R02sOR02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
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)
G47493	TrGAroCN	NCRES1O2 + NO → NCRES1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G47494	TrGAroCN	NCRES1O2 + NO ₂ → NCRES1O + NO ₃	K_C6H5O2_N02	Jagiella and Zabel (2007)*
G47495	TrGAroCN	NCRES1O2 + NO ₃ → NCRES1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G47496	TrGAroCN	NCRES1O2 → NCRES1O	k1_R02sR02	Rickard and Pascoe (2009)
G47497a	TrGAroCN	MNNCATECO2 + HO ₂ → MNNCATCOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47497b	TrGAroCN	MNNCATECO2 + HO ₂ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47498	TrGAroCN	MNNCATECO2 + NO → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47499	TrGAroCN	MNNCATECO2 + NO ₃ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47500	TrGAroCN	MNNCATECO2 → NC4MDCO2HN + HCOCO ₂ H + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)
G47501a	TrGAroCN	MNCATECO2 + HO ₂ → MNCATECOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47501b	TrGAroCN	MNCATECO2 + HO ₂ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47502	TrGAroCN	MNCATECO2 + NO → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47503	TrGAroCN	MNCATECO2 + NO ₃ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47504	TrGAroCN	MNCATECO2 → NC4MDCO2HN + HCOCO ₂ H + HO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47505	TrGAroC	MCATEC1OOH + OH → MCATEC1O2	2.05E-10	Rickard and Pascoe (2009)
G47506	TrGAroCN	NPTLQOOH + OH → NPTLQO2	8.56E-11	Rickard and Pascoe (2009)
G47507	TrGAroC	PTLQOOH + OH → PTLQCO + OH	1.42E-10	Rickard and Pascoe (2009)
G47508	TrGAroC	PTLQCO + OH → C6CO2OHC03	7.95E-11	Rickard and Pascoe (2009)
G47509a	TrGAroCN	NDNCRESO2 + HO ₂ → NDNCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47509b	TrGAroCN	NDNCRESO2 + HO ₂ → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47510	TrGAroCN	NDNCRESO2 + NO → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47511	TrGAroCN	NDNCRESO2 + NO ₃ → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47512	TrGAroCN	NDNCRESO2 → NC4MDCO2HN + HNO ₃ + 2 CO + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47513a	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{DNCRESOOH}$	$\text{KR02H02(7)*(1-rchohch2o2_oh)}$	Rickard and Pascoe (2009)
G47513b	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(7)*rchohch2o2_oh}$	Rickard and Pascoe (2009)*
G47514	TrGAroCN	$\text{DNCRESO}_2 + \text{NO} \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47515	TrGAroCN	$\text{DNCRESO}_2 + \text{NO}_3 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47516	TrGAroCN	$\text{DNCRESO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47517	TrGAroCN	$\text{NCRES1OOH} + \text{OH} \rightarrow \text{NCRES1O}_2$	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	$\text{MNNCATCOOH} + \text{OH} \rightarrow \text{MNNCATECO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47519	TrGAroCN	$\text{MNCATECOOH} + \text{OH} \rightarrow \text{MNCATECO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47520	TrGAroC	$\text{C7CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CH}_3\text{C(O)} + \text{HCOCOCHO}$	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	$\text{C6CO2OHCO}_3 + \text{HO}_2 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47521b	TrGAroC	$\text{C6CO2OHCO}_3 + \text{HO}_2 \rightarrow \text{C6COOHCO}_3\text{H}$	KAPH02*(rco3_ooH+rco3_o3)	Rickard and Pascoe (2009)
G47522	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO} \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G47523	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO}_2 \rightarrow \text{C6CO}_2\text{OHPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G47524	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	$\text{C6CO2OHCO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G47526	TrGAroCN	$\text{NDNCRESOOH} + \text{OH} \rightarrow \text{NDNCRESO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47527	TrGAroCN	$\text{DNCRESOOH} + \text{OH} \rightarrow \text{DNCRESO}_2$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47528	TrGAroC	$\text{C6COOHCO}_3\text{H} + \text{OH} \rightarrow \text{C6CO}_2\text{OHCO}_3$	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	$\text{C6CO}_2\text{OHPAN} + \text{OH} \rightarrow \text{C5134CO}_2\text{OH} + \text{CO} + \text{CO} + \text{NO}_2$	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	$\text{C6CO}_2\text{OHPAN} \rightarrow \text{C6CO}_2\text{OHCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	$\text{C85O}_2 \rightarrow \text{C86O}_2$	k1_R02tR02	Rickard and Pascoe (2009)
G48201	TrGTerC	$\text{C85O}_2 + \text{HO}_2 \rightarrow \text{C85OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	$\text{C85O}_2 + \text{NO} \rightarrow \text{C86O}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48203	TrGTerC	$\text{C85OOH} + \text{OH} \rightarrow \text{C85O}_2$	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	$\text{C86O}_2 \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3$	k1_R02tR02	Rickard and Pascoe (2009)
G48205	TrGTerCN	$\text{C86O}_2 + \text{NO} \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48206	TrGTerC	$\text{C86O}_2 + \text{HO}_2 \rightarrow \text{C86OOH}$	KR02H02(8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48207	TrGTerC	$\text{C86OOH} + \text{OH} \rightarrow \text{C86O2}$	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	$\text{C811O2} \rightarrow \text{C812O2}$	k1_R02pR02	Rickard and Pascoe (2009)
G48209	TrGTerC	$\text{C811O2} + \text{HO}_2 \rightarrow 8 \text{ L CARBON}$	KR02H02(8)	Rickard and Pascoe (2009)
G48210	TrGTerCN	$\text{C811O2} + \text{NO} \rightarrow \text{C812O2} + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G48211	TrGTerC	$\text{C812O2} \rightarrow \text{C813O2}$	k1_R02tOR02	Rickard and Pascoe (2009)
G48212	TrGTerCN	$\text{C812O2} + \text{NO} \rightarrow \text{C813O2} + \text{NO}_2$	KR02NO	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	$\text{C813O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{NO}_2$	KR02NO	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	$\text{C721CO3} + \text{NO} \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*
G48223	TrGTerCN	$\text{C721CO3} + \text{NO}_2 \rightarrow \text{C721PAN}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G48224	TrGTerCN	$\text{C721CO3} + \text{NO}_3 \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KR02NO3*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	$\text{C721CO3} \rightarrow \text{C721O2} + \text{CO}_2$	k1_R02RC03*0.9	Taraborrelli (2016)
G48226	TrGTerC	$\text{C721CO3} \rightarrow \text{NORPINIC}$	k1_R02RC03*0.1	Taraborrelli (2016)
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	$\text{C8BCO2} + \text{NO} \rightarrow \text{C89O2} + \text{NO}_2$	KR02NO*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C8BCNO3}$	KR02NO*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)

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

#	labels	reaction	rate coefficient	reference
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)
G48239a	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C810O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48239b	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C89NO3}$	KR02N0*alpha_AN(7,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48240	TrGTerCN	$\text{C89O2} + \text{NO}_3 \rightarrow \text{C810O2} + \text{NO}_2$	KR02N03	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	$\text{C810O2} + \text{HO}_2 \rightarrow \text{C810OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48245a	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(10,3,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48245b	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{C810NO3}$	KR02N0*alpha_AN(10,3,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G48246	TrGTerCN	$\text{C810O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KR02N03	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	$\text{LXYL} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + \text{LCARBON}$	0.401E-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	$\text{NSTYRENO2} + \text{HO}_2 \rightarrow \text{NSTYRENOOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48408	TrGAroCN	$\text{NSTYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N0	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G48409	TrGAroCN	NSTYRENO2 + NO ₃ → NO ₂ + NO ₂ + HCHO + BENZAL	KR02NO3	Rickard and Pascoe (2009)*
G48410	TrGAroCN	NSTYRENO2 → NO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
G48411	TrGAroCN	NSTYRENOOH + OH → NSTYRENO2	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	STYRENO2 + HO ₂ → STYRENOOH	KR02H02(8)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G48412b	TrGAroC	STYRENO2 + HO ₂ → HO ₂ + OH + HCHO + BENZAL	KR02H02(8)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G48413	TrGAroCN	STYRENO2 + NO → NO ₂ + HO ₂ + HCHO + BENZAL	KR02NO	Rickard and Pascoe (2009)*
G48414	TrGAroCN	STYRENO2 + NO ₃ → NO ₂ + HO ₂ + HCHO + BENZAL	KR02NO3	Rickard and Pascoe (2009)*
G48415	TrGAroC	STYRENO2 → HO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard and Pascoe (2009)*
G48416	TrGAroC	STYRENOOH + OH → STYRENO2	6.16E-11	Rickard and Pascoe (2009)
G49200	TrGTerC	C96O2 → C97O2	k1_R02pR02	Rickard and Pascoe (2009)
G49201	TrGTerC	C96O2 + HO ₂ → C96OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49202a	TrGTerCN	C96O2 + NO → C97O2 + NO ₂	KR02NO*(1.-alpha_AN(10,1,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49202b	TrGTerCN	C96O2 + NO → C96NO3	KR02NO*alpha_AN(10,1,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49203	TrGTerCN	C96NO3 + OH → NORPINAL + NO ₂	2.88E-12	Rickard and Pascoe (2009)
G49204a	TrGTerC	C96OOH + OH → C96O2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G49205b	TrGTerC	C96OOH + OH → NORPINAL + OH	1.30E-11	Rickard and Pascoe (2009)
G49206	TrGTerC	C97O2 → C98O2	k1_R02tR02	Rickard and Pascoe (2009)
G49207	TrGTerCN	C97O2 + NO → C98O2 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G49208a	TrGTerC	C97O2 + HO ₂ → C97OOH	KR02H02(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49208b	TrGTerC	C97O2 + HO ₂ → C98O2 + OH	KR02H02(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49209	TrGTerC	C97OOH + OH → C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 → C614O2 + CH ₃ COCH ₃	k1_R02tR02	Rickard and Pascoe (2009)
G49211a	TrGTerCN	C98O2 + NO → C614O2 + CH ₃ COCH ₃ + NO ₂	KR02NO*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49211b	TrGTerCN	C98O2 + NO → 9 LCARBON + LNITROGEN	KR02NO*alpha_AN(12,3,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49212	TrGTerC	C98O2 + HO ₂ → C98OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49213	TrGTerC	C98OOH + OH → C98O2	2.05E-11	Rickard and Pascoe (2009)
G49214	TrGTerC	NORPINAL + OH → C85CO3	2.64E-11	Rickard and Pascoe (2009)
G49215	TrGTerCN	NORPINAL + NO ₃ → C85CO3 + HNO ₃	KN03AL*8.5	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49216	TrGTerC	$\text{C85CO3} \rightarrow \text{C85O2} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G49217	TrGTerCN	$\text{C85CO3} + \text{NO} \rightarrow \text{C85O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G49218	TrGTerCN	$\text{C85CO3} + \text{NO}_2 \rightarrow \text{C9PAN2}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G49219a	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85CO3H}$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G49219b	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G49220	TrGTerCN	$\text{C9PAN2} \rightarrow \text{C85CO3} + \text{NO}_2$	k_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_R02RC03*0.9	Taraborrelli (2016)
G49223b	TrGTerC	$\text{C89CO3} \rightarrow \text{C89CO2H}$	k1_R02RC03*0.1	Taraborrelli (2016)
G49224a	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G49224b	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G49224c	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow .80 \text{ C811CO3} + .20 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G49225	TrGTerCN	$\text{C89CO3} + \text{NO}_2 \rightarrow \text{C89PAN}$	k_CH3C03_N02	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_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_R02RC03*0.9	Taraborrelli (2016)
G49231b	TrGTerC	$\text{C811CO3} \rightarrow \text{PINIC}$	k1_R02RC03*0.1	Taraborrelli (2016)
G49232a	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811CO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G49232b	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{PINIC} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G49232c	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	KAPH02*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_CH3C03_N02	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	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{NOPINDOOH}$	KR02H02(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	$\text{KR02H02(9)*rcoch2o2_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G49239	TrGTerC	$\text{NOPINDO2} \rightarrow \text{C89CO3}$	k1_R02p0R02	Rickard and Pascoe (2009)
G49240	TrGTerC	$\text{NOPINDOOH} \rightarrow \text{NOPINDCO}$	$2.63\text{E-}11$	Rickard and Pascoe (2009)
G49241	TrGTerC	$\text{NOPINDCO} + \text{OH} \rightarrow \text{C89CO3}$	$3.07\text{E-}12$	Rickard and Pascoe (2009)
G49242	TrGTerC	$\text{NOPINOO} \rightarrow \text{NOPINONE} + \text{H}_2\text{O}_2$	$6.00\text{E-}18*\text{c(ind_H2O)}$	Rickard and Pascoe (2009)
G49243	TrGTerC	$\text{NOPINOO} + \text{CO} \rightarrow \text{NOPINONE} + \text{CO}_2$	$1.2\text{E-}15$	Rickard and Pascoe (2009)
G49244	TrGTerCN	$\text{NOPINOO} + \text{NO} \rightarrow \text{NOPINONE} + \text{NO}_2$	$1\text{E-}14$	Rickard and Pascoe (2009)
G49245	TrGTerCN	$\text{NOPINOO} + \text{NO}_2 \rightarrow \text{NOPINONE} + \text{NO}_3$	$1\text{E-}15$	Rickard and Pascoe (2009)
G49246	TrGTerC	$\text{NORPINENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C86O2}$	$\text{k_CH2CHOH_OH_HCOOH}$	Taraborrelli (2016), So et al. (2014)*
G49247	TrGTerC	$\text{NORPINENOL} + \text{HCOOH} \rightarrow \text{NORPINAL} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G49248	TrGTerC	$\text{NORPINAL} + \text{HCOOH} \rightarrow \text{NORPINENOL} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G49249	TrGTerC	$\text{C811CO3H} + \text{OH} \rightarrow \text{C811CO3}$	$1.04\text{E-}11$	Rickard and Pascoe (2009)
G49250	TrGTerCN	$\text{C811PAN} \rightarrow \text{C811CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	$\text{C811PAN} + \text{OH} \rightarrow \text{C721CHO} + \text{CO} + \text{NO}_2$	$6.77\text{E-}12$	Rickard and Pascoe (2009)
G49400a	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + 2 \text{LCARBON}$	$0.827\text{E-}11$	Rickard and Pascoe (2009)*
G49400b	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{C6H5CH2O2} + 2 \text{LCARBON}$	$0.189\text{E-}11$	Rickard and Pascoe (2009)*
G49400c	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{CRESOL} + 2 \text{LCARBON}$	$0.141\text{E-}11$	Rickard and Pascoe (2009)*
G49400d	TrGAroC	$\text{LTMB} + \text{OH} \rightarrow \text{TLBIPERO2} + \text{HO}_2 + 2 \text{LCARBON}$	$2.917\text{E-}11$	Rickard and Pascoe (2009)*
G49401	TrGAroCN	$\text{LTMB} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + 2 \text{LCARBON}$	$1.52\text{E-}15$	Rickard and Pascoe (2009)*
G40200	TrGTerC	$\text{APINENE} + \text{OH} \rightarrow .75 \text{LAPINABO2} + .15 \text{MENTHEN6ONE} + .15 \text{HO}_2 + .10 \text{ROO6R1O2}$	$1.2\text{E-}11*\text{EXP}(440./\text{TEMP})$	Atkinson et al. (2006)*
G40201a	TrGTerCN	$\text{LAPINABO2} + \text{NO} \rightarrow \text{PINAL} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1-(.65*\alpha_{\text{AN}}(11,3,0,0,0,\text{temp},\text{cair})+.35*\alpha_{\text{AN}}(11,2,0,0,0,\text{temp},\text{cair})))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G40201b	TrGTerCN	$\text{LAPINABO2} + \text{NO} \rightarrow \text{LAPINABNO3}$	$\text{KR02N0}*(.65*\alpha_{\text{AN}}(11,3,0,0,0,\text{temp},\text{cair})+.35*\alpha_{\text{AN}}(11,2,0,0,0,\text{temp},\text{cair})))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G40202a	TrGTerC	$\text{LAPINABO2} + \text{HO}_2 \rightarrow \text{LAPINABOOH}$	$\text{KR02H02(10)}*(1-\text{rchohch2o2_oh})$	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G40202b	TrGTerC	LAPINABO2 + HO ₂ → PINAL + HO ₂ + OH	KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40203	TrGTerC	LAPINABO2 → PINAL + HO ₂	R02*(0.65*k1_R02tOR02+.35*k1_R02sOR02)	Rickard and Pascoe (2009)*
G40204	TrGTerC	LAPINABOOH + OH → .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard and Pascoe (2009)*
G40205	TrGTerCN	LAPINABNO3 + OH → .35 PINAL + .65 C96CO3 + NO ₂	4.29E-12	Rickard and Pascoe (2009)*
G40206	TrGTerC	MENTHEN6ONE + OH → OHMENTHEN6ONEO2	6.46E-11	Vereecken et al. (2007)*
G40207	TrGTerCN	OHMENTHEN6ONEO2 + NO → 2OHMENTHEN6ONE + HO ₂ + NO ₂	KR02NO	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO ₂ → 2OHMENTHEN6ONE	KR02H02(10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 → 2OHMENTHEN6ONE + HO ₂	k1_R02tOR02	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH → 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH → .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./TEMP)	Wallington et al. (2017)*
G40212	TrGTerCN	PINAL + NO ₃ → C96CO3 + HNO ₃	2.0E-14	Wallington et al. (2017)*
G40213a	TrGTerC	C96CO3 → C96O2 + CO ₂	k1_R02RC03*0.9	Rickard and Pascoe (2009)
G40213b	TrGTerC	C96CO3 → PINONIC	k1_R02RC03*0.1	Rickard and Pascoe (2009)
G40214a	TrGTerC	C96CO3 + HO ₂ → PERPINONIC	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO ₂ → PINONIC + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO ₂ → C96O2 + OH + CO ₂	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G40215	TrGTerCN	C96CO3 + NO ₂ → C10PAN2	k_CH3CO3_N02	Rickard and Pascoe (2009)
G40216	TrGTerCN	C96CO3 + NO → C96O2 + NO ₂ + CO ₂	KAPNO	Rickard and Pascoe (2009)
G40217	TrGTerCN	C96CO3 + NO ₃ → C96O2 + NO ₂ + CO ₂	KR02NO3*1.60	Rickard and Pascoe (2009)
G40218	TrGTerCN	C10PAN2 → C96CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G40219	TrGTerCN	C10PAN2 + OH → NORPINAL + CO + NO ₂	3.66E-12	Rickard and Pascoe (2009)
G40220	TrGTerC	PINONIC + OH → C96O2 + CO ₂	6.65E-12	Rickard and Pascoe (2009)
G40221	TrGTerC	PERPINONIC + OH → C96CO3	9.73E-12	Rickard and Pascoe (2009)
G40222	TrGTerC	PINALO2 + HO ₂ → PINALOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40223a	TrGTerCN	PINALO2 + NO → C106O2 + NO ₂	KR02NO*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G40223b	TrGTerCN	PINALO2 + NO → PINALNO3	KR02NO*alpha_AN(12,3,0,1,0, temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40224	TrGTerC	PINALO2 → C106O2	k1_R02tR02	Rickard and Pascoe (2009)
G40225	TrGTerC	PINALOOH + OH → PINALO2	2.75E-11	Rickard and Pascoe (2009)
G40226	TrGTerCN	PINALNO3 + OH → CO235C6CHO + CH ₃ COCH ₃ + NO ₂	2.25E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40227	TrGTerC	$\text{C106O2} + \text{HO}_2 \rightarrow \text{C106OOH}$	$\text{KR02H02}(10)$	Rickard and Pascoe (2009)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
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	$\text{APINENE} + \text{O}_3 \rightarrow .09 \text{ APINBOO} + .08 \text{ PINONIC} + .77 \text{ OH} + .33 \text{ NORPINAL} + .33 \text{ CO} + .33 \text{ HO}_2 + .06 \text{ APINAOO} + .44 \text{ C109O2}$	$8.05\text{E-}16 * \text{EXP}(-640./\text{TEMP})$	Wallington et al. (2017)*
G40233	TrGTerC	$\text{APINAOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * \text{c}(\text{ind_H2O})$	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	$\text{APINAOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2$	$1.00\text{E-}14$	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	$\text{APINBOO} \rightarrow \text{PINONIC}$	$1.00\text{E-}17 * \text{c}(\text{ind_H2O}) * (0.08 + 0.15)$	Rickard and Pascoe (2009)
G40237b	TrGTerC	$\text{APINBOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * \text{c}(\text{ind_H2O}) * 0.77$	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	$\text{APINBOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2$	$1.00\text{E-}14$	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_R02pOR02	Rickard and Pascoe (2009)
G40242	TrGTerCN	$\text{C109O2} + \text{NO} \rightarrow \text{C89CO3} + \text{HCHO} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G40243a	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C109OOH}$	$\text{KR02H02}(10) * \text{rcoch2o2_ooh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G40243b	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{HCHO} + \text{OH}$	$\text{KR02H02}(10) * \text{rcoch2o2_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
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. (2017)*
G40247	TrGTerCN	$\text{LNAPINABO2} \rightarrow \text{PINAL} + \text{NO}_2$	$(0.65 * \text{k1_R02tR02} + 0.35 * \text{k1_R02sR02})$	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)
G40250	TrGTerCN	$\text{LNAPINABO2} + \text{NO}_3 \rightarrow \text{PINAL} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G40251	TrGTerCN	$\text{LNAPINABOOH} + \text{OH} \rightarrow \text{LNAPINABO2}$	$(.65 * 6.87\text{E-}12 + .35 * 1.23\text{E-}11)$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40252a	TrGTerC	BPINENE + OH \rightarrow 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 \rightarrow ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO ₂ \rightarrow BPINAOOH	KR02H02(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40253b	TrGTerC	BPINAO2 + HO ₂ \rightarrow NOPINONE + HCHO + HO ₂ + OH	KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40254a	TrGTerCN	BPINAO2 + NO \rightarrow NOPINONE + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(11,3,0,0,0, temp, cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G40254b	TrGTerCN	BPINAO2 + NO \rightarrow BPINANO3	KR02N0*alpha_AN(11,3,0,0,0, temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40255	TrGTerC	BPINAO2 \rightarrow NOPINONE + HCHO + HO ₂	k1_R02tOR02	Rickard and Pascoe (2009)
G40256	TrGTerC	BPINAOOH + OH \rightarrow BPINAO2	1.33E-11	Rickard and Pascoe (2009)
G40257	TrGTerCN	BPINANO3 + OH \rightarrow NOPINONE + HCHO + NO ₂	4.70E-12	Rickard and Pascoe (2009)
G40258a	TrGTerCN	ROO6R1O2 + NO \rightarrow ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	KR02N0*(1.-alpha_AN(13,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO \rightarrow ROO6R1NO3	KR02N0*alpha_AN(13,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40259	TrGTerC	ROO6R1O2 + HO ₂ \rightarrow 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40260	TrGTerC	ROO6R1O2 \rightarrow ROO6R3O2 + CH ₃ COCH ₃	k1_R02tOR02	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO \rightarrow RO6R3O2 + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO \rightarrow RO6R1NO3	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO ₂ \rightarrow 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 \rightarrow RO6R3O2	k1_R02sOR02	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO \rightarrow 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 \rightarrow 10 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO ₂ \rightarrow 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)
G40266	TrGTerC	RO6R3O2 \rightarrow 9 LCARBON + HCHO + HO ₂	k1_R02sR02	Vereecken and Peeters (2012)*
G40267a	TrGTerC	BPINENE + O ₃ \rightarrow NOPINONE + .63 CO + .37 CH ₂ OO + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	Wallington et al. (2017)*

