

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 4.5.0

Date: April 21, 2021

Batch file: latex

Integrator: rosenbrock_posdef

Gas equation file: gas.eqn

Replacement file:

Selected reactions:

“1”

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase: 708

Aqueous phase: 481

All species: 1189

Number of reactions in selected mechanism:

Gas phase (Gnn): 1815

Aqueous phase (Annn): 402

Henry (Hnn): 735

Photolysis (Jnn): 385

Aqueous phase photolysis (PHnn): 27

Heterogeneous (HETnn): 21

Equilibria (EQnn): 138

Isotope exchange (IEXnn): 0

Tagging equations (TAGnn): 0

Dummy (Dnn): 1

All equations: 3524

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)
G3202a	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$(1.-\alpha_{\text{H00NO}}) * k_{\text{N02_OH}}$	Amedro et al. (2020)
G3202b	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HOONO}$	$\alpha_{\text{H00NO}} * k_{\text{N02_OH}}$	Amedro et al. (2020)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$k_{\text{N02_H02}}$	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	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$k_{\text{HN03_OH}}$	Dulitz et al. (2018)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$k_{\text{N02_H02}} / (2.1\text{E}-27 \cdot \text{EXP}(10900./\text{temp}))$	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	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E}-07 \cdot \text{EXP}(-628./\text{temp}) * (\text{temp})^{**(-1.32)}$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E}-09 \cdot \text{EXP}(-356./\text{temp}) * (\text{temp})^{**(-1.12)}$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E}-12 * ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E}-11 * ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E}-11 * ((\text{temp}/298.)^{**(-2.0)})$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E}-11 * ((\text{temp}/298.)^{**(-2.0)})$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{NH}_2 + \text{O}_2$	$1.2\text{E}-14$	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)
G3227	UpStTrGN	$\text{HOONO} \rightarrow \text{NO}_2 + \text{OH}$	$(\alpha_{\text{H00NO}} * k_{\text{N02_OH}}) / (3.5\text{E}-27 \cdot \text{EXP}(10135./\text{temp}))$	see note*
G3228	UpStTrGN	$\text{HOONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$1.3\text{E}-12 \cdot \text{EXP}(380./\text{temp})$	Burkholder et al. (2015)*
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)

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

#	labels	reaction	rate coefficient	reference
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	$1.85\text{E}-20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp}) - 987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{ HCHO} + .85 \text{ HO}_2 + .15 \text{ CH}_3\text{O} + \text{H}_2\text{O}$	$6.38\text{E}-18 \cdot ((\text{temp})^{**2}) \cdot \text{EXP}(144./\text{temp})$	Atkinson et al. (2006)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$3.8\text{E}-13 \cdot \text{EXP}(780./\text{temp}) / (1.+1./498. \cdot \text{EXP}(1160./\text{temp}))$	Atkinson et al. (2006)
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$3.8\text{E}-13 \cdot \text{EXP}(780./\text{temp}) / (1.+498. \cdot \text{EXP}(-1160./\text{temp}))$	Atkinson et al. (2006)
G4104a	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot (1.-\text{beta_CH3NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot \text{beta_CH3NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$	1.2E-12	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{ O}_2$	$7.4\text{E}-13 \cdot \text{EXP}(-520./\text{temp}) \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{ HCHO} + .5 \text{ CH}_3\text{OH} + .5 \text{ O}_2$	$(\text{k_CH3O2} - 7.4\text{E}-13 \cdot \text{EXP}(-520./\text{temp})) \cdot \text{R02} \cdot 2.$	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. (2018)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18 \cdot \text{EXP}(2.03 \cdot \text{LOG}(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13 \cdot \text{EXP}(-1900./\text{temp})$	Burkholder et al. (2015)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E}-13 + \text{cair} \cdot 3.54\text{E}-33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$2.94\text{E}-14 \cdot \exp(786./\text{temp}) + 9.85\text{E}-13 \cdot \text{EXP}(-1036./\text{temp})$	Paulot et al. (2011)
G4112	UpStG	$\text{CO} + \text{O}(^3\text{P}) \rightarrow \text{CO}_2$	$6.60\text{E}-33 \cdot \text{EXP}(-1103./\text{temp})$	Roble (1995)
G4113	UpStG	$\text{CH}_4 + \text{O}(^3\text{P}) \rightarrow .51 \text{ CH}_3 + .51 \text{ OH} + .49 \text{ CH}_3\text{O} + .49 \text{ H}$	$6.03\text{E}-18 \cdot (\text{temp})^{**}(2.17) \cdot \text{EXP}(-3619./\text{temp})$	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	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$\text{k_NO2_CH3O2} / (9.5\text{E}-29 \cdot \text{EXP}(11234./\text{temp}))$	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	$\text{CH}_3\text{ONO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}_2$	$4.0\text{E}-13 \cdot \text{EXP}(-845./\text{temp})$	Atkinson et al. (2006)
G4118	StTrG	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E}-14 \cdot \exp(-663./\text{temp}) \cdot \text{c}(\text{ind_02})$	Chai et al. (2014)

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

#	labels	reaction	rate coefficient	reference
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 8.1\text{E-}29, 4.5, 2.1\text{E-}11, 0., 0.44)$	Atkinson et al. (2006)
G4119b	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$	$9.6\text{E-}12 * \text{EXP}(-1150./\text{temp})$	Atkinson et al. (2006)
G4120a	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 2.6\text{E-}29, 2.8, 3.3\text{E-}11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/900.), \text{SP}))$	Atkinson et al. (2006)
G4120b	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$	$2.3\text{E-}12 * (\text{temp}/300.)^{**}(0.7)$	Atkinson et al. (2006)
G4121	StTrG	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E-}16 * \text{exp}(-1000./\text{temp})$	Burkholder et al. (2015)
G4122	StTrGN	$\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$	$1.\text{E-}10 * \text{exp}(-1764./\text{temp})$	Nielsen et al. (1991)
G4123	StTrG	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$9.7\text{E-}15 * \text{EXP}(625./\text{temp})$	Atkinson et al. (2006)
G4124	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.4\text{E}12 * \text{EXP}(-7000./\text{temp})$	Atkinson et al. (2006)
G4125	StTrG	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2 \text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$	$5.6\text{E-}15 * \text{EXP}(2300./\text{temp})$	Atkinson et al. (2006)
G4126	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$0.7275 * 2.3\text{E-}12 * \text{EXP}(360./\text{temp})$	Atkinson et al. (2006)*
G4127	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$1.2\text{E-}12$	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(k_{\text{CH302}} * 5.5\text{E-}12) ** (0.5) * \text{R02} * 2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(k_{\text{CH302}} * 5.7\text{E-}14 * \text{EXP}(750./\text{temp})) ** (0.5) * \text{R02} * 2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_{R00HRO}	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{R0HRO}} + k_{\text{s*f_s00H*f_sOH}}$	Taraborrelli (2010)*
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$2. * k_{\text{R0HRO}} + k_{\text{s*f_sOH*f_sOH}}$	Taraborrelli (2010)*
G4133	StTrG	$\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$	$1.4\text{E-}10$	Bossolasco et al. (2014)*
G4134	StTrG	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E+}14 * \text{EXP}(-10000./\text{temp})$	see note*
G4135	StTrG	$\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$	$k_{\text{CH200_N02}} * 3.6\text{E-}6$	Ouyang et al. (2013)*
G4136	StTrG	$\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$	$5.2\text{E-}12$	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$	$6.\text{E-}14$	Welz et al. (2012)*
G4138	StTrGN	$\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$	$k_{\text{CH200_N02}}$	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$	$3.6\text{E-}14$	Vereecken et al. (2012)
G4141	StTrG	$\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$	$1.\text{E-}10$	Welz et al. (2014)*
G4142	StTrG	$\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$	$1.7\text{E-}12$	Stone et al. (2014)*
G4143	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$	$5.\text{E-}12$	Vereecken et al. (2012)*
G4144	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$	$5.\text{E-}12$	Vereecken et al. (2012)*
G4145	StTrG	$\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$	$5.\text{E-}12$	Vereecken et al. (2012)

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

#	labels	reaction	rate coefficient	reference
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	1.E-12	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	6.E-11	Buras et al. (2014)
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	k_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)*

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

#	labels	reaction	rate coefficient	reference
G42002	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42003	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13 * \text{EXP}(700./\text{temp})$	Burkholder et al. (2015)
G42004a	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * (1. - \text{beta_C2H5NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * \text{beta_C2H5NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42005	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Wallington et al. (2018)
G42006	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .8 \text{ CH}_3\text{CHO} + .6 \text{ HO}_2 + .2 \text{ C}_2\text{H}_5\text{OH}$	$2. * (7.6\text{E-}14 * \text{k_CH3O2}) ** (.5) * \text{R02}$	Sander et al. (2019), Atkinson et al. (2006)
G42007a	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	k_R00HRO	Sander et al. (2019)
G42007b	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{OH}$	k_s*f_s00H	Sander et al. (2019)
G42008a	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.95$	Atkinson et al. (2006)
G42008b	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.05$	Atkinson et al. (2006)
G42009	TrGCN	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42010	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$	k_CH3CO2H_OH	Atkinson et al. (2006)*
G42011a	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.61$	Groß et al. (2014)
G42011b	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OOH}$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.23$	Groß et al. (2014)
G42011c	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.16$	Groß et al. (2014)
G42012	TrGCN	$\text{CH}_3\text{C(O)OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E-}12 * \text{EXP}(270./\text{temp})$	Tyndall et al. (2001a)
G42013	TrGCN	$\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3CO3_NO2	Burkholder et al. (2015)*
G42014	TrGCN	$\text{CH}_3\text{C(O)OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$	$4.\text{E-}12$	Canosa-Mas et al. (1996)
G42017a	TrGC	$\text{CH}_3\text{C(O)OO} \rightarrow \text{CH}_3 + \text{CO}_2$	$\text{k1_R02RC03} * 0.9$	Sander et al. (2019)
G42017b	TrGC	$\text{CH}_3\text{C(O)OO} \rightarrow \text{CH}_3\text{COOH}$	$\text{k1_R02RC03} * 0.1$	Sander et al. (2019)
G42018	TrGC	$\text{CH}_3\text{C(O)OOH} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O}$	k_R00HRO	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	$\text{PAN} \rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$	k_PAN_M	Burkholder et al. (2015)*
G42022a	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	$\text{k_3rd}(\text{temp}, \text{cair}, 5.5\text{e-}30, 0.0, 8.3\text{e-}13, -2., 0.6) * 0.71$	Burkholder et al. (2015)*
G42022b	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 5.5\text{e-}30, 0.0, 8.3\text{e-}13, -2., 0.6) * 0.29$	Burkholder et al. (2015)*
G42023a	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$	$8.00\text{E-}12 * 0.80$	Atkinson et al. (2006)
G42023b	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$	$8.00\text{E-}12 * 0.20$	Atkinson et al. (2006)
G42024a	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$	$5.1\text{E-}12 * (1. - 1./ (1 + 1.85\text{E-}18 * \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*

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

#	labels	reaction	rate coefficient	reference
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)*
G42025	TrGC	$\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Sander et al. (2019)
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	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	$k1_R02RC03 \cdot 0.9$	Sander et al. (2019)
G42027b	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$k1_R02RC03 \cdot 0.1$	Sander et al. (2019)
G42028a	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	KAPH02*r_C03_OH	Sander et al. (2019), 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*r_C03_00H	Sander et al. (2019), 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*r_C03_03	Sander et al. (2019), 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	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	$KR02N03 \cdot 1.74$	Rickard and Pascoe (2009)
G42032	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{HCHO} + .09 \text{CO}_2 + .91 \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	$k_C02H + k_s \cdot f_s \cdot \text{OH} \cdot f_C02H$	Sander et al. (2019)
G42033a	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	k_R00HRO	Sander et al. (2019)
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	$k_s \cdot f_s \cdot \text{OH} \cdot f_C02H$	Sander et al. (2019)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42035	TrGCN	$\text{PHAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_s \cdot f_s \cdot \text{OH} \cdot f_c \cdot \text{pan} + k_R0HRO$	Sander et al. (2019)
G42036	TrGC	$\text{GLYOX} + \text{OH} \rightarrow \text{HCOCO} + \text{H}_2\text{O}$	$3.1\text{E}-12 \cdot \text{EXP}(340./\text{temp})$	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	$\text{HCOCO} \rightarrow \text{CO} + \text{CO} + \text{HO}_2$	$7.\text{E}11 \cdot \text{EXP}(-3160./\text{temp}) + 5.\text{E}-12 \cdot c(\text{ind_02})$	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	$\text{HCOCO} \rightarrow \text{HCOCO}_3$	$5.\text{E}-12 \cdot c(\text{ind_02}) \cdot 3.2 \cdot \exp(-550./\text{temp})$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	$\text{HCOCO} \rightarrow \text{OH} + \text{CO} + \text{CO}_2$	$5.\text{E}-12 \cdot c(\text{ind_02}) \cdot (1 - 3.2 \cdot \exp(-550./\text{temp}))$	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	$\text{HCOCO}_3 \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2$	$k1_R02RC03 \cdot 0.9$	Sander et al. (2019)
G42039b	TrGC	$\text{HCOCO}_3 \rightarrow \text{HCOCO}_2\text{H}$	$k1_R02RC03 \cdot 0.1$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G42040	TrGC	$\text{HCOCO}_3 + \text{HO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02	Feierabend et al. (2008), Sander et al. (2019)
G42041	TrGCN	$\text{HCOCO}_3 + \text{NO} \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G42042	TrGCN	$\text{HCOCO}_3 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	KR02N03*1.74	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_CH3CO3_N02	Orlando and Tyndall (2001), Sander et al. (2019)
G42044	TrGC	$\text{HCOCO}_2\text{H} + \text{OH} \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	k_CO2H+k_t*f_0*f_CO2H	Sander et al. (2019)
G42045a	TrGC	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3 + \text{H}_2\text{O}$	k_R00HRO	Sander et al. (2019)
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_0*f_CO2H	Sander et al. (2019)
G42046	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 \rightarrow .6 \text{HOCH}_2\text{CH}_2\text{O} + .2 \text{HOCH}_2\text{CHO} + .2 \text{ETHGLY}$	$2. \cdot (7.8\text{E}-14 \cdot \text{EXP}(1000./\text{temp}))$ $\cdot k_{\text{CH3O2}} \cdot (.5) \cdot \text{R02}$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow .25 \text{HO}_2 + .5 \text{HCHO} + .75 \text{HOCH}_2\text{CH}_2\text{O} + \text{NO}_2$	$\text{KR02N0} \cdot (1. - \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G42048	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{ETHOHNO}_3$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair})$	Sander et al. (2019)
G42049a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HYETHO}_2\text{H}$	$1.53\text{E}-13 \cdot \text{EXP}(1300./\text{temp})$ $\cdot (1. - r_{\text{CHOHCH2O2_OH}})$	Rickard and Pascoe (2009)
G42049b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$1.53\text{E}-13 \cdot \text{EXP}(1300./\text{temp})$ $\cdot r_{\text{CHOHCH2O2_OH}}$	Rickard and Pascoe (2009)
G42050	TrGCN	$\text{ETHOHNO}_3 + \text{OH} \rightarrow .93 \text{NO}_3\text{CH}_2\text{CHO} + .93 \text{HO}_2 + .07 \text{HOCH}_2\text{CHO} + .07 \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}} \cdot (f_{\text{sOH}} \cdot f_{\text{CH2ON02}} + f_{\text{ON02}} \cdot f_{\text{pCH2OH}}) + k_{\text{ROHRO}}$	Sander et al. (2019)
G42051a	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	k_R00HRO	Rickard and Pascoe (2009)*
G42051b	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}} \cdot f_{\text{sO0H}} \cdot f_{\text{pCH2OH}}$	Sander et al. (2019)
G42051c	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{s}} \cdot f_{\text{sOH}} \cdot f_{\text{pCH2OH}} + k_{\text{ROHRO}}$	Sander et al. (2019)
G42052a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HOCH}_2\text{CHO}$	$6.00\text{E}-14 \cdot \text{EXP}(-550./\text{temp})$ $\cdot C(\text{ind}_{\text{O2}})$	Rickard and Pascoe (2009)
G42052b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HCHO} + \text{HCHO}$	$9.50\text{E}13 \cdot \text{EXP}(-5988./\text{temp})$	Rickard and Pascoe (2009)
G42053	TrGC	$\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$2. \cdot k_{\text{s}} \cdot f_{\text{sOH}} \cdot f_{\text{pCH2OH}} + 2. \cdot k_{\text{ROHRO}}$	Sander et al. (2019)
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	Sander et al. (2019)
G42055a	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CHO}$	$k_{\text{R02_H02}}(\text{temp}, 2) \cdot r_{\text{COCH2O2_OOH}}$	Sander et al. (2019)
G42055b	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 2) \cdot r_{\text{COCH2O2_OH}}$	Sander et al. (2019)
G42056a	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{KR02N0} \cdot (1. - \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G42056b	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	$\text{KRO2NO}*\alpha_{\text{AN}}(3,1,1,0,0,\text{temp},\text{cair})$	Sander et al. (2019)
G42057	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KRO2NO3	Sander et al. (2019)
G42058a	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2$	k_R00HRO	Sander et al. (2019)
G42058b	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH}$	$0.8*8.E-12$	Sander et al. (2019)*
G42058c	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	k_s*f_s00H*f_CHO	Sander et al. (2019)
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	$\text{HOOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	KAPNO	Sander et al. (2019)
G42061	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	$\text{KRO2NO3}*1.74$	Sander et al. (2019)
G42062a	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 2 \text{OH} + \text{HCHO} + \text{CO}_2$	KAPH02*r_C03_OH	Sander et al. (2019)
G42062b	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	KAPH02*r_C03_00H	Sander et al. (2019)
G42062c	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{O}_3$	KAPH02*r_C03_03	Sander et al. (2019)
G42063a	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2019)
G42063b	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$	k1_R02RC03*0.1	Sander et al. (2019)
G42064a	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$2.*k_{\text{R00HRO}}$	Sander et al. (2019)
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_s00H*f_C02H	Sander et al. (2019)
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_s00H*f_C02H+k_C02H	Sander et al. (2019)
G42066	TrGC	$\text{CH}_2\text{CO} + \text{OH} \rightarrow .6 \text{HCHO} + .6 \text{HO}_2 + .6 \text{CO} + .4 \text{HOOCH}_2\text{CO}_2\text{H}$	$2.8E-12*\exp(510./\text{temp})$	Baulch et al. (2005), Sander et al. (2019)
G42067a	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{OH}$	$(k_{\text{t}}*f_{\text{t00H}}*f_{\text{tOH}} + k_{\text{ROHRO}})$	Sander et al. (2019)
G42067b	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$	k_R00HRO	Sander et al. (2019)
G42068	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$3.46E12*\exp(-12500./(1.98*\text{temp}))$	Hermans et al. (2005), Sander et al. (2019)
G42069	TrGC	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$	$3.46E12*\exp(-12500./(1.98*\text{temp})) / (6.34E26*\exp(-14700./(1.98*\text{temp})))$	Hermans et al. (2005), Sander et al. (2019)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{CH}_3\text{CHOHOOH} + .3 \text{CH}_3\text{COOH} + .2 \text{CH}_3 + .2 \text{HCOOH} + .2 \text{OH}$	$5.6E-15*\exp(2300./\text{temp})$	Sander et al. (2019)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	k1_R02sOR02	Sander et al. (2019)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KRO2NO	Sander et al. (2019)
G42073	TrGCN	$\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$	$6.7E-13*\exp(-395./\text{temp})$	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_CH20NO2*f_CHO	Paulot et al. (2009a), Sander et al. (2019)*
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_0*f_CH20NO2*3.	Paulot et al. (2009a), Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G42075	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{OH}$	KAPH02	Rickard and Pascoe (2009)*
G42076	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G42077	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G42078	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G42079	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42080	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2\text{NO}_2$	k_3rd_iupac(temp, cair, 1.3E-29, 6.2, 8.8E-12, 0.0, 0.31)	Atkinson et al. (2006)
G42081	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$	k_3rd_iupac(temp, cair, REAL(4.8E-4*EXP(-9285./temp), SP), 0.0, REAL(8.8E15*EXP(-10440./temp), SP), 0.0, 0.31)	Atkinson et al. (2006)
G42082	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	9.50E-13*EXP(-650./temp)	Sander et al. (2019)*
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), Beyersdorf 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), Beyersdorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{ C}_2\text{H}_5\text{O}_2 + .95 \text{ HO}_2 + .05 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	3.0E-12*EXP(20./temp)	Sander et al. (2019), 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	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{ CH}_3 + .5 \text{ NCO} + .5 \text{ NCCH}_2\text{O}_2 + .5 \text{ OH}$	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	$\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$	k_R02_H02(temp, 2)	see note*
G42089a	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{HCHO}$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G42089b	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2$	k_CH2CHOH_OH_ALD	Sander et al. (2019), So et al. (2014)
G42090	TrGC	$\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*