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

#	labels	reaction	rate coefficient	reference
G40267b	TrGTerC	BPINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2017)
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. (2017)
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. (2017)
G40268	TrGTerCN	BPINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2017)*
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 → BPINANO3	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	Taraborrelli (2016), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH → PINAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G40278	TrGTerC	PINAL + HCOOH → PINEOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G40279a	TrGC	CARENE + OH → LAPINABO2	8.7E-11*(.50+.25)	Wolfe et al. (2011), Taraborrelli (2016)
G40279b	TrGC	CARENE + OH → MENTHEN6ONE + HO ₂	8.7E-11*.25*.60	Wolfe et al. (2011), Taraborrelli (2016)
G40279c	TrGC	CARENE + OH → ROO6R1O2	8.7E-11*.25*.40	Wolfe et al. (2011), Taraborrelli (2016)
G40280a	TrGC	CARENE + O ₃ → APINBOO	2.E-16*.50*.18	Wolfe et al. (2011), Taraborrelli (2016)
G40280b	TrGC	CARENE + O ₃ → PINONIC	2.E-16*.50*.16	Wolfe et al. (2011), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G40280c	TrGC	CARENE + O ₃ → OH + NORPINAL + CO + HO ₂	2.E-16*.50*.66	Wolfe et al. (2011), Taraborrelli (2016)
G40280d	TrGC	CARENE + O ₃ → APINAOO	2.E-16*.50*.12	Wolfe et al. (2011), Taraborrelli (2016)
G40280e	TrGC	CARENE + O ₃ → OH + C109O2	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Taraborrelli (2016)
G40281	TrGCN	CARENE + NO ₃ → LNAPINABO2	9.5E-12	Wolfe et al. (2011), Taraborrelli (2016)
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. (2017)*
G40283b	TrGTerC	SABINENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2017)
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. (2017)
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. (2017)
G40284	TrGTerCN	SABINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2017)*
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. (2017)*
G40286b	TrGTerC	CAMPHENE + O ₃ → NOPINOO + CO ₂	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), Wallington et al. (2017)
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. (2017)
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. (2017)
G40287	TrGTerCN	CAMPHENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2017)*

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

#	labels	reaction	rate coefficient	reference
G40400	TrGAroC	LHAROM + OH \rightarrow .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 \rightarrow C6H5CH2O2 + HNO ₃ + 4 LCARBON	2.60E-15	Rickard and Pascoe (2009)*
G6100	UpStTrGCl	Cl + O ₃ \rightarrow ClO + O ₂	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + O(³ P) \rightarrow Cl + O ₂	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO \rightarrow Cl ₂ + O ₂	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO \rightarrow 2 Cl + O ₂	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO \rightarrow Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO \rightarrow Cl ₂ O ₂	k_ClO_ClO	Burkholder et al. (2015)
G6103	StTrGCl	Cl ₂ O ₂ \rightarrow ClO + ClO	k_ClO_ClO/(2.16E-27*EXP(8537./temp))	Burkholder et al. (2015)*
G6200	StGCl	Cl + H ₂ \rightarrow HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO ₂ \rightarrow HCl + O ₂	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO ₂ \rightarrow ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H ₂ O ₂ \rightarrow HCl + HO ₂	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH \rightarrow .94 Cl + .94 HO ₂ + .06 HCl + .06 O ₂	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO ₂ \rightarrow HOCl + O ₂	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH \rightarrow Cl + H ₂ O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH \rightarrow ClO + H ₂ O	3.0E-12*EXP(-500./temp)	Burkholder et al. (2015)
G6300	UpStTrGClN	ClO + NO \rightarrow NO ₂ + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGClN	ClO + NO ₂ \rightarrow ClNO ₃	k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGClN	ClNO ₃ \rightarrow ClO + NO ₂	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGClN	ClNO ₃ + O(³ P) \rightarrow ClO + NO ₃	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGClN	ClNO ₃ + Cl \rightarrow Cl ₂ + NO ₃	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH ₄ \rightarrow HCl + CH ₃	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO \rightarrow HCl + CO + HO ₂	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH ₃ OOH \rightarrow HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH ₃ O ₂ \rightarrow HO ₂ + Cl + HCHO	1.8E-12*EXP(-600./temp)	Burkholder et al. (2015)
G6404	StGCl	CCl ₄ + O(¹ D) \rightarrow LCARBON + ClO + 3 Cl	3.3E-10	Burkholder et al. (2015)
G6405	StGCl	CH ₃ Cl + O(¹ D) \rightarrow 0.1 CH ₃ Cl + 0.1 O(³ P) + 0.46 ClO + 0.35 Cl + 0.09 H + 0.9 LCARBON + 0.09 LCHLORINE	1.65E-10	Burkholder et al. (2015)
G6406	StGCl	CH ₃ Cl + OH \rightarrow LCARBON + H ₂ O + Cl	1.96E-12*EXP(-1200./temp)	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 2 \text{LCARBON} + \text{OH} + 3 \text{Cl}$	3.25E-10	Burkholder et al. (2015)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 2 \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E}-12 \cdot \text{EXP}(-1520./\text{temp})$	Burkholder et al. (2015)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 1.85\text{E}-29, 3.3, 6.0\text{E}-10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})$	8.0e-11	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{LCARBON} + \text{CH}_3 + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 6.1\text{e}-30, 3.0, 2.0\text{e}-10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$8.3\text{E}-11 \cdot \text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
G6413	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{HCl} + \text{HCHO} + \text{NO}_2$	$1.3\text{E}-11 \cdot \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6414	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO} \rightarrow \text{HCl} + \text{HCHO} + \text{NO}$	2.1E-12	Sokolov et al. (1999)
G6415	StTrGCl	$\text{Cl} + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ClO} + .5 \text{CH}_3\text{O} + .5 \text{HCl} + .5 \text{CH}_2\text{OO}$	1.6E-10	Burkholder et al. (2015)
G6416	TrGCCIN	$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{NCCH}_2\text{O}_2 + \text{HCl}$	$1.6\text{E}-11 \cdot \text{EXP}(-2104./\text{temp})$	Tyndall et al. (1996), Tyndall et al. (2001b), Taraborrelli (2016)
G6500	StGClF	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + 2 \text{LFLUORINE} + \text{ClO} + \text{Cl}$	1.4E-10	Burkholder et al. (2015)
G6501	StGClF	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + \text{LFLUORINE} + \text{ClO} + 2 \text{Cl}$	2.3E-10	Burkholder et al. (2015)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E}-11 \cdot \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E}-11 \cdot \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E}-14 \cdot \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E}-12 \cdot \text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E}-12 \cdot \text{EXP}(155./\text{temp})$	Atkinson et al. (2007)
G7203	StGBr	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E}-10 \cdot \text{EXP}(-430./\text{temp})$	Atkinson et al. (2007)
G7204	StTrGBr	$\text{Br}_2 + \text{OH} \rightarrow \text{HOBr} + \text{Br}$	$2.0\text{E}-11 \cdot \text{EXP}(240./\text{temp})$	Atkinson et al. (2007)
G7300	TrGBrN	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.7\text{E}-12 \cdot \text{EXP}(260./\text{temp})$	Atkinson et al. (2007)
G7302	StTrGBrN	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$\text{k_BrO_NO2}/(5.44\text{E}-9 \cdot \text{EXP}(14192./\text{temp}) * 1.\text{E}6 * \text{R_gas} * \text{temp}/(\text{atm}2\text{Pa} * \text{N_A}))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.6\text{E}-12 \cdot \text{EXP}(-1600./\text{temp})$	Kondo and Benson (1984)

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

#	labels	reaction	rate coefficient	reference
G7402	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{CH}_2\text{OO}$	$2.42\text{E-}14 \cdot \text{EXP}(1617./\text{temp})$	Shallcross et al. (2015)
G7403	StTrGBr	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + \text{Br}$	$1.42\text{E-}12 \cdot \text{EXP}(-1150./\text{temp})$	Burkholder et al. (2015)
G7404	TrGBrC	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HBr}$	$2.8\text{E-}13 \cdot \text{EXP}(224./\text{temp}) / (1. + 1.13\text{E}24 \cdot \text{EXP}(-3200./\text{temp}) / \text{C}(\text{ind_O2}))$	Atkinson et al. (2006)*
G7405	TrGBrC	$\text{Br} + \text{CH}_3\text{CHO} \rightarrow \text{HBr} + \text{CH}_3\text{C}(\text{O})$	$1.8\text{E-}11 \cdot \text{EXP}(-460./\text{temp})$	Atkinson et al. (2006)
G7406	TrGBrC	$\text{Br} + \text{C}_2\text{H}_2 \rightarrow \text{LCARBON} + \text{CH}_3\text{O}_2 + \text{HBr}$	$6.35\text{E-}15 \cdot \text{EXP}(440./\text{temp})$	Atkinson et al. (2006)
G7407	TrGBr	$\text{CHBr}_3 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 3 \text{ Br}$	$9.0\text{E-}13 \cdot \text{EXP}(-360./\text{temp})$	Burkholder et al. (2015)*
G7408	TrGBr	$\text{CH}_2\text{Br}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	Burkholder et al. (2015)*
G7600	TrGBrCl	$\text{Br} + \text{BrCl} \rightarrow \text{Br}_2 + \text{Cl}$	$3.32\text{E-}15$	Manion et al. (2015)
G7601	TrGBrCl	$\text{Br} + \text{Cl}_2 \rightarrow \text{BrCl} + \text{Cl}$	$1.10\text{E-}15$	Dolson and Leone (1987)
G7602	TrGBrCl	$\text{Br}_2 + \text{Cl} \rightarrow \text{BrCl} + \text{Br}$	$2.3\text{E-}10 \cdot \text{EXP}(135./\text{temp})$	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$1.6\text{E-}12 \cdot \text{EXP}(430./\text{temp})$	Atkinson et al. (2007)
G7603b	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl} + \text{O}_2$	$2.9\text{E-}12 \cdot \text{EXP}(220./\text{temp})$	Atkinson et al. (2007)
G7603c	StTrGBrCl	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl} + \text{O}_2$	$5.8\text{E-}13 \cdot \text{EXP}(170./\text{temp})$	Atkinson et al. (2007)
G7604	TrGBrCl	$\text{BrCl} + \text{Cl} \rightarrow \text{Br} + \text{Cl}_2$	$1.45\text{E-}11$	Clyne and Cruse (1972)
G7605	TrGBrCl	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{LCARBON} + 2 \text{ LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7606	TrGBrCl	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E-}12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7607	TrGBrCl	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{LCARBON} + \text{LCHLORINE} + \text{H}_2\text{O} + \text{Br}$	$2.1\text{E-}12 \cdot \text{EXP}(-880./\text{temp})$	Burkholder et al. (2015)*
G8100	TrGI	$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	$2.1\text{E-}11 \cdot \text{EXP}(-830./\text{temp})$	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	$\text{IO} + \text{IO} \rightarrow .38 \text{ OIO} + 1.62 \text{ I} + .62 \text{ O}_2$	$5.4\text{E-}11 \cdot \text{EXP}(180./\text{temp})$	Atkinson et al. (2007)*
G8200	TrGI	$\text{I} + \text{HO}_2 \rightarrow \text{HI} + \text{O}_2$	$1.5\text{E-}11 \cdot \text{EXP}(-1090./\text{temp})$	Atkinson et al. (2007)
G8201	TrGI	$\text{IO} + \text{HO}_2 \rightarrow \text{HOI} + \text{O}_2$	$1.4\text{E-}11 \cdot \text{EXP}(540./\text{temp})$	Atkinson et al. (2007)
G8202	TrGI	$\text{HI} + \text{OH} \rightarrow \text{I} + \text{H}_2\text{O}$	$1.6\text{E-}11 \cdot \text{EXP}(440./\text{temp})$	Atkinson et al. (2007)
G8203	TrGI	$\text{OIO} + \text{OH} \rightarrow \text{HIO}_3$	$2.2\text{E-}10 \cdot \text{EXP}(243./\text{temp})$	Plane et al. (2006)
G8204	TrGI	$\text{I}_2 + \text{OH} \rightarrow \text{HOI} + \text{I}$	$2.1\text{E-}10$	Atkinson et al. (2007)
G8300	TrGIN	$\text{I} + \text{NO}_2 \rightarrow \text{INO}_2$	$k_{\text{I_NO2}}$	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)

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

#	labels	reaction	rate coefficient	reference
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	$\text{INO}_2 \rightarrow \text{I} + \text{NO}_2$	$k_{\text{I_NO2}} / (3.7\text{E}-7 \cdot \text{EXP}(9568./\text{temp}) \cdot 1.\text{E}6 \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm}2\text{Pa} \cdot N_{\text{A}}))$	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGIN	$\text{INO}_3 \rightarrow \text{IO} + \text{NO}_2$	0.	see note*
G8307	TrGIN	$\text{I}_2 + \text{NO}_3 \rightarrow \text{I} + \text{INO}_3$	$1.5\text{E}-12$	Atkinson et al. (2007)
G8308	TrGIN	$\text{IO} + \text{NO}_3 \rightarrow \text{OIO} + \text{NO}_2$	$9.\text{E}-12$	Dillon et al. (2008)
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	TrGClI	$\text{IO} + \text{ClO} \rightarrow .2 \text{ICl} + .25 \text{Cl} + .55 \text{OClO} + .8 \text{I} + .45 \text{O}_2$	$4.7\text{E}-12 \cdot \text{EXP}(280./\text{temp})$	Atkinson et al. (2007)
G8700	TrGBrI	$\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br}$	$1.2\text{E}-11$	Burkholder et al. (2015)
G8701	TrGBrI	$\text{IO} + \text{BrO} \rightarrow \text{Br} + .8 \text{OIO} + .2 \text{I} + .2 \text{O}_2$	$1.5\text{E}-11 \cdot \text{EXP}(510./\text{temp})$	Atkinson et al. (2007)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0., 0.6)$	Burkholder et al. (2015)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E}-11 \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	$k_{\text{DMS_OH}}$	Atkinson et al. (2004)*
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E}-13 \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGCS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	$1.\text{E}-10$	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3$	$1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	$3.\text{E}-13$	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5.\text{E}-11$	Barone et al. (1995)
G9408	StTrGS	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	$k_{\text{CH200_S02}}$	Welz et al. (2012), Stone et al. (2014)*
G9409	TrGTerCS	$\text{NOPINOO} + \text{SO}_2 \rightarrow \text{NOPINONE} + \text{H}_2\text{SO}_4$	$7.\text{E}-14$	Rickard and Pascoe (2009)
G9410	TrGTerCS	$\text{APINAOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard and Pascoe (2009)
G9411	TrGTerCS	$\text{APINBOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard and Pascoe (2009)
G9412	TrGTerCS	$\text{MBOOO} + \text{SO}_2 \rightarrow \text{IBUTALOH} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard and Pascoe (2009)
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)
G9700	TrGBrCS	$\text{DMS} + \text{Br} \rightarrow \text{CH}_3\text{SO}_2 + \text{HBr} + \text{HCHO}$	$9.\text{E}-11 \cdot \text{EXP}(-2386./\text{temp})$	Jefferson et al. (1994)
G9701	TrGBrCS	$\text{DMS} + \text{BrO} \rightarrow \text{DMSO} + \text{Br}$	$4.4\text{E}-13$	Ingham et al. (1999)
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)
G10100	TrGHg	$\text{Hg} + \text{O}_3 \rightarrow \text{HgO} + \text{O}_2$	$3.0\text{E}-20$	Hall (1995)
G10200	TrGHg	$\text{Hg} + \text{OH} \rightarrow \text{HgO} + \text{H}$	$3.55\text{E}-14 \cdot \text{EXP}(294./\text{temp})$	Pal and Ariya (2004)

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

#	labels	reaction	rate coefficient	reference
G10201	TrGHg	$\text{Hg} + \text{H}_2\text{O}_2 \rightarrow \text{HgO} + \text{H}_2\text{O}$	8.5E-19	Tokos et al. (1998)*
G10600	TrGClHg	$\text{Hg} + \text{Cl} \rightarrow \text{HgCl}$	1.0E-11	Ariya et al. (2002)
G10601	TrGClHg	$\text{Hg} + \text{Cl}_2 \rightarrow \text{HgCl}_2$	2.6E-18	Ariya et al. (2002)
G10700	TrGBrHg	$\text{Hg} + \text{Br} \rightarrow \text{HgBr}$	3.0E-13	Donohoue et al. (2006)
G10701	TrGBrHg	$\text{HgBr} + \text{Br} \rightarrow \text{HgBr}_2$	$2.5\text{E-}10 * (\text{temp}/298.)^{**(-0.57)}$	Goodsite et al. (2004)
G10702	TrGBrHg	$\text{Hg} + \text{Br}_2 \rightarrow \text{HgBr}_2$	9.0E-17	Ariya et al. (2002)
G10703	TrGBrHg	$\text{Hg} + \text{BrO} \rightarrow \text{HgO} + \text{Br}$	1.0E-15	Raofie and Ariya (2003)
G10704	TrGBrHg	$\text{HgBr} + \text{BrO} \rightarrow \text{BrHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10705	TrGBrClHg	$\text{HgCl} + \text{BrO} \rightarrow \text{ClHgOBr}$	3.0E-12	Calvert and Lindberg (2003)
G10706	TrGBrClHg	$\text{HgBr} + \text{Cl} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)
G10707	TrGBrClHg	$\text{HgCl} + \text{Br} \rightarrow \text{ClHgBr}$	3.0E-12	Calvert and Lindberg (2003)

General notes

Three-body reactions

Rate coefficients for three-body reactions are defined via the function `k_3rd`(T , M , k_0^{300} , n , k_{inf}^{300} , m , f_c). In the code, the temperature T is called `temp` and the concentration of “air molecules” M is called `cair`. Using the auxiliary variables $k_0(T)$, $k_{\text{inf}}(T)$, and k_{ratio} , `k_3rd` is defined as:

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by Wallington et al. (2017) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

RO₂ self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times k_{\text{CH3O2}}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_{CH3O2} = second-order rate coefficient of the self reaction of CH_3O_2 , and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

G1002a: The path leading to $2 \text{O}(^3\text{P}) + \text{O}_2$ results in a null cycle regarding odd oxygen and is neglected.

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

G2117: Converted to $\text{Kc} [\text{molec-1 cm}^3] = \text{Kp} \times \text{R} \times \text{T} / \text{NA}$, where R is $82.05736 [\text{cm}^3 \text{atm K}^{-1} \text{mol}^{-1}]$.

G2118: Assuming fast equilibrium.

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

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

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

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

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

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

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

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

G4116: Same value as for $\text{PAN} + \text{OH}$.

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 RO₂.

G4148: Same value as for NO₂+CH₃O₂.

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of CH₃O₂NO₂.

G4150: Value for CH₃O₂NO₂ + OH, H-abstraction enhanced by the HO-group by f_{soh}.

G4154: Products assumed to be CH₃O₂ + O₂ (could also be HCHO + O₂ + OH).

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

G4160c: The NH + 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, CH₂OO, 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: $k_{\text{CH}_3\text{CO}_3\text{NO}_2} = k_{3\text{rd}}(\text{temp}, \text{cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

G42018: The rate coefficient is the same as for the CH₃ channel in G4107 (CH₃OOH+OH).

G42021: The rate coefficient is $k_{\text{PAN}_M} = k_{\text{CH}_3\text{CO}_3\text{NO}_2}/9.0\text{E-}29*\text{EXP}(-14000./\text{temp})$, 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 HOCH₂CH₂O in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + HO₂.

G42051a: Same as for the CH₃O₂ channel in G4107: CH₃OOH+OH.

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

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

G42074b: Factor of 3 to match the estimate of $k = 1.\text{E-}11$ 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 $k=5.2\text{E-}12$ 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 $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH}$, H-abstraction enhanced by the CH_3CO -group by f_{co} .

G43051c: Products approximated with $\text{C}_2\text{H}_5\text{CHO} + \text{HO}_2$.

G43052: Only major H-abstraction channel considered.

G43059: Products approximated with the major end-product CH_3CHO .

G43060b: Products approximated with the major end-product CH_3CHO .

G43061: Products approximated with the likely end-product CH_3CHO .

G43065: As for HCOCO_3 .

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 $\text{CHCH}(\text{OH})_2$.

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

G43420: $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

G43421: Permutation reaction (minor channels removed).

G44000: The $\text{LC}_4\text{H}_9\text{O}_2$ composition ($n\text{C}_4\text{H}_9\text{O}_2:\text{sC}_4\text{H}_9\text{O}_2$ ratio) is assumed to be equal to the ratio of the production rates at 298K: $k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}) = 0.1273$ and $k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}) = 0.8727$.

G44001b: $\text{sC}_4\text{H}_9\text{O}_2$ products are substituted with 0.636 MEK + 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 $n\text{C}_4\text{H}_9\text{O}_2$ 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: LHMVKABO₂ is $0.12 \text{ HMVKAO}_2 + 0.88 \text{ HMVKBO}_2$.

G44019: LMEKO₂ 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 C₂H₅CHO.

G44097a: Branching ratios according to Rickard et al. (1999). CH₃CHO₂CHO is replaced with its major products CH₃CHO + CO + HO₂.

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: CH₃CHOOA products as from C₃H₆ + O₃ 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 CHCH(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 CHCH(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 CHCH(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 CHCH(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.

G44141: Simplified oxidation.

G44142: Simplified oxidation.

G44202: Alkyl nitrate formation neglected.

G44203a: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G44205: Alkyl nitrate formation neglected.

G44210: Alkyl nitrate formation neglected.

G44221: Same k as for MGLYOX + OH (Tyndall et al., 1995).

G44402: KDEC NC₄DCO₂ → MALANHY + NO₂

G44406c: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44407: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44409: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44410: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44412: KDEC BZFUONOOA → .5 BZFUONOO + .5 CO + .5 CO₂ + .5 HCOCH₂O₂ + .5 OH and BZFUONOO → .625 CO₁₄O₃CO₂H + .375 CO₁₄O₃CHO + .375 H₂O₂

G44421: Only major channel.

G44424: KDEC: GLYOOA → .125 HCHO + .18 GLYOO + 0.82 HO₂ + .57 OH + 1.265 CO + .25 CO₂ and H₂O substitution GLYOO → .625 HCOCO₂H + .375 GLYOX + .375 H₂O₂

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCO₃

G44431: KDEC MALANHYO → HCOCOHCO₃

G44432: Only major channel. KDEC MALANHYO → HCOCOHCO₃

G44436: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂

G44437: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂

G44438: KDEC NBZFUO → .5 CO₁₄O₃CHO + .5 NO₂ + .5 NBZFUONE + .5 HO₂ and RO₂ Only major channel.

G44439: KDEC MALDIALCO₂ → .6 MALANHY + HO₂ + .4 GLYOX + .4 CO + .4 CO₂

G44443: KDEC MECOACETO → CH₃CO₃ + HCHO

G44444: KDEC MECOACETO → CH₃CO₃ + HCHO

G44445: KDEC MECOACETO → CH₃CO₃ + HCHO

G44450: KDEC BZFUO → CO₁₄O₃CHO + HO₂

G44451: KDEC BZFUO → CO₁₄O₃CHO + HO₂

G44452: KDEC BZFUO → CO₁₄O₃CHO + HO₂. Only major channel.

G44457: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2

G44458: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2

G44459: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2. Only major channel.

G44461: KBPAN \rightarrow k.PAN_M

G45019d: Delta-1 and delta-2 LIEPOX are not considered and replaced by beta-LIEPOX formed by ISOP-BOOH and ISOPDOOH.

G45021: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 1.1E-11.

G45037: SAR estimate within uncertainty range of the experimentally determined rate constant by Solberg et al. (1997), 4.2E-11.

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant 4.16E-11.

G45047: Alkyl nitrate formation neglected.

G45055: Alkyl nitrate formation neglected.

G45071: Alkyl nitrate formation neglected.

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 DB2O2 and HOCH2 elimination yielding HVMK and HMAK (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.

G45080: Alkyl nitrate formation neglected.

G45092a: ZCODC23DBCOD = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with NO₃ but only one isomer product considered.

G45095: Alkyl nitrate formation neglected.

G45098: Alkyl nitrate formation neglected.

G45100: Alkyl nitrate formation neglected.

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 (ZCODC23DBCOD) 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: ZCPANC23DBCOD 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 = .67 MBOAO2 + .33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2 \rightarrow MMALANHY + NO2

G45404: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45405: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45406: KDEC NTLFUO \rightarrow ACCOMECHO

G45409: KBPAN \rightarrow k.PAN_M(renaming)

G45413: KFPAN \rightarrow k.CH3CO3_NO2 (renaming)

G45422: KDEC MMALANHYO \rightarrow CO2H3CO3

G45423: KDEC MMALANHYO \rightarrow CO2H3CO3

G45424: KDEC MMALANHYO \rightarrow CO2H3CO3 and Only major channel.

G45429: KBPAN \rightarrow k.PAN_M (renamed)

G45430a: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45431: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45432: KFPAN \rightarrow k.CH3CO3_NO2 (renaming)

G45433: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45434: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2 and only major channel.

G45436: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

G45444: KDEC MC3CODBCO2 \rightarrow .35 GLYOX + .35 CH3 + .35 CO + .35 CO2 + .65 MMALANHY + .65 HO2

G45452: KDEC TLFUONOOA \rightarrow .5 CO + .5 OH + .5 MECOACETO2 + .5 TLFUONOO and H2O subs TLFUONOO \rightarrow .625 C24O3CCO2H + .375 ACCOMECHO + .375 H2O2

G45456: KFPAN \rightarrow k.CH3CO3_NO2 (renaming)

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

G45477: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45478: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

G45479: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

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

G45487: KDEC C5DIALO \rightarrow MALDIAL

G45488: KDEC C5DIALO \rightarrow MALDIAL

G45489: KDEC C5DIALO \rightarrow 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 NDNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2.

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

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

G46416: KDEC NDNPHENO \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 .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

G46462: KDEC PHENO \rightarrow .71 MALDALCO₂H + .71 GLYOX + .29 PBZQONE + HO₂

G46463: KDEC PHENO \rightarrow .71 MALDALCO₂H + .71 GLYOX + .29 PBZQONE + HO₂

G46464: KDEC PHENO \rightarrow .71 MALDALCO₂H + .71 GLYOX + .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 .5 EPXC₄DIAL + .5 GLYOX + .5 HO₂ + .5 C₃DIALO₂ + .5 C₃OH₁₃CO.

G46491b: KDEC BZEMUCO \rightarrow .5 EPXC₄DIAL + .5 GLYOX + .5 HO₂ + .5 C₃DIALO₂ + .5 C₃OH₁₃CO.

G46492: KDEC BZEMUCO \rightarrow .5 EPXC₄DIAL + .5 GLYOX + .5 HO₂ + .5 C₃DIALO₂ + .5 C₃OH₁₃CO

G46493: KDEC BZEMUCO \rightarrow .5 EPXC₄DIAL + .5 GLYOX + .5 HO₂ + .5 C₃DIALO₂ + .5 C₃OH₁₃CO 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 + .5 BZFUONE + .5 BZFUONE

G46524: KDEC BZBIPERO \rightarrow GLYOX + HO₂ + .5 BZFUONE + .5 BZFUONE

G46525: KDEC BZBIPERO \rightarrow GLYOX + HO₂ + .5 BZFUONE + .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 rbipero_{2_oh} is set to 0.40 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

G47408a: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO₂ + .2 ZCODC₂₃DBCOD + .2 C₅DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47408b: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO₂ + .2 ZCODC₂₃DB COD + .2 C₅DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47409: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO₂ + .2 ZCODC₂₃DB COD + .2 C₅DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47410: Only major channel and KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO₂ + .2 ZCODC₂₃DB COD + .2 C₅DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47412: KDEC MGLOOB \rightarrow .125 CH₃CHO + .695 CH₃CO + .57 CO + .57 OH + .125 HO₂ + .18 MGLOO + .25 CO₂

G47413: Merged.

G47418b: Reactions with KRO₂HO₂ and KDEC CRESO \rightarrow .68 C₅CO₁₄OH + .68 GLYOX + HO₂ + .32 PTLQONE.

G47419: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

G47420: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

G47421: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .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 .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47440b: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47441: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

G47442: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .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 MNNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNNCATECO \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 NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

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

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

G47512: KDEC NDNCRESO \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: $\text{KDEC CH}_2\text{OOb} \rightarrow .24 \text{CH}_2\text{OO} + .40 \text{CO} + .36 \text{HO}_2 + .36 \text{CO} + .36 \text{OH}$ and $\text{H}_2\text{O}_{\text{subs}} \text{PHCHOO} \rightarrow .625 \text{PHCOOH} + .375 \text{BENZAL} + .375 \text{H}_2\text{O}_2 + .2 \text{CO}_2$

G48408: $\text{KDEC NSTYRENEO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$

G48409: $\text{KDEC NSTYRENEO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$

G48410: $\text{KDEC NSTYRENEO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$

G48412b: $\text{KDEC STYRENO} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$ and reactions with KRO_2HO_2 .

G48413: $\text{KDEC STYRENO} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$

G48414: $\text{KDEC STYRENO} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$

G48415: $\text{KDEC STYRENO} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$

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 $(3.27\text{E-}11 \cdot 0.21 + 3.25\text{E-}11 \cdot 0.30 + 5.67\text{E-}11 \cdot 0.14)/3$, 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). $\text{LAP-INABO}_2 = .65 \text{APINAO}_2 + .35 \text{APINBO}_2$

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, $(k_{\text{ads}} + k_{\text{adt}}) \cdot \text{acoch}_3 = 6.46\text{E-}11$ where $k_{\text{ads}} = 3.0\text{E-}11$, $k_{\text{adt}} = 5.5\text{E-}11$, $\text{acoch}_3 = 0.76$

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).

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).

G40259: $\text{ROO}_6\text{R}_1\text{OOH}$ is produced but no sink for it.

G40262: $\text{RO}_6\text{R}_1\text{OOH}$ is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

G40267a: Products from Nguyen et al. (2009).

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for $\text{RO}_6\text{R}_1\text{NO}_3$ 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 $O_3 + HCl$. 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 .

G7302: The rate coefficient is: $k_{BrO_NO2} = k_{3rd}(temp, cair, 5.2E-31, 3.2, 6.9E-12, 2.9, 0.6)$.

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

G7404: It is assumed that the reaction liberates all Br atoms in the form of HBr .

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

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

G7605: Same value as for G7408: $CH_2Br_2 + OH$ assumed. It is assumed that the reaction liberates all Br atoms but not Cl . The fate of the carbon atom is currently not considered.

G7606: Same value as for G7408: $CH_2Br_2 + OH$ assumed. It is assumed that the reaction liberates all Br atoms but not Cl . The fate of the carbon atom is currently not considered.

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

G8102: It is assumed that the reaction produces new particles.

G8103: The yield of 38 % OIO is from Atkinson et al. (2007). It is assumed here that the remaining 62 % produce $2 I + O_2$.

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

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

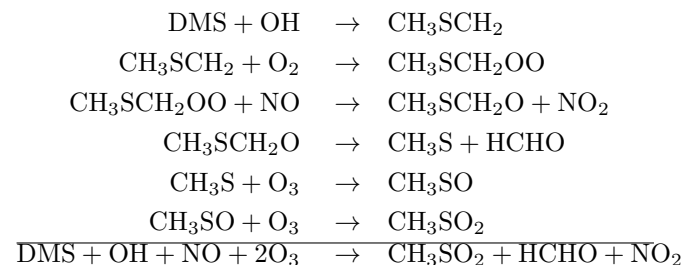
G8306: According to John Plane and John Crowley (pers. comm. 2007), the rate coefficient of $1.1E15 * EXP(-12060./temp)$ suggested by Atkinson et al. (2007) is wrong.

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).

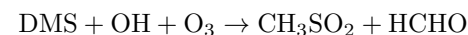
G8402: The products are from Nakano et al. (2005).

G8701: 80% $Br + OIO$ production is from Atkinson et al. (2007). The remaining channels are assumed to produce $Br + I + O_2$.

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



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



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

G9408: Average of $3.9E-11$ and $3.42E-11$.