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

#	labels	reaction	rate coefficient	reference
G42091	TrGC	$\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G42092	TrGC	$\text{HOCCOOH} + \text{OH} \rightarrow 2 \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	2.0 *k_co2h	see note*
G42093a	TrGC	$\text{HOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	k_t*f_toh*f_toh	see note*
G42093b	TrGC	$\text{HOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{CHOCHOHOH} + \text{HO}_2 + \text{H}_2\text{O}$	k_s*f_soh*f_pch2oh	see note*
G42093c	TrGC	$\text{HOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	2.0 * k_rohro	see note*
G42093d	TrGC	$\text{HOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HCHO} + \text{HCOOH} + \text{HO}_2 + \text{H}_2\text{O}$	k_rohro	see note*
G42094a	TrGC	$\text{CH}_3\text{CHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{HO}_2 + \text{H}_2\text{O}$	k_t*f_toh*f_toh	see note*
G42094b	TrGC	$\text{CH}_3\text{CHOHOH} + \text{OH} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{H}_2\text{O}$	2.0 * k_rohro	see note*
G42095a	TrGC	$\text{CHOHOHCOOH} + \text{OH} \rightarrow \text{HOCCOOH} + \text{HO}_2 + \text{H}_2\text{O}$	k_t*f_toh*f_toh*f_co2h	see note*
G42095b	TrGC	$\text{CHOHOHCOOH} + \text{OH} \rightarrow \text{HCOOH} + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	2.0 * k_rohro + k_co2h	see note*
G42096a	TrGC	$\text{CHOHOHCHOHOH} + \text{OH} \rightarrow 2 \text{HCOOH} + \text{HO}_2 + \text{H}_2\text{O}$	4.0 * k_rohro	see note*
G42096b	TrGC	$\text{CHOHOHCHOHOH} + \text{OH} \rightarrow \text{CHOHOHCOOH} + \text{HO}_2 + \text{H}_2\text{O}$	2.0 * k_t*f_toh*f_toh*f_pch2oh	see note*
G42097a	TrGC	$\text{CHOCHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2 + \text{H}_2\text{O}$	2.0 * k_rohro + k_t*f_o*f_pch2oh	see note*
G42097b	TrGC	$\text{CHOCHOHOH} + \text{OH} \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	k_t*f_toh*f_toh*f_cho	see note*
G42098a	TrGC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	k_t*f_toh*f_toh*f_pch2oh	see note*
G42098b	TrGC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	2.0 * k_rohro	see note*
G42098c	TrGC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{CHOCHOHOH} + \text{OH} + \text{H}_2\text{O}$	k_s*f_pch2oh*f_soh	see note*
G43000a	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_s	Sander et al. (2019)
G43000b	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	2.*k_p	Sander et al. (2019)
G43001a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{CHOHOOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	5.5E-15*EXP(-1880./temp)*.57	Atkinson et al. (2006)*
G43001b	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{OO}^*$	5.5E-15*EXP(-1880./temp)*.43	Atkinson et al. (2006)*
G43002	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO}_2$	k_3rd_iupac(temp, cair, 8.6E-27, 3.5, 3.E-11, 1., 0.5)	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO}_3\text{BO}_2$	4.6E-13*EXP(-1155./temp)	Wallington et al. (2018)
G43004	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G43005a	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	2.7E-12*EXP(360./temp)*(1.-alpha_AN(3, 2, 0, 0, 0, temp, cair))	Wallington et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G43005b	TrGCN	$iC_3H_7O_2 + NO \rightarrow iC_3H_7ONO_2$	$2.7E-12*EXP(360./temp)*alpha_AN(3,2,0,0,0,temp,cair)$	Wallington et al. (2018)
G43006	TrGC	$iC_3H_7O_2 \rightarrow .8 CH_3COCH_3 + .2 IPROPOL + .6 HO_2$	$2.*(1.6E-12*EXP(-2200./temp)*k_CH302)**(.5)*R02$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	$iC_3H_7OOH + OH \rightarrow iC_3H_7O_2 + H_2O$	k_R00HR0	Sander et al. (2019)
G43007b	TrGC	$iC_3H_7OOH + OH \rightarrow CH_3COCH_3 + H_2O + OH$	k_t*f_t00H	Sander et al. (2019)
G43008	TrGC	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	$1.9E-13*EXP(1300./temp)$	Atkinson (1997)*
G43009a	TrGCN	$C_3H_7O_2 + NO \rightarrow C_2H_5CHO + HO_2 + NO_2$	$2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,1,0,0,0,temp,cair))$	Wallington et al. (2018)
G43009b	TrGCN	$C_3H_7O_2 + NO \rightarrow C_3H_7ONO_2$	$2.7E-12*EXP(360./temp)*alpha_AN(3,1,0,0,0,temp,cair)$	Wallington et al. (2018)
G43010	TrGC	$C_3H_7O_2 \rightarrow .8 CH_3COCH_3 + .2 NPROPOL + .6 HO_2$	$2.*(k_CH302*3.E-13)**(.5)*R02$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43011	TrGC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	$(8.8E-12*EXP(-1320./temp)+1.7E-14*EXP(423./temp))$	Atkinson et al. (2006)*
G43012a	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	$8.6E-13*EXP(700./temp)*r_C0CH2O_2_00H$	Tyndall et al. (2001a), Sander et al. (2019)
G43012b	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow OH + CH_3C(O) + HCHO$	$8.6E-13*EXP(700./temp)*r_C0CH2O_2_OH$	Tyndall et al. (2001a), Sander et al. (2019)
G43013a	TrGCN	$CH_3COCH_2O_2 + NO \rightarrow CH_3C(O) + HCHO + NO_2$	$2.9E-12*EXP(300./temp)*(1.-alpha_AN(4,1,1,0,0,temp,cair))$	Burkholder et al. (2015)
G43013b	TrGCN	$CH_3COCH_2O_2 + NO \rightarrow NOA$	$2.9E-12*EXP(300./temp)*alpha_AN(4,1,1,0,0,temp,cair)$	Burkholder et al. (2015)
G43014	TrGC	$CH_3COCH_2O_2 \rightarrow .3 CH_3C(O) + .3 HCHO + .5 MGlyOX + .2 CH_3COCH_2OH$	$k1_R02pOR02$	Orlando and Tyndall (2012)
G43015a	TrGC	$CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2 + H_2O$	k_R00HR0	see note*
G43015b	TrGC	$CH_3COCH_2O_2H + OH \rightarrow MGlyOX + OH + H_2O$	$k_s*f_s00H*f_C0$	Sander et al. (2019)
G43016	TrGC	$CH_3COCH_2OH + OH \rightarrow MGlyOX + HO_2 + H_2O$	$1.6E-12*EXP(305./temp)$	Atkinson et al. (2006)
G43017	TrGC	$MGlyOX + OH \rightarrow .4 CH_3 + .6 CH_3C(O) + 1.4 CO + H_2O$	$1.9E-12*EXP(575./temp)$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$iC_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	$6.2E-13*EXP(-230./temp)$	Wallington et al. (2018)
G43021	TrGCN	$CH_3COCH_2O_2 + NO_3 \rightarrow CH_3C(O) + HCHO + NO_2$	$KR02N03$	Rickard and Pascoe (2009)
G43022	TrGC	$HYPPO2 \rightarrow CH_3CHO + HCHO + HO_2$	$k1_R02sOR02$	Rickard and Pascoe (2009)
G43023a	TrGC	$HYPPO2 + HO_2 \rightarrow HYPPO2H$	$k_R02_H02(temp,3)*(1.-r_CHOHCH2O2_OH)$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43023b	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp}, 3) * r_{\text{CHOHCH2O2_OH}}$	Rickard and Pascoe (2009)
G43024a	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02NO} * (1 - \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G43024b	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{PROPOLNO}_3$	$\text{KR02NO} * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G43025	TrGCN	$\text{HYPROPO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)
G43026a	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{HYPROPO}_2$	k_{R00HRO}	Rickard and Pascoe (2009)
G43026b	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{\text{s*f_sOH*f_pCH2OH}} + k_{\text{t*f_t00H*f_pCH2OH}})$	Sander et al. (2019)
G43027	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{HO}_2 \rightarrow \text{PR2O2HNO}_3$	$k_{\text{R02_HO2}}(\text{temp}, 3)$	Rickard and Pascoe (2009)
G43028	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G43029	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)
G43030a	TrGCN	$\text{PR2O2HNO}_3 + \text{OH} \rightarrow \text{PRONO}_3\text{BO}_2$	k_{R00HRO}	Rickard and Pascoe (2009)
G43030b	TrGCN	$\text{PR2O2HNO}_3 + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{\text{t*f_t00H*f_CH2ON02}}$	Sander et al. (2019)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HNO}_3$	$\text{KN03AL} * 2.4$	Rickard and Pascoe (2009)
G43032	TrGCN	$\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$	$(k_{\text{s*f_CO*f_ON02}} + k_{\text{p*f_CO}})$	Sander et al. (2019)
G43033	TrGC	$\text{HOCH}_2\text{COCHO} + \text{OH} \rightarrow .8609 \text{HOCH}_2\text{CO} + .8609 \text{CO} + .1391 \text{HCOCOCHO} + .1391 \text{HO}_2$	$(1.9\text{E}-12 * \text{EXP}(575./\text{temp}) + k_{\text{s*f_sOH*f_CO}})$	Sander et al. (2019)
G43034	TrGCN	$\text{HOCH}_2\text{COCHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL} * 2.4$	Sander et al. (2019)
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E}-14 * \text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Sander et al. (2019)
G43036	TrGC	$\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{HCOCO} + .6 \text{HCHO} + .2 \text{HCOCOCHO} + .2 \text{HOCH}_2\text{COCHO}$	$k1_{\text{R02pOR02}}$	Sander et al. (2019)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02NO	Sander et al. (2019)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{\text{R02_HO2}}(\text{temp}, 3) * r_{\text{COCH2O2_OOH}}$	Sander et al. (2019)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp}, 3) * r_{\text{COCH2O2_OH}}$	Sander et al. (2019)
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02NO3	Sander et al. (2019)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{\text{t*f_CO*f_O}}$	Sander et al. (2019)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s*f_s00H*f_CO}}$	Sander et al. (2019)*
G43040c	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G43041	TrGCN	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	$\text{KN03AL} * 2.4$	Sander et al. (2019)
G43042	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO}$	$k1_{\text{R02pOR02}}$	Sander et al. (2019)
G43043a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$k_{\text{R02_HO2}}(\text{temp}, 3) * r_{\text{COCH2O2_OOH}}$	Sander et al. (2019)
G43043b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp}, 3) * r_{\text{COCH2O2_OH}}$	Sander et al. (2019)
G43044	TrGCN	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02NO	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G43045a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCHO} + \text{OH}$	$k_{\text{s*f_s00H*f_CO}}$	Sander et al. (2019)
G43045b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{O}_2$	k_{R00HRO}	Sander et al. (2019)
G43045c	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E-}12*\text{EXP}(305./\text{temp})$	Sander et al. (2019)*
G43046	TrGC	$\text{CH}_3\text{CHCO} + \text{OH} \rightarrow .72 \text{ CO} + .72 \text{ CH}_3\text{CHO} + .72 \text{ HO}_2 + .21 \text{ CH}_3\text{COCO}_2\text{H} + .07 \text{ CH}_3\text{CHO} + .07 \text{ HO}_2 + .07 \text{ CO}_2$	$7.6\text{E-}11$	Hatakeyama et al. (1985), Sander et al. (2019)
G43047	TrGCN	$\text{PROPOLNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{\text{t*f_ON02*f_pCH2OH}+k_{\text{s*f_sOH*f_CH2ON02}}$	Sander et al. (2019)
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	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E-}13*\text{EXP}(-650./\text{temp})*f_{\text{CO}}$	Sander et al. (2019)*
G43051a	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G43051b	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s*f_s00H}}$	Sander et al. (2019)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f_pCH2OH}}$	Sander et al. (2019)*
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	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}*0.9}$	Sander et al. (2019)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	$k1_{\text{R02RC03}*0.1}$	Sander et al. (2019)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Sander et al. (2019), Groß et al. (2014)
G43055b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$	KAPH02*r_C03_OOH	Sander et al. (2019), Groß et al. (2014)
G43055c	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$	KAPH02*r_C03_O3	Sander et al. (2019), 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	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	$k_{\text{CH3C03_N02}}$	Rickard and Pascoe (2009)
G43058	TrGCN	$\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G43059	TrGC	$\text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$k_{\text{C02H}+k_{\text{p}+k_{\text{s*f_C02H}}}}$	Sander et al. (2019)*
G43060a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G43060b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f_C02H}+k_{\text{p}}}$	Sander et al. (2019)*
G43061	TrGCN	$\text{PPN} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f_cpan}+k_{\text{p}}}$	Sander et al. (2019)*
G43062	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_3 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G43063a	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Sander et al. (2019)
G43063b	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	$\text{KAPH02*(r_C03_OOH+r_C03_O3)}$	Sander et al. (2019)
G43064	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_2$	KAPNO	Sander et al. (2019)
G43065	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_3$	$k_{\text{CH3C03_N02}}$	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G43066	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2 + \text{NO}_2$	$\text{KR02N03} \cdot 1.74$	Sander et al. (2019)
G43067	TrGC	$\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2$	k1_R02RC03	Sander et al. (2019)
G43068	TrGC	$\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{CO} + \text{HO}_2$	$2 \cdot \text{k_t} \cdot \text{f_CO} \cdot \text{f_O}$	Sander et al. (2019)
G43069	TrGC	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$	$2.6\text{E}-12 \cdot \text{EXP}(200./\text{temp})$	Atkinson et al. (2006)
G43070a	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$4.6\text{E}-12 \cdot \text{EXP}(70./\text{temp}) \cdot (\text{k_s} \cdot \text{f_sOH} / (\text{k_p} + \text{k_s} \cdot \text{f_pCH2OH} + \text{k_s} \cdot \text{f_sOH}))$	Atkinson et al. (2006), Sander et al. (2019)*
G43070b	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO2} + \text{H}_2\text{O}$	$4.6\text{E}-12 \cdot \text{EXP}(70./\text{temp}) \cdot ((\text{k_p} + \text{k_s} \cdot \text{f_pCH2OH}) / (\text{k_p} + \text{k_s} \cdot \text{f_pCH2OH} + \text{k_s} \cdot \text{f_sOH}))$	Atkinson et al. (2006), Sander et al. (2019)*
G43071a	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$	$\text{k_CH2CHOH_OH_HCOOH}$	Sander et al. (2019), 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_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G43073	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G43074	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{k_s} \cdot \text{f_s00H} \cdot \text{f_CO} + \text{k_R00HRO}$	Sander et al. (2019)*
G43075a	TrGC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{HCOOH} + \text{H}_2\text{O}$	$2.0 \cdot \text{k_rohro}$	see note*
G43075b	TrGC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_2\text{H} + \text{H}_2\text{O}$	$\text{k_t} \cdot \text{f_toH} \cdot \text{f_toH} \cdot \text{f_co}$	see note*
G43202	TrGTerC	$\text{HCOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{CO}_3$	$4.29\text{E}-11$	Rickard and Pascoe (2009)
G43203	TrGTerCN	$\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$	$2 \cdot \text{KN03AL} \cdot 2.4$	Rickard and Pascoe (2009)
G43204a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{k1_R02RC03} \cdot 0.9$	Sander et al. (2019)
G43204b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$\text{k1_R02RC03} \cdot 0.1$	Sander et al. (2019)
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_CH3CO3_N02	Rickard and Pascoe (2009)
G43207a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{r_CO3_00H}$	Rickard and Pascoe (2009)
G43207b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{r_CO3_03}$	Rickard and Pascoe (2009)
G43207c	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{r_CO3_OH}$	Rickard and Pascoe (2009)
G43210	TrGTerCN	$\text{C}_3\text{PAN2} \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43211	TrGTerCN	$\text{C}_3\text{PAN2} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	$2.10\text{E}-11$	Rickard and Pascoe (2009)
G43212	TrGTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$2.14\text{E}-11$	Rickard and Pascoe (2009)
G43213a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$\text{k1_R02RC03} \cdot 0.9$	Sander et al. (2019)
G43213b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$\text{k1_R02RC03} \cdot 0.1$	Sander et al. (2019)
G43214	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{r_CO3_00H}$	Rickard and Pascoe (2009)
G43215b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{r_CO3_OH}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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*r_C03_03	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	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{C3DIALOOH}$	k_R02_H02(temp,3)*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G43418b	TrGAroC	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	k_R02_H02(temp,3)*r_C03_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_R02sOR02	Rickard and Pascoe (2009)*
G43422a	TrGAroC	$\text{HCOCOHC}_3 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G43422b	TrGAroC	$\text{HCOCOHC}_3 + \text{HO}_2 \rightarrow \text{HCOCOHC}_3\text{H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G43424	TrGAroCN	$\text{HCOCOHC}_3 + \text{NO} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G43425	TrGAroCN	$\text{HCOCOHC}_3 + \text{NO}_2 \rightarrow \text{HCOCOHPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G43426	TrGAroCN	$\text{HCOCOHC}_3 + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	$\text{HCOCOHC}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2$	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	$\text{HCOCOHPAN} \rightarrow \text{HCOCOHC}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	$\text{C32OH13CO} + \text{OH} \rightarrow \text{HCOCOHC}_3$	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	$\text{HCOCOHC}_3\text{H} + \text{OH} \rightarrow \text{HCOCOHC}_3$	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), Sander et al. (2019)
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), Sander et al. (2019)*
G44002	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	k_R02_H02(temp,4)	Rickard and Pascoe (2009)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	KR02N0*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.1273	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02NO}*(1-(0.1273*\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))) * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2019)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC4H9NO3}$	$\text{KR02NO}*(0.1273*\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})+0.8727*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009)*
G44004a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02NO3} * 0.1273$	Rickard and Pascoe (2009), Sander et al. (2019)
G44004b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02NO3} * 0.8727$	Rickard and Pascoe (2009), Sander et al. (2019)
G44005a	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{ROOHR0}	Sander et al. (2019)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}}*f_{\text{tOOH}}*f_{\text{alk}}*(k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2019)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t}}*f_{\text{tOOH}}*f_{\text{alk}}*(k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2019)
G44006a	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp}) * k_{\text{t}}/(3.*k_{\text{p}}+k_{\text{t}})$	Atkinson (2003)
G44006b	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(213./\text{temp}) * 3.*k_{\text{p}}/(3.*k_{\text{p}}+k_{\text{t}})$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$k_{1\text{R02tR02}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G44008	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{TC}_4\text{H}_9\text{OOH}$	$k_{\text{R02_H02}}(\text{temp}, 4)$	Rickard and Pascoe (2009)
G44009a	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02NO}*(1-\alpha_{\text{AN}}(4,3,0,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2019)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC4H9NO3}$	$\text{KR02NO}*\alpha_{\text{AN}}(4,3,0,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G44010a	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{ROOHR0}	Sander et al. (2019)
G44010b	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$3.*k_{\text{p}}*f_{\text{tCH2OH}}$	Sander et al. (2019)*
G44011	TrGCN	$\text{TC4H9NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$3.*k_{\text{p}}*f_{\text{CH2ON02}}$	Sander et al. (2019)*
G44012	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k_{1\text{R02sR02}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G44013	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$	$k_{\text{R02_H02}}(\text{temp}, 4)$	Rickard and Pascoe (2009)
G44014a	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$	$\text{KR02NO}*(1-\alpha_{\text{AN}}(4,2,0,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2019)
G44014b	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC4H9NO3}$	$\text{KR02NO}*\alpha_{\text{AN}}(4,2,0,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G44015a	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	k_{ROOHR0}	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{s00H}}+2.*k_{\text{s}}+k_{\text{t}}*f_{\text{pCH2OH}}$	Sander et al. (2019)*
G44016	TrGCN	$\text{IC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{ON02}}+2.*k_{\text{p}}+k_{\text{t}}*f_{\text{CH2ON02}}$	Sander et al. (2019)*
G44017	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .87 \text{ MGLYOX} + .5481 \text{ CO} + .1392 \text{ HO}_2 + .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .13 \text{ HCHO} + .04680 \text{ OH} + .04680 \text{ CO} + .07280 \text{ CH}_3\text{C(O)} + .026 \text{ CH}_3\text{CHO} + .026 \text{ CO}_2 + .026 \text{ HCHO} + .026 \text{ HO}_2 + .02402 \text{ MGLYOX} + .02402 \text{ H}_2\text{O}_2 + .00718 \text{ CH}_3\text{COCO}_2\text{H}$	$8.5\text{E}-16*\text{EXP}(-1520./\text{temp})$	Sander et al. (2019)
G44018	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{LHMVKABO}_2$	$2.6\text{E}-12*\text{EXP}(610./\text{temp})$	Sander et al. (2019), 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), Sander et al. (2019)*
G44020	TrGC	$\text{LMEKO}_2 + \text{HO}_2 \rightarrow \text{LMEKOOH}$	$k_{\text{R02_HO2}}(\text{temp}, 4)$	Sander et al. (2019)
G44021a	TrGCN	$\text{LMEKO}_2 + \text{NO} \rightarrow .62 \text{ CH}_3\text{CHO} + .62 \text{ CH}_3\text{C(O)} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{KR02NO}*(1-(.62*\alpha_{\text{AN}}(4, 2, 1, 0, 0, \text{temp}, \text{cair})+.38*\alpha_{\text{AN}}(4, 1, 0, 1, 0, \text{temp}, \text{cair})))$	Sander et al. (2019)*
G44021b	TrGCN	$\text{LMEKO}_2 + \text{NO} \rightarrow \text{LMEKNO}_3$	$\text{KR02NO}*(.62*\alpha_{\text{AN}}(4, 2, 1, 0, 0, \text{temp}, \text{cair})+.38*\alpha_{\text{AN}}(4, 1, 0, 1, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44022a	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow \text{LMEKO}_2 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G44022b	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow .62 \text{ BIACET} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O} + \text{OH}$	$(.62*k_{\text{t}}*f_{\text{t00H}}*f_{\text{CO}}+.38*k_{\text{s}}*f_{\text{s00H}})$	Sander et al. (2019)
G44023a	TrGCN	$\text{LC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{t}}*f_{\text{ON02}}*f_{\text{alk}}+k_{\text{p}}*f_{\text{alk}}+k_{\text{s}}*f_{\text{CH2ON02}}+k_{\text{p}})*(k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2019)*
G44023b	TrGCN	$\text{LC}_4\text{H}_9\text{NO}_3 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{p}}+k_{\text{s}}*(1+f_{\text{CH2ON02}}+f_{\text{ON02}})*f_{\text{alk}})*(k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2019)*
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*
G44026	TrGC	$\text{LMEKO}_2 \rightarrow .538 \text{ HCHO} + .538 \text{ CO}_2 + .459 \text{ HOCH}_2\text{CH}_2\text{O}_2 + .079 \text{ C}_2\text{H}_5\text{O}_2 + .462 \text{ CH}_3\text{C(O)} + .462 \text{ CH}_3\text{CHO}$	$(.62*k_{\text{R02s0R02}}+.38*k_{\text{R02p0R02}})$	Rickard and Pascoe (2009)*
G44027	TrGC	$\text{MACR} + \text{OH} \rightarrow .45 \text{ MACO}_3 + .55 \text{ MACRO}_2$	$8.\text{E}-12*\text{EXP}(380./\text{temp})$	Orlando et al. (1999b), Sander et al. (2019)
G44028	TrGC	$\text{MACR} + \text{O}_3 \rightarrow .5481 \text{ CO} + .1392 \text{ HO}_2 + .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .87 \text{ MGLYOX} + .13 \text{ HCHO} + .13 \text{ OH} + .065 \text{ HCOCOCH}_2\text{O}_2 + .065 \text{ CO} + .065 \text{ CH}_3\text{C(O)}$	$1.36\text{E}-15*\text{EXP}(-2112./\text{temp})$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44029	TrGCN	$\text{MACR} + \text{NO}_3 \rightarrow \text{MACO3} + \text{HNO}_3$	$\text{KN03AL} \times 2.0$	Rickard and Pascoe (2009)
G44030a	TrGC	$\text{MACO3} \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{CO}_2$	$\text{k1_R02RC03} \times 0.9$	Sander et al. (2019)
G44030b	TrGC	$\text{MACO3} \rightarrow \text{MACO2H}$	$\text{k1_R02RC03} \times 0.1$	Sander et al. (2019)
G44031a	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO2} + \text{OH}$	$\text{KAPH02} \times \text{r_C03_OH}$	Sander et al. (2019)