G10201: Upper limit.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J0001	UpGJ	$O(^3P) \rightarrow O^+ + e^-$	$jx(ip_0p_em) + jx(ip_se_0p_em)$	Fuller-Rowell (1993)
J0002a	UpGJ	$O_2 \rightarrow O_2^+ + e^-$	$jx(ip_02p_em) + jx(ip_se_02_b1)$	Fuller-Rowell (1993)
J0002b	UpGJ	$O_2 \rightarrow O^+ + O(^3P) + e^-$	$jx(ip_0p_0_em) + jx(ip_se_02_b2)$	Fuller-Rowell (1993)
J0003a	UpGJN	$N_2 \rightarrow N_2^+ + e^-$	$jx(ip_N2p_em) + jx(ip_se_N2_b1)$	Fuller-Rowell (1993)
J0003b	UpGJN	$N_2 \rightarrow N^+ + N + e^-$	$jx(ip_Np_N_em) + jx(ip_se_N2_b2)$	Fuller-Rowell (1993)
J0003c	UpGJN	$N_2 \rightarrow N^+ + N(^2D) + e^-$	$jx(ip_Np_N2D_em) + jx(ip_se_N2_b3)$	Fuller-Rowell (1993)
J0003d	UpGJN	$N_2 \rightarrow N + N(^2D)$	$jx(ip_N_N2D_em) + jx(ip_se_N2_b4)$	Fuller-Rowell (1993)
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	$jx(ip_02)$	Sander et al. (2014)
J1000b	UpGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^1D)$	$jx(ip_03P01D)$	Sander et al. (2014)
J1000c	UpGJ	$O_2 + h\nu \rightarrow O_2^+ + e^-$	$jx(ip_02_b1)$	Sander et al. (2014)
J1000d	UpGJ	$O_2 + h\nu \rightarrow O^+ + O(^3P) + e^-$	$jx(ip_02_b2)$	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)
J1002	UpGJ	$O(^3P) + h\nu \rightarrow O^+ + e^-$	$jx(ip_03Pp)$	Sander et al. (2014)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	$jx(ip_H2O)$	Sander et al. (2014)
J2100b	UpGJ	$H_2O + h\nu \rightarrow H_2 + O(^1D)$	$jx(ip_H201D)$	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	$jx(ip_H202)$	Sander et al. (2014)
J3000a	UpGJN	$N_2 + h\nu \rightarrow N_2^+ + e^-$	$jx(ip_N2_b1)$	Sander et al. (2014)
J3000b	UpGJN	$N_2 + h\nu \rightarrow N^+ + N + e^-$	$jx(ip_N2_b2)$	Sander et al. (2014)
J3000c	UpGJN	$N_2 + h\nu \rightarrow N^+ + N(^2D) + e^-$	$jx(ip_N2_b3)$	Sander et al. (2014)
J3000d	UpGJN	$N_2 + h\nu \rightarrow N + N(^2D)$	$jx(ip_NN2D)$	Sander et al. (2014)
J3100	UpStGJN	$N_2O + h\nu \rightarrow O(^1D) + N_2$	$jx(ip_N2O)$	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	$jx(ip_NO2)$	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow N + O(^3P)$	$jx(ip_NO)$	Sander et al. (2014)
J3102b	UpGJN	$NO + h\nu \rightarrow NO^+ + e^-$	$jx(ip_NOp)$	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	$jx(ip_NO2O)$	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	$jx(ip_NO02)$	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	$jx(ip_N2O5)$	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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41002	StGJ	$\text{CO}_2 + h\nu \rightarrow \text{CO} + \text{O}(^3\text{P})$	jx(ip_CO2)	Sander et al. (2014)
J41003	StGJ	$\text{CH}_4 + h\nu \rightarrow .42 \text{CH}_3 + .42 \text{H} + .6912 \text{H}_2 + .0864 \text{HCHO} + .0864 \text{O}(^3\text{P}) + .1584 \text{OH} + .1584 \text{HO}_2 + .2112 \text{CO}_2 + .1824 \text{CO} + .024 \text{H}_2\text{O} + .10 \text{LCARBON}$	jx(ip_CH4)	Sander et al. (2014)*
J41004	StTrGJN	$\text{CH}_3\text{ONO} + h\nu \rightarrow \text{CH}_3\text{O} + \text{NO}$	jx(ip_CH3ON0)	Sander et al. (2014)
J41005	StTrGJN	$\text{CH}_3\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	jx(ip_CH3NO3)	Sander et al. (2014)
J41006	StTrGJN	$\text{CH}_3\text{O}_2\text{NO}_2 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{CH}_3\text{O}_2 + .333 \text{NO}_3 + .333 \text{CH}_3\text{O}$	jx(ip_CH3O2N02)	Sander et al. (2014)*
J41007	StTrGJ	$\text{HOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOOH} + \text{OH} + \text{HO}_2$	jx(ip_CH300H)	Sander et al. (2014)
J41008	StTrGJ	$\text{CH}_3\text{O}_2 + h\nu \rightarrow \text{HCHO} + \text{OH}$	jx(ip_CH302)	Sander et al. (2014)
J41009	StTrGJ	$\text{HCOOH} + h\nu \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	jx(ip_HCOOH)	Sander et al. (2014)
J41010	StTrGJN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{HOCH}_2\text{O}_2 + .333 \text{NO}_3 + .333 \text{HCOOH} + .333 \text{HO}_2$	jx(ip_CH3O2N02)	Sander et al. (2014)
J42000	TrGJC	$\text{C}_2\text{H}_5\text{OOH} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	von Kuhlmann (2001)
J42001a	TrGJC	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_3 + \text{HO}_2 + \text{CO}$	jx(ip_CH3CHO)	Sander et al. (2014)
J42001b	TrGJC	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHOH}$	jx(ip_CH3CHO2VINY)	Clubb et al. (2012)
J42002	TrGJC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + h\nu \rightarrow \text{CH}_3 + \text{OH} + \text{CO}_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J42004	TrGJCN	$\text{PAN} + h\nu \rightarrow .7 \text{CH}_3\text{C}(\text{O}) + .7 \text{NO}_2 + .3 \text{CH}_3 + .3 \text{CO}_2 + .3 \text{NO}_3$	jx(ip_PAN)	Sander et al. (2014)*
J42005a	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{HCHO} + 2 \text{HO}_2 + \text{CO}$	jx(ip_HOCH2CHO)*0.83	Sander et al. (2014)*
J42005b	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCOCH}_2\text{O}_2$	jx(ip_HOCH2CHO)*0.07	Sander et al. (2014)*
J42005c	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{CH}_3\text{OH} + \text{CO}$	jx(ip_HOCH2CHO)*0.10	Sander et al. (2014)*
J42006	TrGJC	$\text{HOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J42007	TrGJCN	$\text{PHAN} + h\nu \rightarrow .7 \text{HOCH}_2\text{CO} + .7 \text{NO}_2 + .3 \text{HCHO} + .3 \text{HO}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	jx(ip_PAN)	see note*
J42008	TrGJC	$\text{GLYOX} + h\nu \rightarrow 2 \text{CO} + 2 \text{HO}_2$	jx(ip_GLYOX)	Sander et al. (2014)
J42009	TrGJC	$\text{HCOCO}_2\text{H} + h\nu \rightarrow 2 \text{HO}_2 + \text{CO} + \text{CO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J42010	TrGJC	$\text{HCOCO}_3\text{H} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J42011	TrGJC	$\text{HYETHO}_2\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J42012	TrGJCN	$\text{ETHOHNO}_3 + h\nu \rightarrow \text{HO}_2 + 2 \text{HCHO} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)
J42013	TrGJC	$\text{HOOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	2*jx(ip_CH300H)	Taraborrelli (2016)
J42014	TrGC	$\text{HOOCH}_2\text{CO}_2\text{H} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2$	jx(ip_CH300H)	Taraborrelli (2016)
J42015	TrGC	$\text{CH}_2\text{CO} + h\nu \rightarrow .4 \text{CO}_2 + .8 \text{H} + .34 \text{CO} + .34 \text{OH} + .34 \text{HO}_2 + .16 \text{HCHO} + .16 \text{O}(^3\text{P}) + .1 \text{HCOOH} + \text{CO}$	J_ketene* 0.36	Taraborrelli (2016)
J42016	TrGC	$\text{CH}_3\text{CHOHOHOOH} + h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42017	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	$(\text{jx}(\text{ip_C2H5N03}) + \text{jx}(\text{ip_CH3CHO}))$ $\cdot (\text{jx}(\text{ip_NOA}) + 1\text{E-10}) / (0.59 \cdot \text{J_}$ $\text{IC3H7N03} + \text{jx}(\text{ip_CH3COCH3}) + 1\text{E-10})$	Taraborrelli (2016)*
J42018	TrGJC	$\text{HOOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Taraborrelli (2016)
J42019	TrGJCN	$\text{C}_2\text{H}_5\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{jx}(\text{ip_C2H5N03})$	Taraborrelli (2016)
J42020	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow .7 \text{ NO}_3\text{CH}_2\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ HCHO} +$ $.3 \text{ NO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Taraborrelli (2016)*
J42021	StTrGJCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + h\nu \rightarrow .667 \text{ NO}_2 + .667 \text{ C}_2\text{H}_5\text{O}_2 + .333 \text{ NO}_3 +$ $.333 \text{ CH}_3\text{CHO} + .333 \text{ HO}_2$	$\text{jx}(\text{ip_CH302N02})$	Taraborrelli (2016)*
J43000	TrGJC	$\text{iC}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43001	TrGJC	$\text{CH}_3\text{COCH}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CH}_3$	$\text{jx}(\text{ip_CH3C0CH3})$	Sander et al. (2014)
J43002	TrGJC	$\text{CH}_3\text{COCH}_2\text{OH} + h\nu \rightarrow .5 \text{ CH}_3\text{C}(\text{O}) + .5 \text{ HCHO} + .5 \text{ HO}_2 + .5$ $\text{HOCH}_2\text{CO} + .5 \text{ CH}_3$	J_ACETOL	Sander et al. (2014)*
J43003	TrGJC	$\text{MGLYOX} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2014)
J43004	TrGJC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Rickard and Pascoe (2009)
J43005	TrGJC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Taraborrelli (2016)
J43006	TrGJCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	J_IC3H7N03	von Kuhlmann et al. (2003)*
J43007	TrGJCN	$\text{NOA} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	$\text{jx}(\text{ip_NOA})$	Barnes et al. (1993)
J43009	TrGJC	$\text{HYPROPO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J43010	TrGJCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J43011	TrGJC	$\text{HOCH}_2\text{COCHO} + h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J43012	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{J_ACETOL}$	Taraborrelli (2016)
J43013	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Taraborrelli (2016)
J43014	TrGJTerC	$\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) \cdot 2.$	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	$\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$	$2 \cdot \text{jx}(\text{ip_MGLYOX})$	Taraborrelli (2016)
J43018	TrGJC	$\text{CH}_3\text{COCO}_2\text{H} + h\nu \rightarrow .32 \text{ CH}_3\text{CHO} + .16 \text{ CH}_2\text{CHOH} + .54 \text{ CO}_2$ $+ .38 \text{ CH}_3\text{C}(\text{O}) + .38 \text{ HO}_2 + .38 \text{ CO}_2 + .07 \text{ CH}_3\text{COOH} + .07$ $\text{CO} + .05 \text{ CH}_3\text{C}(\text{O}) + .05 \text{ CO} + .05 \text{ OH}$	$\text{JX}(\text{IP_CH3C0C02H})$	Taraborrelli (2016)*
J43019	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{CO}_2$	$\text{JX}(\text{IP_MGLYOX}) + \text{jx}(\text{ip_CH300H})$	Taraborrelli (2016)
J43020	TrGC	$\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{J_ketene} \cdot 0.36 \cdot 2.$	Taraborrelli (2016)
J43021	TrGCN	$\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7N03	Taraborrelli (2016)
J43022	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$	$\text{jx}(\text{ip_CH302N02}) + \text{jx}(\text{ip_CH3C0CH3})$	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43023	TrGJC	$C_3H_7OOH + h\nu \rightarrow C_2H_5CHO + HO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J43024	TrGJCN	$C_3H_7ONO_2 + h\nu \rightarrow C_2H_5CHO + NO_2 + HO_2$	0.59*J_IC3H7N03	see note*
J43025a	TrGJC	$C_2H_5CHO + h\nu \rightarrow C_2H_5O_2 + HO_2 + CO$	jx(ip_C2H5CH02HC0)	see note*
J43025b	TrGJC	$C_2H_5CHO + h\nu \rightarrow CH_2CHCH_2OH$	jx(ip_C2H5CH02EN0L)	Andrews et al. (2012), Taraborrelli (2016)*
J43026	TrGJCN	$PPN + h\nu \rightarrow .7 C_2H_5CO_3 + .7 NO_2 + .3 C_2H_5O_2 + .3 CO_2 + .3 NO_3$	jx(ip_PAN)	Sander et al. (2014)
J43027	TrGJC	$C_2H_5CO_3H + h\nu \rightarrow C_2H_5O_2 + CO_2 + OH$	jx(ip_CH300H)	von Kuhlmann (2001)
J43028a	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HOOCH_2CO_3 + CO + HO_2$	jx(ip_MGLY0X)	Taraborrelli (2016)
J43028b	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HCOCO + HCHO + OH$	jx(ip_H0CH2CH0)+jx(ip_CH300H)	Taraborrelli (2016)
J43200	TrGJTerC	$HCOCH_2CO_3H + h\nu \rightarrow HCOCH_2O_2 + CO_2 + OH$	jx(ip_H0CH2CH0)+jx(ip_CH300H)	Rickard and Pascoe (2009)
J43400	TrGJAroC	$C3DIALOOH + h\nu \rightarrow GLYOX + CO + HO_2 + OH$	jx(ip_H0CH2CH0)*2+jx(ip_CH300H)	Rickard and Pascoe (2009)*
J43401	TrGJAroC	$C32OH13CO + h\nu \rightarrow GLYOX + HO_2 + HO_2 + CO$	jx(ip_H0CH2CH0)*2	Rickard and Pascoe (2009)
J43402	TrGJAroC	$HCOCOCH_2CO_3H + h\nu \rightarrow GLYOX + HO_2 + CO_2 + OH$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44000a	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + C_3H_7CHO + HO_2$	jx(ip_CH300H)*(k_p/(k_p+k_s))	Rickard and Pascoe (2009), Taraborrelli (2016)
J44000b	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 C_2H_5O_2$	jx(ip_CH300H)*(k_s/(k_p+k_s))	Rickard and Pascoe (2009), Taraborrelli (2016)
J44001	TrGJC	$MVK + h\nu \rightarrow .5 C_3H_6 + .5 CH_3C(O) + .5 HCHO + CO + .5 HO_2$	jx(ip_MVK)	Sander et al. (2014)
J44002	TrGJC	$MEK + h\nu \rightarrow CH_3C(O) + C_2H_5O_2$	0.42*jx(ip_CH0H)	von Kuhlmann et al. (2003)
J44003	TrGJC	$LMEKOOH + h\nu \rightarrow .62 CH_3C(O) + .62 CH_3CHO + .38 HCHO + .38 CO_2 + .38 HOCH_2CH_2O_2 + OH$	jx(ip_CH300H)+0.42*jx(ip_CH0H)	Taraborrelli (2016)
J44004	TrGJC	$BIACET + h\nu \rightarrow 2 CH_3C(O)$	2.15*jx(ip_MGLY0X)	see note*
J44005a	TrGJCN	$LC4H9NO_3 + h\nu \rightarrow NO_2 + C_3H_7CHO + HO_2$	J_IC3H7N03*(k_p/(k_p+k_s))	see note*
J44005b	TrGJCN	$LC4H9NO_3 + h\nu \rightarrow NO_2 + MEK + HO_2$	J_IC3H7N03*(k_s/(k_p+k_s))	see note*
J44006	TrGJCN	$MPAN + h\nu \rightarrow .7 MACO_3 + .7 NO_2 + .3 MACO_2 + .3 NO_3$	jx(ip_PAN)	see note*
J44007a	TrGJC	$CO_2H_3CO_3H + h\nu \rightarrow MGLYOX + HO_2 + OH + CO_2$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44007b	TrGJC	$CO_2H_3CO_3H + h\nu \rightarrow CH_3C(O) + HO_2 + HCOCO_3H$	J_ACET0L	Rickard and Pascoe (2009)
J44008	TrGJC	$MACR + h\nu \rightarrow .5 MACO_3 + .5 CH_3C(O) + .5 HCHO + .5 CO + HO_2$	jx(ip_MACR)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44009	TrGJC	MACROOH + $h\nu$ → MACRO + OH	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)	Taraborrelli (2016)*
J44010	TrGJC	MACROH + $h\nu$ → CH ₃ COCH ₂ OH + CO + HO ₂ + HO ₂	2.77*jx(ip_HOCH2CHO)	see note*
J44011	TrGJC	MACO3H + $h\nu$ → MACO2 + OH	jx(ip_CH300H)	Taraborrelli (2016)
J44012	TrGJC	LHMKABOOH + $h\nu$ → .12 MGLYOX + .12 HO ₂ + .88 CH ₃ C(O) + .88 HOCH ₂ CHO + .12 HCHO + OH	jx(ip_CH300H)+J_ACETOL	Taraborrelli (2016)
J44013	TrGJC	CO2H3CHO + $h\nu$ → MGLYOX + CO + HO ₂ + HO ₂	jx(ip_HOCH2CHO)+J_ACETOL	Taraborrelli (2016)
J44014	TrGJC	HO12CO3C4 + $h\nu$ → CH ₃ C(O) + HOCH ₂ CHO + HO ₂	J_ACETOL	Rickard and Pascoe (2009)
J44015	TrGJC	BIACETOH + $h\nu$ → CH ₃ C(O) + HOCH ₂ CO	2.15*jx(ip_MGLYOX)	see note*
J44016	TrGC	HCOCCH ₃ CO + $h\nu$ → .5 OH + .5 CH ₃ CHO + CO + .5 CH ₃ CHCO + .5 CO	J_KETENE	Taraborrelli (2016)
J44017a	TrGC	CH ₃ COCHCO + $h\nu$ → .0192 CH ₃ COCO ₂ H + .1848 H ₂ O ₂ + .2208 MGLYOX + .36 OH + .36 CO + .56 CH ₃ C(O) + .2 CH ₃ CHO + .2 CO ₂ + .2 HCHO + .2 HO ₂ + CO	J_KETENE*0.5	Taraborrelli (2016),Rickard and Pascoe (2009)*
J44017b	TrGC	CH ₃ COCHCO + $h\nu$ → CH ₃ CHCO + CO	J_KETENE*0.5	Taraborrelli (2016)
J44018a	TrGJC	CH ₃ COCOCHO + $h\nu$ → CH ₃ C(O) + 2 CO + HO ₂	jx(ip_MGLYOX)	Taraborrelli (2016)
J44018b	TrGJC	CH ₃ COCOCHO + $h\nu$ → HCOCO + CH ₃ C(O)	2.15*jx(ip_MGLYOX)	Taraborrelli (2016)
J44019	TrGJC	CH ₃ COCOCO2H + $h\nu$ → CH ₃ C(O) + CO + CO ₂ + HO ₂	3.15*jx(ip_MGLYOX)	Taraborrelli (2016)
J44020a	TrGJTerC	CH ₃ COCOCH ₂ OOH + $h\nu$ → CH ₃ C(O) + OH + HCHO + CO	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J44020b	TrGJTerC	CH ₃ COCOCH ₂ OOH + $h\nu$ → CH ₃ C(O) + HCOCO	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44021	TrGJTerC	C44OOH + $h\nu$ → HCOCH ₂ CHO + CO ₂ + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44022	TrGJTerC	C413COOOH + $h\nu$ → HCOCH ₂ CO3 + HCHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)
J44023a	TrGJTerC	C4CODIAL + $h\nu$ → HCOCOCH ₂ O ₂ + HO ₂ + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44023b	TrGJTerC	C4CODIAL + $h\nu$ → HCOCH ₂ CO3 + HO ₂ + CO	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44024	TrGJTerC	C312COCO3H + $h\nu$ → HCOCOCH ₂ O ₂ + CO ₂ + OH	jx(ip_CH300H)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44025	TrGJCN	LMEKNO3 + $h\nu$ → .62 CH ₃ C(O) + .62 CH ₃ CHO + .38 HCHO + .38 CO ₂ + .38 HOCH ₂ CH ₂ O ₂ + NO ₂	jx(ip_MEKN03)	Barnes et al. (1993), Taraborrelli (2016)*
J44026	TrGJCN	MVKNO3 + $h\nu$ → CH ₃ C(O) + HOCH ₂ CHO + NO ₂	jx(ip_MEKN03)	Barnes et al. (1993), Taraborrelli (2016)*
J44027	TrGJCN	MACRN + $h\nu$ → CH ₃ COCH ₂ OH + 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), Taraborrelli (2016)*
J44028	TrGJCN	TC4H9NO3 + $h\nu$ → CH ₃ COCH ₃ + CH ₃ + NO ₂	2.84*J_IC3H7N03	Taraborrelli (2016)
J44029	TrGJC	TC ₄ H ₉ OOH + $h\nu$ → CH ₃ COCH ₃ + CH ₃ + OH	jx(ip_CH300H)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44030	TrGJCN	$\text{IBUTOLBNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 \cdot \text{J_IC3H7N03}$	Taraborrelli (2016)
J44031	TrGJC	$\text{IBUTOLBOOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J44032	TrGJC	$\text{LBUT1ENOOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J44033	TrGJCN	$\text{LBUT1ENNO}_3 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7N03	Taraborrelli (2016)
J44034	TrGJC	$\text{BUT2OLOOH} + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J44035	TrGJCN	$\text{BUT2OLNO}_3 + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	J_IC3H7N03	Taraborrelli (2016)
J44036	TrGJC	$\text{BUT2OLO} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HOCH}_2\text{CO}$	J_ACETOL	Taraborrelli (2016)
J44037a	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx(ip_C3H7CHO2HCO)}$	Taraborrelli (2016)
J44037b	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{CHOH}$	$\text{jx(ip_C3H7CHO2VINY)}$	Taraborrelli (2016)*
J44038	TrGJC	$\text{IPRCHO} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	jx(ip_IPRCHO2HCO)	Taraborrelli (2016)
J44039	TrGJCN	$\text{IC4H9NO}_3 + h\nu \rightarrow \text{IPRCHO} + \text{NO}_2$	J_IC3H7N03	Taraborrelli (2016)
J44040	TrGJC	$\text{IC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{IPRCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J44041	TrGJC	$\text{PERIBUACID} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J44042	TrGJCN	$\text{PIP}_N + h\nu \rightarrow .7 \text{IPRCO}_3 + .7 \text{NO}_2 + .3 \text{iC}_3\text{H}_7\text{O}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	jx(ip_PAN)	Taraborrelli (2016), Sander et al. (2014)
J44043	TrGJC	$\text{HVMK} + h\nu \rightarrow \text{MGlyOX} + \text{CO} + 2 \text{OH}$	jx(ip_PeDI0NE24)	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	$\text{HMAC} + h\nu \rightarrow \text{HCOCCH}_3\text{CO} + 2 \text{OH}$	jx(ip_PeDI0NE24)	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx(ip_C2H5CHO2HCO)}$	Rickard and Pascoe (2009)
J44045b	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$	$\text{jx(ip_C2H5CHO2ENOL)}$	Andrews et al. (2012), Taraborrelli (2016)
J44046a	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{jx(ip_C2H5CHO2HCO)} \cdot 2.$	see note*
J44046b	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$	$\text{jx(ip_C2H5CHO2ENOL)} \cdot 2.$	Andrews et al. (2012), Taraborrelli (2016)
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	$\text{IPRHOCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44400a	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{C}_3\text{O}_2\text{H}_{13}\text{CO} + \text{CO} + \text{OH} + \text{HO}_2$	$\text{jx(ip_HOCH2CHO)} \cdot 2$	Rickard and Pascoe (2009)
J44400b	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44401	TrGJAroC	BZFUOOH + $h\nu$ → CO14O3CHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44402	TrGJAroC	HOCOC4DIAL + $h\nu$ → HCOCO3HCO3 + HO ₂ + CO	jx(ip_MGLY0X)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44403	TrGJAroCN	NBZFUOOH + $h\nu$ → .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	MALDALCO3H + $h\nu$ → HCOCO ₃ H + HO ₂ + CO + HO ₂ + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J44404b	TrGJAroC	MALDALCO3H + $h\nu$ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44405	TrGJAroC	EPXDLCO2H + $h\nu$ → C3DIALO2 + CO ₂ + HO ₂	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44406	TrGJAroC	MALDIAL + $h\nu$ → .4 BZFUONE + .6 MALDIALCO3 + .6 HO ₂	jx(ip_NO2)*0.14	Rickard and Pascoe (2009)
J44407	TrGJAroC	MALANHYOOH + $h\nu$ → HCOCO3HCO3 + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J44408	TrGJAroC	EPXDLCO3H + $h\nu$ → C3DIALO2 + OH + CO ₂	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44409	TrGJAroC	CO2C4DIAL + $h\nu$ → CO + CO + HO ₂ + HO ₂ + CO + CO	jx(ip_MGLY0X)*2	Rickard and Pascoe (2009)
J44410	TrGJAroC	MALDALCO2H + $h\nu$ → HCOCO ₂ H + HO ₂ + CO + HO ₂ + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J44411	TrGJAroC	EPXC4DIAL + $h\nu$ → C3DIALO2 + CO + HO ₂	2.77*jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J44412	TrGJAroC	CO14O3CHO + $h\nu$ → HO ₂ + CO + HCOCH ₂ O ₂ + CO ₂	jx(ip_MGLY0X)	Rickard and Pascoe (2009)
J44414	TrGJAroC	MECOACEOOH + $h\nu$ → CH ₃ C(O) + HCHO + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45002	TrGJC	LISOPACOOH + $h\nu$ → LISOPACO + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45003	TrGJCN	LISOPACNO3 + $h\nu$ → LISOPACO + NO ₂	0.59*J_IC3H7N03	see note*
J45004	TrGJC	ISOPBOOH + $h\nu$ → MVK + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45005	TrGJCN	ISOPBNO3 + $h\nu$ → MVK + HCHO + HO ₂ + NO ₂	2.84*J_IC3H7N03	see note*
J45006	TrGJC	ISOPDOOH + $h\nu$ → MACR + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45007	TrGJCN	ISOPDNO3 + $h\nu$ → 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 + $h\nu$ → LHC4ACCO3 + 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), Taraborrelli (2016)*
J45010	TrGJCN	LNISOOH + $h\nu$ → NOA + OH + .5 HOCHCHO + .5 CO + .5 HO ₂ + .5 CO ₂	jx(ip_CH300H)	Taraborrelli et al. (2009), Taraborrelli (2016)
J45011	TrGJC	LHC4ACCHO + $h\nu$ → .5 LHC4ACCO3 + .5 HO ₂ + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2	jx(ip_MACR)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45012	TrGJC	$\text{LC578OOH} + h\nu \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 2.77 * \text{jx}(\text{ip_HOCH2CHO})$	Taraborrelli (2016)
J45013	TrGJC	$\text{LHC4ACCO3H} + h\nu \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{OH} + \text{CO}_2$	J_HPALD	Taraborrelli (2016)
J45014	TrGJCN	$\text{LC5PAN1719} + h\nu \rightarrow .7 \text{ LHC4ACCO3} + .7 \text{ NO}_2 + .15 \text{ MACRO2} + .15 \text{ LHMVKABO2} + .3 \text{ CO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Taraborrelli (2016)
J45015	TrGJC	$\text{HCOC5} + h\nu \rightarrow .65 \text{ CH}_3 + .65 \text{ CO} + .65 \text{ HCHO} + .35 \text{ OH} + .35 \text{ CH}_3\text{COCH}_2\text{O}_2 + \text{HOCH2CO}$	$0.5 * \text{jx}(\text{ip_MVK})$	Taraborrelli (2016)*
J45016	TrGJC	$\text{C59OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH2CO} + \text{OH}$	$\text{J_ACETOL} + \text{jx}(\text{ip_CH300H})$	Taraborrelli (2016)
J45017	TrGJTerC	$\text{C511OOH} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCH2CHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J45018a	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J45018b	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCH2CO3}$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J45019	TrGJTerC	$\text{CO23C4CO3H} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J45020	TrGJTerC	$\text{C512OOH} + h\nu \rightarrow \text{C513O2} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J45021	TrGJTerC	$\text{CO13C4CHO} + h\nu \rightarrow \text{CHOC3COO2} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard and Pascoe (2009)
J45022	TrGJTerC	$\text{C513OOH} + h\nu \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J45023	TrGJTerC	$\text{C513CO} + h\nu \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 + \text{CO} + \text{CO}$	$\text{jx}(\text{ip_MGLYOX}) + 2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J45024	TrGJTerC	$\text{C514OOH} + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard and Pascoe (2009)
J45025	TrGJTerCN	$\text{C514NO3} + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	$\text{J_IC3H7N03} + \text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard and Pascoe (2009)
J45026a	TrGJC	$\text{ZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HVMK} + \text{OH}$	$\text{J_HPALD} * 0.6 * 0.5$	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	$\text{ZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CH}_3\text{C(O)} + \text{HOCH}_2\text{CHO}$	$\text{J_HPALD} * 0.6 * 0.5$	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	$\text{ZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HMAC} + \text{OH}$	$\text{J_HPALD} * 0.4 * 0.5$	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	$\text{ZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2$	$\text{J_HPALD} * 0.4 * 0.5$	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	$\text{ZCO3HC23DBCOD} + h\nu \rightarrow .62 \text{ EZCH3CO2CHCHO} + .38 \text{ EZCHOCCH3CHO2} + \text{OH} + \text{CO}_2$	J_HPALD	Taraborrelli (2016)
J45028a	TrGJC	$\text{C10OHC2OOHC4OD} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} + 2 \text{ CO} + \text{HO}_2$	$2.77 * \text{JX}(\text{IP_HOCH2CHO})$	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45028b	TrGJC	$\text{C1OOHC2OOHC4OD} + h\nu \rightarrow .5 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .5 \text{ HOCHCHO} + .5 \text{ CO}_2\text{H}_3\text{CHO} + .5 \text{ HCHO} + 1.5 \text{ OH}$	$2.*\text{JX}(\text{IP_CH300H})$	Taraborrelli (2016)
J45029	TrGC	$\text{DB1OOH} + h\nu \rightarrow \text{DB1O}_2 + \text{OH}$	$\text{JX}(\text{IP_CH300H})$	Taraborrelli (2016)
J45030	TrGC	$\text{DB2OOH} + h\nu \rightarrow .48 \text{ CH}_3\text{COCH}_2\text{OH} + .52 \text{ HOCH}_2\text{CHO} + .52 \text{ MGLYOX} + .48 \text{ GLYOX} + \text{HO}_2 + \text{OH}$	$\text{JX}(\text{ip_CH300H})$	Taraborrelli (2016)
J45031a	TrGJC	$\text{C1ODC2OOHC4OD} + h\nu \rightarrow \text{MGLYOX} + \text{HOCHCHO} + \text{OH}$	$\text{JX}(\text{ip_CH300H})$	Taraborrelli (2016)
J45031b	TrGJC	$\text{C1ODC2OOHC4OD} + h\nu \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$2.*2.77*\text{JX}(\text{IP_HOCH}_2\text{CHO})$	Taraborrelli (2016)
J45032	TrGJC	$\text{ZCODC23DBCOD} + h\nu \rightarrow .5 \text{ CH}_3\text{COCHCO} + .5 \text{ HCOCCH}_3\text{CO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_N02})*0.1*0.5$	Taraborrelli (2016)*
J45033	TrGCN	$\text{DB1NO}_3 + h\nu \rightarrow \text{DB1O}_2 + \text{NO}_2$	J_IC3H7N03	Taraborrelli (2016)
J45034	TrGJTerC	$\text{CHOC3COOOH} + h\nu \rightarrow \text{CHOC3COO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})+\text{jx}(\text{ip_HOCH}_2\text{CHO})+\text{J_ACETOL}$	Rickard and Pascoe (2009)
J45200a	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})*.67$	Rickard and Pascoe (2009), Taraborrelli (2016)
J45200b	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})*.33$	Rickard and Pascoe (2009), Taraborrelli (2016)
J45201	TrGJTerC	$\text{MBOACO} + h\nu \rightarrow \text{HCHO} + \text{HO}_2 + \text{IPRHOCO}_3$	J_ACETOL	Rickard and Pascoe (2009)
J45202	TrGJTerC	$\text{MBOCOCO} + h\nu \rightarrow \text{CO} + \text{HO}_2 + \text{IPRHOCO}_3$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J45203a	TrGJTerCN	$\text{LNMBOABOOH} + h\nu \rightarrow \text{NO}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})*.65$	Rickard and Pascoe (2009), Taraborrelli (2016)
J45203b	TrGJTerCN	$\text{LNMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})*.35$	Rickard and Pascoe (2009), Taraborrelli (2016)
J45204	TrGJTerCN	$\text{NC4OHCO}_3\text{H} + h\nu \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45400	TrGJAroC	$\text{C54CO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{CO} + \text{CO} + \text{CH}_3\text{C}(\text{O})$	$\text{jx}(\text{ip_MGLYOX})+2.15*\text{jx}(\text{ip_MGLYOX})*2$	Rickard and Pascoe (2009)
J45401	TrGJAroC	$\text{C5134CO}_2\text{OH} + h\nu \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH}_2\text{CHO})+2.15*\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J45402	TrGJAroC	$\text{C5DIALOOH} + h\nu \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})+\text{jx}(\text{ip_MACR})$	Rickard and Pascoe (2009)*
J45406	TrGJAroC	$\text{C5CO14OH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MVK})$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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	MMALNHOOH + $h\nu$ → 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)
J46402	TrGJAroC	C5CO2DCO3H + $h\nu$ → CH ₃ C(O) + HCOCOCHO + CO ₂ + OH	jx(ip_CH300H)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46403	TrGJAroCN	NDNPHENOOH + $h\nu$ → NC4DCO2H + HNO ₃ + CO + CO + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	BZBIPERNO3 + $h\nu$ → GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE + NO ₂	J_IC3H7N03	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	HOC6H4NO2 + $h\nu$ → HONO + CPDKETENE	jx(ip_HOC6H4NO2)	Chen et al. (2011)*
J46406	TrGJAroC	CPDKETENE + $h\nu$ → CO ₂ + CO + 2 HO ₂ + MALDIAL	J_KETENE	see note*
J46407	TrGJAroC	C5COOHCO3H + $h\nu$ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46408	TrGJAroC	BZEPOXMUC + $h\nu$ → .5 C5DIALO2 + 1.5 HO ₂ + 1.5 CO + .5 MALDIAL	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46409	TrGJAroCN	NPHEN1OOH + $h\nu$ → NPHEN1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46410	TrGJAroC	BZEMUCCO + $h\nu$ → HCOCO ₂ HCO ₃ + C3DIALO ₂	jx(ip_HOCH ₂ CHO)*2+J_ACETOL	Rickard and Pascoe (2009)
J46411	TrGJAroC	BZEMUCCO ₂ H + $h\nu$ → C5DIALO ₂ + CO ₂ + HO ₂	jx(ip_MACR)	Rickard and Pascoe (2009)
J46412	TrGJAroCN	NNCATECOOH + $h\nu$ → NC4DCO ₂ H + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46413	TrGJAroC	C615CO ₂ OOH + $h\nu$ → C5DICARB + CO + HO ₂ + OH	jx(ip_MVK)+jx(ip_CH300H)	Rickard and Pascoe (2009)
J46414	TrGJAroCN	NPHENOOH + $h\nu$ → MALDALCO ₂ H + GLYOX + OH + NO ₂	J_IC3H7N03 + jx(ip_CH300H)	Rickard and Pascoe (2009)
J46415	TrGJAroCN	NCATECOOH + $h\nu$ → NC4DCO ₂ H + HCOCO ₂ H + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46416	TrGJAroC	PBZQOOH + $h\nu$ → C5CO ₂ OHCO ₃ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46417	TrGJAroC	BZOBIPEROH + $h\nu$ → MALDIALCO ₃ + GLYOX + HO ₂	J_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	BZBIPEROOH + $h\nu$ → GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	NBZQOOH + $h\nu$ → C6CO ₄ DB + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46420	TrGJAroC	CATEC1OOH + $h\nu$ → CATEC1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46421	TrGJAroC	C6125CO + $h\nu$ → C5CO ₁₄ O ₂ + CO + HO ₂	jx(ip_MGLYOX)+jx(ip_MVK)	Rickard and Pascoe (2009)
J46422	TrGJAroCN	DNPHENOOH + $h\nu$ → NC4DCO ₂ H + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46423	TrGJAroC	BZEMUCCO ₃ H + $h\nu$ → C5DIALO ₂ + CO ₂ + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46424	TrGJAroC	C6H ₅ OOH + $h\nu$ → C6H ₅ O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46425	TrGJAroC	BZEMUCOOH + $h\nu$ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO ₂ + .5 C32OH13CO + OH	jx(ip_CH300H)+jx(ip_HOCH ₂ CHO)*2	Rickard and Pascoe (2009)*
J46427	TrGJAroCN	BZEMUCNO ₃ + $h\nu$ → EPXC4DIAL + NO ₂ + GLYOX + HO ₂	2.77*jx(ip_HOCH ₂ CHO)	Rickard and Pascoe (2009)
J46428	TrGJAroCN	DNPHEN + $h\nu$ → HONO + NCPDKETENE	jx(ip_HOC6H4N02)	Taraborrelli (2016)
J46429	TrGJAroCN	NCPDKETENE + $h\nu$ → CO ₂ + CO + 2 HO ₂ + NC4DCO ₂ H	J_KETENE	see note*
J47200	TrGJTerC	CO235C6CHO + $h\nu$ → CHOC3COCO ₃ + CH ₃ C(O)	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47201	TrGJTerC	C235C6CO ₃ H + $h\nu$ → CO235C6O ₂ + CO ₂ + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47202	TrGJTerC	C716OOH + $h\nu$ → CO13C4CHO + CH ₃ C(O) + OH	jx(ip_CH300H)+jx(ip_HOCH ₂ CHO)	Rickard and Pascoe (2009)
J47203	TrGJTerC	C721OOH + $h\nu$ → C722O ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47204	TrGJTerC	C722OOH + $h\nu$ → CH ₃ COCH ₃ + C44O ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47400	TrGJAroC	TLEPOXMUC + $h\nu$ → .5 C615CO ₂ O ₂ + HO ₂ + CO + .5 EPXC4DIAL + .5 CH ₃ C(O)	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47401	TrGJAroC	$\text{C6H5CH2OOH} + h\nu \rightarrow \text{BENZAL} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47402	TrGJAroCN	$\text{C6H5CH2NO3} + h\nu \rightarrow \text{BENZAL} + \text{HO}_2 + \text{NO}_2$	$0.59 \cdot \text{J_IC3H7N03}$	Rickard and Pascoe (2009)*
J47403	TrGJAroC	$\text{BENZAL} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{C6H5O2}$	jx(ip_BENZAL)	Wallington et al. (2017)
J47404	TrGJAroC	$\text{TLBIPEROOH} + h\nu \rightarrow .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47405	TrGJAroCN	$\text{TLBIPERNO3} + h\nu \rightarrow .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ ZCODC23DBCOD} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)*
J47406	TrGJAroC	$\text{TLOBIPEROH} + h\nu \rightarrow \text{C5CO14O2} + \text{GLYOX} + \text{HO}_2$	J_ACETOL	Rickard and Pascoe (2009)
J47407	TrGJAroC	$\text{CRESOOH} + h\nu \rightarrow .68 \text{ C5CO14OH} + .68 \text{ GLYOX} + \text{HO}_2 + .32 \text{ PTLQONE} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47408a	TrGJAroCN	$\text{NCRESOOH} + h\nu \rightarrow .68 \text{ C5CO14OH} + .68 \text{ GLYOX} + \text{HO}_2 + .32 \text{ PTLQONE} + \text{OH} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)*
J47408b	TrGJAroCN	$\text{NCRESOOH} + h\nu \rightarrow \text{C5CO14OH} + \text{GLYOX} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	$\text{TOL1OHNO2} + h\nu \rightarrow \text{HONO} + \text{MCPDKETENE}$	$\text{jx(ip_HOPh3Me2N02)}$	see note*
J47410	TrGJAroC	$\text{TLEMUCCO2H} + h\nu \rightarrow \text{C615CO2O2} + \text{CO}_2 + \text{HO}_2$	jx(ip_MACR)	Rickard and Pascoe (2009)
J47411	TrGJAroC	$\text{TLEMUCCO3H} + h\nu \rightarrow \text{C615CO2O2} + \text{CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_MACR)}$	Rickard and Pascoe (2009)
J47412	TrGJAroC	$\text{TLEMUCOOH} + h\nu \rightarrow .5 \text{ C3DIALO2} + .5 \text{ CO2H3CHO} + .5 \text{ EPXC4DIAL} + .5 \text{ MGLYOX} + .5 \text{ HO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + 2.77 \cdot \text{jx(ip_HOCH2CHO)} + \text{J_ACETOL}$	Rickard and Pascoe (2009)*
J47413	TrGJAroCN	$\text{TLEMUCNO3} + h\nu \rightarrow \text{EPXC4DIAL} + \text{NO}_2 + \text{CH}_3\text{C(O)} + \text{CO} + \text{HO}_2$	$2.77 \cdot \text{jx(ip_HOCH2CHO)} + \text{J_ACETOL}$	Rickard and Pascoe (2009)
J47414	TrGJAroC	$\text{TLEMUCCO} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{EPXC4DIAL} + \text{CO} + \text{HO}_2$	$2.77 \cdot \text{jx(ip_HOCH2CHO)} + 2.15 \cdot \text{jx(ip_MGLYOX)}$	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	$\text{MCPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{ HO}_2 + \text{ZCODC23DBCOD}$	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*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47421	TrGJAroC	MCATEC1OOH + $h\nu$ → MCATEC1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47422	TrGJAroCN	NPTLQOOH + $h\nu$ → C7CO4DB + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47423	TrGJAroC	PTLQOOH + $h\nu$ → C6CO2OHCO3 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47424	TrGJAroCN	NCRES1OOH + $h\nu$ → NCRES1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47425	TrGJAroCN	MNNCATCOOH + $h\nu$ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47426	TrGJAroCN	MNCATECOOH + $h\nu$ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47427	TrGJAroC	C7CO4DB + $h\nu$ → C5CO2DBCO3 + HO ₂ + CO	jx(ip_MGLY0X)*2	Rickard and Pascoe (2009)
J47428	TrGJAroCN	NDNCRESOOH + $h\nu$ → NC4MDCO2HN + HNO ₃ + CO + CO + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47429	TrGJAroCN	DNCRESOOH + $h\nu$ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47430	TrGJAroC	C6COOHCO3H + $h\nu$ → C5134CO2OH + HO ₂ + CO + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48200	TrGJTerC	C86OOH + $h\nu$ → C511O2 + CH ₃ COCH ₃ + OH	jx(ip_CH300H)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48201	TrGJTerC	C812OOH + $h\nu$ → C813O2 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48202	TrGJTerC	C813OOH + $h\nu$ → CH ₃ COCH ₃ + C512O2 + OH	jx(ip_CH300H)+jx(ip_MGLY0X)	Rickard and Pascoe (2009)
J48203	TrGJTerC	C721CHO + $h\nu$ → C721O2 + CO + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48204	TrGJTerC	C721CO3H + $h\nu$ → C721O2 + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48205	TrGJTerC	C8BCOOH + $h\nu$ → C89O2 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48206	TrGJTerC	C89OOH + $h\nu$ → C810O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48207	TrGJTerCN	C89NO3 + $h\nu$ → C810O2 + NO ₂	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48208	TrGJTerC	C810OOH + $h\nu$ → CH ₃ COCH ₃ + C514O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48209	TrGJTerCN	C810NO3 + $h\nu$ → CH ₃ COCH ₃ + C514O2 + NO ₂	2.84*J_IC3H7N03+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48210	TrGJTerCN	C8BCNO3 + $h\nu$ → C89O2 + NO ₂	J_IC3H7N03	Rickard and Pascoe (2009)
J48211	TrGJTerC	C85OOH + $h\nu$ → C86O2 + OH	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J48400	TrGJAroC	STYRENOOH + $h\nu$ → HO ₂ + HCHO + BENZAL + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J49200	TrGJTerC	C96OOH + $h\nu$ → C97O2 + OH	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J49201	TrGJTerC	C97OOH + $h\nu$ → C98O2 + OH	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J49202	TrGJTerC	C98OOH + $h\nu$ → C614O2 + CH ₃ COCH ₃ + OH	(jx(ip_CH300H)+2.15*jx(ip_MGLY0X))	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J49203a	TrGJTerC	NORPINAL + $h\nu$ → C85O2 + CO + HO ₂	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009), Taraborrelli (2016)
J49203b	TrGJTerC	NORPINAL + $h\nu$ → NORPINENOL	jx(ip_PINAL2ENOL)	Taraborrelli (2016), Andrews et al. (2012)
J49204	TrGJTerC	C85CO3H + $h\nu$ → C85O2 + CO ₂ + OH	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J49205	TrGJTerC	C89CO2H + $h\nu$ → .8 C811CO3 + .2 C89O2 + .2 CO ₂ + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49206	TrGJTerC	C89CO3H + $h\nu$ → .8 C811CO3 + .2 C89O2 + .2 CO ₂ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49207	TrGJTerC	C811CO3H + $h\nu$ → C811O2 + CO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J49208	TrGJTerC	NOPINDOOH + $h\nu$ → C89CO3 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40200	TrGJTerC	LAPINABOOH + $h\nu$ → PINAL + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40201	TrGJTerC	MENTHEN6ONE + $h\nu$ → RO6R1O2 + OH	jx(ip_CH300H)	Vereecken et al. (2007)
J40202	TrGJTerC	2OHMENTHEN6ONE + $h\nu$ → 10 LCARBON + OH	jx(ip_CH300H)	Vereecken et al. (2007)
J40203a	TrGJTerC	PINAL + $h\nu$ → C96O2 + CO + HO ₂	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009)
J40203b	TrGJTerC	PINAL + $h\nu$ → PINEOL	jx(ip_PINAL2ENOL)	Taraborrelli (2016), Andrews et al. (2012)*
J40204	TrGJTerC	PERPINONIC + $h\nu$ → C96O2 + CO ₂ + OH	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J40205	TrGJTerC	PINALOOH + $h\nu$ → C106O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40206	TrGJTerCN	PINALNO3 + $h\nu$ → C106O2 + NO ₂	J_IC3H7N03+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40207	TrGJTerC	C106OOH + $h\nu$ → C716O2 + CH ₃ COCH ₃ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40208	TrGJTerCN	C106NO3 + $h\nu$ → C716O2 + CH ₃ COCH ₃ + NO ₂	J_IC3H7N03+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40209	TrGJTerC	C109OOH + $h\nu$ → C89CO3 + HCHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40210	TrGJTerC	C109CO + $h\nu$ → C89CO3 + CO + HO ₂	jx(ip_MGLY0X)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40211	TrGJTerCN	LNAPINABOOH + $h\nu$ → PINAL + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40212	TrGJTerC	BPINAOOH + $h\nu$ → NOPINONE + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40213	TrGJTerCN	LNBPINABOOH + $h\nu$ → NOPINONE + HCHO + NO ₂ + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J40214	TrGJTerCN	ROO6R1NO3 + $h\nu$ → ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	2.84*J_IC3H7N03+jx(ip_CH300H)	Taraborrelli (2016)
J40215	TrGJTerCN	RO6R1NO3 + $h\nu$ → 9 LCARBON + HCHO + HO ₂ + NO ₂	2.84*J_IC3H7N03	Taraborrelli (2016)
J6000	StTrGJCl	Cl ₂ + $h\nu$ → Cl + Cl	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	Cl ₂ O ₂ + $h\nu$ → 2 Cl	jx(ip_Cl202)	Sander et al. (2014)
J6101	StTrGJCl	OClo + $h\nu$ → Clo + O(³ P)	jx(ip_OC10)	Sander et al. (2014)
J6200	StGJCl	HCl + $h\nu$ → Cl + H	jx(ip_HCl)	Sander et al. (2014)
J6201	StTrGJCl	HOCl + $h\nu$ → OH + Cl	jx(ip_HOCl)	Sander et al. (2014)
J6300	TrGJCIN	ClNO ₂ + $h\nu$ → Cl + NO ₂	jx(ip_ClN02)	Sander et al. (2014)
J6301a	StTrGJCIN	ClNO ₃ + $h\nu$ → Cl + NO ₃	jx(ip_ClN03)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6301b	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	$\text{jx}(\text{ip_ClON02})$	Sander et al. (2014)
J6400	StGJCl	$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3$	$\text{jx}(\text{ip_CH3Cl})$	Sander et al. (2014)
J6401	StGJCl	$\text{CCl}_4 + h\nu \rightarrow \text{LCARBON} + 4 \text{ Cl}$	$\text{jx}(\text{ip_CCl4})$	Sander et al. (2014)
J6402	StGJCCl	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 2 \text{ LCARBON} + 3 \text{ Cl}$	$\text{jx}(\text{ip_CH3CCl3})$	Sander et al. (2014)
J6500	StGJCIF	$\text{CFCl}_3 + h\nu \rightarrow \text{LCARBON} + \text{LFLUORINE} + \text{Cl} + 2 \text{ LCHLORINE}$	$\text{jx}(\text{ip_CFCl3})$	Sander et al. (2014)*
J6501	StGJCIF	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ LFLUORINE} + \text{Cl} + \text{LCHLORINE}$	$\text{jx}(\text{ip_CF2Cl2})$	Sander et al. (2014)*
J7000	StTrGJBr	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	$\text{jx}(\text{ip_Br2})$	Sander et al. (2014)
J7100	StTrGJBr	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip_Br0})$	Sander et al. (2014)
J7200	StTrGJBr	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	$\text{jx}(\text{ip_HOBr})$	Sander et al. (2014)
J7300	TrGJBrN	$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$	$\text{jx}(\text{ip_BrNO2})$	Sander et al. (2014)
J7301	StTrGJBrN	$\text{BrNO}_3 + h\nu \rightarrow .85 \text{ Br} + .85 \text{ NO}_3 + .15 \text{ BrO} + .15 \text{ NO}_2$	$\text{jx}(\text{ip_BrNO3})$	Sander et al. (2014)*
J7400	StGJBr	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3$	$\text{jx}(\text{ip_CH3Br})$	Sander et al. (2014)
J7401	TrGJBr	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br}$	$\text{jx}(\text{ip_CH2Br2})$	Sander et al. (2014)
J7402	TrGJBr	$\text{CHBr}_3 + h\nu \rightarrow \text{LCARBON} + 3 \text{ Br}$	$\text{jx}(\text{ip_CHBr3})$	Sander et al. (2014)
J7500	StGJBrF	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{LCARBON} + 3 \text{ LFLUORINE} + \text{Br}$	$\text{jx}(\text{ip_CF3Br})$	Sander et al. (2014)
J7600	StTrGJBrCl	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_BrCl})$	Sander et al. (2014)
J7601	StGJBrClF	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + 2 \text{ LFLUORINE} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CF2ClBr})$	Sander et al. (2014)
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CH2ClBr})$	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{LCARBON} + \text{Br} + 2 \text{ Cl}$	$\text{jx}(\text{ip_CHCl2Br})$	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br} + \text{Cl}$	$\text{jx}(\text{ip_CHClBr2})$	Sander et al. (2014)
J8000	TrGJI	$\text{I}_2 + h\nu \rightarrow \text{I} + \text{I}$	$\text{jx}(\text{ip_I2})$	Sander et al. (2014)
J8100	TrGJI	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip_IO})$	Sander et al. (2014)
J8200	TrGJI	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	$\text{jx}(\text{ip_HOI})$	Sander et al. (2014)
J8300	TrGJIN	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$	$\text{jx}(\text{ip_IN02})$	Sander et al. (2014)
J8301	TrGJIN	$\text{INO}_3 + h\nu \rightarrow \text{I} + \text{NO}_3$	$\text{jx}(\text{ip_IN03})$	Sander et al. (2014)
J8400	TrGJI	$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2 \text{ I} + 2 \text{ HO}_2 + \text{CO}$	$\text{jx}(\text{ip_CH2I2})$	Sander et al. (2014)
J8401	TrGJI	$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3$	$\text{jx}(\text{ip_CH3I})$	Sander et al. (2014)
J8402	TrGJCI	$\text{CH}_3\text{CHICH}_3 + h\nu \rightarrow 2 \text{ LCARBON} + \text{I} + \text{CH}_3$	$\text{jx}(\text{ip_C3H7I})$	Sander et al. (2014)
J8403	TrGJCII	$\text{CH}_2\text{CII} + h\nu \rightarrow \text{I} + \text{Cl} + 2 \text{ HO}_2 + \text{CO}$	$\text{jx}(\text{ip_CH2CII})$	Sander et al. (2014)
J8600	TrGJCII	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	$\text{jx}(\text{ip_ICl})$	Sander et al. (2014)
J8700	TrGJBrI	$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$	$\text{jx}(\text{ip_IBr})$	Sander et al. (2014)
PH3200_a01	TrAa01JN	$\text{NO}_3^-(\text{aq}) + h\nu \rightarrow \text{NO}_2(\text{aq}) + \text{OH}(\text{aq}) + \text{OH}^-(\text{aq})$	$\text{xaer}(01)*\text{jx}(\text{ip_N02}) * 1.4\text{E-}4$	see note*
PH10200_a01	TrAa01JHg	$\text{Hg}(\text{OH})_2(\text{aq}) + h\nu \rightarrow \text{Hg}(\text{aq})$	$\text{xaer}(01)*6\text{E-}5*\text{jx}(\text{ip_N02})$	see note*

General notes

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

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

J(11) \rightarrow jx(ip_COH2)
J(12) \rightarrow jx(ip_CHOH)
J(15) \rightarrow jx(ip_HOCH2CHO)
J(18) \rightarrow jx(ip_MACR)
J(22) \rightarrow jx(ip_ACETOL)
J(23)+J(24) \rightarrow jx(ip_MVK)
J(31)+J(32)+J(33) \rightarrow jx(ip_GLYOX)
J(34) \rightarrow jx(ip_MGLYOX)
J(41) \rightarrow jx(ip_CH3OOH)
J(53) \rightarrow J(isopropyl nitrate)
J(54) \rightarrow J(isopropyl nitrate)
J(55) \rightarrow J(isopropyl nitrate)
J(56)+J(57) \rightarrow jx(ip_NOA)

Specific notes

J41003: CH₃- and CH₂-channels are considered only and with their branching ratios being 0.42 and 0.48, respectively (Gans et al., 2011). CH-production is neglected. CH₂ is assumed to react only with O₂ yielding 1.44 H₂ + .18 HCHO + .18 O(³P) + .33 OH + .33 HO₂ + .44 CO₂ + .38 CO + .05 H₂O as assumed in the WACCM model by J. Orlando (Doug Kinnison, pers. comm. with D. Taraborrelli).