G44031b	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO3H}$	$\text{KAPH02} \times \text{r_C03_OOH}$	Sander et al. (2019)
G44031c	TrGC	$\text{MACO3} + \text{HO}_2 \rightarrow \text{MACO2H} + \text{O}_3$	$\text{KAPH02} \times \text{r_C03_O3}$	Sander et al. (2019)
G44032	TrGCN	$\text{MACO3} + \text{NO} \rightarrow \text{MACO2} + \text{NO}_2$	$8.70\text{E-}12 \times \text{EXP}(290./\text{temp})$	Sander et al. (2019)
G44033	TrGCN	$\text{MACO3} + \text{NO}_2 \rightarrow \text{MPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G44034	TrGCN	$\text{MACO3} + \text{NO}_3 \rightarrow \text{MACO2} + \text{NO}_2$	$\text{KR02N03} \times 1.74$	Sander et al. (2019)
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	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACRO} + \text{OH}$	$\text{k_R02_HO2}(\text{temp}, 4) \times \text{r_COCH202_OH}$	Sander et al. (2019)
G44036b	TrGC	$\text{MACRO2} + \text{HO}_2 \rightarrow \text{MACROOH}$	$\text{k_R02_HO2}(\text{temp}, 4) \times \text{r_COCH202_OOH}$	Sander et al. (2019)
G44037a	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRO} + \text{NO}_2$	$\text{KR02N0} \times (1. - \alpha_{\text{AN}}(6, 3, 1, 0, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44037b	TrGCN	$\text{MACRO2} + \text{NO} \rightarrow \text{MACRNO3}$	$\text{KR02N0} \times \alpha_{\text{AN}}(6, 3, 1, 0, 0, \text{temp}, \text{cair})$	Sander et al. (2019)
G44038	TrGCN	$\text{MACRO2} + \text{NO}_3 \rightarrow \text{MACRO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44039a	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{MACRO2}$	k_R00HRO	Sander et al. (2019)
G44039b	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$\text{k_t} \times \text{f_0} \times \text{f_tCH20H} \times \text{f_alk}$	Sander et al. (2019)
G44039c	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$(\text{k_s} \times \text{f_sOH} \times \text{f_pCH20H} + \text{k_R0HRO})$	Sander et al. (2019)
G44040	TrGC	$\text{MACROH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2$	$\text{k_t} \times \text{f_0} \times \text{f_tCH20H} \times \text{f_alk}$	Sander et al. (2019)
G44041	TrGC	$\text{MACRO} \rightarrow .885 \text{ CH}_3\text{COCH}_2\text{OH} + .885 \text{ CO} + .115 \text{ MGLYOX} + .115 \text{ HCHO} + \text{HO}_2$	KDEC	Sander et al. (2019)
G44042	TrGC	$\text{MACO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2 + \text{CO}_2$	$(\text{k_adt} + \text{k_adp}) \times \text{a_C02H} + \text{k_C02H}$	Sander et al. (2019)
G44043a	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{OH}$	$(\text{k_adt} + \text{k_adp}) \times \text{a_C02H}$	Sander et al. (2019)
G44043b	TrGC	$\text{MACO3H} + \text{OH} \rightarrow \text{MACO3}$	k_R00HRO	Sander et al. (2019)
G44044	TrGC	$\text{LHMKABO2} \rightarrow .024 \text{ CO2H3CHO} + .072 \text{ MGLYOX} + .072 \text{ HO}_2 + .072 \text{ HCHO} + .5280 \text{ CH}_3\text{C(O)} + .5280 \text{ HOCH}_2\text{CHO} + .176 \text{ BIACETOH} + .2 \text{ HO12CO3C4}$	$(.12 \times \text{k1_R02p0R02} + .88 \times \text{k1_R02s0R02})$	Sander et al. (2019)
G44045a	TrGC	$\text{LHMKABO2} + \text{HO}_2 \rightarrow \text{OH} + \text{HOCH}_2\text{CHO} + \text{CH}_3\text{C(O)}$	$\text{k_R02_HO2}(\text{temp}, 4) \times .88 \times \text{r_COCH202_OH}$	Sander et al. (2019)
G44045b	TrGC	$\text{LHMKABO2} + \text{HO}_2 \rightarrow \text{LHMKABOOH}$	$\text{k_R02_HO2}(\text{temp}, 4) \times (.12 + .88 \times \text{r_COCH202_OOH})$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44046a	TrGCN	$\text{LHMKABO}_2 + \text{NO} \rightarrow .12 \text{ MGLYOX} + .12 \text{ HO}_2 + .88 \text{ HOCH}_2\text{CHO} + .88 \text{ CH}_3\text{C(O)} + .12 \text{ HCHO} + \text{NO}_2$	$\text{KRO2NO} * (1 - (.12 * \alpha_{\text{AN}}(6, 1, 0, 1, 0, \text{temp}, \text{cair}) + .88 * \alpha_{\text{AN}}(6, 2, 1, 0, 0, \text{temp}, \text{cair})))$	Sander et al. (2019)
G44046b	TrGCN	$\text{LHMKABO}_2 + \text{NO} \rightarrow \text{MVKNO}_3$	$\text{KRO2NO} * (.12 * \alpha_{\text{AN}}(6, 1, 0, 1, 0, \text{temp}, \text{cair}) + .88 * \alpha_{\text{AN}}(6, 2, 1, 0, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)*
G44047	TrGCN	$\text{LHMKABO}_2 + \text{NO}_3 \rightarrow .12 \text{ MGLYOX} + .12 \text{ HO}_2 + .88 \text{ HOCH}_2\text{CHO} + .88 \text{ CH}_3\text{C(O)} + .12 \text{ HCHO} + .12 \text{ HO}_2 + \text{NO}_2$	KRO2NO_3	Sander et al. (2019)
G44048a	TrGC	$\text{LHMKABOOH} + \text{OH} \rightarrow \text{LHMKABO}_2$	k_{ROOHR0}	Sander et al. (2019)
G44048b	TrGC	$\text{LHMKABOOH} + \text{OH} \rightarrow .12 \text{ CO}_2\text{H}_3\text{CHO} + .88 \text{ BIACETOH} + \text{OH}$	$(.12 * k_{\text{s}} * f_{\text{s00H}} * f_{\text{pCH20H}} + .88 * k_{\text{t}} * f_{\text{t00H}} * f_{\text{pCH20H}} * f_{\text{CO}})$	Sander et al. (2019)
G44049a	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	$k_{\text{t}} * f_{\text{O}} * f_{\text{alk}}$	Sander et al. (2019)
G44049b	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{t}} * f_{\text{CO}} * f_{\text{tOH}} * f_{\text{CHO}}$	Sander et al. (2019)
G44050	TrGCN	$\text{CO}_2\text{H}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{HNO}_3$	$\text{KN03AL} * 4.0$	Rickard and Pascoe (2009)
G44051	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	$k_{\text{1}} \text{RO2RCO}_3$	Sander et al. (2019)
G44052a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	$\text{KAPH02} * r_{\text{CO}_3\text{OH}}$	Sander et al. (2019)
G44052b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} * r_{\text{CO}_3\text{O}_3}$	Sander et al. (2019)
G44052c	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3\text{H}$	$\text{KAPH02} * r_{\text{CO}_3\text{OOH}}$	Sander et al. (2019)
G44053	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	KAPNO	Sander et al. (2019)
G44054	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$\text{KRO2NO}_3 * 1.74$	Sander et al. (2019)
G44055a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	k_{ROOHR0}	Sander et al. (2019)
G44055b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{CO}_2 + \text{OH}$	$(k_{\text{t}} * f_{\text{CO}_2\text{H}} * f_{\text{CO}} * f_{\text{tOH}})$	Sander et al. (2019)
G44056	TrGC	$\text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCOCO}_2\text{H} + \text{HO}_2$	$k_{\text{t}} * f_{\text{CO}_2\text{H}} * f_{\text{CO}} * f_{\text{tOH}} + k_{\text{CO}_2\text{H}}$	Sander et al. (2019)
G44057a	TrGC	$\text{HO}_2\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{BIACETOH} + \text{HO}_2$	$k_{\text{t}} * f_{\text{tOH}} * f_{\text{alk}} * f_{\text{CO}}$	Sander et al. (2019)
G44057b	TrGC	$\text{HO}_2\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$	$k_{\text{s}} * f_{\text{sOH}} * f_{\text{alk}}$	Sander et al. (2019)
G44058	TrGC	$\text{MACO}_2 \rightarrow .65 \text{ CH}_3 + .65 \text{ CO} + .65 \text{ HCHO} + .35 \text{ OH} + .35 \text{ CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$	KDEC	Sander et al. (2019)
G44059	TrGC	$\text{LHMKABO}_2 \rightarrow .88 \text{ MGLYOX} + .88 \text{ HCHO} + .12 \text{ HOOCH}_2\text{CHO} + .12 \text{ CH}_3\text{C(O)} + \text{OH}$	k_{hsd}	Sander et al. (2019)
G44060	TrGC	$\text{MACRO}_2 \rightarrow \text{MGLYOX} + \text{HCHO} + \text{OH}$	k_{hsb}	Sander et al. (2019)
G44061a	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}} * f_{\text{s00H}} * f_{\text{CH20NO}_2} + k_{\text{ROHR0}}$	Sander et al. (2019)*
G44061b	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{BIACETOH} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t}} * f_{\text{ON}_2} * f_{\text{CO}} * f_{\text{pCH20H}}$	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G44062a	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t*f}_0\text{*f_CH2ON02}}$	Sander et al. (2019)*
G44062b	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{ROHRO}+k_{\text{s*f}_\text{s00H*f_CH2ON02}}$	Sander et al. (2019)*
G44063	TrGC	$\text{MACRO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH} + \text{CO}$	$k_{14\text{hsal}}$	Sander et al. (2019)
G44064	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow .9 \text{CH}_3\text{COCHCO} + .1 \text{CH}_3\text{C(O)} + .01 \text{GLYOX} + .18 \text{CO} + .09 \text{HO}_2 + \text{OH}$	$k_{15\text{hs24vynal}}$	Sander et al. (2019)
G44065	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOHCHCHO}$	$k_{\text{R02_H02}(\text{temp}, 4)}$	Sander et al. (2019)
G44066	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G44067	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44068	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO}$	$k_{1_R02\text{sOR02}}$	Sander et al. (2019)
G44069	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCCH}_3\text{CO} + \text{OH}$	$k_{15\text{hs24vynal}}$	Sander et al. (2019)
G44070	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G44071	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{HO}_2 \rightarrow \text{HCOCCH}_3\text{CHOOH}$	$k_{\text{R02_H02}(\text{temp}, 4)}$	Sander et al. (2019)
G44072	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO}_3 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44073	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO}$	$k_{1_R02\text{pOR02}}$	Sander et al. (2019)
G44074	TrGC	$\text{CH}_3\text{COOHCHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{OH}$	k_{hydec}	Sander et al. (2019)
G44075	TrGC	$\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{OH}$	k_{hydec}	Sander et al. (2019)
G44076	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G44077	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44078	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX} + \text{OH}$	$k_{\text{R02_H02}(\text{temp}, 4)}$	Sander et al. (2019)*
G44079	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} \rightarrow \text{CH}_3\text{C(O)} + \text{GLYOX}$	$k_{1_R02\text{sOR02}}$	Sander et al. (2019)
G44080	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$	$k_{1_R02\text{tOR02}}$	Sander et al. (2019)
G44081	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G44082	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}(\text{temp}, 4)}$	Sander et al. (2019)*
G44083	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44084	TrGC	$\text{HCOCCH}_3\text{CO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$1\text{E-}10\text{*a_CH0}$	Hatakeyama et al. (1985), Sander et al. (2019)
G44085	TrGC	$\text{CH}_3\text{COCHCO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$7.6\text{E-}11\text{*a_COCH3}$	Hatakeyama et al. (1985), Sander et al. (2019)*
G44086	TrGCN	$\text{LMEKNO}_3 + \text{OH} \rightarrow .62 \text{MGLYOX} + .62 \text{HCHO} + .62 \text{HO}_2 + .62 \text{NO}_2 + .38 \text{CH}_3\text{C(O)} + .38 \text{NO}_3\text{CH}_2\text{CHO}$	$.62\text{*}(k_{\text{p}}\text{*}(\text{f_CO}+\text{f_CH2ON02}))$ $+ .38\text{*}(k_{\text{s}}\text{*f_CH2ON02*f_CO})$	Sander et al. (2019)*
G44087	TrGC	$\text{MEPROPENE} + \text{OH} \rightarrow \text{IBUTOLBO}_2$	$9.4\text{E-}12\text{*EXP}(505./\text{temp})$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G44088a	TrGC	MEPROPENE + O ₃ → CH ₃ COCH ₃ + CH ₂ OO*	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Sander et al. (2019)
G44088b	TrGC	MEPROPENE + O ₃ → CH ₃ COCH ₂ O ₂ + OH + HCHO	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Sander et al. (2019)
G44089	TrGCN	MEPROPENE + NO ₃ → CH ₃ COCH ₃ + HCHO + NO ₂	3.4E-13	Atkinson et al. (2006), Sander et al. (2019)*
G44090	TrGC	IBUTOLBO2 → CH ₃ COCH ₃ + HCHO + HO ₂	k1_R02tOR02	Sander et al. (2019)
G44091a	TrGC	IBUTOLBO2 + HO ₂ → IBUTOLBOOH	k_R02_H02(temp,4)*r_COCH202_OOH	Sander et al. (2019)
G44091b	TrGC	IBUTOLBO2 + HO ₂ → CH ₃ COCH ₃ + HCHO + HO ₂ + OH	k_R02_H02(temp,4)*r_COCH202_OH	Sander et al. (2019)
G44092a	TrGCN	IBUTOLBO2 + NO → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02NO*(1.-alpha_AN(5,3,0,0,0, temp, cair))	Sander et al. (2019)
G44092b	TrGCN	IBUTOLBO2 + NO → IBUTOLBNO3	KR02NO*alpha_AN(5,3,0,0,0,temp, cair)	Sander et al. (2019)
G44093	TrGCN	IBUTOLBO2 + NO ₃ → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	KR02NO3	Sander et al. (2019)
G44094a	TrGC	IBUTOLBOOH + OH → IBUTOLBO2	k_R00HRO	Sander et al. (2019)
G44094b	TrGC	IBUTOLBOOH + OH → CH ₃ COCH ₃ + HCHO + HO ₂	k_s*f_s00H*f_pCH20H	Sander et al. (2019)
G44095	TrGCN	IBUTOLBNO3 + OH → CH ₃ COCH ₃ + HCHO + HO ₂ + NO ₂	3.*k_p	Sander et al. (2019)
G44096	TrGC	BUT1ENE + OH → LBUT1ENO2	6.6E-12*EXP(465./temp)	Atkinson et al. (2006)*
G44097a	TrGC	BUT1ENE + O ₃ → HCHO + .5 C ₂ H ₅ CHO + .5 H ₂ O ₂ + .5 CH ₃ CHO + .5 CO + .5 HO ₂	3.35E-15*EXP(-1745./temp)*.57	Atkinson et al. (2006), Sander et al. (2019)*
G44097b	TrGC	BUT1ENE + O ₃ → C ₂ H ₅ CHO + CH ₂ OO*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Sander et al. (2019)*
G44098	TrGCN	BUT1ENE + NO ₃ → C ₂ H ₅ CHO + HCHO + NO ₂	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44099	TrGC	LBUT1ENO2 → C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02sOR02	Sander et al. (2019)
G44100a	TrGC	LBUT1ENO2 + HO ₂ → LBUT1ENOOH	k_R02_H02(temp,4)*r_COCH202_OOH	Sander et al. (2019)
G44100b	TrGC	LBUT1ENO2 + HO ₂ → C ₂ H ₅ CHO + HCHO + HO ₂ + OH	k_R02_H02(temp,4)*r_COCH202_OH	Sander et al. (2019)
G44101a	TrGCN	LBUT1ENO2 + NO → C ₂ H ₅ CHO + HCHO + HO ₂ + NO ₂	KR02NO*(1.-alpha_AN(5,2,0,0,0, temp, cair))	Sander et al. (2019)
G44101b	TrGCN	LBUT1ENO2 + NO → LBUT1ENNO3	KR02NO*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44102	TrGCN	$\text{LBUT1ENO2} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Sander et al. (2019)
G44103a	TrGC	$\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{LBUT1ENO2}$	k_R00HR0	Sander et al. (2019)
G44103b	TrGC	$\text{LBUT1ENOOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HCHO} + \text{HO}_2$	k_t*f_t00H*f_pCH20H	Sander et al. (2019)*
G44104	TrGCN	$\text{LBUT1ENNO3} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	k_s*f_s0H*f_CH20N02	Sander et al. (2019)*
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), Sander et al. (2019)*
G44107	TrGCN	$\text{CBUT2ENE} + \text{NO}_3 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{NO}_2$	3.5E-13	Atkinson et al. (2006), Sander et al. (2019)*
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), Sander et al. (2019)
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), Sander et al. (2019)*
G44111	TrGC	$\text{BUT2OLO2} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2$	k1_R02s0R02	Sander et al. (2019)
G44112a	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow \text{BUT2OLOOH}$	k_R02_H02(temp,4)*r_COCH202_00H	Sander et al. (2019)
G44112b	TrGC	$\text{BUT2OLO2} + \text{HO}_2 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	k_R02_H02(temp,4)*r_COCH202_0H	Sander et al. (2019)
G44113a	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02NO*(1.-alpha_AN(5,2,0,0,0, temp, cair))	Sander et al. (2019)
G44113b	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow \text{BUT2OLNO3}$	KR02NO*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2019)
G44114	TrGCN	$\text{BUT2OLO2} + \text{NO}_3 \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Sander et al. (2019)
G44115a	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO2}$	k_R00HR0	Sander et al. (2019)
G44115b	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{LMEKOOH} + \text{HO}_2$	k_t*f_t0H*f_pCH20H	Sander et al. (2019)
G44115c	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO} + \text{OH}$	k_t*f_t00H*f_pCH20H	Sander et al. (2019)
G44116	TrGCN	$\text{BUT2OLNO3} + \text{OH} \rightarrow \text{LMEKNO3} + \text{HO}_2$	k_t*f_t0H*f_CH20N02	Sander et al. (2019)
G44117	TrGC	$\text{BUT2OLO} + \text{OH} \rightarrow \text{BIACET} + \text{HO}_2$	k_t*f_t0H*f_CO	Sander et al. (2019)
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)
G44119	TrGCN	$\text{IPRCHO} + \text{NO}_3 \rightarrow \text{IPRCO3} + \text{HNO}_3$	$1.67\text{E-}12*\text{EXP}(-1460./\text{temp})$	Atkinson et al. (2006)
G44120	TrGC	$\text{IPRCO3} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G44121a	TrGC	$\text{IPRCO3} + \text{HO}_2 \rightarrow \text{PERIBUACID}$	KAPH02*r_C03_00H	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44121b	TrGC	$\text{IPRCO}_3 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*(1.-\text{r_CO3_00H})$	Rickard and Pascoe (2009), Sander et al. (2019)
G44122	TrGCN	$\text{IPRCO}_3 + \text{NO}_2 \rightarrow \text{PIP}_\text{N}$	k_CH3CO3_N02	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	$\text{PERIBUACID} + \text{OH} \rightarrow \text{IPRCO}_3 + \text{H}_2\text{O}$	k_R00HRO	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	Sander et al. (2019)*
G44125	TrGCN	$\text{PIP}_\text{N} \rightarrow \text{IPRCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	$\text{PIP}_\text{N} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{NO}_2$	k_s*f_cpan	Sander et al. (2019)*
G44127	TrGC	$\text{MPROPENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{COCH}_3$	$\text{k_CH2CHOH_OH_HCOOH}$	Sander et al. (2019), So et al. (2014)*
G44128	TrGC	$\text{MPROPENOL} + \text{HCOOH} \rightarrow \text{IPRCHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44129	TrGC	$\text{IPRCHO} + \text{HCOOH} \rightarrow \text{MPROPENOL} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44130	TrGC	$\text{BUTENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C}_2\text{H}_5\text{CHO}$	$\text{k_CH2CHOH_OH_HCOOH}$	Sander et al. (2019), So et al. (2014)*
G44131	TrGC	$\text{BUTENOL} + \text{HCOOH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44132	TrGC	$\text{C}_3\text{H}_7\text{CHO} + \text{HCOOH} \rightarrow \text{BUTENOL} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44133	TrGC	$\text{HVMK} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Sander et al. (2019), 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	Sander et al. (2019), da Silva (2010)*
G44135	TrGC	$\text{CO}_2\text{C}_3\text{CHO} + \text{HCOOH} \rightarrow \text{HVMK} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44136	TrGC	$\text{HMAC} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{MGLYOX}$	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	$\text{HMAC} + \text{HCOOH} \rightarrow \text{IBUTDIAL} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44138	TrGC	$\text{IBUTDIAL} + \text{HCOOH} \rightarrow \text{HMAC} + \text{HCOOH}$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44139	TrGC	$\text{CO}_2\text{C}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{k_t*f_0*f_alk} + \text{k_s*f_CHO*f_CO}$	Sander et al. (2019)*
G44140	TrGCN	$\text{CO}_2\text{C}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2 + \text{HNO}_3$	KN03AL*4.0	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G44141	TrGC	IBUTDIAL + OH \rightarrow CH ₃ CHO + CO + HO ₂ + CO ₂ + H ₂ O	2.*k_t*f_0*f_alk+k_t*f_CHO*f_CHO	Sander et al. (2019)*
G44142	TrGCN	IBUTDIAL + NO ₃ \rightarrow CH ₃ CHO + CO + HO ₂ + CO ₂ + HNO ₃	2.*KN03AL*4.0	Sander et al. (2019)*
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	k_R02_H02(temp,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_s00H	Rickard and Pascoe (2009)*
G44203b	TrGTerC	CH ₃ COCOCH ₂ OOH + OH \rightarrow CH ₃ COCOCH ₂ O ₂	k_R00HRO	Rickard and Pascoe (2009)
G44204	TrGTerC	C44O2 + HO ₂ \rightarrow C44OOH	k_R02_H02(temp,4)	Rickard and Pascoe (2009)
G44205	TrGTerCN	C44O2 + NO \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O2 \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂	k1_R02sOR02	Rickard and Pascoe (2009)
G44207	TrGTerC	C44OOH + OH \rightarrow C44O2	7.46E-11	Rickard and Pascoe (2009)
G44208	TrGTerC	CHOC3COO2 \rightarrow HCOCH ₂ CO3 + HCHO	k1_R02pOR02	Rickard and Pascoe (2009)
G44209	TrGTerC	CHOC3COO2 + HO ₂ \rightarrow C413COOOH	k_R02_H02(temp,4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	CHOC3COO2 + NO \rightarrow HCOCH ₂ CO3 + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44211	TrGTerC	C413COOOH + OH \rightarrow CHOC3COO2	8.33E-11	Rickard and Pascoe (2009)
G44212	TrGTerC	C4CODIAL + OH \rightarrow C312COCO3	3.39E-11	Rickard and Pascoe (2009)
G44213	TrGTerCN	C4CODIAL + NO ₃ \rightarrow C312COCO3 + HNO ₃	2.*KN03AL*4.0	Rickard and Pascoe (2009)
G44214	TrGTerC	C312COCO3 \rightarrow HCOCOCH ₂ O ₂ + CO ₂	k1_R02RCO3	Rickard and Pascoe (2009)
G44215a	TrGTerC	C312COCO3 + HO ₂ \rightarrow C312COCO3H	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G44215b	TrGTerC	C312COCO3 + HO ₂ \rightarrow HCOCOCH ₂ O ₂ + CO ₂ + OH	KAPH02*(1.-r_C03_00H)	Rickard and Pascoe (2009)
G44216	TrGTerCN	C312COCO3 + NO ₂ \rightarrow C312COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44217	TrGTerCN	C312COCO3 + NO \rightarrow HCOCOCH ₂ O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44218	TrGTerC	C312COCO3H + OH \rightarrow C312COCO3	1.63E-11	Rickard and Pascoe (2009)
G44219	TrGTerCN	C312COPAN \rightarrow C312COCO3 + 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)	Sander et al. (2019)*
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 IPRHOCO3	1.4E-11	Rickard and Pascoe (2009)
G44224a	TrGTerC	IPRHOCO3 + HO ₂ \rightarrow CH ₃ COCH ₃ + CO ₂ + HO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G44224b	TrGTerC	IPRHOCO3 + HO ₂ \rightarrow IPRHOCO2H + O ₃	KAPH02*r_C03_O3	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44224c	TrGTerC	IPRHOCO3 + HO ₂ → IPRHOCO3H	KAPH02*r_C03_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G44225	TrGTerCN	IPRHOCO3 + NO → CH ₃ COCH ₃ + CO ₂ + HO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44226	TrGTerCN	IPRHOCO3 + NO ₂ → C4PAN5	k_CH3C03_N02	Rickard and Pascoe (2009)
G44227	TrGTerCN	IPRHOCO3 + NO ₃ → CH ₃ COCH ₃ + CO ₂ + HO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G44228a	TrGTerC	IPRHOCO3 → CH ₃ COCH ₃ + CO ₂ + HO ₂	k1_R02RC03*0.7	Rickard and Pascoe (2009)
G44228b	TrGTerC	IPRHOCO3 → IPRHOCO2H	k1_R02RC03*0.3	Rickard and Pascoe (2009)
G44229	TrGTerC	IPRHOCO2H + OH → CH ₃ COCH ₃ + CO ₂ + HO ₂ + H ₂ O	1.72E-12	Rickard and Pascoe (2009)
G44230	TrGTerC	OH + IPRHOCO3H → IPRHOCO3	4.80E-12	Rickard and Pascoe (2009)
G44231	TrGTerCN	C4PAN5 → IPRHOCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	C4PAN5 + OH → CH ₃ COCH ₃ + CO + NO ₂	4.75E-13	Rickard and Pascoe (2009)
G44233a	TrGTerC	MBOOO → IPRHOCO2H	1.60E-17*C(ind_H20)*(0.08+0.15)	Rickard and Pascoe (2009), Sander et al. (2019)
G44233b	TrGTerC	MBOOO → IBUTALOH + H ₂ O ₂	1.60E-17*C(ind_H20)*0.77	Rickard and Pascoe (2009), Sander et al. (2019)
G44234	TrGTerC	MBOOO + CO → IBUTALOH + CO ₂	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	MBOOO + NO → IBUTALOH + NO ₂	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	MBOOO + NO ₂ → IBUTALOH + NO ₃	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	MALANHY + OH → MALANHYO2	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	MALDIALOOH + OH → HOCOC4DIAL + OH	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	MALDIALOOH + OH → MALDIALO2	k_R00HRO	Rickard and Pascoe (2009)
G44402	TrGAroCN	NC4DCO2H + OH → MALANHY + NO ₂	k_R00HRO	Rickard and Pascoe (2009)*
G44403	TrGAroC	CO14O3CO2H + OH → HCOCH ₂ O ₂ + 2 CO ₂	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	BZFUOOH + OH → BZFUO2	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	HOCOC4DIAL + OH → CO2C4DIAL + HO ₂	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	MALDIALCO3 + HO ₂ → MALDALCO2H + O ₃	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G44406b	TrGAroC	MALDIALCO3 + HO ₂ → MALDALCO3H	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G44406c	TrGAroC	MALDIALCO3 + HO ₂ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)*
G44407	TrGAroCN	MALDIALCO3 + NO → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)*
G44408	TrGAroCN	MALDIALCO3 + NO ₂ → MALDIALPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO3 + NO ₃ → .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44410	TrGAroC	MALDIALCO3 \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO ₃ \rightarrow NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O ₃ \rightarrow .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H ₂ O ₂ + .5 CO + .5 CO ₂ + .5 HCOCH ₂ O ₂ + .5 OH	2.20E-19	see note*
G44413	TrGAroC	BZFUONE + OH \rightarrow BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH \rightarrow NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH \rightarrow MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH \rightarrow C3DIALO2 + CO ₂	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow C3DIALO2 + CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO2H + O ₃	KAPH02*r_C03_O3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO3H	KAPH02*r_C03_OOH	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO \rightarrow C3DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G44419	TrGAroCN	EPXDLCO3 + NO ₂ \rightarrow EPXDLPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G44420	TrGAroCN	EPXDLCO3 + NO ₃ \rightarrow C3DIALO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G44421	TrGAroC	EPXDLCO3 \rightarrow C3DIALO2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G44422	TrGAroC	MALNHYOHCO + OH \rightarrow CO + CO + CO + CO ₂ + HO ₂	5.68E-12	Rickard and Pascoe (2009)