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(NO₃CH₂CHO) is the same as J(PAN).

J42021: In analogy to what is assumed for CH₃O₂NO₂ photolysis as in (Sander et al., 2014).

J43002: Following von Kuhlmann et al. (2003), we use J(CH₃COCH₂OH) = 0.11*jx(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(iC₃H₇ONO₂) = 3.7*jx(ip_PAN).

J43018: One third of the acetaldehyde channel is considered to be CH₂CHOH according to Hjorth (2002) EUPHORE Report.

J43024: Assuming J(C₃H₇ONO₂) = 0.59 \times J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J43025a: Photolysis frequencies very similar to the ones of CH₃CHO.

J43025b: Photolysis frequencies very similar to the ones of CH₃CHO.

J43400: KDEC C3DIALO \rightarrow GLYOX + CO + HO₂

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(iC₃H₇ONO₂).

J44005b: It is assumed that J(LC4H₉NO₃) is the same as J(iC₃H₇ONO₂).

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(HOCH₂CHO), 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(HOCH₂CHO), 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 CH₃COCH which upon reaction with O₂ 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*J(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 HO₂ 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: KDEC MALDIALO \rightarrow GLYOX + GLYOX + HO2

J44401: KDEC BZFUO \rightarrow CO14O3CHO + HO2

J44403: KDEC NBZFUO \rightarrow .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2

J44404b: KDEC MALDIALCO2 \rightarrow .6 MALANHY + HO2 + .4 GLYOX + .4 CO

J44407: KDEC MALANHYO \rightarrow HCOCO2HCO3

J44414: KDEC MECOACETO \rightarrow CH3CO3 + 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 $J(\text{ISOPDNO}_3)$ is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J45009: $0.59 \times J_{\text{IC3H7NO3}}$ 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 $J(\text{HCOC5})$ is half as large as $J(\text{MVK})$. With exception of HOCH2CO the products of MACO2 decomposition without CO2.

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

J45402: KDEC C5DIALO \rightarrow MALDIAL + CO + HO2

J45407: KDEC TLFUONE \rightarrow .6 C5CO14O2 + .6 HO2 + .4 TLFUONE

J45410: KDEC MMALANHYO \rightarrow CO2H3CO3

J45411: KDEC C5DICARBO \rightarrow MGLYOX + GLYOX + HO2

J45412: KDEC NTLFUO \rightarrow ACCOMECHO + NO2

J45414: KDEC C5CO14CO2 \rightarrow .83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

J45415: KDEC TLFUO \rightarrow ACCOMECHO + HO2

J46400: KDEC PHENO \rightarrow .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

J46403: KDEC NDNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2

J46404: KDEC BZBIPERO \rightarrow GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

J46415: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

J46416: KDEC PBZQO \rightarrow C5CO2OHCO3

J46418: KDEC BZBIPERO \rightarrow GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

J46419: KDEC NBZQO \rightarrow C6CO4DB + NO2

J46422: KDEC DNPHEO \rightarrow NC4DCO2H + HCOCO2H + NO2

J46425: KDEC BZEMUCO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

J46429: new channel

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

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

J47404: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

J47405: KDEC TLBIPERO \rightarrow .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

J47407: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

J47408a: KDEC CRESO \rightarrow .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE

J47408b: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

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

J47412: KDEC TLEMUCO \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .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 \rightarrow C7CO4DB + NO2

J47423: KDEC PTLQO \rightarrow C6CO2OHCO3

J47425: KDEC MNNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

J47426: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

J47428: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2

J47429: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

J48400: KDEC STYRENO \rightarrow HO2 + HCHO + BEN-	muth, 1993).	for the entire spectrum.
ZAL		
J40203b: Substituted vinyl alcohol in analogy to	J6501: Only 1 Cl atom is produced in analogy to	PH3200_a01: Scaled to J(NO ₂) so that its lifetime is
CH ₃ CHO photolysis.	CFC1 ₃ .	about 10.5 days, as suggested by Zellner et al. (1990).
J6500: Only 1 Cl atom is produced (Felder and De-	J7301: The quantum yields are recommended by	PH10200_a01: Scaled to J(NO ₂) so that it produces
Burkholder et al. (2015) for $\lambda > 300\text{nm}$ and used here		about 3.0×10^{-7} .

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

#	labels	reaction	rate coefficient	reference
H1000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	$k_{\text{exf}}(01, \text{ind_O2})$	see general notes*
H1000b_a01	TrAa01Sc	$O_2(aq) \rightarrow O_2$	$k_{\text{exb}}(01, \text{ind_O2})$	see general notes*
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(01, \text{ind_O3})$	see general notes*
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(01, \text{ind_O3})$	see general notes*
H2100f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	$k_{\text{exf}}(01, \text{ind_OH})$	see general notes*
H2100b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	$k_{\text{exb}}(01, \text{ind_OH})$	see general notes*
H2101f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	$k_{\text{exf}}(01, \text{ind_HO2})$	see general notes*
H2101b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	$k_{\text{exb}}(01, \text{ind_HO2})$	see general notes*
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(01, \text{ind_H2O2})$	see general notes*
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(01, \text{ind_H2O2})$	see general notes*
H3101f_a01	TrAa01ScN	$NO_2 \rightarrow NO_2(aq)$	$k_{\text{exf}}(01, \text{ind_NO2})$	see general notes*
H3101b_a01	TrAa01ScN	$NO_2(aq) \rightarrow NO_2$	$k_{\text{exb}}(01, \text{ind_NO2})$	see general notes*
H3102f_a01	TrAa01ScN	$NO_3 \rightarrow NO_3(aq)$	$k_{\text{exf}}(01, \text{ind_NO3})$	see general notes*
H3102b_a01	TrAa01ScN	$NO_3(aq) \rightarrow NO_3$	$k_{\text{exb}}(01, \text{ind_NO3})$	see general notes*
H3200f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(01, \text{ind_NH3})$	see general notes*
H3200b_a01	TrAa01MblScScmN	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(01, \text{ind_NH3})$	see general notes*
H3201_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf_N2O5}}(01)*C(\text{ind_H2O_a01})$	Behnke et al. (1994), Behnke et al. (1997)
H3202f_a01	TrAa01ScN	$HONO \rightarrow HONO(aq)$	$k_{\text{exf}}(01, \text{ind_HONO})$	see general notes*
H3202b_a01	TrAa01ScN	$HONO(aq) \rightarrow HONO$	$k_{\text{exb}}(01, \text{ind_HONO})$	see general notes*
H3203f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(01, \text{ind_HNO3})$	see general notes*
H3203b_a01	TrAa01MblScScmN	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(01, \text{ind_HNO3})$	see general notes*
H3204f_a01	TrAa01ScN	$HNO_4 \rightarrow HNO_4(aq)$	$k_{\text{exf}}(01, \text{ind_HNO4})$	see general notes*
H3204b_a01	TrAa01ScN	$HNO_4(aq) \rightarrow HNO_4$	$k_{\text{exb}}(01, \text{ind_HNO4})$	see general notes*
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(01, \text{ind_CO2})$	see general notes*
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(01, \text{ind_CO2})$	see general notes*
H4101f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	$k_{\text{exf}}(01, \text{ind_HCHO})$	see general notes*
H4101b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	$k_{\text{exb}}(01, \text{ind_HCHO})$	see general notes*
H4102f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	$k_{\text{exf}}(01, \text{ind_CH3O2})$	see general notes*
H4102b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	$k_{\text{exb}}(01, \text{ind_CH3O2})$	see general notes*
H4103f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	$k_{\text{exf}}(01, \text{ind_HCOOH})$	see general notes*
H4103b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	$k_{\text{exb}}(01, \text{ind_HCOOH})$	see general notes*
H4104f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	$k_{\text{exf}}(01, \text{ind_CH3OOH})$	see general notes*
H4104b_a01	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	$k_{\text{exb}}(01, \text{ind_CH3OOH})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H6000f_a01	TrAa01MblScCl	$\text{Cl}_2 \rightarrow \text{Cl}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_Cl2})$	see general notes*
H6000b_a01	TrAa01MblScCl	$\text{Cl}_2(\text{aq}) \rightarrow \text{Cl}_2$	$k_{\text{exb}}(01, \text{ind_Cl2})$	see general notes*
H6200f_a01	TrAa01MblScScmCl	$\text{HCl} \rightarrow \text{HCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCl})$	see general notes*
H6200b_a01	TrAa01MblScScmCl	$\text{HCl}(\text{aq}) \rightarrow \text{HCl}$	$k_{\text{exb}}(01, \text{ind_HCl})$	see general notes*
H6201f_a01	TrAa01MblScCl	$\text{HOCl} \rightarrow \text{HOCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCl})$	see general notes*
H6201b_a01	TrAa01MblScCl	$\text{HOCl}(\text{aq}) \rightarrow \text{HOCl}$	$k_{\text{exb}}(01, \text{ind_HOCl})$	see general notes*
H6300_a01	TrAa01MblClN	$\text{N}_2\text{O}_5 + \text{Cl}^-(\text{aq}) \rightarrow \text{ClNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_N2O5}}(01) * 5.E2$	Behnke et al. (1994), Behnke et al. (1997)
H6301_a01	TrAa01MblClN	$\text{ClNO}_3 \rightarrow \text{HOCl}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf_ClNO3}}(01) * C(\text{ind_H2O_a01})$	see general notes*
H6302_a01	TrAa01MblClN	$\text{ClNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{Cl}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(01) * 5.E2$	see general notes*
H7000f_a01	TrAa01MblScBr	$\text{Br}_2 \rightarrow \text{Br}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_Br2})$	see general notes*
H7000b_a01	TrAa01MblScBr	$\text{Br}_2(\text{aq}) \rightarrow \text{Br}_2$	$k_{\text{exb}}(01, \text{ind_Br2})$	see general notes*
H7200f_a01	TrAa01MblScScmBr	$\text{HBr} \rightarrow \text{HBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HBr})$	see general notes*
H7200b_a01	TrAa01MblScScmBr	$\text{HBr}(\text{aq}) \rightarrow \text{HBr}$	$k_{\text{exb}}(01, \text{ind_HBr})$	see general notes*
H7201f_a01	TrAa01MblScBr	$\text{HOBr} \rightarrow \text{HOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOBr})$	see general notes*
H7201b_a01	TrAa01MblScBr	$\text{HOBr}(\text{aq}) \rightarrow \text{HOBr}$	$k_{\text{exb}}(01, \text{ind_HOBr})$	see general notes*
H7300_a01	TrAa01MblBrN	$\text{N}_2\text{O}_5 + \text{Br}^-(\text{aq}) \rightarrow \text{BrNO}_2 + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_N2O5}}(01) * 3.E5$	Behnke et al. (1994), Behnke et al. (1997)
H7301_a01	TrAa01MblBrN	$\text{BrNO}_3 \rightarrow \text{HOBr}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * C(\text{ind_H2O_a01})$	see general notes*
H7302_a01	TrAa01MblBrN	$\text{BrNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{Br}_2(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * 3.E5$	see general notes*
H7600f_a01	TrAa01MblScBrCl	$\text{BrCl} \rightarrow \text{BrCl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_BrCl})$	see general notes*
H7600b_a01	TrAa01MblScBrCl	$\text{BrCl}(\text{aq}) \rightarrow \text{BrCl}$	$k_{\text{exb}}(01, \text{ind_BrCl})$	see general notes*
H7601_a01	TrAa01MblBrClN	$\text{ClNO}_3 + \text{Br}^-(\text{aq}) \rightarrow \text{BrCl}(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_ClNO3}}(01) * 3.E5$	see general notes*
H7602_a01	TrAa01MblBrClN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl}(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * 5.E2$	see general notes*
H8000f_a01	TrAa01ScI	$\text{I}_2 \rightarrow \text{I}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_I2})$	see general notes*
H8000b_a01	TrAa01ScI	$\text{I}_2(\text{aq}) \rightarrow \text{I}_2$	$k_{\text{exb}}(01, \text{ind_I2})$	see general notes*
H8100f_a01	TrAa01MblScI	$\text{IO} \rightarrow \text{IO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_IO})$	see general notes*
H8100b_a01	TrAa01MblScI	$\text{IO}(\text{aq}) \rightarrow \text{IO}$	$k_{\text{exb}}(01, \text{ind_IO})$	see general notes*
H8101_a01	TrAa01I	$\text{OIO} \rightarrow \text{HOI}(\text{aq}) + \text{HO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_OIO})$	see general notes*
H8102_a01	TrAa01I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI}(\text{aq}) + \text{H}^+(\text{aq}) + \text{IO}_2^-(\text{aq})$	$k_{\text{exf}}(01, \text{ind_I2O2})$	see general notes*
H8200f_a01	TrAa01MblScI	$\text{HOI} \rightarrow \text{HOI}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOI})$	see general notes*
H8200b_a01	TrAa01MblScI	$\text{HOI}(\text{aq}) \rightarrow \text{HOI}$	$k_{\text{exb}}(01, \text{ind_HOI})$	see general notes*
H8201_a01	TrAa01MblScI	$\text{HI} \rightarrow \text{H}^+(\text{aq}) + \text{I}^-(\text{aq})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H8202_a01	TrAa01ScI	$\text{HIO}_3 \rightarrow \text{IO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{mt}}(\text{HIO}_3) \cdot lwc$	see general notes*
H8300_a01	TrAa01IN	$\text{INO}_2 \rightarrow \text{HOI}(\text{aq}) + \text{HONO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_INO2})$	see general notes*
H8301_a01	TrAa01MblIN	$\text{INO}_3 \rightarrow \text{HOI}(\text{aq}) + \text{HNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_INO3})$	see general notes*
H8600f_a01	TrAa01MblScClI	$\text{ICl} \rightarrow \text{ICl}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ICl})$	see general notes*
H8600b_a01	TrAa01MblScClI	$\text{ICl}(\text{aq}) \rightarrow \text{ICl}$	$k_{\text{exb}}(01, \text{ind_ICl})$	see general notes*
H8700f_a01	TrAa01MblScBrI	$\text{IBr} \rightarrow \text{IBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_IBr})$	see general notes*
H8700b_a01	TrAa01MblScBrI	$\text{IBr}(\text{aq}) \rightarrow \text{IBr}$	$k_{\text{exb}}(01, \text{ind_IBr})$	see general notes*
H9100f_a01	TrAa01MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_SO2})$	see general notes*
H9100b_a01	TrAa01MblScScmS	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(01, \text{ind_SO2})$	see general notes*
H9200_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$xnom7\text{sulf} * k_{\text{exf}}(01, \text{ind_H2SO4})$	see general notes*
H9400f_a01	TrAa01CS	$\text{DMSO} \rightarrow \text{DMSO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_DMSO})$	see general notes*
H9400b_a01	TrAa01CS	$\text{DMSO}(\text{aq}) \rightarrow \text{DMSO}$	$k_{\text{exb}}(01, \text{ind_DMSO})$	see general notes*
H9401_a01	TrAa01MblS	$\text{CH}_3\text{SO}_3\text{H} \rightarrow \text{CH}_3\text{SO}_3^-(\text{aq}) + \text{H}^+(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3SO3H})$	see general notes*
H9402f_a01	TrAa01CS	$\text{DMS} \rightarrow \text{DMS}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_DMS})$	see general notes*
H9402b_a01	TrAa01CS	$\text{DMS}(\text{aq}) \rightarrow \text{DMS}$	$k_{\text{exb}}(01, \text{ind_DMS})$	see general notes*
H10000f_a01	TrAa01Hg	$\text{Hg} \rightarrow \text{Hg}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_Hg})$	see general notes*
H10000b_a01	TrAa01Hg	$\text{Hg}(\text{aq}) \rightarrow \text{Hg}$	$k_{\text{exb}}(01, \text{ind_Hg})$	see general notes*
H10100f_a01	TrAa01Hg	$\text{HgO} \rightarrow \text{HgO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HgO})$	see general notes*
H10100b_a01	TrAa01Hg	$\text{HgO}(\text{aq}) \rightarrow \text{HgO}$	$k_{\text{exb}}(01, \text{ind_HgO})$	see general notes*
H10600f_a01	TrAa01ClHg	$\text{HgCl}_2 \rightarrow \text{HgCl}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HgCl2})$	see general notes*
H10600b_a01	TrAa01ClHg	$\text{HgCl}_2(\text{aq}) \rightarrow \text{HgCl}_2$	$k_{\text{exb}}(01, \text{ind_HgCl2})$	see general notes*
H10700f_a01	TrAa01BrHg	$\text{HgBr}_2 \rightarrow \text{HgBr}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HgBr2})$	see general notes*
H10700b_a01	TrAa01BrHg	$\text{HgBr}_2(\text{aq}) \rightarrow \text{HgBr}_2$	$k_{\text{exb}}(01, \text{ind_HgBr2})$	see general notes*
H10701f_a01	TrAa01BrClHg	$\text{ClHgBr} \rightarrow \text{ClHgBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ClHgBr})$	see general notes*
H10701b_a01	TrAa01BrClHg	$\text{ClHgBr}(\text{aq}) \rightarrow \text{ClHgBr}$	$k_{\text{exb}}(01, \text{ind_ClHgBr})$	see general notes*
H10702f_a01	TrAa01BrHg	$\text{BrHgOBr} \rightarrow \text{BrHgOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_BrHgOBr})$	see general notes*
H10702b_a01	TrAa01BrHg	$\text{BrHgOBr}(\text{aq}) \rightarrow \text{BrHgOBr}$	$k_{\text{exb}}(01, \text{ind_BrHgOBr})$	see general notes*
H10703f_a01	TrAa01BrClHg	$\text{ClHgOBr} \rightarrow \text{ClHgOBr}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ClHgOBr})$	see general notes*
H10703b_a01	TrAa01BrClHg	$\text{ClHgOBr}(\text{aq}) \rightarrow \text{ClHgOBr}$	$k_{\text{exb}}(01, \text{ind_ClHgOBr})$	see general notes*

General notes

The forward (k_{exf}) and backward (k_{exb}) rate coefficients are calculated in sub-

routine `mecca_aero_calc_k_ex` in the file `chemprop.pdf`.
`messy_mecca_aero.f90` using accommodation coef-

ficients and Henry’s law constants from chemprop (see

For uptake of X (X = N_2O_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 = liq-

uid 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
HET200	StHetN	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2 \text{HNO}_3$	<code>khet_St(ihs_N2O5_H2O)</code>	see general notes*
HET201	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^-(\text{aq}) + 2 \text{H}^+(\text{aq})$	<code>khet_Tr(iht_N2O5)</code>	see general notes*
HET410	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see general notes*
HET420	StHetClN	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see general notes*
HET421	StHetClN	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_H2O)</code>	see general notes*
HET422	StHetClN	$\text{N}_2\text{O}_5 + \text{HCl} \rightarrow \text{ClNO}_2 + \text{HNO}_3$	<code>khet_St(ihs_N2O5_HCl)</code>	see general notes*
HET510	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see general notes*
HET520	StHetBrN	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_H2O)</code>	see general notes*
HET540	StHetBrClN	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see general notes*
HET541	StHetBrClN	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see general notes*
HET542	StHetBrCl	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see general notes*
HET543	StHetBrCl	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HCl)</code>	see general notes*
HET1001	StTrHetHg	$\text{Hg} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_Hg) + khet_St(ihs_Hg)</code>	see general notes*
HET1002	StTrHetHg	$\text{HgO} \rightarrow \text{Hg}(\text{aq})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1003	StTrHetClHg	$\text{HgCl} \rightarrow \text{Hg}(\text{aq}) + \text{LCHLORINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1004	StTrHetClHg	$\text{HgCl}_2 \rightarrow \text{Hg}(\text{aq}) + 2 \text{LCHLORINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1005	StTrHetBrHg	$\text{HgBr} \rightarrow \text{Hg}(\text{aq}) + \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1006	StTrHetBrHg	$\text{HgBr}_2 \rightarrow \text{Hg}(\text{aq}) + 2 \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1007	StTrHetBrClHg	$\text{ClHgBr} \rightarrow \text{Hg}(\text{aq}) + \text{LCHLORINE} + \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1008	StTrHetBrHg	$\text{BrHgOBr} \rightarrow \text{Hg}(\text{aq}) + 2 \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1009	StTrHetBrClHg	$\text{ClHgOBr} \rightarrow \text{Hg}(\text{aq}) + \text{LCHLORINE} + \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*