G44423	TrGAroCN	MALDIAL + NO ₃ \rightarrow MALDIALCO3 + HNO ₃	2.*KN03AL*2.0	Rickard and Pascoe (2009)
G44424	TrGAroC	MALDIAL + O ₃ \rightarrow 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 \rightarrow .83 MALDIALCO3 + .17 MALDIALO2	5.20E-11	Rickard and Pascoe (2009)*
G44426	TrGAroC	MALANHYOOH + OH \rightarrow MALNHYOHCO + OH	4.66E-11	Rickard and Pascoe (2009)
G44427	TrGAroCN	MALDIALPAN + OH \rightarrow GLYOX + CO + CO + NO ₂	3.70E-11	Rickard and Pascoe (2009)
G44428	TrGAroCN	MALDIALPAN \rightarrow MALDIALCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G44429a	TrGAroC	MALANHYO2 + HO ₂ \rightarrow MALANHYOOH	k_R02_H02(temp,4)*(1.-r_COCH2O2_OH-r_CHOCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44429b	TrGAroC	MALANHYO2 + HO ₂ \rightarrow HCOCOHC03 + CO ₂ + OH	k_R02_H02(temp,4)*(r_COCH2O2_OH+r_CHOCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44430	TrGAroCN	MALANHYO2 + NO \rightarrow HCOCOHC03 + CO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G44431	TrGAroCN	MALANHYO2 + NO ₃ \rightarrow HCOCOHC03 + CO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 \rightarrow HCOCOHC03 + CO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G44433	TrGAroC	EPXDLCO3H + OH \rightarrow EPXDLCO3	2.62E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44434	TrGAroC	$\text{CO2C4DIAL} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CO} + \text{CO} + \text{HO}_2$	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	$\text{NBZFUO2} + \text{HO}_2 \rightarrow \text{NBZFUOOH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * (1 - r_{\text{COCH202_OH}})$	Rickard and Pascoe (2009), Sander et al. (2019)
G44435b	TrGAroCN	$\text{NBZFUO2} + \text{HO}_2 \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * r_{\text{COCH202_OH}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G44436	TrGAroCN	$\text{NBZFUO2} + \text{NO} \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44437	TrGAroCN	$\text{NBZFUO2} + \text{NO}_3 \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44438	TrGAroCN	$\text{NBZFUO2} \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2$	k1_R02sOR02	Rickard and Pascoe (2009)*
G44439	TrGAroC	$\text{MALDALCO2H} + \text{OH} \rightarrow .6 \text{ MALANHY} + \text{HO}_2 + .4 \text{ GLYOX} + .4 \text{ CO} + .4 \text{ CO}_2$	3.70E-11	Rickard and Pascoe (2009)*
G44440	TrGAroCN	$\text{EPXC4DIAL} + \text{NO}_3 \rightarrow \text{EPXDLCO3} + \text{HNO}_3$	2.*KN03AL*4.0	Rickard and Pascoe (2009)
G44441	TrGAroC	$\text{EPXC4DIAL} + \text{OH} \rightarrow \text{EPXDLCO3}$	4.32E-11	Rickard and Pascoe (2009)
G44442a	TrGAroC	$\text{MECOACETO2} + \text{HO}_2 \rightarrow \text{MECOACEOOH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * (1 - r_{\text{COCH202_OH}})$	Rickard and Pascoe (2009), Sander et al. (2019)
G44442b	TrGAroC	$\text{MECOACETO2} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{CO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * r_{\text{COCH202_OH}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G44443	TrGAroCN	$\text{MECOACETO2} + \text{NO} \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44444	TrGAroCN	$\text{MECOACETO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44445	TrGAroC	$\text{MECOACETO2} \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{CO}_2$	k1_R02pOR02	Rickard and Pascoe (2009)*
G44446	TrGAroCN	$\text{CO14O3CHO} + \text{NO}_3 \rightarrow \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{HNO}_3$	KN03AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	$\text{CO14O3CHO} + \text{OH} \rightarrow \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	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	$\text{BZFUO2} + \text{HO}_2 \rightarrow \text{BZFUOOH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * (1 - r_{\text{COCH202_OH}} - r_{\text{CHOHCH202_OH}})$	Rickard and Pascoe (2009), Sander et al. (2019)
G44449b	TrGAroC	$\text{BZFUO2} + \text{HO}_2 \rightarrow \text{CO14O3CHO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 4) * (r_{\text{COCH202_OH}} + r_{\text{CHOHCH202_OH}})$	Rickard and Pascoe (2009), Sander et al. (2019)
G44450	TrGAroCN	$\text{BZFUO2} + \text{NO} \rightarrow \text{CO14O3CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44451	TrGAroCN	$\text{BZFUO2} + \text{NO}_3 \rightarrow \text{CO14O3CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G44452	TrGAroC	$\text{BZFUO2} \rightarrow \text{CO14O3CHO} + \text{HO}_2$	k1_R02sOR02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44453	TrGAroC	BZFUCO + OH \rightarrow CO14O3CHO + HO ₂	1.78E-11	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO ₂ \rightarrow MALDIALOOH	k_R02_H02(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO ₂ \rightarrow GLYOX + GLYOX + HO ₂ + OH	k_R02_H02(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G44457	TrGAroCN	MALDIALO2 + NO \rightarrow GLYOX + GLYOX + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G44458	TrGAroCN	MALDIALO2 + NO ₃ \rightarrow GLYOX + GLYOX + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G44459	TrGAroC	MALDIALO2 \rightarrow GLYOX + GLYOX + HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH \rightarrow HCOCOCHO + CO + NO ₂	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN \rightarrow EPXDLCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH \rightarrow MECOACETO2	3.59E-12	Rickard and Pascoe (2009)
G45000	TrGC	C ₅ H ₈ + O ₃ \rightarrow .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), Sander et al. (2019)
G45001	TrGC	C ₅ H ₈ + OH \rightarrow .63 LISOPAB + .30 LISOPCD + .07 LISOPEFO2	2.7E-11*EXP(390./temp)	Atkinson et al. (2006), Sander et al. (2019)
G45002	TrGCN	C ₅ H ₈ + NO ₃ \rightarrow NISOPO2	3.0E-12*EXP(-450./temp)	Atkinson et al. (2006)
G45003a	TrGC	LISOPAB + O ₂ \rightarrow LISOPACO2	5.530E-13	Sander et al. (2019)
G45003b	TrGC	LISOPAB + O ₂ \rightarrow ISOPBO2	3.E-12	Sander et al. (2019)
G45004a	TrGC	LISOPCD + O ₂ \rightarrow LDISOPACO2	6.780E-13	Sander et al. (2019)
G45004b	TrGC	LISOPCD + O ₂ \rightarrow ISOPDO2	3.E-12	Sander et al. (2019)
G45005	TrGC	LISOPACO2 \rightarrow LISOPAB + O ₂	3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4	Sander et al. (2019)
G45006	TrGC	ISOPBO2 \rightarrow LISOPAB + O ₂	3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp)	Sander et al. (2019)
G45007	TrGC	LDISOPACO2 \rightarrow LISOPCD + O ₂	5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58	Sander et al. (2019)
G45008	TrGC	ISOPDO2 \rightarrow LISOPCD + O ₂	5.0E14*exp(-10120./temp)+8.25E14*exp(-10220./temp)	Sander et al. (2019)
G45009a	TrGC	LISOPACO2 \rightarrow C1ODC2O2C4OOH	k_16hsz14 * 2./3.*(1.-f_HPAL)	Sander et al. (2019)
G45009b	TrGC	LISOPACO2 \rightarrow LZCODC23DBCOOH + HO ₂	k_16hsz14 * (2./3.*f_HPAL + 1./3.)	Sander et al. (2019)
G45010a	TrGC	LDISOPACO2 \rightarrow C1OOHC3O2C4OD	k_16hsz41 * 2./3.*(1.-f_HPAL)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45010b	TrGC	$\text{LISOPACO}_2 \rightarrow \text{LZCODC23DBCOOH} + \text{HO}_2$	$k_{16\text{hsz41}} * (2./3.*f_{\text{HPAL}} + 1./3.)$	Sander et al. (2019)
G45011	TrGC	$\text{LISOPACO}_2 \rightarrow .9 \text{ LISOPACO} + .1 \text{ ISOPAHO}$	$k_{1_R02\text{LISOPACO}_2}$	Rickard and Pascoe (2009), Sander et al. (2019)
G45012	TrGC	$\text{LISOPACO}_2 + \text{HO}_2 \rightarrow \text{LISOPACOOH}$	$k_{R02_H02}(\text{temp}, 5)$	Rickard and Pascoe (2009)
G45013a	TrGCN	$\text{LISOPACO}_2 + \text{NO} \rightarrow \text{LISOPACO} + \text{NO}_2$	$\text{KR02NO}*(1.-\alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45013b	TrGCN	$\text{LISOPACO}_2 + \text{NO} \rightarrow \text{LISOPACNO}_3$	$\text{KR02NO}*\alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair})$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45014	TrGCN	$\text{LISOPACO}_2 + \text{NO}_3 \rightarrow \text{LISOPACO} + \text{NO}_2$	KR02NO_3	Rickard and Pascoe (2009)
G45015	TrGC	$\text{LISOPACO}_2 \rightarrow .9 \text{ LISOPACO} + .1 \text{ ISOPAHO}$	$k_{1_R02\text{LISOPACO}_2}$	Rickard and Pascoe (2009), Sander et al. (2019)
G45016	TrGC	$\text{LISOPACO}_2 + \text{HO}_2 \rightarrow \text{LISOPACOOH}$	$k_{R02_H02}(\text{temp}, 5)$	Rickard and Pascoe (2009)
G45017a	TrGCN	$\text{LISOPACO}_2 + \text{NO} \rightarrow \text{LISOPACO} + \text{NO}_2$	$\text{KR02NO}*(1.-\alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45017b	TrGCN	$\text{LISOPACO}_2 + \text{NO} \rightarrow \text{LISOPACNO}_3$	$\text{KR02NO}*\alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair})$	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45018	TrGCN	$\text{LISOPACO}_2 + \text{NO}_3 \rightarrow \text{LISOPACO} + \text{NO}_2$	KR02NO_3	Rickard and Pascoe (2009)
G45019a	TrGC	$\text{LISOPACOOH} + \text{OH} \rightarrow \text{LISOPACO}_2$	k_{ROOHRO}	Sander et al. (2019)
G45019b	TrGC	$\text{LISOPACOOH} + \text{OH} \rightarrow \text{LZCODC23DBCOOH} + \text{HO}_2$	$k_{s*f_allyl*f_sOH}$	Sander et al. (2019)
G45019c	TrGC	$\text{LISOPACOOH} + \text{OH} \rightarrow \text{LHC4ACCHO} + \text{OH}$	$(k_{s*f_s00H*f_allyl} + k_{\text{ROHRO}})$	Sander et al. (2019)
G45019d	TrGC	$\text{LISOPACOOH} + \text{OH} \rightarrow \text{LIEPOX} + \text{OH}$	$(k_{\text{adt}} + k_{\text{ads}})*a_{\text{CH2OH}}*a_{\text{CH2OOH}}$	Sander et al. (2019)*
G45020	TrGC	$\text{ISOPAHO} + \text{OH} \rightarrow \text{LHC4ACCHO} + \text{HO}_2$	$(k_{\text{adt}} + k_{\text{ads}})*a_{\text{CH2OH}}*a_{\text{CH2OH}} + k_{s*f_sOH*f_allyl} + k_{\text{ROHRO}}$	Sander et al. (2019)
G45021	TrGCN	$\text{LISOPACNO}_3 + \text{OH} \rightarrow \text{LISOPACNO}_3\text{O}_2$	$(k_{\text{adt}} + k_{\text{ads}})*a_{\text{CH2ONO}_2}*a_{\text{CH2OH}}$	Sander et al. (2019)*
G45022	TrGC	$\text{ISOPBO}_2 \rightarrow .8 \text{ MVK} + .8 \text{ HCHO} + .8 \text{ HO}_2 + .2 \text{ ISOPBOH}$	$k_{1_R02\text{ISOPBO}_2}$	Rickard and Pascoe (2009)
G45023a	TrGC	$\text{ISOPBO}_2 + \text{HO}_2 \rightarrow \text{ISOPBOOH}$	$k_{R02_H02}(\text{temp}, 5)*(1.-r_{\text{CHOHCH2O}_2_OH})$	Sander et al. (2019)
G45023b	TrGC	$\text{ISOPBO}_2 + \text{HO}_2 \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$k_{R02_H02}(\text{temp}, 5)*r_{\text{CHOHCH2O}_2_OH}$	Sander et al. (2019)
G45024a	TrGCN	$\text{ISOPBO}_2 + \text{NO} \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02NO}*(1.-\alpha_{\text{AN}}(6, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Lockwood et al. (2010), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45024b	TrGCN	ISOPBO2 + NO → ISOPBNO3	KR02N0*alpha_AN(6,3,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45025	TrGCN	ISOPBO2 + NO ₃ → MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45026a	TrGC	ISOPBOOH + OH → LIEPOX + OH	(k_ads+k_adp)*a_CH200H	Paulot et al. (2009b), Sander et al. (2019)
G45026b	TrGC	ISOPBOOH + OH → ISOPBO2	k_R00HRO	Sander et al. (2019)
G45026c	TrGC	ISOPBOOH + OH → MGLYOX + HOCH ₂ CHO	k_ROHRO+k_s*f_alk*f_sOH	Sander et al. (2019)
G45027	TrGC	ISOPBOOH + O ₃ → .1368 MACROOH + .1368 H ₂ O ₂ + .2280 HO ₂ + .4332 CH ₃ COCH ₂ OH + .2280 CO ₂ + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO ₂ + .06880 OH + .2709 CO + .1591 CH ₂ OO	1.E-17	Sander et al. (2019)
G45028	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃	k_s*f_alk*f_sOH+(k_adp+k_ads)*a_CH2OH	Sander et al. (2019)
G45029	TrGCN	ISOPBNO3 + OH → ISOPBDNO3O2	(k_adt+k_adp)*f_CH20N02	Sander et al. (2019)
G45030	TrGC	ISOPDO2 → .8 MACR + .8 HCHO + .8 HO ₂ + .1 HCOC5 + .1 ISOPDOH	k1_R02ISOPDO2	Rickard and Pascoe (2009)
G45031a	TrGC	ISOPDO2 + HO ₂ → ISOPDOOH	k_R02_HO2(temp,5)*(1-r_CHOCH202_OH)	Sander et al. (2019)
G45031b	TrGC	ISOPDO2 + HO ₂ → MACR + HCHO + HO ₂ + OH	k_R02_HO2(temp,5)*r_CHOCH202_OH	Sander et al. (2019)
G45032a	TrGCN	ISOPDO2 + NO → MACR + HCHO + HO ₂ + NO ₂	KR02N0*(1-alpha_AN(6,2,0,0,0, temp, cair))	Lockwood et al. (2010), Sander et al. (2019)
G45032b	TrGCN	ISOPDO2 + NO → ISOPDNO3	KR02N0*alpha_AN(6,2,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45033	TrGCN	ISOPDO2 + NO ₃ → MACR + HCHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45034a	TrGC	ISOPDOOH + OH → LIEPOX + OH	(k_adt+k_adp)*a_CH200H	Paulot et al. (2009b), Sander et al. (2019)
G45034b	TrGC	ISOPDOOH + OH → ISOPDO2	k_R00HRO	Sander et al. (2019)
G45034c	TrGC	ISOPDOOH + OH → HCOC5 + OH	k_t*f_t0OH*f_allyl*f_pCH2OH	Sander et al. (2019)
G45034d	TrGC	ISOPDOOH + OH → CH ₃ COCH ₂ OH + GLYOX + OH	k_s*f_pCH2OH*f_sOH	Sander et al. (2019)
G45035	TrGC	ISOPDOOH + O ₃ → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO ₂ + .2079 CO + .1221 CH ₂ OO	1.E-17	Sander et al. (2019)
G45036	TrGC	ISOPDOH + OH → HCOC5 + HO ₂	2.*k_ROHRO+(k_t*f_tOH*f_allyl+k_s*f_sOH)*f_pCH2OH+(k_adt+k_adp)*a_CH2OH	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45037	TrGCN	ISOPDNO3 + OH → ISOPBDNO3O2	(k _{adp} +k _{ads})*a _{CH2ON02}	Sander et al. (2019)*
G45038	TrGCN	NISOP02 → .8 NC4CHO + .6 HO ₂ + .2 LISOPACNO3	k1_R02LISOPAC02	Rickard and Pascoe (2009)
G45039	TrGCN	NISOP02 + HO ₂ → NISOP0OH	k_R02_H02(temp,5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOP02 + NO → NC4CHO + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOP02 + NO ₃ → NC4CHO + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G45042	TrGCN	NISOP0OH + OH → NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC4CHO + OH → LNISO3	(k _{adt} +k _{ads})*a _{CH0} *a _{CH2ON02}	Sander et al. (2019)*
G45044	TrGCN	NC4CHO + O ₃ → .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	Sander et al. (2019)
G45045	TrGCN	NC4CHO + NO ₃ → LNISO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO3 + HO ₂ → LNISOOH	0.5*k_R02_H02(temp,5)+0.5*KAPH02	Rickard and Pascoe (2009)
G45047	TrGCN	LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	0.5*KAPN0+0.5*KR02N0	Rickard and Pascoe (2009)*
G45048	TrGCN	LNISO3 + NO ₃ → NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	KR02N03*1.37	Rickard and Pascoe (2009)
G45049	TrGCN	LNISOOH + OH → LNISO3	2.65E-11	Rickard and Pascoe (2009)
G45050a	TrGC	LHC4ACCHO + OH → LC578O2	(k _{adtertprim} +k _{ads})*a _{CH0} *a _{CH2OH}	Sander et al. (2019)
G45050b	TrGC	LHC4ACCHO + OH → LHC4ACCO3	k _t *f ₀	Sander et al. (2019)
G45050c	TrGC	LHC4ACCHO + OH → C4MDIAL + HO ₂	k _s *f _{sOH} *f _{allyl}	Sander et al. (2019)
G45051	TrGC	LHC4ACCHO + O ₃ → .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 → LHC4ACCO3 + HNO ₃	KN03AL*4.25	Rickard and Pascoe (2009)
G45053	TrGC	LC578O2 → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂	k1_R02tOR02	Rickard and Pascoe (2009)
G45054a	TrGC	LC578O2 + HO ₂ → MGLYOX + HOCH ₂ CHO + OH	k_R02_H02(temp,5)*r _{COCH202_OH}	Rickard and Pascoe (2009)
G45054b	TrGC	LC578O2 + HO ₂ → LC578OOH	k_R02_H02(temp,5)*r _{COCH202_OOH}	Rickard and Pascoe (2009)
G45055	TrGCN	LC578O2 + NO → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH ₂ CHO + .75 HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
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	$\text{LC578O2} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCH}_2\text{CHO} + .75 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	k_hsb	Sander et al. (2019)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	k_R00HR0	Sander et al. (2019)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C10DC2OOHC4OD} + \text{HO}_2$	k_t*f_0*f_tCH2OH*f_alk+k_t*f_tOH*f_pCH2OH*f_pCH2OH+k_s*f_sOH*f_pCH2OH	Sander et al. (2019)
G45059a	TrGC	$\text{LHC4ACCO3} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2019)
G45059b	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LHC4ACCO2H}$	k1_R02RC03*0.1	Sander et al. (2019)
G45060a	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 2 \text{ OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	KAPH02*r_C03_OH	Sander et al. (2019)
G45060b	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO3H}$	KAPH02*r_C03_OOH	Sander et al. (2019)
G45060c	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$	KAPH02*r_C03_O3	Sander et al. (2019)
G45061	TrGCN	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KAPNO	Sander et al. (2019)
G45062	TrGCN	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45063	TrGCN	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KR02N03*1.74	Sander et al. (2019)
G45064a	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	2.52E-11	Sander et al. (2019)
G45064b	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	2.88E-11	Rickard and Pascoe (2009)
G45065	TrGCN	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45066	TrGCN	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	2.52E-11	Rickard and Pascoe (2009)
G45067	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	3.81E-11	Rickard and Pascoe (2009)
G45068	TrGC	$\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{ H}_2\text{O}_2 + .67 \text{ HCHO} + .2079 \text{ CO} + .1221 \text{ CH}_2\text{OO} + .05280 \text{ OH}$	$7.51\text{E-16} * \text{EXP}(-1521./\text{temp})$	Sander et al. (2019)
G45069	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	k1_R02t0R02	Sander et al. (2019)
G45070a	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	k_R02_H02(temp,5)*r_COCH202_OH	Sander et al. (2019)
G45070b	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	k_R02_H02(temp,5)*r_COCH202_OOH	Sander et al. (2019)
G45071	TrGCN	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G45072	TrGCN	$\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G45073	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	9.7E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45074	TrGC	LIEPOX + OH \rightarrow DBIO2 + H ₂ O	5.78E-11*EXP(-400./temp) *(1.52/3.+0.98*2./3.)/1.51	Paulot et al. (2009b), Bates et al. (2014), Sander et al. (2019)*
G45075	TrGC	ISOPBO2 \rightarrow MVK + HCHO + OH	k_hsb	Sander et al. (2019)
G45076	TrGC	ISOPDO2 \rightarrow MACR + HCHO + OH	k_hsd	Sander et al. (2019)
G45077a	TrGC	LZCODC23DBCOOH + OH \rightarrow .6 C1ODC2O2C4OOH + .4 C1OOHC2O2C4OD	k_adt*a_CH0*a_CH200H	Sander et al. (2019)
G45077b	TrGC	LZCODC23DBCOOH + OH \rightarrow .6 C1ODC3O2C4OOH + .4 C1OOHC3O2C4OD	k_ads*a_CH0*a_CH200H	Sander et al. (2019)
G45077c	TrGC	LZCODC23DBCOOH + OH \rightarrow LZCO3HC23DBCOD	k_t*f_0*f_alk+k_R00HR0	Sander et al. (2019)
G45077d	TrGC	LZCODC23DBCOOH + OH \rightarrow C4MDIAL + OH	k_s*f_s00H*f_allyl	Sander et al. (2019)
G45078	TrGC	LZCODC23DBCOOH + O ₃ \rightarrow .4672 OH + .2336 HCOCOCH ₂ O ₂ + .2336 CO + .2336 CH ₃ C(O) + .4672 HOOCH ₂ CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH ₂ CHO + .02765 H ₂ O ₂ + .02592 CH ₃ OOH + .02592 CO ₂ + .01037 HCOCO + .01555 CH ₂ OO + .01555 CO + .006908 HOOCH ₂ CO ₃ + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH ₂ OOH + .2628 GLYOX + .0972 CH ₃ COCH ₂ O ₂ H + .00972 HCOCO ₂ H + .005832 GLYOX + .005832 H ₂ O ₂ + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO ₂ + .01458 HCOOH + .01458 CO	2.4E-17	Sander et al. (2019)
G45079	TrGC	C1OOHC2O2C4OD \rightarrow .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH	k1_R02t0R02	Sander et al. (2019)
G45080	TrGCN	C1OOHC2O2C4OD + NO \rightarrow .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH + NO ₂	KR02N0	Sander et al. (2019)*
G45081a	TrGC	C1OOHC2O2C4OD + HO ₂ \rightarrow C1OOHC2OOHC4OD	k_R02_H02(temp,5)*r_COCH202_OOH	Sander et al. (2019)
G45081b	TrGC	C1OOHC2O2C4OD + HO ₂ \rightarrow .78 CH ₃ COCH ₂ O ₂ H + .78 HOCHCHO + .22 CO ₂ H ₃ CHO + .22 HCHO + 1.22 OH	k_R02_H02(temp,5)*r_COCH202_OH	Sander et al. (2019)
G45082	TrGC	C1OOHC2O2C4OD \rightarrow CH ₃ COCH ₂ O ₂ H + GLYOX + OH	k_hsb	Sander et al. (2019)
G45083	TrGC	C1ODC2O2C4OOH \rightarrow OH + C1ODC2OOHC4OD	k_15hsdhb	Sander et al. (2019)
G45084a	TrGC	C1OOHC2OOHC4OD + OH \rightarrow C1ODC2OOHC4OD + OH	2.*k_s*f_s00H*f_tCH20H	Sander et al. (2019)
G45084b	TrGC	C1OOHC2OOHC4OD + OH \rightarrow CH ₃ COCH ₂ O ₂ H + 2 CO + 2 HO ₂ + OH	k_t*f_t0H*f_pCH20H*f_pCH20H	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45084c	TrGC	$\text{C1OOHC2OOHC4OD} + \text{OH} \rightarrow \text{C1OOHC2O2C4OD}$	k_{R00HR0}	Sander et al. (2019)
G45085	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{CO2H3CHO} + \text{CO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t*f}_0\text{*f}_\text{tCH2OH}+\text{k}_\text{t*f}_\text{tOH*f}_\text{tOH*f}_\text{tCH0}}$	Sander et al. (2019)
G45086	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{HOOCH2CHO} + \text{HO}_2$	$k1_{\text{R02s0R02}}$	Sander et al. (2019)
G45087	TrGCN	$\text{C1ODC3O2C4OOH} + \text{NO} \rightarrow \text{MGLYOX} + \text{HOOCH2CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Sander et al. (2019)
G45088	TrGC	$\text{C1ODC3O2C4OOH} + \text{HO}_2 \rightarrow .5 \text{ CH}_3\text{C(O)} + .5 \text{ CO} + .5 \text{ MGLYOX} + .5 \text{ HO}_2 + \text{HOOCH}_2\text{CO}_3$	$k_{\text{R02_HO2}}(\text{temp}, 5)$	Sander et al. (2019)
G45089	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{OH} + \text{HOOCH2CHO}$	k_{hsd}	Sander et al. (2019)
G45090	TrGC	$\text{C1OOHC3O2C4OD} \rightarrow .625 \text{ MGLYOX} + 2 \text{ CO} + 1.625 \text{ HO}_2 + .375 \text{ CH}_3\text{C(O)} + .375 \text{ CO}_2 + \text{OH}$	$k_{15\text{hsd}hb}$	Sander et al. (2019)
G45091	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LZCO3HC23DBCOD} + \text{HO}_2$	k_{16hs}	Sander et al. (2019)
G45092a	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{C1ODC2O2C4OD}$	$(k_{\text{adt}}+k_{\text{ads}})*a_{\text{CH0}}*a_{\text{CH0}}$	Sander et al. (2019)*
G45092b	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{LZCO3C23DBCOD}$	$2.*k_{\text{t*f}_0\text{*f}_\text{alk}}$	Sander et al. (2019)*
G45093	TrGCN	$\text{C4MDIAL} + \text{NO}_3 \rightarrow \text{LZCO3C23DBCOD} + \text{HNO}_3$	KN03AL*4.25*2.	Sander et al. (2019)*
G45094a	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$	$k_{\text{R02_HO2}}(\text{temp}, 5)*r_{\text{COCH2O2_OH}}$	Sander et al. (2019)
G45094b	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1ODC2OOHC4OD}$	$k_{\text{R02_HO2}}(\text{temp}, 5)*r_{\text{COCH2O2_OOH}}$	Sander et al. (2019)
G45095	TrGCN	$\text{C1ODC2O2C4OD} + \text{NO} \rightarrow \text{NO}_2 + \text{MGLYOX} + \text{HOCHCHO}$	KR02N0	Sander et al. (2019)*
G45096	TrGC	$\text{C1ODC2O2C4OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$	$k1_{\text{R02t0R02}}$	Sander et al. (2019)
G45097a	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO}$	$(2.*k_{\text{t*f}_0\text{*f}_\text{tCH2OH*f}_\text{alk}+k_{\text{t*f}_\text{tOH*f}_\text{CH0*f}_\text{pCH2OH}})*.5$	Sander et al. (2019)
G45097b	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + \text{OH}$	$(2.*k_{\text{t*f}_0\text{*f}_\text{tCH2OH*f}_\text{alk}+k_{\text{t*f}_\text{tOH*f}_\text{CH0*f}_\text{pCH2OH}})*.5$	Sander et al. (2019)
G45098	TrGCN	$\text{LISOPACNO3O2} + \text{NO} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH2CHO} + .225 \text{ H}_2\text{O}_2 + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G45099	TrGCN	$\text{LISOPACNO3O2} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH2CHO} + .225 \text{ H}_2\text{O}_2$	$k1_{\text{R02t0R02}}+k_{\text{R02_HO2}}(\text{temp}, 5)*c(\text{ind_HO2})$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45100	TrGCN	ISOPBDNO3O2 + NO → .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRNO ₃ + .14 MVKNO ₃ + .4 HCHO + .4 HO ₂ + 1.6 NO ₂	KR02N0	Sander et al. (2019)*
G45101	TrGCN	ISOPBDNO3O2 → .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 MACRNO ₃ + .14 MVKNO ₃ + .4 HCHO + .4 HO ₂ + .6 NO ₂	k1_R02sOR02+k_R02_H02(temp,5) *c(ind_H02)	Sander et al. (2019)
G45102	TrGCN	LISOPACNO ₃ + O ₃ → .8704 OH + .365 HO ₂ + .73 MGLYOX + .4325 NO ₃ CH ₂ CHO + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .4325 NO ₂ + .0891 H ₂ O ₂ + .135 NOA + .0675 HOCHCHO + .3866 HOCH ₂ CHO + .0405 CH ₃ OH + .0405 CO + .0054 HOCH ₂ CO	2.8E-17	Feierabend et al. (2008), Sander et al. (2019)
G45103	TrGC	DB1O2 → DB1O2	k1_R02sOR02	Sander et al. (2019)
G45104a	TrGC	DB1O2 + HO ₂ → DB1OOH	k_R02_H02(temp,5)*(1-r_ CHOHCH2O2_OH)	Sander et al. (2019)*
G45104b	TrGC	DB1O2 + HO ₂ → DB1O2 + OH	k_R02_H02(temp,5)*r_CHOHCH2O2_OH	Sander et al. (2019)
G45105a	TrGCN	DB1O2 + NO → DB1O2 + NO ₂	KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair))	Sander et al. (2019)
G45105b	TrGCN	DB1O2 + NO → DB1NO ₃	KR02N0*alpha_AN(7,2,0,0,0,temp, cair)	Sander et al. (2019)
G45106	TrGCN	DB1O2 + NO ₃ → DB1O2 + NO ₂	KR02N03	Sander et al. (2019)
G45107	TrGC	DB1O2 → DB1O2 + OH	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 → DB1O2	KDEC*0.72	see note*
G45108b	TrGC	DB1O2 → .5 HVMK + .5 HMAc + HCHO + HO ₂	KDEC*0.28	see note*
G45109	TrGC	DB1O2 → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂	k1_R02sOR02	Sander et al. (2019)
G45110a	TrGC	DB1O2 + HO ₂ → DB2OOH	k_R02_H02(temp,5)*(1-r_ CHOHCH2O2_OH)	Sander et al. (2019)
G45110b	TrGC	DB1O2 + HO ₂ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + OH	k_R02_H02(temp,5)*r_CHOHCH2O2_OH	Sander et al. (2019)
G45111	TrGCN	DB1O2 + NO → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02N0	see note*