General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA_KHET) and then supplied to the MECCA chemistry (see www.messy-interface.org for details)

Table 5: Acid-base and other equilibria

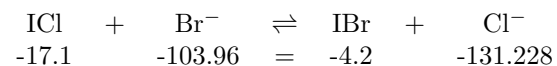
#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ20_a01	TrAa01Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a01	TrAa01MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
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)
EQ70_a01	TrAa01Br	$\text{Br}_2^- \rightleftharpoons \text{Br} + \text{Br}^-$	2.54E-6	-2256	Liu et al. (2002)
EQ71_a01	TrAa01MblScScmBr	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ72_a01	TrAa01ScBr	$\text{HOBr} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ73_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01MblBrCl	$\text{Br}_2 + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01MblBrCl	$\text{Br}^- + \text{Cl}_2 \rightleftharpoons \text{BrCl}_2^-$	4.2E6	14072	Wang et al. (1994)
EQ80_a01	TrAa01MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ81_a01	TrAa01MblScBrI	$\text{IBr} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2.9E2		Troy and Margerum (1991)
EQ82_a01	TrAa01MblScBrClI	$\text{ICl} + \text{Br}^- \rightleftharpoons \text{IBr} + \text{Cl}^-$	3.3E2		see note*
EQ90_a01	TrAa01MblScScmS	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01MblScScmS	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01MblScScmS	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ100_a01	TrAa01Hg	$\text{Hg}^{2+} + \text{OH}^- \rightleftharpoons \text{HgOH}^+$	4.0E10		Ammann and Pöschl (2007)
EQ101_a01	TrAa01Hg	$\text{HgOH}^+ + \text{OH}^- \rightleftharpoons \text{Hg}(\text{OH})_2$	1.58E11		Ammann and Pöschl (2007)
EQ102_a01	TrAa01ClHg	$\text{Hg}^{2+} + \text{Cl}^- \rightleftharpoons \text{HgCl}^+$	5.8E6		Ammann and Pöschl (2007)
EQ103_a01	TrAa01ClHg	$\text{HgCl}^+ + \text{Cl}^- \rightleftharpoons \text{HgCl}_2$	2.5E6		Ammann and Pöschl (2007)
EQ104_a01	TrAa01ClHg	$\text{HgOH}^+ + \text{Cl}^- \rightleftharpoons \text{Hg}(\text{OH})\text{Cl}$	2.69E7		Ammann and Pöschl (2007)
EQ105_a01	TrAa01BrHg	$\text{Hg}^{2+} + \text{Br}^- \rightleftharpoons \text{HgBr}^+$	1.1E9		Raofie and Ariya (2004)
EQ106_a01	TrAa01BrHg	$\text{HgBr}^+ + \text{Br}^- \rightleftharpoons \text{HgBr}_2$	2.5E8		Raofie and Ariya (2004)
EQ107_a01	TrAa01HgS	$\text{Hg}^{2+} + \text{SO}_3^{2-} \rightleftharpoons \text{HgSO}_3$	2.E13		van Loon et al. (2001)
EQ108_a01	TrAa01HgS	$\text{HgSO}_3 + \text{SO}_3^{2-} \rightleftharpoons \text{Hg}(\text{SO}_3)_2^{2-}$	1.E10		van Loon et al. (2001)

Specific notes

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

EQ72_a01: For $pK_a(\text{HOBr})$, see also Keller-Rudek et al. (1992).

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



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

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

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

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
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)
A7000_a01	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2 Br^- + Br_2$	1.9E9		Ross et al. (1992)
A7100_a01	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A7101_a01	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A7102_a01	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2 Br^-$	1.7E8		Wagner and Strehlow (1987)
A7200_a01	TrAa01Br	$Br^- + OH \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)
A7201_a01	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A7202_a01	TrAa01MblBr	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7203_a01	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A7204_a01	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2 Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A7205_a01	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A7206_a01	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999)
A7207_a01	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A7208_a01	TrAa01MblBr	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7209a_a01	TrAa01Br	$BrOH^- \rightarrow Br^- + OH$	3.3E7		Zehavi and Rabani (1972)
A7209b_a01	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A7210_a01	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A7300_a01	TrAa01BrN	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A7301_a01	TrAa01BrN	$Br_2^- + NO_2^- \rightarrow 2 Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A7400_a01	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2 Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*
A7601_a01	TrAa01BrCl	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A7602_a01	TrAa01MblBrCl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A7603_a01	TrAa01MblBrCl	$\text{HOBr} + \text{Cl}^- + \text{H}^+ \rightarrow \text{BrCl}$	2.3E10		Liu and Margerum (2001)*
A7604_a01	TrAa01MblBrCl	$\text{BrCl} \rightarrow \text{Cl}^- + \text{HOBr} + \text{H}^+$	3.0E6		Liu and Margerum (2001)
A8100_a01	TrAa01MbII	$\text{I}^- + \text{O}_3 \rightarrow \text{HOI} + \text{OH}^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a01	TrAa01MbII	$\text{IO} + \text{IO} \rightarrow \text{HOI} + \text{IO}_2^- + \text{H}^+$	1.5E9		Buxton et al. (1986)
A8200_a01	TrAa01MbII	$\text{IO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{IO}_3^-$	6.0E1		Furrow (1987)
A8201_a01	TrAa01I	$\text{HOI} + \text{IO}_2^- \rightarrow \text{IO}_3^- + \text{I}^- + \text{H}^+$	6.0E2		Chinake and Simoyi (1996)
A8202_a01	TrAa01MbII	$\text{HOI} + \text{I}^- + \text{H}^+ \rightarrow \text{I}_2$	4.4E12		Eigen and Kustin (1962)
A8203_a01	TrAa01MbII	$\text{IO}_2^- + \text{I}^- + \text{H}^+ \rightarrow 2 \text{HOI} + \text{OH}^-$	2.0E10		Edblom et al. (1987)
A8600_a01	TrAa01MblClII	$\text{ICl} \rightarrow \text{HOI} + \text{Cl}^- + \text{H}^+$	2.4E6		Wang et al. (1989)
A8601_a01	TrAa01MblClII	$\text{I}^- + \text{HOCl} + \text{H}^+ \rightarrow \text{ICl}$	3.5E11		Nagy et al. (1988)
A8602_a01	TrAa01ClII	$\text{IO}_2^- + \text{HOCl} \rightarrow \text{IO}_3^- + \text{Cl}^- + \text{H}^+$	1.5E3		Lengyel et al. (1996)
A8603_a01	TrAa01MblClII	$\text{HOI} + \text{Cl}^- + \text{H}^+ \rightarrow \text{ICl}$	2.9E10		Wang et al. (1989)
A8604_a01	TrAa01ClII	$\text{HOI} + \text{Cl}_2 \rightarrow \text{IO}_2^- + 2 \text{Cl}^- + 3\text{H}^+$	1.0E6		Lengyel et al. (1996)
A8605_a01	TrAa01ClII	$\text{HOI} + \text{HOCl} \rightarrow \text{IO}_2^- + \text{Cl}^- + 2 \text{H}^+$	5.0E5		Citri and Epstein (1988)
A8606_a01	TrAa01ClII	$\text{ICl} + \text{I}^- \rightarrow \text{I}_2 + \text{Cl}^-$	1.1E9		Margerum et al. (1986)
A8700_a01	TrAa01MblBrI	$\text{IBr} \rightarrow \text{HOI} + \text{H}^+ + \text{Br}^-$	8.0E5		Troy et al. (1991)
A8701_a01	TrAa01MblBrI	$\text{I}^- + \text{HOBr} \rightarrow \text{IBr} + \text{OH}^-$	5.0E9		Troy and Margerum (1991)
A8702_a01	TrAa01BrI	$\text{IO}_2^- + \text{HOBr} \rightarrow \text{IO}_3^- + \text{Br}^- + \text{H}^+$	1.0E6		Chinake and Simoyi (1996)
A8703_a01	TrAa01MblBrI	$\text{HOI} + \text{Br}^- + \text{H}^+ \rightarrow \text{IBr}$	3.3E12		Troy et al. (1991)
A8704_a01	TrAa01BrI	$\text{HOI} + \text{HOBr} \rightarrow \text{IO}_2^- + \text{Br}^- + 2 \text{H}^+$	1.0E6		Chinake and Simoyi (1996)
A8705_a01	TrAa01BrI	$\text{IBr} + \text{I}^- \rightarrow \text{I}_2 + \text{Br}^-$	2.0E9		Faria et al. (1993)
A9100_a01	TrAa01ScS	$\text{SO}_3^- + \text{O}_2 \rightarrow \text{SO}_5^-$	1.5E9		Huie and Neta (1987)
A9101_a01	TrAa01MblScScmS	$\text{SO}_3^{2-} + \text{O}_3 \rightarrow \text{SO}_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a01	TrAa01ScS	$\text{SO}_4^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a01	TrAa01ScS	$\text{SO}_4^- + \text{SO}_3^{2-} \rightarrow \text{SO}_3^- + \text{SO}_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a01	TrAa01ScS	$\text{SO}_5^- + \text{O}_2^- \rightarrow \text{HSO}_5^- + \text{OH}^-$	2.3E8		Buxton et al. (1996)
A9105_a01	TrAa01S	$\text{SO}_5^- + \text{SO}_3^{2-} \rightarrow .72 \text{SO}_4^- + .72 \text{SO}_4^{2-} + .28 \text{SO}_3^- + .28 \text{HSO}_5^- + .28 \text{OH}^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A9106_a01	TrAa01S	$\text{SO}_5^- + \text{SO}_5^- \rightarrow \text{O}_2 + \text{SO}_4^{2-} + \text{LSULFUR}$	1.0E8		Ross et al. (1992)*
A9200_a01	TrAa01ScS	$\text{SO}_3^{2-} + \text{OH}^- \rightarrow \text{SO}_3^- + \text{OH}^-$	5.5E9		Buxton et al. (1988)
A9201_a01	TrAa01ScS	$\text{SO}_4^- + \text{OH}^- \rightarrow \text{HSO}_5^-$	1.0E9		Jiang et al. (1992)
A9202_a01	TrAa01ScS	$\text{SO}_4^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.5E9		Jiang et al. (1992)
A9203_a01	TrAa01ScS	$\text{SO}_4^- + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{OH}^-$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a01	TrAa01ScS	$\text{SO}_4^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{HO}_2$	1.2E7		Wine et al. (1989)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9205_a01	TrAa01ScS	$\text{HSO}_3^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-} + \text{OH}$	3.0E3		see note*
A9206_a01	TrAa01MblScScmS	$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a01	TrAa01ScS	$\text{HSO}_3^- + \text{OH} \rightarrow \text{SO}_3^-$	4.5E9		Buxton et al. (1988)
A9208_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{OH} + \text{H}^+$	3.0E3		see note*
A9209_a01	TrAa01MblScScmS	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a01	TrAa01ScS	$\text{HSO}_3^- + \text{SO}_4^- \rightarrow \text{SO}_3^- + \text{SO}_4^{2-} + \text{H}^+$	8.0E8		Huie and Neta (1987)
A9211_a01	TrAa01S	$\text{HSO}_3^- + \text{SO}_5^- \rightarrow .75 \text{SO}_4^- + .75 \text{SO}_4^{2-} + .75 \text{H}^+ + .25 \text{SO}_3^- + .25 \text{HSO}_5^-$	1.0E5		Huie and Neta (1987)
A9212_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HSO}_5^- + \text{H}^+ \rightarrow 2 \text{HSO}_4^- + \text{H}^+$	7.1E6		Betterton and Hoffmann (1988)
A9301_a01	TrAa01ScNS	$\text{SO}_4^- + \text{NO}_3^- \rightarrow \text{SO}_4^{2-} + \text{NO}_3$	5.0E4		Exner et al. (1992)
A9302_a01	TrAa01ScNS	$\text{SO}_4^{2-} + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{SO}_4^-$	1.0E5		Logager et al. (1993)
A9304_a01	TrAa01ScNS	$\text{HSO}_3^- + \text{NO}_3 \rightarrow \text{SO}_3^- + \text{NO}_3^- + \text{H}^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a01	TrAa01ScNS	$\text{HSO}_3^- + \text{HNO}_4 \rightarrow \text{HSO}_4^- + \text{NO}_3^- + \text{H}^+$	3.1E5		Warneck (1999)
A9400_a01	TrAa01ScS	$\text{SO}_3^{2-} + \text{HCHO} \rightarrow \text{CH}_2\text{OH}\text{SO}_3^- + \text{OH}^-$	1.4E4		Boyce and Hoffmann (1984)*
A9401_a01	TrAa01ScS	$\text{SO}_3^{2-} + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A9402_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HCHO} \rightarrow \text{CH}_2\text{OH}\text{SO}_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A9403_a01	TrAa01ScS	$\text{HSO}_3^- + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{HSO}_4^- + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A9404_a01	TrAa01ScS	$\text{CH}_2\text{OH}\text{SO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^{2-} + \text{HCHO}$	3.6E3		Seinfeld and Pandis (1998)
A9600_a01	TrAa01ClS	$\text{SO}_3^{2-} + \text{Cl}_2^- \rightarrow \text{SO}_3^- + 2 \text{Cl}^-$	6.2E7		Jacobi et al. (1996)
A9601_a01	TrAa01MblClS	$\text{SO}_3^{2-} + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a01	TrAa01ClS	$\text{SO}_4^- + \text{Cl}^- \rightarrow \text{SO}_4^{2-} + \text{Cl}$	2.5E8		Buxton et al. (1999a)
A9603_a01	TrAa01ClS	$\text{SO}_4^{2-} + \text{Cl} \rightarrow \text{SO}_4^- + \text{Cl}^-$	2.1E8		Buxton et al. (1999a)
A9604_a01	TrAa01ClS	$\text{HSO}_3^- + \text{Cl}_2^- \rightarrow \text{SO}_3^- + 2 \text{Cl}^- + \text{H}^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a01	TrAa01MblClS	$\text{HSO}_3^- + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^- + \text{H}^+$	7.6E8		see note*
A9606_a01	TrAa01ClS	$\text{HSO}_5^- + \text{Cl}^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9700_a01	TrAa01BrS	$\text{SO}_3^{2-} + \text{Br}_2^- \rightarrow 2 \text{Br}^- + \text{SO}_3^-$	2.2E8	-649	Shoute et al. (1991)
A9701_a01	TrAa01BrS	$\text{SO}_3^{2-} + \text{BrO}^- \rightarrow \text{Br}^- + \text{SO}_4^{2-}$	1.0E8		Troy and Margerum (1991)
A9702_a01	TrAa01MblBrS	$\text{SO}_3^{2-} + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^-$	5.0E9		Troy and Margerum (1991)
A9703_a01	TrAa01BrS	$\text{SO}_4^- + \text{Br}^- \rightarrow \text{Br} + \text{SO}_4^{2-}$	2.1E9		Jacobi (1996)
A9704_a01	TrAa01BrS	$\text{HSO}_3^- + \text{Br}_2^- \rightarrow 2 \text{Br}^- + \text{H}^+ + \text{SO}_3^-$	6.3E7	-782	Shoute et al. (1991)
A9705_a01	TrAa01MblBrS	$\text{HSO}_3^- + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^- + \text{H}^+$	5.0E9		see note*
A9706_a01	TrAa01BrS	$\text{HSO}_5^- + \text{Br}^- \rightarrow \text{HOBr} + \text{SO}_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)
A9800_a01	TrAa01IS	$\text{HSO}_3^- + \text{I}_2 \rightarrow 2 \text{I}^- + \text{HSO}_4^- + 2 \text{H}^+$	1.7E9		Yiin and Margerum (1990)
A10100_a01	TrAa01Hg	$\text{Hg} + \text{O}_3 \rightarrow \text{HgO} + \text{O}_2$	4.7E7		Munthe (1992)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A10200_a01	TrAa01Hg	$\text{HgO} + \text{H}^+ \rightarrow \text{Hg}^{2+} + \text{OH}^-$	1.0E10		Pleijel and Munthe (1995)
A10201_a01	TrAa01Hg	$\text{Hg} + \text{OH} \rightarrow \text{Hg}^+ + \text{OH}^-$	2.0E9		Lin and Pehkonen (1997)
A10202_a01	TrAa01Hg	$\text{Hg}^+ + \text{OH} \rightarrow \text{Hg}^{2+} + \text{OH}^-$	1.0E10		Lin and Pehkonen (1997)
A10203_a01	TrAa01Hg	$\text{Hg}^{2+} + \text{HO}_2 \rightarrow \text{Hg}^+ + \text{O}_2 + \text{H}^+$	1.7E4		Enami et al. (2007)
A10204_a01	TrAa01Hg	$\text{Hg}^+ + \text{HO}_2 \rightarrow \text{Hg} + \text{O}_2 + \text{H}^+$	1.0E10		Lin and Pehkonen (1997)
A10600_a01	TrAa01ClHg	$\text{Hg} + \text{HOCl} \rightarrow \text{Hg}^{2+} + \text{Cl}^- + \text{OH}^-$	2.09E6		Lin and Pehkonen (1998)
A10601_a01	TrAa01ClHg	$\text{Hg} + \text{ClO}^- \rightarrow \text{Hg}^{2+} + \text{Cl}^- + 2 \text{OH}^-$	1.99E6		Lin and Pehkonen (1998)
A10700_a01	TrAa01BrHg	$\text{Hg} + \text{HOBr} \rightarrow \text{Hg}^{2+} + \text{Br}^- + \text{OH}^-$	0.279		Wang and Pehkonen (2004)
A10701_a01	TrAa01BrHg	$\text{Hg} + \text{BrO}^- \rightarrow \text{Hg}^{2+} + \text{Br}^- + 2 \text{OH}^-$	0.273		Wang and Pehkonen (2004)
A10702_a01	TrAa01BrHg	$\text{Hg} + \text{Br}_2 \rightarrow \text{Hg}^{2+} + 2 \text{Br}^-$	0.196		Wang and Pehkonen (2004)
A10900_a01	TrAa01HgS	$\text{HgSO}_3 \rightarrow \text{Hg} + \text{HSO}_4^- + \text{H}^+$	0.0106		van Loon et al. (2000)

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.

A7400_a01: Assumed to be the same as for $\text{Br}_2^- + \text{H}_2\text{O}_2$.

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

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 $\text{SO}_3^{2-} + \text{HOCl}$.

A9705_a01: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOBr}$.

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.
- Ammann, M. and Pöschl, U.: Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions - Part 2: exemplary practical applications and numerical simulations, *Atmos. Chem. Phys.*, 7, 6025–6045, 2007.
- 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, 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.
- Ariya, P. A., Khalizov, A., and Gidas, A.: Reactions of gaseous mercury with atomic and molecular halogens: Kinetics, product studies, and atmospheric implications, *J. Phys. Chem. A*, 106, 7310–7320, 2002.
- 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, 1997.
- Atkinson, R.: Kinetics of the gas-phase reactions of OH radicals with alkanes and cycloalkanes, *Atmos. Chem. Phys.*, 3, 2233–2307, 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, 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, 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, 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.
- Bailey, S. M., Barth, C. A., and Solomon, S. C.: A model of nitric oxide in the lower thermosphere, *J. Geophys. Res.*, 107, doi:10.1029/2001JA000258, 2002.
- 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, 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, 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, 1993.
- Barone, S. B., Turnipseed, A. A., and Ravishankara, A. R.: Role of adducts in the atmospheric oxidation of dimethyl sulfide, *Faraday Discuss.*, 100, 39–54, 1995.
- Barth, C. A.: Nitric oxide in the lower thermosphere, *Planet. Space Sci.*, 40, 315–336, 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: Supplement II, *J. Phys. Chem. Ref. Data*, 34, 757–1397, 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.
- Beckwith, R. C., Wang, T. X., and Margerum, D. W.: Equilibrium and kinetics of bromine hydrolysis, *Inorg. Chem.*, 35, 995–1000, 1996.
- Bedjanian, Y., Laverdet, G., and Le Bras, G.: Low-pressure study of the reaction of Cl atoms with isoprene, *J. Phys. Chem. A*, 102, 953–959, 1998.
- 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, 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, 1997.
- Betterton, E. A. and Hoffmann, M. R.: Oxidation of aqueous SO₂ by peroxydisulfate, *J. Phys. Chem.*, 92, 5962–5965, 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.
- Bichsel, Y. and von Gunten, U.: Oxidation of iodide and hypiodous acid in the disinfection of natural waters, *Environ. Sci. Technol.*, 33, 4040–4045, 1999.
- 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, 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.
- 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, 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, 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· + SO₄^{2−}, *Phys. Chem. Chem. Phys.*, 1, 269–273, 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, 1999b.
- Calvert, J. G. and Lindberg, S. E.: A modeling study of the mechanism of the halogen-ozone-mercury homogeneous reactions in the troposphere during the polar spring, *Atmos. Environ.*, 37, 4467–4481, 2003.
- 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, 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, 2001.
- 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.
- Chameides, W. L.: The photochemistry of a remote marine stratiform cloud, *J. Geophys. Res.*, 89D, 4739–4755, 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, 1996.
- Christensen, H. and Sehested, K.: HO_2 and O_2^- radicals at elevated temperatures, *J. Phys. Chem.*, 92, 3007–3011, 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, 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, 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.
- Clyne, M. A. A. and Cruse, H. W.: Atomic resonance fluorescence spectrometry for the rate constants of rapid bimolecular reactions. Part 2. Reactions $\text{Cl} + \text{BrCl}$, $\text{Cl} + \text{Br}_2$, $\text{Cl} + \text{ICl}$, $\text{Br} + \text{IBr}$, $\text{Br} + \text{ICl}$, *J. Chem. Soc. Faraday Trans. 2*, 68, 1377–1387, 1972.
- 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.
- 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, 1983.
- 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 , $\text{H}_2\text{SO}_4(\text{g})$, $\text{MSA}(\text{g})$, and $\text{MSA}(\text{p})$, *J. Geophys. Res.*, 103D, 1657–1678, 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, 1964.
- daSilva, G.: Carboxylic acid catalyzed keto-enol tautomerizations in the gas phase, *Angew. Chem.*, 122, 7685–7687, doi:10.1002/ange.201003530, 2010.
- Deister, U. and Warneck, P.: Photooxidation of SO_3^{2-} in aqueous solution, *J. Phys. Chem.*, 94, 2191–2198, 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 CH_3SCH_3 : Products and temperature dependent rate coefficients by laser induced fluorescence, *Phys. Chem. Chem. Phys.*, 8, 847–855, 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 CH_3O_2 , CF_3O_2 and O_3 , *Phys. Chem. Chem. Phys.*, 8, 5185–5198, 2006b.
- Dillon, T. J., Tucceri, M. E., Sander, R., and Crowley, J. N.: LIF studies of iodine oxide chemistry, part 3. Reactions $\text{IO} + \text{NO}_3 \rightarrow \text{OIO} + \text{NO}_2$, $\text{I} + \text{NO}_3 \rightarrow \text{IO}$

- + NO₂, and CH₂I + O₂ → (products): Implications for the chemistry of the marine atmosphere at night., *Phys. Chem. Chem. Phys.*, 10, 1540–1554, 2008.
- Dolson, D. A. and Leone, S. R.: A reinvestigation of the laser-initiated chlorine/hydrogen bromide chain reaction: absolute rate constants and the $v = 2/v = 1$ ratio from chlorine atom + hydrogen bromide → hydrogen chloride(v) + bromine atom, *J. Phys. Chem.*, 91, 3543–3550, 1987.
- Donohoue, D. L., Bauer, D., Cossairt, B., and Hynes, A. J.: Temperature and pressure dependent rate coefficients for the reaction of Hg with Br and the reaction of Br with Br: a pulsed laser photolysis-pulsed laser induced fluorescence study, *J. Phys. Chem. A*, 110, 6623–6632, 2006.
- 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.
- 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, 1987.
- Eigen, M. and Kustin, K.: The kinetics of halogen hydrolysis, *J. Am. Chem. Soc.*, 84, 1355–1361, 1962.
- Enami, S., Hoshino, Y., and Kawasaki, M.: A kinetic study of the gas-phase reactions of OIO with NO, NO₂, and Cl₂, *Int. J. Chem. Kinetics*, 39, 688–693, 2007.
- Espinosa-Garcia, J. and Garcia-Bernáldez, J. C.: Analytical potential energy surface for the CH₄ + O(³P) → CH₃ + OH reaction. Thermal rate constants and kinetic isotope effects, *Phys. Chem. Chem. Phys.*, 2, 2345–2351, doi:10.1039/b001038n, 2000.
- 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, 1992.
- Faria, R. B., Lengyel, I., Epstein, I. R., and Kustin, K.: Combined mechanism explaining nonlinear dynamics in bromine(III) and bromine(V) oxidations of iodide ion, *J. Phys. Chem.*, 97, 1164–1171, 1993.
- 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, 2008.
- Felder, P. and Demuth, C.: Photodissociation of CFC1₃ at 193 nm investigated by photofragment translational spectroscopy, *Chem. Phys. Lett.*, 208, 21–26, doi:10.1016/0009-2614(93)80070-6, 1993.
- Fell, C., Steinfeld, J. I., and Miller, S.: Quenching of N(²D) by O(³P), *J. Chem. Phys.*, 92, 4768–4777, 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, 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, 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, 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, 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, 1987.
- Gans, B., Boyé-Peronne, S., Broquier, M., Delsaut, M., Douin, S., Fellows, C. E., Halvick, P., Loison, J.-C., Lucchese, R. R., and Gauyacq, D.: Photolysis of methane revisited at 121.6 nm and at 118.2 nm: quantum yields of the primary products, measured by mass spectrometry, *Phys. Chem. Chem. Phys.*, 13, 8140–8152, doi:10.1039/c0cp02627a, 2011.
- 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, 2006.
- Garton, D. J., Minton, T. K., Troya, D., Pascual, R., and Schatz, G. C.: Hyperthermal reactions of O(³P) with alkanes: Observations of novel reaction pathways in crossed-beams and theoretical studies, *J. Phys. Chem. A*, 107, 4583–4587, doi:10.1021/jp0226026, 2003.

- 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 O₂ in atmospheric association reactions, *Science*, 337, 1066–1069, doi:10.1126/science.1224106, 2012.
- Goodsite, M., Plane, J. M. C., and Skov, H.: A theoretical study of the oxidation of Hg⁰ to HgBr₂ in the troposphere, *Environ. Sci. Technol.*, 38, 1772–1776, 2004.
- 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 O₃ formation in the Reaction of CH₃C(O)O₂ with HO₂, *J. Phys. Chem. A*, 1, 974–985, doi:10.1021/jp412380z, 2014.
- Gruzdev, A. N., Elokho, 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, 1993.
- Haag, W. R. and Hoigné, J.: Ozonation of bromide-containing waters: Kinetics of formation of hypobromous acid and bromate, *Environ. Sci. Technol.*, 17, 261–267, 1983.
- Hall, B.: The gas phase oxidation of elemental mercury by ozone, *Water Air Soil Pollut.*, 80, 301–315, 1995.
- 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, 1985.
- Hermans, I., Müller, J.-F., Nguyen, T. L., Jacobs, P. A., and Peeters, J.: Kinetics of α -hydroxy-alkylperoxyl radicals in oxidation processes. HO₂-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, 1995.
- Herrmann, H., Ervens, B., Nowacki, P., Wolke, R., and Zellner, R.: A chemical aqueous phase radical mechanism for tropospheric chemistry, *Chemosphere*, 38, 1223–1232, 1999.
- Hoffmann, M. R.: On the kinetics and mechanism of oxidation of aquated sulfur dioxide by ozone, *Atmos. Environ.*, 20, 1145–1154, 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, 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, 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, 1996.
- Ingham, T., Bauer, D., Sander, R., Crutzen, P. J., and Crowley, J. N.: Kinetics and products of the reactions BrO + DMS and Br + DMS at 298 K, *J. Phys. Chem. A*, 103, 7199–7209, 1999.
- 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, 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 Cl₂⁻ radical in the aqueous phase, in: *Air Pollution Research Report 57: Homogenous and heterogenous chemical Processes in the Troposphere*, edited by Mirabel, P., pp. 172–176, Office for official Publications of the European Communities, Luxembourg, 1996.
- Jagiella, S. and Zabel, F.: Reaction of phenylperoxy radicals with NO₂ at 298 K, *Phys. Chem. Chem. Phys.*, 9, 5036–5051, doi:10.1039/B705193J, 2007.
- Jefferson, A., Nicovich, J. M., and Wine, P. H.: Temperature-dependent kinetics studies of the reactions Br(²P_{3/2}) + CH₃SCH₃ ↔ CH₃SCH₂ + HBr. Heat of formation of the CH₃SCH₂ radical, *J. Phys. Chem.*, 98, 7128–7135, 1994.
- 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, 1997.
- Jenkin, M. E., Young, J. C., and Rickard, A. R.: The MCM v3.3.1 degradation scheme for isoprene, *Atmos. Chem. Phys.*, 15, 11433–11459, 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, 1992.
- Keller-Rudek, H., Koschel, D., Merlet, P., Ohms-Bredemann, U., Wagner, J., and Wietelmann, A.: *Gmelin Handbook of Inorganic and Organometallic Chemistry*, 8th Edition, Br, Bromine, Supplement Volume B2, Compounds with Oxygen and Nitrogen, Springer Verlag, Berlin, 1992.
- Kelley, C. M. and Tartar, H. V.: On the system: bromine-water, *J. Am. Chem. Soc.*, 78, 5752–5756, 1956.
- 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.
- 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, 1999.
- Kondo, O. and Benson, S. W.: Kinetics and equilibria in the system $\text{Br} + \text{CH}_3\text{OOH} \rightleftharpoons \text{HBr} + \text{CH}_3\text{OO}$. An upper limit for the heat of formation of the methylperoxy radical, *J. Phys. Chem.*, 88, 6675–6680, 1984.
- Kumar, K. and Margerum, D. W.: Kinetics and mechanism of general-acid-assisted oxidation of bromide by hypochlorite and hypochlorous acid, *Inorg. Chem.*, 26, 2706–2711, 1987.
- Lax, E.: *Taschenbuch für Chemiker und Physiker*, Springer Verlag, Berlin, 1969.
- 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, 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 dioxide/chlorite reaction, *J. Am. Chem. Soc.*, 118, 3708–3719, 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.
- 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, 2013.
- Lin, C.-J. and Pehkonen, S. O.: Aqueous free radical chemistry of mercury in the presence of iron oxides and ambient aerosol, *Atmos. Environ.*, 31, 4125–4137, 1997.
- Lin, C.-J. and Pehkonen, S. O.: Oxidation of elemental mercury by aqueous chlorine (HOCl/OCl^-): Implications for tropospheric mercury chemistry, *J. Geophys. Res.*, 103D, 28 093–28 102, 1998.
- 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, 1987.
- Liu, Q. and Margerum, D. W.: Equilibrium and kinetics of bromine chloride hydrolysis, *Environ. Sci. Technol.*, 35, 1127–1133, 2001.
- Liu, Y., Pimentel, A. S., Antoku, Y., Giles, B. J., and Barker, J. R.: Temperature-dependent rate and equilibrium constants for $\text{Br} \cdot (\text{aq}) + \text{Br}^- (\text{aq}) \rightleftharpoons \text{Br}_2^- \cdot (\text{aq})$, *J. Phys. Chem. A*, 106, 11 075–11 082, 2002.
- Lockhart, J., Blitz, M., Heard, D., Seakins, P., and Shannon, R.: Kinetic study of the $\text{OH} + \text{glyoxal}$ 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.
- Logager, 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, 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, 1980.
- 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, 1997.

- Manion, J. A., Huie, R. E., Levin, R. D., Burgess, Jr., D. R., Orkin, V. L., Tsang, W., McGivern, W. S., Hudgens, J. W., Knyazev, V. D., Atkinson, D. B., Chai, E., Tereza, A. M., Lin, C.-Y., Allison, T. C., Mallard, W. G., Westley, F., Herron, J. T., Hampson, R. F., and Frizzell, D. H.: NIST Chemical Kinetics Database, NIST Standard Reference Database 17 (Web Version), <http://kinetics.nist.gov>, 2015.
- 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, 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, 1985.
- Martin, L. R. and Damschen, D. E.: Aqueous oxidation of sulfur dioxide by hydrogen peroxide at low pH, *Atmos. Environ.*, 15, 1615–1621, 1981.
- Matthew, B. M., George, I., and Anastasio, C.: Hydroperoxyl radical ($\text{HO}_2\cdot$) oxidizes dibromide radical anion ($\cdot\text{Br}_2^-$) to bromine (Br_2) in aqueous solution: Implications for the formation of Br_2 in the marine boundary layer, *Geophys. Res. Lett.*, 30, doi:10.1029/2003GL018572, 2003.
- 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, 2001.
- 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.
- 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, 1999.
- Munthe, J.: The aqueous oxidation of elemental mercury by ozone, *Atmos. Environ.*, 26A, 1461–1468, 1992.
- 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, 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 NO_3 with CH_3I measured with use of cavity ring-down spectroscopy, *J. Phys. Chem. A*, 109, 6527–6531, 2005.
- Neta, P. and Huie, R. E.: Rate constants for reactions of NO_3 radicals in aqueous solutions, *J. Phys. Chem.*, 90, 4644–4648, 1986.
- Nguyen, T. L., Peeters, J., and Vereecken, L.: Theoretical study of the gas-phase ozonolysis of β -pinene ($\text{C}_{10}\text{H}_{16}$), *Phys. Chem. Chem. Phys.*, 11, 5643–5656, doi:10.1039/b822984h, 2009.
- 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.
- 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, 1997.
- Orlando, J. J. and Tyndall, G. S.: Rate coefficients for the thermal decomposition of BrONO_2 and the heat of formation of BrONO_2 , *J. Phys. Chem.*, 100, 19 398–19 405, 1996.
- Orlando, J. J. and Tyndall, G. S.: The atmospheric chemistry of the HC(O)CO radical, *Int. J. Chem. Kinetics*, 33, 149–156, 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, 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, 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, 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, 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.
- Pal, B. and Ariya, P. A.: Gas-phase HO-initiated reactions of elemental mercury: Kinetics, product studies, and atmospheric implications, *Environ. Sci. Technol.*, 38, 5555–5566, 2004.
- 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, 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.
- 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, 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.
- Pleijel, K. and Munthe, J.: Modelling the atmospheric mercury cycle – Chemistry in fog droplets, *Atmos. Environ.*, 29, 1441–1457, 1995.
- Raofie, F. and Ariya, P. A.: Kinetics and products study of the reaction of BrO radicals with gaseous mercury, *J. Phys. IV France*, 107, 1119–1121, 2003.
- Raofie, F. and Ariya, P. A.: Product study of the gas-phase BrO-initiated oxidation of Hg^0 : Evidence for stable Hg^{1+} compounds, *Environ. Sci. Technol.*, 38, 4319–4326, 2004.
- 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, 1999.
- 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.
- 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, <http://www.geosci-model-dev.net/7/2653>, 2014.
- Sander, S. P., Finlayson-Pitts, B. J., Friedl, R. R., Golden, D. M., Huie, R. E., Kolb, C. E., Kurylo, M. J., Molina, M. J., Moortgat, G. K., Orkin, V. L., and Ravishankara, A. R.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 14, JPL Publication 02-25, Jet Propulsion Laboratory, Pasadena, CA, 2003.
- 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.
- Schwarz, H. A. and Bielski, B. H. J.: Reactions of HO_2 and O_2^- with iodine and bromine and the I_2^- and I atom reduction potentials, *J. Phys. Chem.*, 90, 1445–1448, 1986.
- 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, 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, 1983.
- Seinfeld, J. H. and Pandis, S. N.: *Atmospheric Chemistry and Physics*, John Wiley & Sons, Inc., 1998.
- Shallcross, D. E., Leather, K. E., Bacak, A., Xiao, P., Lee, E. P. F., Ng, M., Mok, D. K. W., Dyke, J. M., Hossaini, R., Chipperfield, M. P., Khan, M. A. H., and Percival, C. J.: Reaction between CH_3O_2 and BrO radicals: a new source of upper troposphere lower stratosphere hydroxyl radicals, *J. Phys. Chem. A*, 119, 4618–4632, 2015.
- 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, 1991.
- 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, 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, 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, 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.
- Sutton, H. C. and Downes, M. T.: Reactions of the HO_2 radical in aqueous solution with bromine and related compounds, *J. Chem. Soc. Faraday Trans. 1*, 68, 1498–1507, 1972.
- Swaminathan, P. K., Strobel, D. F., Kupperman, D. G., Acton, L., DeMajistre, R., Yee, J.-H., Paxton, L., Anderson, D. E., Strickland, D. J., and Duff, J. W.: Nitric oxide abundance in the mesosphere/lower thermosphere region: Roles of solar soft X rays, suprathermal $\text{N}(^4\text{S})$ atoms, and vertical transport, *J. Geophys. Res.*, 103A, 11 579–11 594, 1998.
- 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.: The Mainz Organics Mechanism (MOM), Geosci. Model Dev., (in preparation), 2016.
- 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, <http://www.atmos-chem-phys.net/9/2751>, 2009.
- Tokos, J. J. S., Hall, B., Calhoun, J. A., and Prestbo, E. M.: Homogeneous gas-phase reaction of Hg^0 with H_2O_2 , O_3 , CH_3I , and $(\text{CH}_3)_2\text{S}$: Implications for atmospheric Hg cycling, *Atmos. Environ.*, 32, 823–827, 1998.
- Troy, R. C. and Margerum, D. W.: Non-metal redox kinetics: Hypobromite and hypobromous acid reactions with iodide and with sulfite and the hydrolysis of bromosulfate, *Inorg. Chem.*, 30, 3538–3543, 1991.
- Troy, R. C., Kelley, M. D., Nagy, J. C., and Margerum, D. W.: Non-metal redox kinetics: Iodine monobromide reaction with iodide ion and the hydrolysis of IBr , *Inorg. Chem.*, 30, 4838–4845, 1991.
- 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, 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, 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 CH_3CN , *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 INO_2 intermediate complexes in iodine recombination, *J. Chem. Phys.*, 64, 736–742, 1976.
- van Loon, L., Mader, E., and Scott, S. L.: Reduction of the aqueous mercuric ion by sulfite: UV spectrum of HgSO_3 and its intramolecular redox reaction, *J. Phys. Chem. A*, 104, 1621–1626, 2000.
- van Loon, L. L., Mader, E. A., and Scott, S. L.: Sulfite stabilization and reduction of the aqueous mercuric ion: Kinetic determination of sequential formation constants, *J. Phys. Chem. A*, 105, 3190–3195, 2001.
- 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 ($\text{C}_{10}\text{H}_{16}$): 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 , RO_2 , and SO_2 , 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.
- 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.
- Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H., Halow, I., Bailey, S. M., Churney, K. L., and Nuttall, R. L.: The NBS tables of chemical thermodynamic properties; Selected values for inorganic and C_1 and C_2 organic substances in SI units, *J. Phys. Chem. Ref. Data*, 11, suppl. 2, 1982.

- Wagner, I. and Strehlow, H.: On the flash photolysis of bromide ions in aqueous solution, *Ber. Bunsenges. Phys. Chem.*, 91, 1317–1321, 1987.
- 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>, 2017.
- 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, 1994.
- Wang, T. X., Kelley, M. D., Cooper, J. N., Beckwith, R. C., and Margerum, D. W.: Equilibrium, kinetic, and UV-spectral characteristics of aqueous bromine chloride, bromine, and chlorine species, *Inorg. Chem.*, 33, 5872–5878, 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, 1989.
- Wang, Z. and Pehkonen, S. O.: Oxidation of elemental mercury by aqueous bromine: atmospheric implications, *Atmos. Environ.*, 38, 3675–3688, 2004.
- Warneck, P.: Chemical reactions in clouds, *Fresenius J. Anal. Chem.*, 340, 585–590, 1991.
- Warneck, P.: The relative importance of various pathways for the oxidation of sulfur dioxide and nitrogen dioxide in sunlit continental fair weather clouds, *Phys. Chem. Chem. Phys.*, 1, 5471–5483, 1999.
- Wayne, R. P., Barnes, I., Biggs, P., Burrows, J. P., Canosa-Mas, C. E., Hjorth, J., Le Bras, G., Moortgat, G. K., Perner, D., Poulet, G., Restelli, G., and Sidebottom, H.: The nitrate radical: Physics, chemistry, and the atmosphere, *Atmos. Environ.*, 25A, 1–203, 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 cloudwater: H_2O_2 production and destruction, *Environ. Sci. Technol.*, 25, 791–800, 1991.
- Welz, O., Savee, J. D., Osborn, D. L., Vasu, S. S., Percival, C. J., Shallcross, D. E., and Taatjes, C. A.: Direct kinetic measurements of Criegee intermediate (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 reactions with formic and acetic acid near the collision limit: Direct kinetics measurements and atmospheric 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, 1989.
- Wingenter, O. W., Sive, B. C., Blake, N. J., and Rowland, F. S.: Atomic chlorine concentrations determined from ethane and hydroxyl measurements made over the Central Pacific Ocean, *Eos, Trans. AGU (Abstract Supplement)*, 80, F149–F150, 1999.
- Wolfe, G. M., Thornton, J. A., Bouvier-Brown, N. C., Goldstein, A. H., Park, J.-H., McKay, M., Matross, D. M., Mao, J., Brune, W. H., LaFranchi, B. W., Browne, E. C., Min, K.-E., Wooldridge, P. J., Cohen, R. C., Crounse, J. D., Faloona, I. C., Gilman, J. B., Kuster, W. C., de Gouw, J. A., Huisman, A., and Keutsch, F. N.: The chemistry of atmosphere-forest exchange (CAFE) model - part 2: application to BEARPEX-2007 observations, *Atmos. Chem. Phys.*, 11, 1269–1294, doi:10.5194/acp-11-1269-2011, 2011.
- Wu, D., Wong, D., and Di Bartolo, B.: Evolution of Cl_2^- in aqueous NaCl solutions, *J. Photochem.*, 14, 303–310, 1980.
- Yiin, B. S. and Margerum, D. W.: Nonmetal redox kinetics: reactions of iodine and triiodide with sulfite and hydrogen sulfite and the hydrolysis of iodosulfate, *Inorg. Chem.*, 29, 1559–1564, 1990.
- Yin, F., Grosjean, D., and Seinfeld, J. H.: Photooxidation of dimethyl sulfide and dimethyl disulfide. I: Mechanism development, *J. Atmos. Chem.*, 11, 309–364, 1990.
- Yoon, M.-C., Choi, Y. S., and Kim, S. K.: The OH production from the $\pi - \pi^*$ transition of acetylacetone, *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 photolysis in acidic aqueous solutions containing chloride ions, *J. Phys. Chem. Ref. Data*, 33, 747–763, 2004.

Zehavi, D. and Rabani, J.: The oxidation of aqueous bromide by hydroxyl radicals. A pulse radiolytic investigation, *J. Phys. Chem.*, 76, 312–319, 1972.

Zellner, R., Hartmann, D., Karthäuser, J., Rhäsa, D.,

and Weibring, G.: A laser photolysis/LIF study of the reactions of $O(^3P)$ atoms with CH_3 and CH_3O_2 radicals, *J. Chem. Soc. Faraday Trans. 2*, 84, 549–568, doi:10.1039/f29888400549, 1988.

Zellner, R., Exner, M., and Herrmann, H.: Absolute OH quantum yield in the laser photolysis of nitrate, nitrite and dissolved H_2O_2 at 308 and 351 nm in the temperature range 278–353 K, *J. Atmos. Chem.*, 10, 411–425, 1990.