G45112	TrGCN	DB1O2 + NO ₃ → .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02N03	Sander et al. (2019)
G45113	TrGC	DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH	k_14hsa1	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45114a	TrGC	DB1OOH + OH \rightarrow DB1O2	k_R00HR0	Sander et al. (2019)
G45114b	TrGC	DB1OOH + OH \rightarrow HCOOH + HO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2019)*
G45115	TrGC	DB1OOH + HCOOH \rightarrow C1ODC2OOHC4OD + HCOOH	4.67E-26*(temp)**(3.286) *EXP(4509./(1.987*temp))	Sander et al. (2019), da Silva (2010)*
G45116	TrGCN	DB1NO3 + OH \rightarrow HCOOH + NO ₂ + CH ₃ COCHO ₂ CHO	k_adt	Sander et al. (2019)*
G45117	TrGC	DB2OOH + OH \rightarrow DB1O2	k_R00HR0	Sander et al. (2019)*
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	Sander et al. (2019)
G45119a	TrGC	LZCO3HC23DBCOD + 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_CH0*a_CO2H	Sander et al. (2019)
G45119b	TrGC	LZCO3HC23DBCOD + 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_CH0*a_CO2H	Sander et al. (2019)
G45120	TrGC	LISOPEFO2 \rightarrow LISOPEFO	k1_R02pOR02	Sander et al. (2019)
G45121a	TrGCN	LISOPEFO2 + NO \rightarrow LISOPEFO + NO ₂	KR02NO*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Sander et al. (2019)
G45121b	TrGCN	LISOPEFO2 + NO \rightarrow ISOPDNO3	KR02NO*alpha_AN(6,1,0,0,0,temp, cair)	Sander et al. (2019)*
G45122a	TrGC	LISOPEFO2 + HO ₂ \rightarrow .7143 ISOPDOOH + .2857 ISOPBOOH	k_R02_H02(temp,5)*(1.-r_CHOCH202_OH)	Sander et al. (2019)
G45122b	TrGC	LISOPEFO2 + HO ₂ \rightarrow LISOPEFO + OH	k_R02_H02(temp,5)*r_CHOCH202_OH	Sander et al. (2019)
G45123	TrGCN	LISOPEFO2 + NO ₃ \rightarrow LISOPEFO + NO ₂	KR02NO3	Sander et al. (2019)
G45124	TrGC	LISOPEFO2 \rightarrow .7143 MACR + .2857 MVK + HCHO + OH	0.7143*k_hsd+.2857*k_hsb	Sander et al. (2019)
G45125	TrGC	LISOPEFO \rightarrow .7143 MACR + .2857 MVK + HCHO + HO ₂	KDEC	Sander et al. (2019)
G45126a	TrGC	LISOPACO \rightarrow 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G45126b	TrGC	LISOPACO \rightarrow .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO \rightarrow 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	LISOPACO \rightarrow .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	3METHYLFURAN + OH \rightarrow L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Sander et al. (2019)*
G45129	TrGCN	3METHYLFURAN + NO ₃ \rightarrow L3METHYLFURANO2 + NO ₂	1.9E-11	Sander et al. (2019), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 \rightarrow C4MDIAL + HO ₂	k1_R02sOR02	Sander et al. (2019)
G45131	TrGCN	L3METHYLFURANO2 + NO \rightarrow C4MDIAL + HO ₂ + NO ₂	KR02NO	Sander et al. (2019)*
G45132	TrGC	L3METHYLFURANO2 + HO ₂ \rightarrow C4MDIAL + HO ₂	k_R02_H02(temp,5)	Sander et al. (2019)*
G45133	TrGC	LZCO3C23DBCOD \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂	k1_R02RC03	Sander et al. (2019)
G45134a	TrGC	LZCO3C23DBCOD + HO ₂ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH	KAPH02*r_C03_OH	Sander et al. (2019)
G45134b	TrGC	LZCO3C23DBCOD + HO ₂ \rightarrow LZCO3HC23DBCOD	KAPH02*(r_C03_00H+r_C03_03)	Sander et al. (2019)*
G45135	TrGCN	LZCO3C23DBCOD + NO \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KAPNO	Sander et al. (2019)
G45136	TrGCN	LZCO3C23DBCOD + NO ₂ \rightarrow LZCPANC23DBCOD	k_CH3C03_N02	Rickard and Pascoe (2009)
G45137	TrGCN	LZCO3C23DBCOD + NO ₃ \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KR02N03*1.74	Sander et al. (2019)
G45138	TrGCN	LZCPANC23DBCOD \rightarrow LZCO3C23DBCOD + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	LZCPANC23DBCOD + OH \rightarrow .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	2.52E-11	Sander et al. (2019)*
G45200	TrGTerC	C511O2 \rightarrow CH ₃ C(O) + HCOCH2CHO	k1_R02sOR02	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO \rightarrow CH ₃ C(O) + HCOCH2CHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G45202a	TrGTerC	C511O2 + HO ₂ \rightarrow C511OOH	k_R02_H02(temp,5)*r_COCH202_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G45202b	TrGTerC	C511O2 + HO ₂ \rightarrow CH ₃ C(O) + HCOCH2CHO + OH	k_R02_H02(temp,5)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
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_R02RC03	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_CH3C03_N02	Rickard and Pascoe (2009)
G45209a	TrGTerC	$\text{CO23C4CO3} + \text{HO}_2 \rightarrow \text{CO23C4CO3H}$	KAPH02*(r_C03_00H+r_C03_03)	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*r_C03_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	$\text{C512O2} + \text{HO}_2 \rightarrow \text{C512OOH}$	k_R02_H02(temp, 5)	Rickard and Pascoe (2009)
G45214	TrGTerCN	$\text{C512O2} + \text{NO} \rightarrow \text{C513O2} + \text{NO}_2$	KR02NO	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	$\text{C513O2} + \text{NO} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G45218a	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{C513OOH}$	k_R02_H02(temp, 5)*r_COCH202_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G45218b	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	k_R02_H02(temp, 5)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
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.*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_R02RC03	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_CH3C03_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	$\text{C514O2} + \text{HO}_2 \rightarrow \text{C514OOH}$	k_R02_H02(temp, 5)	Rickard and Pascoe (2009)
G45228a	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02NO*(1.-alpha_AN(7, 2, 0, 1, 0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G45228b	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{C514NO3}$	KR02NO*alpha_AN(7, 2, 0, 1, 0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G45229	TrGTerCN	$\text{C514O2} + \text{NO}_3 \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)
G45230	TrGTerC	$\text{C514O2} \rightarrow \text{CO13C4CHO} + \text{HO}_2$	k1_R02sR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45231	TrGTerC	$\text{C514OOH} + \text{OH} \rightarrow \text{C013C4CHO} + \text{OH}$	$1.10\text{E}-10$	Rickard and Pascoe (2009)
G45232	TrGTerCN	$\text{C514NO3} + \text{OH} \rightarrow \text{C013C4CHO} + \text{NO}_2$	$4.33\text{E}-11$	Rickard and Pascoe (2009)
G45233	TrGTerC	$\text{CHOC3COOOH} + \text{OH} \rightarrow \text{CHOC3COCO3}$	$7.55\text{E}-11$	Rickard and Pascoe (2009)
G45234	TrGTerCN	$\text{CHOC3COPAN} \rightarrow \text{CHOC3COCO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G45235	TrGTerCN	$\text{CHOC3COPAN} + \text{OH} \rightarrow \text{C4CODIAL} + \text{CO} + \text{NO}_2$	$7.19\text{E}-11$	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), Sander et al. (2019)*
G45237a	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{COCH}_3 + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH} + .84 \text{MBOOO}$	$1.0\text{E}-17 * 0.57$	Rickard and Pascoe (2009), Sander et al. (2019)
G45237b	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{IBUTALOH} + .63 \text{CO} + .37 \text{HOCH}_2\text{OOH} + .16 \text{OH} + .16 \text{HO}_2$	$1.0\text{E}-17 * 0.43$	Rickard and Pascoe (2009), Sander et al. (2019)
G45238	TrGTerCN	$\text{MBO} + \text{NO}_3 \rightarrow \text{LMBOABO2}$	$4.6\text{E}-14 * \text{EXP}(-400./\text{temp})$	Rickard and Pascoe (2009), Sander et al. (2019)
G45239	TrGTerC	$\text{LMBOABO2} + \text{HO}_2 \rightarrow \text{LMBOABOOH}$	$k_{\text{R02_H02}}(\text{temp}, 5)$	Rickard and Pascoe (2009), Sander et al. (2019)
G45240a	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{LMBOABNO3}$	$\text{KR02N0} * (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Sander et al. (2019)
G45240b	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .67$	Rickard and Pascoe (2009), Sander et al. (2019)
G45240c	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .33$	Rickard and Pascoe (2009), Sander et al. (2019)
G45241a	TrGTerC	$\text{LMBOABO2} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2$	$k1_{\text{R02sOR02}} * .67$	Rickard and Pascoe (2009), Sander et al. (2019)
G45241b	TrGTerC	$\text{LMBOABO2} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2$	$k1_{\text{R02pOR02}} * .33$	Rickard and Pascoe (2009), Sander et al. (2019)
G45242a	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{MBOACO}$	$0.67 * 2.93\text{E}-11 + .33 * 2.05\text{E}-12$	Rickard and Pascoe (2009), Sander et al. (2019)
G45242b	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{LMBOABO2}$	k_{R00HRO}	Rickard and Pascoe (2009), Sander et al. (2019)
G45243	TrGTerCN	$\text{LMBOABNO3} + \text{OH} \rightarrow \text{MBOACO} + \text{NO}_2$	$0.67 * 1.75\text{E}-12 + .33 * 2.69\text{E}-12$	Rickard and Pascoe (2009), Sander et al. (2019)
G45244	TrGTerC	$\text{MBOACO} + \text{OH} \rightarrow \text{MBOCOCO} + \text{HO}_2$	$3.79\text{E}-12$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45245	TrGTerC	MBOCOCO + OH \rightarrow CO + IPRHOCO3	1.38E-11	Rickard and Pascoe (2009)
G45246	TrGTerCN	LNMBOABO2 + HO ₂ \rightarrow LNMBOABOOH	k_R02_H02(temp,5)	Rickard and Pascoe (2009), Sander et al. (2019)
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	KR02N0	Rickard and Pascoe (2009), Sander et al. (2019)*
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	KR02N03	Rickard and Pascoe (2009), Sander et al. (2019)
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_R02s0R02	Rickard and Pascoe (2009), Sander et al. (2019)
G45250a	TrGTerCN	LNMBOABOOH + OH \rightarrow .65 C4MCONO3OH + .35 NMBOBCO	0.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45250b	TrGTerCN	LNMBOABOOH + OH \rightarrow LNMBOABO2	k_R00HRO	Rickard and Pascoe (2009), Sander et al. (2019)
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*r_C03_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45252b	TrGTerCN	NC4OHCO3 + HO ₂ \rightarrow NC4OHCO3H	KAPH02*(r_C03_03+r_C03_00H)	Rickard and Pascoe (2009), Sander et al. (2019)
G45253	TrGTerCN	NC4OHCO3 + NO \rightarrow IBUTALOH + CO ₂ + NO ₂ + NO ₂	KAPN0	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	KR02N03*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), Sander et al. (2019)
G45400	TrGAroCN	NC4MDCO2HN + OH \rightarrow MMALANHY + NO ₂	k_R00HRO	Rickard and Pascoe (2009)*
G45401	TrGAroCN	C54CO + NO ₃ \rightarrow 3 CO + CH ₃ C(O)OO + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	C54CO + OH \rightarrow 3 CO + CH ₃ C(O)OO	1.72E-11	Rickard and Pascoe (2009)
G45403a	TrGAroCN	NTLFUO2 + HO ₂ \rightarrow NTLFUOOH	k_R02_H02(temp,5)*(1.-r_COCH202_ OH)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	NTLFUO2 + HO ₂ \rightarrow ACCOMECHO + NO ₂ + OH	k_R02_H02(temp,5)*r_COCH202_OH	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45404	TrGAroCN	$\text{NTLFUO}_2 + \text{NO} \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G45405	TrGAroCN	$\text{NTLFUO}_2 + \text{NO}_3 \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)*
G45406	TrGAroCN	$\text{NTLFUO}_2 \rightarrow \text{ACCOMMECHO} + \text{NO}_2$	k1_R02tOR02	Rickard and Pascoe (2009)*
G45407	TrGAroC	$\text{C5134CO}_2\text{OH} + \text{OH} \rightarrow \text{C54CO} + \text{HO}_2$	7.48E-11	Rickard and Pascoe (2009)
G45408	TrGAroCN	$\text{C5COO}_2\text{NO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{CO} + \text{NO}_2$	5.43E-11	Rickard and Pascoe (2009)
G45409	TrGAroCN	$\text{C5COO}_2\text{NO}_2 \rightarrow \text{C5CO14O}_2 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45410	TrGAroC	$\text{C5DIALOOH} + \text{OH} \rightarrow \text{C5DIALCO} + \text{OH}$	7.52E-11	Rickard and Pascoe (2009)
G45411a	TrGAroC	$\text{C4CO}_2\text{DBC}_3 + \text{HO}_2 \rightarrow \text{C4CO}_2\text{DC}_3\text{H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G45411b	TrGAroC	$\text{C4CO}_2\text{DBC}_3 + \text{HO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45412	TrGAroCN	$\text{C4CO}_2\text{DBC}_3 + \text{NO} \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G45413	TrGAroCN	$\text{C4CO}_2\text{DBC}_3 + \text{NO}_2 \rightarrow \text{C4CO}_2\text{DBPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$\text{C4CO}_2\text{DBC}_3 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KR02NO3*1.74	Rickard and Pascoe (2009)
G45415	TrGAroC	$\text{C4CO}_2\text{DBC}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45416	TrGAroC	$\text{MMALANHY} + \text{OH} \rightarrow \text{MMALANHYO}_2$	1.50E-12	Rickard and Pascoe (2009)
G45421a	TrGAroC	$\text{MMALANHYO}_2 + \text{HO}_2 \rightarrow \text{MMALNHYOOH}$	k_R02_H02(temp,5)*(1.-r_COCH202_OH-r_CHOCH202_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45421b	TrGAroC	$\text{MMALANHYO}_2 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{CO}_2 + \text{OH}$	k_R02_H02(temp,5)*(r_COCH202_OH+r_CHOCH202_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45422	TrGAroCN	$\text{MMALANHYO}_2 + \text{NO} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{CO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$\text{MMALANHYO}_2 + \text{NO}_3 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{CO}_2 + \text{NO}_2$	KR02NO3	Rickard and Pascoe (2009)*
G45424	TrGAroC	$\text{MMALANHYO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{CO}_2$	k1_R02tOR02	Rickard and Pascoe (2009)*
G45428	TrGAroCN	$\text{C4CO}_2\text{DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO}_2 + \text{CO} + \text{NO}_2$	2.74E-11	Rickard and Pascoe (2009)
G45429	TrGAroCN	$\text{C4CO}_2\text{DBPAN} \rightarrow \text{C4CO}_2\text{DBC}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	$\text{C5CO14O}_2 + \text{HO}_2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard and Pascoe (2009)*
G45430b	TrGAroC	$\text{C5CO14O}_2 + \text{HO}_2 \rightarrow \text{C5CO14OH} + \text{O}_3$	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G45430c	TrGAroC	$\text{C5CO14O}_2 + \text{HO}_2 \rightarrow \text{C5CO14OOH}$	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G45431	TrGAroCN	$\text{C5CO14O}_2 + \text{NO} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)*
G45432	TrGAroCN	$\text{C5CO14O}_2 + \text{NO}_2 \rightarrow \text{C5COO}_2\text{NO}_2$	k_CH3C03_N02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45433	TrGAroCN	$C5CO14O2 + NO_3 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	$C5CO14O2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G45436	TrGAroC	$C5CO14OH + OH \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	$C5DICARB + NO_3 \rightarrow C5CO14O2 + HNO_3$	KN03AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	$C5DICARB + O_3 \rightarrow .5338 \text{ GLYOX} + .063 \text{ CH}_3\text{CHO} + .348 \text{ CH}_3\text{C(O)OO} + .918 \text{ CO} + .57 \text{ OH} + .473 \text{ HO}_2 + .0563 \text{ CH}_3\text{COCO}_2\text{H} + .5338 \text{ MGLYOX} + .676 \text{ H}_2\text{O}_2 + .063 \text{ HCHO} + .0563 \text{ HCOCO}_2\text{H} + .2465 \text{ CO}_2$	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	$C5DICARB + OH \rightarrow .48 \text{ C5CO14O2} + .52 \text{ C5DICARBO2}$	6.2E-11	Rickard and Pascoe (2009)
G45444	TrGAroC	$MC3ODBCO2H + OH \rightarrow .35 \text{ GLYOX} + .35 \text{ CH}_3 + .35 \text{ CO} + .35 \text{ CO}_2 + .65 \text{ MMALANHY} + .65 \text{ HO}_2$	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	$TLFUONE + NO_3 \rightarrow NTLFUO2$	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	$TLFUONE + O_3 \rightarrow .5 \text{ CO} + .5 \text{ OH} + .5 \text{ MECOACETO2} + .3125 \text{ C24O3CCO2H} + .1875 \text{ ACCOMECHO} + .1875 \text{ H}_2\text{O}_2$	8.00E-19	see note*
G45453	TrGAroC	$TLFUONE + OH \rightarrow TLFUO2$	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	$ACCOMECO3 + HO_2 \rightarrow ACCOMECHO3H$	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G45454b	TrGAroC	$ACCOMECO3 + HO_2 \rightarrow MECOACETO2 + CO_2 + OH$	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G45455	TrGAroCN	$ACCOMECO3 + NO \rightarrow MECOACETO2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	$ACCOMECO3 + NO_2 \rightarrow ACCOMECHAN$	k_CH3C03_N02	Rickard and Pascoe (2009)*
G45457	TrGAroCN	$ACCOMECO3 + NO_3 \rightarrow MECOACETO2 + CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	$ACCOMECO3 \rightarrow MECOACETO2 + CO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45459	TrGAroC	$C4CO2DCO3H + OH \rightarrow C4CO2DBCO3$	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	$ACCOMEECHO + NO_3 \rightarrow ACCOMECHO3 + HNO_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	$ACCOMEECHO + OH \rightarrow ACCOMECHO3$	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	$MMALNHYOOH + OH \rightarrow MMALANHYO2$	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	$C5DICAROOH + OH \rightarrow C5134CO2OH + OH$	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	$C5DICAROOH + OH \rightarrow C5DICARBO2$	k_R00HR0	Rickard and Pascoe (2009)
G45468	TrGAroC	$C24O3CCO2H + OH \rightarrow MECOACETO2 + CO_2$	8.76E-13	Rickard and Pascoe (2009)
G45469	TrGAroCN	$NTLFUOOH + OH \rightarrow NTLFUO2$	4.44E-12	Rickard and Pascoe (2009)
G45470	TrGAroCN	$ACCOMEPAN + OH \rightarrow METACETHO + CO + CO + NO_2$	1.00E-14	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45471	TrGAroCN	ACCOMEPAN \rightarrow ACCOMECO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G45476a	TrGAroC	TLFUO2 + HO ₂ \rightarrow TLFUOOH	k_R02_H02(temp,5)*(1.-r_COCH202_OH-r_CHOHCH202_OH)	Rickard and Pascoe (2009)
G45476b	TrGAroC	TLFUO2 + HO ₂ \rightarrow ACCOMECHO + HO ₂ + OH	k_R02_H02(temp,5)*(r_COCH202_OH+r_CHOHCH202_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_R02t0R02	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	k_R02_H02(temp,5)*(1.-r_COCH202_OH)	Rickard and Pascoe (2009)
G45486b	TrGAroC	C5DIALO2 + HO ₂ \rightarrow MALDIAL + CO + HO ₂ + OH	k_R02_H02(temp,5)*r_COCH202_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_R02s0R02	Rickard and Pascoe (2009)*
G45490a	TrGAroC	C5DICARBO2 + HO ₂ \rightarrow C5DICAROOH	k_R02_H02(temp,5)*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G45491b	TrGAroC	C5DICARBO2 + HO ₂ \rightarrow MGLYOX + GLYOX + HO ₂ + OH	k_R02_H02(temp,5)*r_C03_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_R02s0R02	Rickard and Pascoe (2009)*
G46200a	TrGTerC	CO235C6O2 + HO ₂ \rightarrow CO235C6OOH	k_R02_H02(temp,6)*r_COCH202_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G46200b	TrGTerC	CO235C6O2 + HO ₂ \rightarrow CO23C4CO3 + HCHO + OH	k_R02_H02(temp,6)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G46201	TrGTerCN	CO235C6O2 + NO \rightarrow CO23C4CO3 + HCHO + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46202	TrGTerC	CO235C6O2 \rightarrow CO23C4CO3 + HCHO	k1_R02p0R02	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_R02s0R02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46205a	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KRO2NO} * (1 - \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G46205b	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{C614NO3}$	$\text{KRO2NO} * \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G46206a	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{C614OOH}$	$\text{k_R02_HO2}(\text{temp}, 6) * (1 - \text{r_CHOHCH2O2_OH})$	Rickard and Pascoe (2009), Sander et al. (2019)
G46206b	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{k_R02_HO2}(\text{temp}, 6) * \text{r_CHOHCH2O2_OH}$	Rickard and Pascoe (2009), Sander et al. (2019)
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	$\text{NDNPHENOOH} + \text{OH} \rightarrow \text{NDNPHENO2}$	k_R00HRO	Rickard and Pascoe (2009)
G46404a	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C615CO2OOH}$	$\text{k_R02_HO2}(\text{temp}, 6) * (1 - \text{r_COCH2O2_OH})$	Rickard and Pascoe (2009)
G46404b	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{k_R02_HO2}(\text{temp}, 6) * \text{r_COCH2O2_OH}$	Rickard and Pascoe (2009)*
G46405	TrGAroCN	$\text{C615CO2O2} + \text{NO} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KRO2NO	Rickard and Pascoe (2009)*
G46406	TrGAroCN	$\text{C615CO2O2} + \text{NO}_3 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KRO2NO3	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_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	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NDNPHENOOH}$	$\text{k_R02_HO2}(\text{temp}, 6) * (1 - \text{r_CHOHCH2O2_OH})$	Rickard and Pascoe (2009)
G46413b	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	$\text{k_R02_HO2}(\text{temp}, 6) * \text{r_CHOHCH2O2_OH}$	Rickard and Pascoe (2009)*
G46414	TrGAroCN	$\text{NDNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{NO}_2$	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46415	TrGAroCN	NDNPHEO2 + NO ₃ → NC4DCO2H + HNO ₃ + CO + CO + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46416	TrGAroCN	NDNPHEO2 → NC4DCO2H + HNO ₃ + CO + CO + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46417	TrGAroC	PBZQCO + OH → C5CO2OHCO3	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	CATECHOL + NO ₃ → CATEC1O + HNO ₃	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	CATECHOL + O ₃ → MALDALCO2H + HCOCO ₂ H + HO ₂ + OH	9.2E-18	Rickard and Pascoe (2009)
G46420	TrGAroC	CATECHOL + OH → CATEC1O	1.0E-10	Rickard and Pascoe (2009)
G46421	TrGAroC	C5COOHCO3H + OH → C5CO2OHCO3	8.01E-11	Rickard and Pascoe (2009)
G46422	TrGAroCN	NCATECHOL + NO ₃ → NNCATECO2	2.60E-12	Rickard and Pascoe (2009)
G46423	TrGAroCN	NCATECHOL + OH → NCATECO2	3.47E-12	Rickard and Pascoe (2009)
G46424a	TrGAroC	C5CO2OHCO3 + HO ₂ → C5COOHCO3H	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G46424b	TrGAroC	C5CO2OHCO3 + HO ₂ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G46425	TrGAroCN	C5CO2OHCO3 + NO → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G46426	TrGAroCN	C5CO2OHCO3 + NO ₂ → C5CO2OHPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46427	TrGAroCN	C5CO2OHCO3 + NO ₃ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G46428	TrGAroC	C5CO2OHCO3 → HOCOC4DIAL + HO ₂ + CO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46429	TrGAroCN	BZEPOXMUC + NO ₃ → BZEMUCCO3 + HNO ₃	2.*KN03AL*2.75	Rickard and Pascoe (2009)
G46430	TrGAroC	BZEPOXMUC + O ₃ → 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 → .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard and Pascoe (2009)
G46432a	TrGAroCN	NCATECO2 + HO ₂ → NCATECOOH	k_R02_H02(temp,6)*(1-r_CHOHCH202_OH)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	NCATECO2 + HO ₂ → NC4DCO2H + HCOCO ₂ H + HO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard and Pascoe (2009)*
G46433	TrGAroCN	NCATECO2 + NO → NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46434	TrGAroCN	NCATECO2 + NO ₃ → NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46435	TrGAroCN	NCATECO2 \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46436	TrGAroCN	NPHEN1OOH + OH \rightarrow NPHEN1O2	9.00E-13	Rickard and Pascoe (2009)
G46437a	TrGAroCN	NPHENO2 + HO ₂ \rightarrow NPHENOOH	k_R02_H02(temp,6)*(1.-r_ CHOHCH202_OH)	Rickard and Pascoe (2009)
G46437b	TrGAroCN	NPHENO2 + HO ₂ \rightarrow MALDALCO2H + GLYOX + NO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard and Pascoe (2009)*
G46438	TrGAroCN	NPHENO2 + NO \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46439	TrGAroCN	NPHENO2 + NO ₃ \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46440	TrGAroCN	NPHENO2 \rightarrow MALDALCO2H + GLYOX + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46441	TrGAroC	BENZENE + OH \rightarrow .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO ₂ + .53 PHENOL + .53 HO ₂	2.3E-12*EXP(-190./temp)	Rickard and Pascoe (2009)*
G46442	TrGAroCN	C5CO2OHPAN + OH \rightarrow HOCOC4DIAL + CO + CO + NO ₂	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	C5CO2OHPAN \rightarrow C5CO2OHCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G46444	TrGAroCN	CATEC1O + NO ₂ \rightarrow NCATECHOL	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46445	TrGAroC	CATEC1O + O ₃ \rightarrow CATEC1O2	k_C6H50_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46446	TrGAroC	BZEMUCCO + OH \rightarrow EPXDLCO3 + GLYOX	9.20E-11	Rickard and Pascoe (2009)
G46447a	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NNCATECOOH	k_R02_H02(temp,6)*(1.-r_ CHOHCH202_OH)	Rickard and Pascoe (2009)
G46447b	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard and Pascoe (2009)*
G46448	TrGAroCN	NNCATECO2 + NO \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G46449	TrGAroCN	NNCATECO2 + NO ₃ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G46450	TrGAroCN	NNCATECO2 \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46451	TrGAroC	BZEMUCCO2H + OH \rightarrow C5DIALO2 + CO ₂	4.06E-11	Rickard and Pascoe (2009)
G46452	TrGAroCN	NNCATECOOH + OH \rightarrow NNCATECO2	k_R00HRO	Rickard and Pascoe (2009)
G46453	TrGAroCN	NPHEN1O + NO ₂ \rightarrow DNPEN	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)

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

#	labels	reaction	rate coefficient	reference
G46454	TrGAroCN	NPHEN1O + O ₃ → NPHEN1O2	k_C6H5O_03	Rickard and Pascoe (2009), Tao and Li (1999)
G46455	TrGAroCN	DNPHEN + NO ₃ → NDNPHENO2	2.25E-15	Rickard and Pascoe (2009)
G46456	TrGAroCN	DNPHEN + OH → DNPHEO2	3.00E-14	Rickard and Pascoe (2009)
G46457	TrGAroCN	PHENOL + NO ₃ → .742 C6H5O + .742 HNO ₃ + .258 NPHENO2	3.8E-12	Rickard and Pascoe (2009)*
G46458	TrGAroC	PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 HO ₂ + .14 PHENO2	4.7E-13*EXP(1220./temp)	Rickard and Pascoe (2009)*
G46459	TrGAroCN	PBZQONE + NO ₃ → NBZQO2	3.00E-13	Rickard and Pascoe (2009)
G46460	TrGAroC	PBZQONE + OH → PBZQO2	4.6E-12	Rickard and Pascoe (2009)
G46461a	TrGAroC	PHENO2 + HO ₂ → PHENO2OH	k_R02_HO2(temp,6)*(1.-r_CHOCH2O2_OH)	Rickard and Pascoe (2009)
G46461b	TrGAroC	PHENO2 + HO ₂ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + OH	k_R02_HO2(temp,6)*r_CHOCH2O2_OH	Rickard and Pascoe (2009)*
G46462	TrGAroCN	PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G46463	TrGAroCN	PHENO2 + NO ₃ → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)*
G46464	TrGAroC	PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46465	TrGAroC	C615CO2OOH + OH → C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
G46466a	TrGAroC	C5CO2DBCO3 + HO ₂ → C5CO2DCO3H	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBCO3 + HO ₂ → CH ₃ C(O) + HCOCOCHO + CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBCO3 + NO → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBCO3 + NO ₂ → C5CO2DBPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBCO3 + NO ₃ → CH ₃ C(O) + HCOCOCHO + CO ₂ + NO ₂	KR02NO3*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBCO3 → CH ₃ C(O) + HCOCOCHO + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G46471	TrGAroCN	NPHEN1O2 + HO ₂ → NPHEN1OOH	k_R02_HO2(temp,6)	Rickard and Pascoe (2009)
G46472a	TrGAroCN	NPHEN1O2 + NO → NPHEN1O + NO ₂	KR02NO	Rickard and Pascoe (2009)
G46472b	TrGAroCN	NPHEN1O2 + NO ₂ → NPHEN1O + NO ₃	k_C6H5O2_N02	Jagiella and Zabel (2007)*
G46473	TrGAroCN	NPHEN1O2 + NO ₃ → NPHEN1O + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G46474	TrGAroCN	NPHEN1O2 → NPHEN1O	k1_R02sR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46475	TrGAroCN	NPHENOOH + OH \rightarrow NPHENO2	1.07E-10	Rickard and Pascoe (2009)
G46476	TrGAroCN	C6H5O + NO ₂ \rightarrow HOC6H4NO2	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O ₃ \rightarrow C6H5O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46478	TrGAroCN	NCATECOOH + OH \rightarrow NCATECO2	k_R00HRO	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH \rightarrow PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)
G46480a	TrGAroC	PBZQO2 + HO ₂ \rightarrow PBZQOOH	k_R02_HO2(temp,6)*(1-r_CHOHCH2O2_OH-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G46480b	TrGAroC	PBZQO2 + HO ₂ \rightarrow C5CO2OHCO3 + OH	k_R02_HO2(temp,6)*(r_CHOHCH2O2_OH+r_COCH2O2_OH)	Rickard and Pascoe (2009)*
G46481	TrGAroCN	PBZQO2 + NO \rightarrow C5CO2OHCO3 + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G46482	TrGAroCN	PBZQO2 + NO ₃ \rightarrow C5CO2OHCO3 + NO ₂	KR02NO3	Rickard and Pascoe (2009)*
G46483	TrGAroC	PBZQO2 \rightarrow C5CO2OHCO3	k1_R02sOR02	Rickard and Pascoe (2009)*
G46484	TrGAroC	BZOBIPEROH + OH \rightarrow MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	DNPHEO2 + HO ₂ \rightarrow DNPHEOOH	k_R02_HO2(temp,6)*(1-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46485b	TrGAroCN	DNPHEO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	k_R02_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46486	TrGAroCN	DNPHEO2 + NO \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G46487	TrGAroCN	DNPHEO2 + NO ₃ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)*
G46488	TrGAroCN	DNPHEO2 \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46489	TrGAroC	BZBIPEROOH + OH \rightarrow BZOBIPEROH + OH	9.77E-11	Rickard and Pascoe (2009)
G46490a	TrGAroC	BZEMUCO2 + HO ₂ \rightarrow BZEMUCOOH	k_R02_HO2(temp,6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	BZEMUCO2 + HO ₂ \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + OH	k_R02_HO2(temp,6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	BZEMUCO2 + NO \rightarrow BZEMUCNO3	KR02NO*alpha_AN(10,2,0,1,0,temp,cair)	Rickard and Pascoe (2009)
G46491b	TrGAroCN	BZEMUCO2 + NO \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + NO ₂	KR02NO*(1-alpha_AN(10,2,0,1,0,temp,cair))	Rickard and Pascoe (2009)*
G46492	TrGAroCN	BZEMUCO2 + NO ₃ \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO + NO ₂	KR02NO3	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46493	TrGAroC	BZEMUCO2 \rightarrow .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO2 + .5 C32OH13CO	k1_R02sOR02	Rickard and Pascoe (2009)*
G46494	TrGAroCN	C5CO2DBPAN + OH \rightarrow HCOCOCHO + CH ₃ CHO + CO ₂ + NO ₂	3.28E-11	Rickard and Pascoe (2009)
G46495	TrGAroCN	C5CO2DBPAN \rightarrow C5CO2DBCO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	NBZQOOH + OH \rightarrow NBZQO2	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	CATEC1OOH + OH \rightarrow CATEC1O2	k_R00HRO	Rickard and Pascoe (2009)
G46498	TrGAroC	C6125CO + OH \rightarrow C5CO14O2 + CO	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	NBZQO2 + HO ₂ \rightarrow NBZQOOH	k_R02_H02(temp,6)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G46499b	TrGAroCN	NBZQO2 + HO ₂ \rightarrow C6CO4DB + NO ₂ + OH	k_R02_H02(temp,6)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G46500	TrGAroCN	NBZQO2 + NO \rightarrow C6CO4DB + NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G46501	TrGAroCN	NBZQO2 + NO ₃ \rightarrow C6CO4DB + NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)*
G46502	TrGAroCN	NBZQO2 \rightarrow C6CO4DB + NO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G46503	TrGAroCN	DNPHENO2 + OH \rightarrow DNPHENO2	k_R00HRO	Rickard and Pascoe (2009)
G46504	TrGAroC	CATEC1O2 + HO ₂ \rightarrow CATEC1OOH	k_R02_H02(temp,6)	Rickard and Pascoe (2009)
G46505a	TrGAroCN	CATEC1O2 + NO \rightarrow CATEC1O + NO ₂	KR02NO	Rickard and Pascoe (2009)
G46505b	TrGAroCN	CATEC1O2 + NO ₂ \rightarrow CATEC1O + NO ₃	k_C6H5O2_N02	Jagiella and Zabel (2007)*
G46506	TrGAroCN	CATEC1O2 + NO ₃ \rightarrow CATEC1O + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G46507	TrGAroC	CATEC1O2 \rightarrow CATEC1O	k1_R02sOR02	Rickard and Pascoe (2009)
G46508	TrGAroC	BZEMUCCO3H + OH \rightarrow BZEMUCCO3	4.37E-11	Rickard and Pascoe (2009)
G46509	TrGAroC	C6H5OOH + OH \rightarrow C6H5O2	3.60E-12	Rickard and Pascoe (2009)
G46510	TrGAroC	BZEMUCOOH + OH \rightarrow BZEMUCCO + OH	1.31E-10	Rickard and Pascoe (2009)
G46511a	TrGAroC	BZEMUCCO3 + HO ₂ \rightarrow BZEMUCCO2H + O ₃	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G46511b	TrGAroC	BZEMUCCO3 + HO ₂ \rightarrow BZEMUCCO3H	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G46511c	TrGAroC	BZEMUCCO3 + HO ₂ \rightarrow C5DIALO2 + CO ₂ + OH	KAPH02*r_C03_0H	Rickard and Pascoe (2009)
G46512	TrGAroCN	BZEMUCCO3 + NO \rightarrow C5DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G46513	TrGAroCN	BZEMUCCO3 + NO ₂ \rightarrow BZEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G46514	TrGAroCN	BZEMUCCO3 + NO ₃ \rightarrow C5DIALO2 + CO ₂ + NO ₂	KR02NO3*1.74	Rickard and Pascoe (2009)
G46515	TrGAroC	BZEMUCCO3 \rightarrow C5DIALO2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G46516	TrGAroC	C6H5O2 + HO ₂ \rightarrow C6H5OOH	k_R02_H02(temp,6)	Rickard and Pascoe (2009)
G46517	TrGAroCN	C6H5O2 + NO \rightarrow C6H5O + NO ₂	KR02NO	Rickard and Pascoe (2009)
G46518	TrGAroCN	C6H5O2 + NO ₃ \rightarrow C6H5O + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G46519	TrGAroC	C6H5O2 \rightarrow C6H5O	k1_R02sR02	Rickard and Pascoe (2009)
G46520	TrGAroCN	C6H5O2 + NO ₂ \rightarrow C6H5O + NO ₃	k_C6H5O2_N02	Jagiella and Zabel (2007)

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

#	labels	reaction	rate coefficient	reference
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO ₂	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	BZBIPERO2 + HO ₂ → BZBIPEROOH	k_R02_H02(temp,6)*(1-r_BIPERO2_OH)	Rickard and Pascoe (2009)
G46522b	TrGAroC	BZBIPERO2 + HO ₂ → OH + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	k_R02_H02(temp,6)*r_BIPERO2_OH	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G46523a	TrGAroCN	BZBIPERO2 + NO → BZBIPERNO3	KR02N0*alpha_AN(9,2,0,0,1,temp,cair)	Rickard and Pascoe (2009)
G46523b	TrGAroCN	BZBIPERO2 + NO → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N0*(1.-alpha_AN(9,2,0,0,1,temp,cair))	Rickard and Pascoe (2009)*
G46524	TrGAroCN	BZBIPERO2 + NO ₃ → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02N03	Rickard and Pascoe (2009)*
G46525	TrGAroC	BZBIPERO2 → GLYOX + HO ₂ + BZFUONE	k1_R02sOR02	Rickard and Pascoe (2009)*
G47200	TrGTerCN	CO235C6CHO + NO ₃ → CO235C6CO3 + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	CO235C6CO3 + HO ₂ → C235C6CO3H	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO ₂ → CO235C6O2 + CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G47203	TrGTerCN	CO235C6CO3 + NO → CO235C6O2 + CO ₂ + NO ₂	KAPN0	Rickard and Pascoe (2009)
G47204	TrGTerCN	CO235C6CO3 + NO ₂ → C7PAN3	k_CH3C03_N02	Rickard and Pascoe (2009)
G47205	TrGTerC	CO235C6CO3 → CO235C6O2 + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)
G47206	TrGTerC	C235C6CO3H + OH → CO235C6CO3	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	C7PAN3 + OH → CO235C5CHO + CO + NO ₂	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	C7PAN3 → CO235C6CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G47209a	TrGTerC	C716O2 + HO ₂ → C716OOH	k_R02_H02(temp,7)*r_COCH202_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G47209b	TrGTerC	C716O2 + HO ₂ → CO13C4CHO + CH ₃ C(O) + OH	k_R02_H02(temp,7)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G47210	TrGTerCN	C716O2 + NO → CO13C4CHO + CH ₃ C(O) + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47211	TrGTerC	C716O2 → CO13C4CHO + CH ₃ C(O)	k1_R02sOR02	Rickard and Pascoe (2009)
G47212	TrGTerC	C716OOH + OH → CO235C6CHO + OH	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	C721O2 + HO ₂ → C721OOH	k_R02_H02(temp,7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	C721O2 + NO → C722O2 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47215	TrGTerC	C721O2 → C722O2	k1_R02pR02	Rickard and Pascoe (2009)
G47216	TrGTerC	C721OOH + OH → C721O2	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	C722O2 + HO ₂ → C722OOH	k_R02_H02(temp,7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	C722O2 + NO → CH ₃ COCH ₃ + C44O2 + NO ₂	KR02N0	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47219	TrGTerC	$C722O2 \rightarrow CH_3COCH_3 + C44O2$	k1_R02tR02	Rickard and Pascoe (2009)
G47220	TrGTerC	$C722OOH + OH \rightarrow C722O2$	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	$ROO6R3O2 \rightarrow ROO6R5O2$	$5.68E10 \cdot \exp(-8745./temp)$	Vereecken and Peeters (2012)
G47222	TrGTerCN	$ROO6R3O2 + NO \rightarrow ROO6R3O + NO_2$	KR02N0	Vereecken and Peeters (2012)*
G47223	TrGTerC	$ROO6R3O2 + HO_2 \rightarrow 7 \text{ L CARBON}$	k_R02_H02(temp, 7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	$ROO6R3O2 \rightarrow ROO6R3O$	k1_R02sR02	Vereecken and Peeters (2012)
G47225	TrGTerC	$ROO6R3O \rightarrow 7 \text{ L CARBON} + HO_2$	$5.7E10 \cdot \exp(-2949./temp)$	Vereecken and Peeters (2012)*
G47226	TrGTerC	$ROO6R5O2 \rightarrow 7 \text{ L CARBON} + OH$	$9.17E10 \cdot \exp(-8706./temp)$	Vereecken and Peeters (2012)*
G47400	TrGAroC	$TOLUENE + OH \rightarrow .07 \text{ C6H5CH2O2} + .18 \text{ CRESOL} + .18 \text{ HO}_2 + .65 \text{ TLBIPERO2} + .10 \text{ TLEPOXMUC} + .10 \text{ HO}_2$	$1.8E-12 \cdot \exp(340./temp)$	Rickard and Pascoe (2009)*
G47401	TrGAroC	$C6H5CH2O2 + HO_2 \rightarrow C6H5CH2OOH$	$1.5E-13 \cdot \exp(1310./temp)$	Rickard and Pascoe (2009)
G47402a	TrGAroCN	$C6H5CH2O2 + NO \rightarrow C6H5CH2NO3$	$KR02N0 \cdot \alpha_AN(7, 1, 0, 0, 0, temp, cair)$	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	$C6H5CH2O2 + NO \rightarrow BENZAL + HO_2 + NO_2$	$KR02N0 \cdot (1 - \alpha_AN(7, 1, 0, 0, 0, temp, cair))$	Rickard and Pascoe (2009)*
G47403	TrGAroCN	$C6H5CH2O2 + NO_3 \rightarrow BENZAL + HO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)*
G47404	TrGAroC	$C6H5CH2O2 \rightarrow BENZAL + HO_2$	$2 \cdot (k_CH302 \cdot 2.4E-14 \cdot \exp(1620./temp)) \cdot (0.5) \cdot R02$	Rickard and Pascoe (2009)*
G47405	TrGAroCN	$CRESOL + NO_3 \rightarrow .103 \text{ CRESO2} + .103 \text{ HNO}_3 + .506 \text{ NCRESO2} + .391 \text{ TOL1O} + .391 \text{ HNO}_3$	1.4E-11	Rickard and Pascoe (2009)*
G47406	TrGAroC	$CRESOL + OH \rightarrow .2 \text{ CRESO2} + .727 \text{ MCATECHOL} + .727 \text{ HO}_2 + .073 \text{ TOL1O}$	4.65E-11	Rickard and Pascoe (2009)*
G47407a	TrGAroC	$TLBIPERO2 + HO_2 \rightarrow TLBIPEROOH$	$k_R02_H02(temp, 7) \cdot (1 - r_BIPERO2_OH)$	Rickard and Pascoe (2009)
G47407b	TrGAroC	$TLBIPERO2 + HO_2 \rightarrow OH + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + HO_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	$k_R02_H02(temp, 7) \cdot r_BIPERO2_OH$	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G47408a	TrGAroCN	$TLBIPERO2 + NO \rightarrow NO_2 + .6 \text{ GLYOX} + .4 \text{ MGLYOX} + HO_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL}$	$KR02N0 \cdot (1 - \alpha_AN(11, 2, 0, 0, 1, temp, cair))$	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	$TLBIPERO2 + NO \rightarrow TLBIPERNO3$	$KR02N0 \cdot \alpha_AN(11, 2, 0, 0, 1, temp, cair)$	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47409	TrGAroCN	TLBIPERO2 + NO ₃ → NO ₂ + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KR02N03	Rickard and Pascoe (2009)*
G47410	TrGAroC	TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k1_R02s0R02	Rickard and Pascoe (2009)*
G47411	TrGAroCN	TLEPOXMUC + NO ₃ → TLEMUCCO3 + HNO ₃	KN03AL*2.75	Rickard and Pascoe (2009)
G47412	TrGAroC	TLEPOXMUC + O ₃ → EPXC4DIAL + .125 CH ₃ CHO + .695 CH ₃ C(O) + .57 CO + .57 OH + .125 HO ₂ + .1125 CH ₃ COCO ₂ H + .0675 MGLYOX + .0675 H ₂ O ₂ + .25 CO ₂	5.00E-18	Rickard and Pascoe (2009)*
G47413	TrGAroC	TLEPOXMUC + OH → .31 TLEMUCCO3 + .69 TLEMUCO2	7.99E-11	Rickard and Pascoe (2009)*
G47414	TrGAroC	C6H5CH2OOH + OH → BENZAL + OH	2.05E-11	Rickard and Pascoe (2009)
G47415	TrGAroCN	C6H5CH2NO3 + OH → BENZAL + NO ₂	6.03E-12	Rickard and Pascoe (2009)
G47416	TrGAroCN	BENZAL + NO ₃ → C6H5CO3 + HNO ₃	2.40E-15	Rickard and Pascoe (2009)
G47417	TrGAroC	BENZAL + OH → C6H5CO3	5.9E-12*EXP(225./temp)	Rickard and Pascoe (2009)
G47418a	TrGAroC	CRESO2 + HO ₂ → CRESOOH	k_R02_H02(temp,7)*(1.-r_CHOHCH202_OH)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO2 + HO ₂ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO2 + NO ₃ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47421	TrGAroC	CRESO2 → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO2 + HO ₂ → NCRESOOH	k_R02_H02(temp,7)*(1.-r_CHOHCH202_OH)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO2 + HO ₂ → C5CO14OH + GLYOX + NO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO2 + NO → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO2 + NO ₃ → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO2 → C5CO14OH + GLYOX + NO ₂	k1_R02IS0PD02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47426	TrGAroCN	TOLIO + NO ₂ → TOLIOHNO ₂	k_C6H5O_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOLIO + O ₃ → OXYLIO ₂	k_C6H5O_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47428	TrGAroCN	MCATECHOL + NO ₃ → MCATEC1O + HNO ₃	1.7E-10*1.0	Rickard and Pascoe (2009)
G47429	TrGAroC	MCATECHOL + O ₃ → 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 → C5CO14O ₂ + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO ₃ + HO ₂ → C615CO ₂ O ₂ + CO ₂ + OH	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₂ H + O ₃	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO ₃ + HO ₂ → TLEMUCCO ₃ H	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO ₃ + NO → C615CO ₂ O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO ₃ + NO ₂ → TLEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO ₃ + NO ₃ → C615CO ₂ O ₂ + CO ₂ + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009)
G47438	TrGAroC	TLEMUCCO ₃ → C615CO ₂ O ₂ + CO ₂	k1_R02RC03	Rickard and Pascoe (2009)*
G47439a	TrGAroC	TLEMUCO ₂ + HO ₂ → TLEMUCOOH	k_R02_H02(temp,7)*(1.-r_CHOHCH202_OH-r_COCH202_OH)	Rickard and Pascoe (2009)
G47439b	TrGAroC	TLEMUCO ₂ + HO ₂ → .5 C3DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH	k_R02_H02(temp,7)*(r_CHOHCH202_OH+r_COCH202_OH)	Rickard and Pascoe (2009)*
G47440a	TrGAroCN	TLEMUCO ₂ + NO → TLEMUCNO ₃	KR02N0*alpha_AN(11,2,1,0,0,temp,cair)	Rickard and Pascoe (2009)
G47440b	TrGAroCN	TLEMUCO ₂ + NO → .5 C3DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(11,2,1,0,0,temp,cair))	Rickard and Pascoe (2009)*
G47441	TrGAroCN	TLEMUCO ₂ + NO ₃ → .5 C3DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47442	TrGAroC	TLEMUCO ₂ → .5 C3DIALO ₂ + .5 CO ₂ H ₃ CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂	k1_R02s0R02	Rickard and Pascoe (2009)*
G47443a	TrGAroC	C6H5CO ₃ + HO ₂ → C6H5CO ₃ H	1.1E-11*EXP(364./temp)*0.65	Roth et al. (2010)
G47443b	TrGAroC	C6H5CO ₃ + HO ₂ → C6H5O ₂ + CO ₂ + OH	1.1E-11*EXP(364./temp)*0.20	Roth et al. (2010)
G47443c	TrGAroC	C6H5CO ₃ + HO ₂ → PHCOOH + O ₃	1.1E-11*EXP(364./temp)*0.15	Roth et al. (2010)
G47444	TrGAroCN	C6H5CO ₃ + NO → C6H5O ₂ + CO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G47445	TrGAroCN	C6H5CO ₃ + NO ₂ → PBZN	k_CH3C03_N02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47446	TrGAroCN	$\text{C6H5CO3} + \text{NO}_3 \rightarrow \text{C6H5O2} + \text{CO}_2 + \text{NO}_2$	$\text{KR02N03} \cdot 1.74$	Rickard and Pascoe (2009)
G47447	TrGAroC	$\text{C6H5CO3} \rightarrow \text{C6H5O2} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G47448	TrGAroC	$\text{CRESOOH} + \text{OH} \rightarrow \text{CRESO2}$	$1.15\text{E-}10$	Rickard and Pascoe (2009)
G47449	TrGAroCN	$\text{NCRESOOH} + \text{OH} \rightarrow \text{NCRESO2}$	$1.07\text{E-}10$	Rickard and Pascoe (2009)
G47450	TrGAroCN	$\text{TOL1OHNO2} + \text{NO}_3 \rightarrow \text{NCRES1O} + \text{HNO}_3$	$3.13\text{E-}13 \cdot 1.0$	Rickard and Pascoe (2009)
G47451	TrGAroCN	$\text{TOL1OHNO2} + \text{OH} \rightarrow \text{NCRES1O}$	$2.8\text{E-}12$	Rickard and Pascoe (2009)
G47452	TrGAroC	$\text{OXYL1O2} + \text{HO}_2 \rightarrow \text{OXYL1OOH}$	$\text{k_R02_H02}(\text{temp}, 7)$	Rickard and Pascoe (2009)
G47453	TrGAroCN	$\text{OXYL1O2} + \text{NO} \rightarrow \text{TOL1O} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G47454	TrGAroCN	$\text{OXYL1O2} + \text{NO}_2 \rightarrow \text{TOL1O} + \text{NO}_3$	k_C6H5O2_N02	Jagiella and Zabel (2007)*
G47455	TrGAroCN	$\text{OXYL1O2} + \text{NO}_3 \rightarrow \text{TOL1O} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G47456	TrGAroC	$\text{OXYL1O2} \rightarrow \text{TOL1O}$	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	$\text{MCATEC1O} + \text{O}_3 \rightarrow \text{MCATEC1O2}$	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47459	TrGAroC	$\text{TLEMUCCO2H} + \text{OH} \rightarrow \text{C615CO2O2} + \text{CO}_2$	$5.98\text{E-}11$	Rickard and Pascoe (2009)
G47460	TrGAroC	$\text{TLEMUCCO3H} + \text{OH} \rightarrow \text{TLEMUCCO3}$	$6.29\text{E-}11$	Rickard and Pascoe (2009)
G47461	TrGAroCN	$\text{TLEMUCPAN} + \text{OH} \rightarrow \text{C5DICARB} + \text{CO} + \text{CO}_2 + \text{NO}_2$	$5.96\text{E-}11$	Rickard and Pascoe (2009)
G47462	TrGAroCN	$\text{TLEMUCPAN} \rightarrow \text{TLEMUCCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G47463	TrGAroC	$\text{TLEMUCOOH} + \text{OH} \rightarrow \text{TLEMUCCO} + \text{OH}$	$7.04\text{E-}11$	Rickard and Pascoe (2009)
G47464	TrGAroCN	$\text{TLEMUCNO3} + \text{OH} \rightarrow \text{TLEMUCCO} + \text{NO}_2$	$3.06\text{E-}11$	Rickard and Pascoe (2009)
G47465	TrGAroC	$\text{TLEMUCCO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{EPXC4DIAL} + \text{CO}$	$4.06\text{E-}11$	Rickard and Pascoe (2009)
G47466	TrGAroC	$\text{C6H5CO3H} + \text{OH} \rightarrow \text{C6H5CO3}$	$4.66\text{E-}12$	Rickard and Pascoe (2009)
G47467	TrGAroC	$\text{PHCOOH} + \text{OH} \rightarrow \text{C6H5O2} + \text{CO}_2$	$1.10\text{E-}12$	Rickard and Pascoe (2009)
G47468	TrGAroCN	$\text{PBZN} + \text{OH} \rightarrow \text{C6H5OOH} + \text{CO} + \text{NO}_2$	$1.06\text{E-}12$	Rickard and Pascoe (2009)
G47469	TrGAroCN	$\text{PBZN} \rightarrow \text{C6H5CO3} + \text{NO}_2$	$\text{k_PAN_M} \cdot 0.67$	Rickard and Pascoe (2009)
G47470	TrGAroCN	$\text{PTLQONE} + \text{NO}_3 \rightarrow \text{NPTLQO2}$	$1.00\text{E-}12$	Rickard and Pascoe (2009)
G47471	TrGAroC	$\text{PTLQONE} + \text{OH} \rightarrow \text{PTLQO2}$	$2.3\text{E-}11$	Rickard and Pascoe (2009)
G47472	TrGAroCN	$\text{NCRES1O} + \text{NO}_2 \rightarrow \text{DNCRES}$	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	$\text{NCRES1O} + \text{O}_3 \rightarrow \text{NCRES1O2}$	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47474	TrGAroC	$\text{OXYL1OOH} + \text{OH} \rightarrow \text{OXYL1O2}$	$4.65\text{E-}11$	Rickard and Pascoe (2009)
G47475	TrGAroCN	$\text{MNCATECH} + \text{NO}_3 \rightarrow \text{MNNCATECO2}$	$5.03\text{E-}12$	Rickard and Pascoe (2009)
G47476	TrGAroCN	$\text{MNCATECH} + \text{OH} \rightarrow \text{MNCATECO2}$	$6.83\text{E-}12$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47477	TrGAroC	MCATEC1O2 + HO ₂ → MCATEC1OOH	k_R02_H02(temp, 7)	Rickard and Pascoe (2009)
G47478	TrGAroCN	MCATEC1O2 + NO → MCATEC1O + NO ₂	KR02N0	Rickard and Pascoe (2009)
G47479	TrGAroCN	MCATEC1O2 + NO ₂ → MCATEC1O + NO ₃	k_C6H5O2_N02	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO ₃ → MCATEC1O + NO ₂	KR02N03	Rickard and Pascoe (2009)
G47481	TrGAroC	MCATEC1O2 → MCATEC1O	k1_R02sOR02	Rickard and Pascoe (2009)
G47482a	TrGAroCN	NPTLQO2 + HO ₂ → NPTLQOOH	k_R02_H02(temp, 7)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO ₂ → C7CO4DB + NO ₂ + OH	k_R02_H02(temp, 7)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G47483	TrGAroCN	NPTLQO2 + NO → C7CO4DB + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47484	TrGAroCN	NPTLQO2 + NO ₃ → C7CO4DB + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47485	TrGAroCN	NPTLQO2 → C7CO4DB + NO ₂	k1_R02sOR02	Rickard and Pascoe (2009)*
G47486a	TrGAroC	PTLQO2 + HO ₂ → PTLQOOH	k_R02_H02(temp, 7)*(1.-r_CHOCH2O2_OH-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO ₂ → C6CO2OHCO3 + OH	k_R02_H02(temp, 7)*(r_CHOCH2O2_OH+r_COCH2O2_OH)	Rickard and Pascoe (2009)*
G47487	TrGAroCN	PTLQO2 + NO → C6CO2OHCO3 + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G47488	TrGAroCN	PTLQO2 + NO ₃ → C6CO2OHCO3 + NO ₂	KR02N03	Rickard and Pascoe (2009)*
G47489	TrGAroC	PTLQO2 → C6CO2OHCO3	k1_R02sOR02	Rickard and Pascoe (2009)*
G47490	TrGAroCN	DNCRES + NO ₃ → DNCRESO2	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	k_R02_H02(temp, 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	k_R02_H02(temp, 7)*(1.-r_CHOCH2O2_OH)	Rickard and Pascoe (2009)
G47497b	TrGAroCN	MNNCATECO2 + HO ₂ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	k_R02_H02(temp, 7)*r_CHOCH2O2_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_R02ISOPD02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47501a	TrGAroCN	$\text{MNCATECO}_2 + \text{HO}_2 \rightarrow \text{MNCATECOOH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * (1 - r_{\text{CHOHCH202_OH}})$	Rickard and Pascoe (2009)
G47501b	TrGAroCN	$\text{MNCATECO}_2 + \text{HO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * r_{\text{CHOHCH202_OH}}$	Rickard and Pascoe (2009)*
G47502	TrGAroCN	$\text{MNCATECO}_2 + \text{NO} \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47503	TrGAroCN	$\text{MNCATECO}_2 + \text{NO}_3 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47504	TrGAroCN	$\text{MNCATECO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{HO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47505	TrGAroC	$\text{MCATEC1OOH} + \text{OH} \rightarrow \text{MCATEC1O}_2$	2.05E-10	Rickard and Pascoe (2009)
G47506	TrGAroCN	$\text{NPTLQOOH} + \text{OH} \rightarrow \text{NPTLQO}_2$	8.56E-11	Rickard and Pascoe (2009)
G47507	TrGAroC	$\text{PTLQOOH} + \text{OH} \rightarrow \text{PTLQCO} + \text{OH}$	1.42E-10	Rickard and Pascoe (2009)
G47508	TrGAroC	$\text{PTLQCO} + \text{OH} \rightarrow \text{C6CO}_2\text{OHC}_3$	7.95E-11	Rickard and Pascoe (2009)
G47509a	TrGAroCN	$\text{NDNCRESO}_2 + \text{HO}_2 \rightarrow \text{NDNCRESOOH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * (1 - r_{\text{CHOHCH202_OH}})$	Rickard and Pascoe (2009)
G47509b	TrGAroCN	$\text{NDNCRESO}_2 + \text{HO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HNO}_3 + 2 \text{CO} + \text{NO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * r_{\text{CHOHCH202_OH}}$	Rickard and Pascoe (2009)*
G47510	TrGAroCN	$\text{NDNCRESO}_2 + \text{NO} \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HNO}_3 + 2 \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G47511	TrGAroCN	$\text{NDNCRESO}_2 + \text{NO}_3 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HNO}_3 + 2 \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G47512	TrGAroCN	$\text{NDNCRESO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HNO}_3 + 2 \text{CO} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47513a	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{DNCRESOOH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * (1 - r_{\text{CHOHCH202_OH}})$	Rickard and Pascoe (2009)
G47513b	TrGAroCN	$\text{DNCRESO}_2 + \text{HO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 7) * r_{\text{CHOHCH202_OH}}$	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_R02IS0PD02	Rickard and Pascoe (2009)*
G47517	TrGAroCN	$\text{NCRES1OOH} + \text{OH} \rightarrow \text{NCRES1O}_2$	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	$\text{MNNCATCOOH} + \text{OH} \rightarrow \text{MNNCATECO}_2$	k_ROOHR0	Rickard and Pascoe (2009)
G47519	TrGAroCN	$\text{MNCATECOOH} + \text{OH} \rightarrow \text{MNCATECO}_2$	k_ROOHR0	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47520	TrGAroC	$C7CO4DB + OH \rightarrow CO + CO + CH_3C(O) + HCOCOCHO$	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	$C6CO2OHCO3 + HO_2 \rightarrow C5134CO2OH + HO_2 + CO + CO_2 + OH$	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G47521b	TrGAroC	$C6CO2OHCO3 + HO_2 \rightarrow C6COOHCO3H$	KAPH02*(r_C03_00H+r_C03_03)	Rickard and Pascoe (2009)
G47522	TrGAroCN	$C6CO2OHCO3 + NO \rightarrow C5134CO2OH + HO_2 + CO + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G47523	TrGAroCN	$C6CO2OHCO3 + NO_2 \rightarrow C6CO2OHPAN$	k_CH3C03_N02	Rickard and Pascoe (2009)
G47524	TrGAroCN	$C6CO2OHCO3 + NO_3 \rightarrow C5134CO2OH + HO_2 + CO + CO_2 + NO_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	$C6CO2OHCO3 \rightarrow C5134CO2OH + HO_2 + CO + CO_2$	k1_R02RC03	Rickard and Pascoe (2009)
G47526	TrGAroCN	$NDNCRESOOH + OH \rightarrow NDNCRESO2$	k_R00HRO	Rickard and Pascoe (2009)
G47527	TrGAroCN	$DNCRESOOH + OH \rightarrow DNCRESO2$	k_R00HRO	Rickard and Pascoe (2009)
G47528	TrGAroC	$C6COOHCO3H + OH \rightarrow C6CO2OHCO3$	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	$C6CO2OHPAN + OH \rightarrow C5134CO2OH + CO + CO + NO_2$	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	$C6CO2OHPAN \rightarrow C6CO2OHCO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	$C85O2 \rightarrow C86O2$	k1_R02tR02	Rickard and Pascoe (2009)
G48201	TrGTerC	$C85O2 + HO_2 \rightarrow C85OOH$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	$C85O2 + NO \rightarrow C86O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48203	TrGTerC	$C85OOH + OH \rightarrow C85O2$	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	$C86O2 \rightarrow C511O2 + CH_3COCH_3$	k1_R02tR02	Rickard and Pascoe (2009)
G48205	TrGTerCN	$C86O2 + NO \rightarrow C511O2 + CH_3COCH_3 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48206	TrGTerC	$C86O2 + HO_2 \rightarrow C86OOH$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)
G48207	TrGTerC	$C86OOH + OH \rightarrow C86O2$	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	$C811O2 \rightarrow C812O2$	k1_R02pR02	Rickard and Pascoe (2009)
G48209	TrGTerC	$C811O2 + HO_2 \rightarrow 8 \text{ L CARBON}$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)
G48210	TrGTerCN	$C811O2 + NO \rightarrow C812O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48211	TrGTerC	$C812O2 \rightarrow C813O2$	k1_R02tOR02	Rickard and Pascoe (2009)
G48212	TrGTerCN	$C812O2 + NO \rightarrow C813O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48213	TrGTerC	$C812O2 + HO_2 \rightarrow C812OOH$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)
G48214	TrGTerC	$C812OOH + OH \rightarrow C812O2$	1.09E-11	Rickard and Pascoe (2009)
G48215	TrGTerC	$C813O2 \rightarrow CH_3COCH_3 + C512O2$	k1_R02tR02	Rickard and Pascoe (2009)
G48216	TrGTerCN	$C813O2 + NO \rightarrow CH_3COCH_3 + C512O2 + NO_2$	KR02NO	Rickard and Pascoe (2009)*
G48217	TrGTerC	$C813O2 + HO_2 \rightarrow C813OOH$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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*r_C03_00H	Rickard and Pascoe (2009)
G48221b	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G48221c	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{NORPINIC} + \text{O}_3$	KAPH02*r_C03_03	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_CH3C03_N02	Rickard and Pascoe (2009)
G48224	TrGTerCN	$\text{C721CO3} + \text{NO}_3 \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	$\text{C721CO3} \rightarrow \text{C721O2} + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2019)
G48226	TrGTerC	$\text{C721CO3} \rightarrow \text{NORPINIC}$	k1_R02RC03*0.1	Sander et al. (2019)
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	$\text{C8BCO2} + \text{HO}_2 \rightarrow \text{C8BCOOH}$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)
G48233a	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C89O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C8BCNO3}$	KR02N0*alpha_AN(8,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48234	TrGTerC	$\text{C8BCO2} \rightarrow \text{C89O2}$	k1_R02sR02	Rickard and Pascoe (2009)
G48235	TrGTerC	$\text{C8BCOOH} + \text{OH} \rightarrow \text{C8BCCO} + \text{OH}$	1.62E-11	Rickard and Pascoe (2009)
G48236	TrGTerCN	$\text{C8BCNO3} + \text{OH} \rightarrow \text{C8BCCO} + \text{NO}_2$	1.84E-12	Rickard and Pascoe (2009)
G48237	TrGTerC	$\text{C8BCCO} + \text{OH} \rightarrow \text{C89O2}$	3.94E-12	Rickard and Pascoe (2009)
G48238	TrGTerC	$\text{C89O2} + \text{HO}_2 \rightarrow \text{C89OOH}$	k_R02_H02(temp,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	$\text{C810O2} + \text{HO}_2 \rightarrow \text{C810OOH}$	k_R02_H02(temp,8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48245a	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(10, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G48245b	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{C810NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(10, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G48246	TrGTerCN	$\text{C810O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	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	$\text{NSTYRENO2} + \text{HO}_2 \rightarrow \text{NSTYRENOOH}$	k_R02_H02(temp, 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)*
G48409	TrGAroCN	$\text{NSTYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N03	Rickard and Pascoe (2009)*
G48410	TrGAroCN	$\text{NSTYRENO2} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	k1_R02sR02	Rickard and Pascoe (2009)*
G48411	TrGAroCN	$\text{NSTYRENOOH} + \text{OH} \rightarrow \text{NSTYRENO2}$	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	$\text{STYRENO2} + \text{HO}_2 \rightarrow \text{STYRENOOH}$	$k_{\text{R02_H02}}(\text{temp}, 8) * (1 - r_{\text{CHOHCH2O2_OH}})$	Rickard and Pascoe (2009)
G48412b	TrGAroC	$\text{STYRENO2} + \text{HO}_2 \rightarrow \text{HO}_2 + \text{OH} + \text{HCHO} + \text{BENZAL}$	$k_{\text{R02_H02}}(\text{temp}, 8) * r_{\text{CHOHCH2O2_OH}}$	Rickard and Pascoe (2009)*
G48413	TrGAroCN	$\text{STYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N0	Rickard and Pascoe (2009)*
G48414	TrGAroCN	$\text{STYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N03	Rickard and Pascoe (2009)*
G48415	TrGAroC	$\text{STYRENO2} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	k1_R02sR02	Rickard and Pascoe (2009)*
G48416	TrGAroC	$\text{STYRENOOH} + \text{OH} \rightarrow \text{STYRENO2}$	6.16E-11	Rickard and Pascoe (2009)
G49200	TrGTerC	$\text{C96O2} \rightarrow \text{C97O2}$	k1_R02pR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49201	TrGTerC	$\text{C96O2} + \text{HO}_2 \rightarrow \text{C96OOH}$	$k_{\text{R02_H02}}(\text{temp}, 9)$	Rickard and Pascoe (2009)
G49202a	TrGTerCN	$\text{C96O2} + \text{NO} \rightarrow \text{C97O2} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(10, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G49202b	TrGTerCN	$\text{C96O2} + \text{NO} \rightarrow \text{C96NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(10, 1, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G49203	TrGTerCN	$\text{C96NO3} + \text{OH} \rightarrow \text{NORPINAL} + \text{NO}_2$	$2.88\text{E-}12$	Rickard and Pascoe (2009)
G49204a	TrGTerC	$\text{C96OOH} + \text{OH} \rightarrow \text{C96O2}$	k_{R00HRO}	Rickard and Pascoe (2009)
G49205b	TrGTerC	$\text{C96OOH} + \text{OH} \rightarrow \text{NORPINAL} + \text{OH}$	$1.30\text{E-}11$	Rickard and Pascoe (2009)
G49206	TrGTerC	$\text{C97O2} \rightarrow \text{C98O2}$	$k_{1_R02tR02}$	Rickard and Pascoe (2009)
G49207	TrGTerCN	$\text{C97O2} + \text{NO} \rightarrow \text{C98O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G49208a	TrGTerC	$\text{C97O2} + \text{HO}_2 \rightarrow \text{C97OOH}$	$k_{\text{R02_H02}}(\text{temp}, 9) * r_{\text{COCH202_00H}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G49208b	TrGTerC	$\text{C97O2} + \text{HO}_2 \rightarrow \text{C98O2} + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 9) * r_{\text{COCH202_0H}}$	Rickard and Pascoe (2009), Sander et al. (2019)
G49209	TrGTerC	$\text{C97OOH} + \text{OH} \rightarrow \text{C97O2}$	$1.05\text{E-}11$	Rickard and Pascoe (2009)
G49210	TrGTerC	$\text{C98O2} \rightarrow \text{C614O2} + \text{CH}_3\text{COCH}_3$	$k_{1_R02tR02}$	Rickard and Pascoe (2009)
G49211a	TrGTerCN	$\text{C98O2} + \text{NO} \rightarrow \text{C614O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)
G49211b	TrGTerCN	$\text{C98O2} + \text{NO} \rightarrow 9 \text{ L CARBON} + \text{LNITROGEN}$	$\text{KR02N0} * \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G49212	TrGTerC	$\text{C98O2} + \text{HO}_2 \rightarrow \text{C98OOH}$	$k_{\text{R02_H02}}(\text{temp}, 9)$	Rickard and Pascoe (2009)
G49213	TrGTerC	$\text{C98OOH} + \text{OH} \rightarrow \text{C98O2}$	$2.05\text{E-}11$	Rickard and Pascoe (2009)
G49214	TrGTerC	$\text{NORPINAL} + \text{OH} \rightarrow \text{C85CO3}$	$2.64\text{E-}11$	Rickard and Pascoe (2009)
G49215	TrGTerCN	$\text{NORPINAL} + \text{NO}_3 \rightarrow \text{C85CO3} + \text{HNO}_3$	$\text{KN03AL} * 8.5$	Rickard and Pascoe (2009)
G49216	TrGTerC	$\text{C85CO3} \rightarrow \text{C85O2} + \text{CO}_2$	$k_{1_R02RC03}$	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	$\text{C85CO3} + \text{NO}_2 \rightarrow \text{C9PAN2}$	$k_{\text{CH3CO3_N02}}$	Rickard and Pascoe (2009)
G49219a	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85CO3H}$	$\text{KAPH02} * (r_{\text{C03_00H}} + r_{\text{C03_03}})$	Rickard and Pascoe (2009)
G49219b	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02} * r_{\text{C03_0H}}$	Rickard and Pascoe (2009)
G49220	TrGTerCN	$\text{C9PAN2} \rightarrow \text{C85CO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard and Pascoe (2009)
G49221	TrGTerCN	$\text{C9PAN2} + \text{OH} \rightarrow \text{C85OOH} + \text{CO} + \text{NO}_2$	$6.60\text{E-}12$	Rickard and Pascoe (2009)
G49222	TrGTerC	$\text{C85CO3H} + \text{OH} \rightarrow \text{C85CO3}$	$1.02\text{E-}11$	Rickard and Pascoe (2009)
G49223a	TrGTerC	$\text{C89CO3} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	$k_{1_R02RC03} * 0.9$	Sander et al. (2019)
G49223b	TrGTerC	$\text{C89CO3} \rightarrow \text{C89CO2H}$	$k_{1_R02RC03} * 0.1$	Sander et al. (2019)
G49224a	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO3H}$	$\text{KAPH02} * r_{\text{C03_00H}}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49224b	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO2H} + \text{O}_3$	KAPH02*r_C03_03	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*r_C03_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	Sander et al. (2019)
G49231b	TrGTerC	$\text{C811CO3} \rightarrow \text{PINIC}$	k1_R02RC03*0.1	Sander et al. (2019)
G49232a	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811CO3H}$	KAPH02*r_C03_00H	Rickard and Pascoe (2009)
G49232b	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{PINIC} + \text{O}_3$	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G49232c	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_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	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{NOPINDOOH}$	k_R02_H02(temp,9)*r_COCH202_00H	Rickard and Pascoe (2009), Sander et al. (2019)
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	k_R02_H02(temp,9)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)*
G49239	TrGTerC	$\text{NOPINDO2} \rightarrow \text{C89CO3}$	k1_R02p0R02	Rickard and Pascoe (2009)
G49240	TrGTerC	$\text{NOPINDOOH} \rightarrow \text{NOPINDCO}$	2.63E-11	Rickard and Pascoe (2009)
G49241	TrGTerC	$\text{NOPINDCO} + \text{OH} \rightarrow \text{C89CO3}$	3.07E-12	Rickard and Pascoe (2009)
G49242	TrGTerC	$\text{NOPINOO} \rightarrow \text{NOPINONE} + \text{H}_2\text{O}_2$	6.00E-18*c(ind_H2O)	Rickard and Pascoe (2009)
G49243	TrGTerC	$\text{NOPINOO} + \text{CO} \rightarrow \text{NOPINONE} + \text{CO}_2$	1.2E-15	Rickard and Pascoe (2009)
G49244	TrGTerCN	$\text{NOPINOO} + \text{NO} \rightarrow \text{NOPINONE} + \text{NO}_2$	1.E-14	Rickard and Pascoe (2009)
G49245	TrGTerCN	$\text{NOPINOO} + \text{NO}_2 \rightarrow \text{NOPINONE} + \text{NO}_3$	1.E-15	Rickard and Pascoe (2009)
G49246	TrGTerC	$\text{NORPINENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C86O2}$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
G49247	TrGTerC	NORPINENOL + HCOOH \rightarrow NORPINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G49248	TrGTerC	NORPINAL + HCOOH \rightarrow NORPINENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G49249	TrGTerC	C811CO3H + OH \rightarrow C811CO3	1.04E-11	Rickard and Pascoe (2009)
G49250	TrGTerCN	C811PAN \rightarrow C811CO3 + NO ₂	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	C811PAN + OH \rightarrow C721CHO + CO + NO ₂	6.77E-12	Rickard and Pascoe (2009)
G49400a	TrGAroC	LTMB + OH \rightarrow TLEPOXMUC + HO ₂ + 2 LCARBON	0.827E-11	Rickard and Pascoe (2009)*
G49400b	TrGAroC	LTMB + OH \rightarrow C6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard and Pascoe (2009)*
G49400c	TrGAroC	LTMB + OH \rightarrow CRESOL + 2 LCARBON	0.141E-11	Rickard and Pascoe (2009)*
G49400d	TrGAroC	LTMB + OH \rightarrow TLBIPERO2 + HO ₂ + 2 LCARBON	2.917E-11	Rickard and Pascoe (2009)*
G49401	TrGAroCN	LTMB + NO ₃ \rightarrow C6H5CH2O2 + HNO ₃ + 2 LCARBON	1.52E-15	Rickard and Pascoe (2009)*
G40200	TrGTerC	APINENE + OH \rightarrow .75 LAPINABO2 + .15 MENTHEN6ONE + .15 HO ₂ + .10 ROO6R1O2	1.2E-11*EXP(440./temp)	Atkinson et al. (2006)*
G40201a	TrGTerCN	LAPINABO2 + NO \rightarrow PINAL + HO ₂ + NO ₂	KR02NO*(1-(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)))	Rickard and Pascoe (2009), Sander et al. (2019)
G40201b	TrGTerCN	LAPINABO2 + NO \rightarrow LAPINABNO3	KR02NO*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40202a	TrGTerC	LAPINABO2 + HO ₂ \rightarrow LAPINABOOH	k_R02_H02(temp,10)*(1-r_CHOCH202_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G40202b	TrGTerC	LAPINABO2 + HO ₂ \rightarrow PINAL + HO ₂ + OH	k_R02_H02(temp,10)*r_CHOCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40203	TrGTerC	LAPINABO2 \rightarrow PINAL + HO ₂	R02*(0.65*k1_R02tOR02+.35*k1_R02sOR02)	Rickard and Pascoe (2009)*
G40204	TrGTerC	LAPINABOOH + OH \rightarrow .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard and Pascoe (2009)*
G40205	TrGTerCN	LAPINABNO3 + OH \rightarrow .35 PINAL + .65 C96CO3 + NO ₂	4.29E-12	Rickard and Pascoe (2009)*
G40206	TrGTerC	MENTHEN6ONE + OH \rightarrow OHMENTHEN6ONEO2	6.46E-11	Vereecken et al. (2007)*
G40207	TrGTerCN	OHMENTHEN6ONEO2 + NO \rightarrow 2OHMENTHEN6ONE + HO ₂ + NO ₂	KR02NO	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO ₂ \rightarrow 2OHMENTHEN6ONE	k_R02_H02(temp,10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 \rightarrow 2OHMENTHEN6ONE + HO ₂	k1_R02tOR02	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH \rightarrow 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH \rightarrow .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./temp)	Wallington et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G40212	TrGTerCN	PINAL + NO ₃ → C96CO3 + HNO ₃	2.0E-14	Wallington et al. (2018)*
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*r_C03_00H	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO ₂ → PINONIC + O ₃	KAPH02*r_C03_03	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO ₂ → C96O2 + OH + CO ₂	KAPH02*r_C03_OH	Rickard and Pascoe (2009)
G40215	TrGTerCN	C96CO3 + NO ₂ → C10PAN2	k_CH3C03_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	KR02N03*1.74	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	k_R02_H02(temp,10)	Rickard and Pascoe (2009)
G40223a	TrGTerCN	PINALO2 + NO → C106O2 + NO ₂	KR02N0*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40223b	TrGTerCN	PINALO2 + NO → PINALNO3	KR02N0*alpha_AN(12,3,0,1,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
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)
G40227	TrGTerC	C106O2 + HO ₂ → C106OOH	k_R02_H02(temp,10)	Rickard and Pascoe (2009)
G40228a	TrGTerCN	C106O2 + NO → C716O2 + CH ₃ COCH ₃ + NO ₂	KR02N0*0.875*(1.-alpha_AN(13,3,0,0,0,temp, cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40228b	TrGTerCN	C106O2 + NO → C106NO3	KR02N0*0.875*alpha_AN(13,3,0,0,0,temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40229	TrGTerC	C106O2 → C716O2 + CH ₃ COCH ₃	k1_R02tR02	Rickard and Pascoe (2009)
G40230	TrGTerC	C106OOH + OH → C106O2	8.01E-11	Rickard and Pascoe (2009)
G40231	TrGTerCN	C106NO3 + OH → CO235C6CHO + CH ₃ COCH ₃ + NO ₂	7.03E-11	Rickard and Pascoe (2009)
G40232	TrGTerC	APINENE + O ₃ → .09 APINBOO + .08 PINONIC + .77 OH + .33 NORPINAL + .33 CO + .33 HO ₂ + .06 APINAOO + .44 C109O2	8.05E-16*EXP(-640./temp)	Wallington et al. (2018)*
G40233	TrGTerC	APINAOO → PINAL + H ₂ O ₂	1.00E-17*c(ind_H2O)	Rickard and Pascoe (2009)
G40234	TrGTerC	APINAOO + CO → PINAL + CO ₂	1.20E-15	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40235	TrGTerCN	APINAOO + NO → PINAL + NO ₂	1.00E-14	Rickard and Pascoe (2009)
G40236	TrGTerCN	APINAOO + NO ₂ → PINAL + NO ₃	1.00E-15	Rickard and Pascoe (2009)
G40237a	TrGTerC	APINBOO → PINONIC	1.00E-17*c(ind_H20)*(0.08+0.15)	Rickard and Pascoe (2009)
G40237b	TrGTerC	APINBOO → PINAL + H ₂ O ₂	1.00E-17*c(ind_H20)*0.77	Rickard and Pascoe (2009)
G40238	TrGTerC	APINBOO + CO → PINAL + CO ₂	1.20E-15	Rickard and Pascoe (2009)
G40239	TrGTerCN	APINBOO + NO → PINAL + NO ₂	1.00E-14	Rickard and Pascoe (2009)
G40240	TrGTerCN	APINBOO + NO ₂ → PINAL + NO ₃	1.00E-15	Rickard and Pascoe (2009)
G40241	TrGTerC	C109O2 → C89CO3 + HCHO	k1_R02pOR02	Rickard and Pascoe (2009)
G40242	TrGTerCN	C109O2 + NO → C89CO3 + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G40243a	TrGTerC	C109O2 + HO ₂ → C109OOH	k_R02_H02(temp,10)*r_COCH202_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G40243b	TrGTerC	C109O2 + HO ₂ → C89CO3 + HCHO + OH	k_R02_H02(temp,10)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40244	TrGTerC	C109OOH + OH → C109CO + OH	5.47E-11	Rickard and Pascoe (2009)
G40245	TrGTerC	C109CO + OH → C89CO3 + CO	5.47E-11	Rickard and Pascoe (2009)
G40246	TrGTerCN	APINENE + NO ₃ → LNAPINABO2	1.2E-12*EXP(490./temp)	Wallington et al. (2018)*
G40247	TrGTerCN	LNAPINABO2 → PINAL + NO ₂	(0.65*k1_R02tR02 + 0.35*k1_R02sR02)	Rickard and Pascoe (2009)
G40248	TrGTerCN	LNAPINABO2 + NO → PINAL + NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G40249	TrGTerCN	LNAPINABO2 + HO ₂ → LNAPINABOOH	k_R02_H02(temp,10)	Rickard and Pascoe (2009)
G40250	TrGTerCN	LNAPINABO2 + NO ₃ → PINAL + NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009)
G40251	TrGTerCN	LNAPINABOOH + OH → LNAPINABO2	(.65*6.87E-12+.35*1.23E-11)	Rickard and Pascoe (2009)
G40252a	TrGTerC	BPINENE + OH → BPINAO2	1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40252b	TrGTerC	BPINENE + OH → ROO6R1O2	1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068)	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO ₂ → BPINAOOH	k_R02_H02(temp,10)*r_COCH202_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G40253b	TrGTerC	BPINAO2 + HO ₂ → NOPINONE + HCHO + HO ₂ + OH	k_R02_H02(temp,10)*r_COCH202_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40254a	TrGTerCN	BPINAO2 + NO → NOPINONE + HCHO + HO ₂ + NO ₂	KR02NO*(1.-alpha_AN(11,3,0,0,0, temp, cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KR02NO*alpha_AN(11,3,0,0,0, temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO ₂	k1_R02tOR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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	k_R02_H02(temp, 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	k_R02_H02(temp, 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	k_R02_H02(temp, 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. (2018)*
G40267b	TrGTerC	BPINENE + O ₃ \rightarrow NOPINOO + CO ₂	1.35E-15*EXP(-1270./temp) * .368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267c	TrGTerC	BPINENE + O ₃ \rightarrow NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./temp) * .283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267d	TrGTerC	BPINENE + O ₃ \rightarrow C8BC + 2 CO ₂	1.35E-15*EXP(-1270./temp) * (.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40268	TrGTerCN	BPINENE + NO ₃ \rightarrow LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40269	TrGTerCN	LNBPINABO2 + HO ₂ \rightarrow LNBPINABOOH	k_R02_H02(temp, 10)	Rickard and Pascoe (2009)
G40270	TrGTerCN	LNBPINABO2 + NO \rightarrow NOPINONE + HCHO + NO ₂ + NO ₂	KR02N0	Rickard and Pascoe (2009)*
G40271	TrGTerCN	LNBPINABO2 + NO ₃ \rightarrow NOPINONE + HCHO + NO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G40272a	TrGTerCN	LNBPINABO2 \rightarrow NOPINONE + HCHO + NO ₂	k1_R02tR02*0.7	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40272b	TrGTerCN	LNBPINABO2 \rightarrow BPINANO3	k1_R02tR02*0.3	Rickard and Pascoe (2009)
G40273	TrGTerCN	LNBPINABOOH + OH \rightarrow LNBPINABO2	9.58E-12	Rickard and Pascoe (2009)
G40274	TrGTerCN	ROO6R1NO3 + OH \rightarrow ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40275	TrGTerCN	RO6R1NO3 + OH \rightarrow 9 LCARBON + HCHO + HO ₂ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)
G40276	TrGTerC	PINEOL + OH \rightarrow HCOOH + OH + NORPINAL	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH \rightarrow PINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G40278	TrGTerC	PINAL + HCOOH \rightarrow PINEOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G40279a	TrGC	CARENE + OH \rightarrow LAPINABO2	8.8E-11*(.50+.25)	Atkinson and Arey (2003)
G40279b	TrGC	CARENE + OH \rightarrow MENTHEN6ONE + HO ₂	8.8E-11*.25*.60	Atkinson and Arey (2003)
G40279c	TrGC	CARENE + OH \rightarrow ROO6R1O2	8.8E-11*.25*.40	Atkinson and Arey (2003)
G40280a	TrGC	CARENE + O ₃ \rightarrow APINBOO	3.7E-17*.50*.18	Atkinson and Arey (2003)
G40280b	TrGC	CARENE + O ₃ \rightarrow PINONIC	3.7E-17*.50*.16	Atkinson and Arey (2003)
G40280c	TrGC	CARENE + O ₃ \rightarrow OH + NORPINAL + CO + HO ₂	3.7E-17*.50*.66	Atkinson and Arey (2003)
G40280d	TrGC	CARENE + O ₃ \rightarrow APINAOO	3.7E-17*.50*.12	Atkinson and Arey (2003)
G40280e	TrGC	CARENE + O ₃ \rightarrow OH + C109O2	3.7E-17*.50*(.22+.66)	Atkinson and Arey (2003)
G40281	TrGCN	CARENE + NO ₃ \rightarrow LNAPINABO2	9.1E-12	Atkinson and Arey (2003)
G40282a	TrGTerC	SABINENE + OH \rightarrow 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 \rightarrow 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 \rightarrow NOPINONE + .63 CO + .37 HOCH ₂ OOH + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./temp) *.051/(1.-.027)	Wallington et al. (2018)*
G40283b	TrGTerC	SABINENE + O ₃ \rightarrow NOPINOO + CO ₂	1.35E-15*EXP(-1270./temp) *.368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283c	TrGTerC	SABINENE + O ₃ \rightarrow NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283d	TrGTerC	SABINENE + O ₃ \rightarrow C8BC + 2 CO ₂	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40284	TrGTerCN	SABINENE + NO ₃ \rightarrow LNBPINABO2	2.51E-12	Wallington et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G40285a	TrGTerC	CAMPHENE + OH \rightarrow 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 \rightarrow 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 \rightarrow NOPINONE + .63 CO + .37 HOCH ₂ OOH + .16 OH + .16 HO ₂	1.35E-15*EXP(-1270./temp) *.051/(1.-.027)	Wallington et al. (2018)*
G40286b	TrGTerC	CAMPHENE + O ₃ \rightarrow NOPINOO + CO ₂	1.35E-15*EXP(-1270./temp) *.368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286c	TrGTerC	CAMPHENE + O ₃ \rightarrow NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286d	TrGTerC	CAMPHENE + O ₃ \rightarrow C8BC + 2 CO ₂	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40287	TrGTerCN	CAMPHENE + NO ₃ \rightarrow LNBPINABO2	2.51E-12	Wallington et al. (2018)*
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)

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

#	labels	reaction	rate coefficient	reference
G6301	StTrGCIN	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 1.6\text{E-}31, 3.4, 7\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G6302	TrGCIN	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	$6.918\text{E-}7 * \text{EXP}(-10909./\text{temp}) * \text{cair}$	Anderson and Fahey (1990)
G6303	StGCIN	$\text{ClNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{ClO} + \text{NO}_3$	$4.5\text{E-}12 * \text{EXP}(-900./\text{temp})$	Atkinson et al. (2007)
G6304	StTrGCIN	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	$6.2\text{E-}12 * \text{EXP}(145./\text{temp})$	Atkinson et al. (2007)
G6400	StTrGCl	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$	$6.6\text{E-}12 * \text{EXP}(-1240./\text{temp})$	Atkinson et al. (2006)
G6401	StTrGCl	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$	$8.1\text{E-}11 * \text{EXP}(-34./\text{temp})$	Atkinson et al. (2006)
G6402	StTrGCl	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{HCl} + \text{OH}$	$5.9\text{E-}11$	Atkinson et al. (2006)*
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$1.8\text{E-}12 * \text{EXP}(-600./\text{temp})$	Burkholder et al. (2015)
G6404	StGCl	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + \text{ClO} + 3 \text{ Cl}$	$3.3\text{E-}10$	Burkholder et al. (2015)
G6405	StGCl	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow 0.1 \text{ CH}_3\text{Cl} + 0.1 \text{ O}(^3\text{P}) + 0.46 \text{ ClO} + 0.35 \text{ Cl} + 0.09 \text{ H} + 0.9 \text{ LCARBON} + 0.09 \text{ LCHLORINE}$	$1.65\text{E-}10$	Burkholder et al. (2015)
G6406	StGCl	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{LCARBON} + \text{H}_2\text{O} + \text{Cl}$	$1.96\text{E-}12 * \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6407	StGCCl	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow 2 \text{ LCARBON} + \text{OH} + 3 \text{ Cl}$	$3.25\text{E-}10$	Burkholder et al. (2015)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 2 \text{ LCARBON} + \text{H}_2\text{O} + 3 \text{ Cl}$	$1.64\text{E-}12 * \text{EXP}(-1520./\text{temp})$	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	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})$	$8.0\text{E-}11$	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{LCARBON} + \text{CH}_3 + \text{HCl}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 6.1\text{E-}30, 3.0, 2.0\text{E-}10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$8.3\text{E-}11 * \text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)
G6413	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{HCl} + \text{HCHO} + \text{NO}_2$	$1.3\text{E-}11 * \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6414	StTrGCIN	$\text{Cl} + \text{CH}_3\text{ONO} \rightarrow \text{HCl} + \text{HCHO} + \text{NO}$	$2.1\text{E-}12$	Sokolov et al. (1999)
G6415	StTrGCl	$\text{Cl} + \text{CH}_3\text{O}_2 \rightarrow .5 \text{ ClO} + .5 \text{ CH}_3\text{O} + .5 \text{ HCl} + .5 \text{ CH}_2\text{OO}$	$1.6\text{E-}10$	Burkholder et al. (2015)
G6416	TrGCCIN	$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{NCCH}_2\text{O}_2 + \text{HCl}$	$1.6\text{E-}11 * \text{EXP}(-2104./\text{temp})$	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019)
G6500	StGCIF	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + 2 \text{ LFLUORINE} + \text{ClO} + \text{Cl}$	$1.4\text{E-}10$	Burkholder et al. (2015)
G6501	StGCIF	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{LCARBON} + \text{LFLUORINE} + \text{ClO} + 2 \text{ Cl}$	$2.3\text{E-}10$	Burkholder et al. (2015)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E-}11 * \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7101	StGBr	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E-}11 * \text{EXP}(230./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{ Br} + \text{O}_2$	$2.7\text{E-}12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E-}14 * \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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	$\text{Br} + \text{BrNO}_3 \rightarrow \text{Br}_2 + \text{NO}_3$	$4.9\text{E}-11$	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	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO_NO2}} / (5.44\text{E}-9 \cdot \text{EXP}(14192./\text{temp}) \cdot 1.\text{E}6 \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm}2\text{Pa} \cdot N_{\text{A}}))$	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-580./\text{temp})$	Atkinson et al. (2006)
G7401	TrGBr	$\text{Br} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HBr}$	$2.6\text{E}-12 \cdot \text{EXP}(-1600./\text{temp})$	Kondo and Benson (1984)
G7402	TrGBr	$\text{BrO} + \text{CH}_3\text{O}_2 \rightarrow \text{HOBr} + \text{CH}_2\text{OO}$	$2.42\text{E}-14 \cdot \text{EXP}(1617./\text{temp})$	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	$\text{Br} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HBr}$	$2.8\text{E}-13 \cdot \text{EXP}(224./\text{temp}) / (1. + 1.13\text{E}24 \cdot \text{EXP}(-3200./\text{temp}) / C(\text{ind_O2}))$	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	$\text{CHCl}_2\text{Br} + \text{OH} \rightarrow \text{LCARBON} + 2 \text{ Cl} + \text{H}_2\text{O} + \text{Br}$	$2.0\text{E}-12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7606	TrGBrCl	$\text{CHClBr}_2 + \text{OH} \rightarrow \text{LCARBON} + \text{Cl} + \text{H}_2\text{O} + 2 \text{ Br}$	$2.0\text{E}-12 \cdot \text{EXP}(-840./\text{temp})$	see note*
G7607	TrGBrCl	$\text{CH}_2\text{ClBr} + \text{OH} \rightarrow \text{LCARBON} + \text{Cl} + \text{H}_2\text{O} + \text{Br}$	$2.1\text{E}-12 \cdot \text{EXP}(-880./\text{temp})$	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)*

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

#	labels	reaction	rate coefficient	reference
G8200	TrGI	$I + HO_2 \rightarrow HI + O_2$	$1.5E-11*EXP(-1090./temp)$	Atkinson et al. (2007)
G8201	TrGI	$IO + HO_2 \rightarrow HOI + O_2$	$1.4E-11*EXP(540./temp)$	Atkinson et al. (2007)
G8202	TrGI	$HI + OH \rightarrow I + H_2O$	$1.6E-11*EXP(440./temp)$	Atkinson et al. (2007)
G8203	TrGI	$OIO + OH \rightarrow HIO_3$	$2.2E-10*EXP(243./temp)$	Plane et al. (2006)
G8204	TrGI	$I_2 + OH \rightarrow HOI + I$	$2.1E-10$	Atkinson et al. (2007)
G8205	TrGI	$HOI + OH \rightarrow IO + H_2O$	$5.0E-12$	Riffault et al. (2005)
G8300	TrGIN	$I + NO_2 \rightarrow INO_2$	k_I_NO2	Atkinson et al. (2007)*
G8301	TrGIN	$I + NO_3 \rightarrow IO + NO_2$	$1.E-10$	Dillon et al. (2008)
G8302	TrGIN	$IO + NO \rightarrow I + NO_2$	$7.15E-12*EXP(300./temp)$	Atkinson et al. (2007)
G8303	TrGIN	$IO + NO_2 \rightarrow INO_3$	$k_3rd_iupac(temp, cair, 7.7E-31, 5., 1.6E-11, 0., 0.4)$	Atkinson et al. (2007)
G8304	TrGIN	$OIO + NO \rightarrow NO_2 + IO$	$1.1E-12*EXP(542./temp)$	Atkinson et al. (2007)
G8305	TrGIN	$INO_2 \rightarrow I + NO_2$	$k_I_NO2/(3.7E-7*EXP(9568./temp) * 1.E6*R_gas*temp/(atm2Pa*N_A))$	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGIN	$INO_3 \rightarrow IO + NO_2$	$2.1e15*EXP(-13670./temp)$	Kaltsayannis and Plane (2008)
G8307	TrGIN	$I_2 + NO_3 \rightarrow I + INO_3$	$1.5E-12$	Atkinson et al. (2007)
G8308	TrGIN	$IO + NO_3 \rightarrow OIO + NO_2$	$9.E-12$	Dillon et al. (2008)
G8309	TrGIN	$I + INO_3 \rightarrow I_2 + NO_3$	$9.1E-11*EXP(-146./temp)$	Kaltsayannis and Plane (2008)
G8400	TrGCI	$CH_3CHICH_3 + OH \rightarrow 2\text{ L CARBON} + CH_3O_2 + I$	$1.22E-12$	Carl and Crowley (2001)
G8401	TrGI	$CH_3O_2 + IO \rightarrow .4\text{ I} + .6\text{ OIO} + HCHO + HO_2$	$2.E-12$	Dillon et al. (2006b), Bale et al. (2005)*
G8402	TrGIN	$CH_3I + NO_3 \rightarrow HNO_3 + HCHO + IO$	$3.4E-17$	Wayne et al. (1991)*
G8600	TrGCII	$IO + ClO \rightarrow .2\text{ ICl} + .25\text{ Cl} + .55\text{ OClO} + .8\text{ I} + .45\text{ O}_2$	$4.7E-12*EXP(280./temp)$	Atkinson et al. (2007)
G8700	TrGBrI	$I + BrO \rightarrow IO + Br$	$1.2E-11$	Burkholder et al. (2015)
G8701	TrGBrI	$IO + BrO \rightarrow Br + .8\text{ OIO} + .2\text{ I} + .2\text{ O}_2$	$1.5E-11*EXP(510./temp)$	Atkinson et al. (2007)*
G8702	TrGBrI	$IBr + OH \rightarrow .84\text{ HOI} + .84\text{ Br} + .16\text{ HOBr} + .16\text{ I}$	$1.4E-10$	Riffault et al. (2005)
G8703	TrGBrI	$IO + Br \rightarrow I + BrO$	$2.3E-11$	Bedjanian et al. (1997)
G8704	TrGBrI	$I_2 + Br \rightarrow IBr + I$	$1.2E-10$	Bedjanian et al. (1997)
G9200	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	$k_3rd(temp, cair, 3.3E-31, 4.3, 1.6E-12, 0., 0.6)$	Burkholder et al. (2015)
G9400a	TrGCS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	$1.13E-11*EXP(-253./temp)$	Atkinson et al. (2004)*
G9400b	TrGCS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGCNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	$1.9E-13*EXP(520./temp)$	Atkinson et al. (2004)
G9402	TrGCS	$DMSO + OH \rightarrow .6\text{ SO}_2 + HCHO + .6\text{ CH}_3 + .4\text{ HO}_2 + .4\text{ CH}_3\text{SO}_3\text{H}$	$1.E-10$	Hynes and Wine (1996)*

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

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

General notes

Three-body reactions

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

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by Wallington et al. (2018) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

Structure-Activity Relationships (SAR)

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

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

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

RO₂ self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \text{k_CH3O2}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH3O2 = second-order rate coefficient of the self reaction of CH_3O_2 , and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

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

G2110: The rate coefficient is: $k_{\text{H02_H02}} = (3.0\text{E-}13 \cdot \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 \cdot \text{EXP}(920./\text{temp}) \cdot \text{cair}) \cdot (1 + 1.4\text{E-}21 \cdot \text{EXP}(2200./\text{temp}) \cdot \text{C}(\text{ind_H2O}))$.

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

G2118: Assuming fast equilibrium.

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

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

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

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

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

G3227: Backward reaction divided by equilibrium constant from Burkholder et al. (2015).

G3228: Same as for $\text{OH} + \text{HNO}_4$.

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

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

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

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

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

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

G4130a: SAR for H-abstraction by OH.

G4130b: SAR for H-abstraction by OH.

G4132: SAR for H-abstraction by OH.

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

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

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

G4136: Average of two measurements.

G4137: Upper limit.

G4138: Average of $7\text{E-}12$ and $1.5\text{E-}12$.

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

G4142: High-pressure limit.

G4143: Generic estimate for reaction with alcohols.

G4144: Generic estimate for reaction with RO_2 .

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

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

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

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

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

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

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

G4164: Upper limit. Dominant pathway under atmospheric conditions.

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

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

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

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

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

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

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

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

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

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

promptly. The decomposition products are $2 \text{HCHO} + \text{HO}_2$.

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

G42058b: The aldehydic H is assumed to be like the analogous H of HOCH_2CHO .

G42074a: Factor of 3 to match the estimate of $k = 1. \times 10^{-11} \text{ molec/cm}^3/\text{s}$ by Paulot et al. (2009a).

G42074b: Factor of 3 to match the estimate of $k = 1. \times 10^{-11} \text{ molec/cm}^3/\text{s}$ by Paulot et al. (2009a).

G42075: $\text{NO}_3\text{CH}_2\text{CO}_2\text{H}$ and $\text{NO}_3\text{CH}_2\text{CO}_3\text{H}$ neglected.

G42078: $\text{NO}_3\text{CH}_2\text{CO}_2\text{H}$ neglected.

G42082: Same rate constant as for $\text{PAN} + \text{OH}$.

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 $< 0.1 \text{ bar}$.

G42085b: Channel proposed by Hynes and Wine 1991, $\text{OH} + \text{HCHO} + \text{HOCN}$, could not be confirmed by Tyndall et al. (2001b). There is no alternative mechanism at the moment. Products assumed to be $\text{OH} + \text{CH}_3\text{CO}_3 + \text{NO}$

G42086b: Assuming HCN is from channel 2h, $\text{HCO} + \text{H} + \text{HCN}$. HCO is replaced by $\text{H} + \text{CO}$.

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

G42087: HCOCN is produced but replaced here by its likely oxidation products ($\text{HCN} + \text{CO}_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $\text{RO}_2 + \text{NO}$ reaction is used.

G42088: NCCH_2OOH is produced but replaced here by its likely oxidation products ($\text{HCN} + \text{CO}_2$) as studied by Tyndall et al. (2001b). The rate constant for a typical $\text{RO}_2 + \text{HO}_2$ reaction is used.

G42089a: The minor channel with $k = 5.2 \times 10^{-12}$ 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).

G42092: approximated OH reaction for oxalic acid

G42093a: SAR for H-abstraction by OH

G42093b: SAR for H-abstraction by OH, assuming that $-\text{CHOHOH}$ has an effect like $-\text{CH}_2\text{OH}$

G42093c: SAR for H-abstraction by OH

G42093d: SAR for H-abstraction by OH

G42094a: SAR for H-abstraction by OH

G42094b: SAR for H-abstraction by OH

G42095a: SAR for H-abstraction by OH

G42095b: SAR for H-abstraction by OH

G42096a: SAR for H-abstraction by OH

G42096b: SAR for H-abstraction by OH

G42097a: SAR for H-abstraction by OH

G42097b: SAR for H-abstraction by OH

G42098a: SAR for H-abstraction by OH, assuming that $-\text{CH}_2\text{OOH}$ has the same effect as $-\text{CH}_2\text{OH}$

G42098b: SAR for H-abstraction by OH

G42098c: SAR for H-abstraction by OH

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

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

G43004: The value for the generic $\text{RO}_2 + \text{HO}_2$ reaction from Atkinson (1997) is used here.

G43008: The value for the generic $\text{RO}_2 + \text{HO}_2$ 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 ($\text{CH}_3\text{OOH} + \text{OH}$) is used, multiplied by the branching ratio of the CH_3O_2 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.

G43075a: Same value as for methanediol.

G43075b: Same value as for methanediol.

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 ($\text{nC}_4\text{H}_9\text{O}_2:\text{sC}_4\text{H}_9\text{O}_2$ ratio) is assumed to be equal to the ratio of the production rates at 298K: $k_p/(k_p+k_s) = 0.1273$ and $k_s/(k_p+k_s) = 0.8727$.

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

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

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

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

G44015b: Products assumed to be only from H-abstraction from a secondary C bearing the $-\text{OOH}$ group.

G44016: Products assumed to be only from H-abstraction from a secondary C bearing the $-\text{ONO}_2$ group.

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

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

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

G44023a: Products from H-abstraction from the tertiary carbon bearing the ONO_2 group.

G44023b: Products from H-abstraction from the secondary carbon bearing the ONO_2 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 RO_2 .

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 RO_2 is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO_2 isomers mostly $\text{C}_2\text{H}_5\text{CHO}$.

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

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

G44098: The nitrated RO_2 is replaced by its products upon reaction with NO.

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

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

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

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

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

G44127: Only this channel considered as the intermediate radical is likely more stable than 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 → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO₂

G44407: KDEC MALDIALCO₂ → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO₂

G44409: KDEC MALDIALCO₂ → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO₂

G44410: KDEC MALDIALCO₂ → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO + 0.4 CO₂

G44412: KDEC BZFUONOOA → 0.5 BZFUONOO + 0.5 CO + 0.5 CO₂ + 0.5 HCOCH₂O₂ + 0.5 OH and BZFUONOO → 0.625 CO₁₄O₃CO₂H + 0.375 CO₁₄O₃CHO + 0.375 H₂O₂

G44421: Only major channel.

G44424: KDEC: GLYOOA → 0.125 HCHO + 0.18 GLYOO + 0.82 HO₂ + 0.57 OH + 1.265 CO + 0.25 CO₂ and H₂O substitution GLYOO → 0.625 HCOCO₂H + 0.375 GLYOX + 0.375 H₂O₂

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCO₃

G44431: KDEC MALANHYO → HCOCOHCO₃

G44432: Only major channel. KDEC MALANHYO → HCOCOHCO₃

G44436: KDEC NBZFUO → 0.5 CO₁₄O₃CHO + 0.5 NO₂ + 0.5 NBZFUONE + 0.5 HO₂

G44437: KDEC NBZFUO → 0.5 CO₁₄O₃CHO + 0.5 NO₂ + 0.5 NBZFUONE + 0.5 HO₂

G44438: KDEC NBZFUO → 0.5 CO₁₄O₃CHO + 0.5 NO₂ + 0.5 NBZFUONE + 0.5 HO₂ and RO₂ Only major channel.

G44439: KDEC MALDIALCO₂ → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO + 0.4 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 → GLYOX + GLYOX + HO₂

G44458: KDEC MALDIALO → GLYOX + GLYOX + HO₂

G44459: KDEC MALDIALO → GLYOX + GLYOX + HO₂. Only major channel.

G44461: KBPAN → 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), $4.2\text{E-}11$.

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant $4.16\text{E-}11$.

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: C4MDIAL = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with NO_3 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 HO_2 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 RO_2 -to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with O_2 forming HCOOH + HO_2 . Along $\text{CH}_3\text{COCHOHCHO}$ should be produced but not in the mechanism. Only $\text{CH}_3\text{COCHO}_2\text{CHO}$. 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 RO_2 that upon conversion to RO yields 100% 2-methyl-butenedial (C4MDIAL) although Aschmann et al. (2014) quantified a 38% yield of the Z/E mixture.

G45129: As for 3METHYLFURAN + OH but with additional NO_2 production for mass conservation.

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

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

G45139: LZCPANC23DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: $\text{LMBOABO}_2 = 0.67 \text{ MBOAO}_2 + 0.33 \text{ MBOBO}_2$

G45247: Alkyl nitrate formation neglected.

G45400: $\text{KDEC NC4MDCO}_2 \rightarrow \text{MMALANH}_Y + \text{NO}_2$

G45404: $\text{KDEC NTLFUO} \rightarrow \text{ACCOMETCHO} + \text{NO}_2$

G45405: $\text{KDEC NTLFUO} \rightarrow \text{ACCOMETCHO} + \text{NO}_2$

G45406: $\text{KDEC NTLFUO} \rightarrow \text{ACCOMETCHO}$

G45409: $\text{KBPAN} \rightarrow \text{k_PAN_M}(\text{renaming})$

G45413: $\text{KFPAN} \rightarrow \text{k_CH}_3\text{CO}_3\text{NO}_2(\text{renaming})$

G45422: $\text{KDEC MMALANH}_Y\text{O} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$

G45423: $\text{KDEC MMALANH}_Y\text{O} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$

G45424: $\text{KDEC MMALANH}_Y\text{O} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$ and Only major channel.

G45429: $\text{KBPAN} \rightarrow \text{k_PAN_M}(\text{renamed})$

G45430a: $\text{KDEC C}_5\text{CO}_{14}\text{CO}_2 \rightarrow 0.83 \text{ MALANH}_Y + 0.83 \text{ CH}_3 + 0.17 \text{ MGLYOX} + 0.17 \text{ HO}_2 + 0.17 \text{ CO} + 0.17 \text{ CO}_2$

G45431: $\text{KDEC C}_5\text{CO}_{14}\text{CO}_2 \rightarrow 0.83 \text{ MALANH}_Y + 0.83 \text{ CH}_3 + 0.17 \text{ MGLYOX} + 0.17 \text{ HO}_2 + 0.17 \text{ CO} + 0.17 \text{ CO}_2$

G45432: $\text{KFPAN} \rightarrow \text{k_CH}_3\text{CO}_3\text{NO}_2(\text{renaming})$

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

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

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

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

G45452: KDEC TLFUONOOA \rightarrow 0.5 CO + 0.5 OH + 0.5 MECOACETO2 + 0.5 TLFUONOO and H2O subs TLFUONOO \rightarrow 0.625 C24O3CCO2H + 0.375 AC-COMECHO + 0.375 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 ND-NPHENO \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 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

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

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

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

G46468: KFPAN \rightarrow k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO \rightarrow C5CO2OHCO3

G46481: KDEC PBZQO \rightarrow C5CO2OHCO3

G46482: KDEC PBZQO \rightarrow C5CO2OHCO3

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

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

G46486: KDEC DNPHEO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHEO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHEO \rightarrow NC4DCO2H + HCOCO2H + NO2

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

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

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

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

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

G46500: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46501: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46502: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

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

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

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

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

G47210: Alkyl nitrate formation neglected.

G47214: Alkyl nitrate formation neglected.

G47218: Alkyl nitrate formation neglected.

G47222: Alkyl nitrate formation neglected.

G47223: ROO6R3OOH produced but no sink for it.

G47225: ROO6R4P produced but no sink for it.

G47226: ROO6R5P produced but no sink for it

G47400: Merged.

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

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

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

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

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero2_oh is set to 0.4 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

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

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

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

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

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

G47413: Merged.

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

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

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

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

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

G47423: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

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

G47436: KFPAN \rightarrow k_CH3CO3_NO2

G47438: Only major channel.

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

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

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

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

G47445: KFPAN \rightarrow k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

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

G47483: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47484: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47485: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO \rightarrow C6CO2OHCO3

G47487: KDEC PTLQO \rightarrow C6CO2OHCO3

G47488: KDEC PTLQO \rightarrow C6CO2OHCO3

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

G47494: New channel.

G47497b: Reactions with KRO2HO2 and KDEC MN-NCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47498: KDEC MN-NCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MN-NCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47501b: Reactions with KRO2HO2 and KDEC MN-NCATECO \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 ND-NCRESO \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: KDEC CH₂O₂B → 0.24 CH₂O + 0.40 CO + 0.36 HO₂ + 0.36 CO + 0.36 OH and H₂O + PH-CHOO → 0.625 PHCOOH + 0.375 BENZAL + 0.375 H₂O₂ + 0.2 CO₂

G48408: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

G48409: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

G48410: KDEC NSTYRENEO → NO₂ + HCHO + BENZAL

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

G48413: KDEC STYRENO → HO₂ + HCHO + BENZAL

G48414: KDEC STYRENO → HO₂ + HCHO + BENZAL

G48415: KDEC STYRENO → HO₂ + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

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

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

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

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11 \cdot 0.21 + 3.25\text{E-}11 \cdot 0.30 + 5.67\text{E-}11 \cdot 0.14)/3$, 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). LAP-INABO₂ = 0.65 APINAO₂ + 0.35 APINBO₂

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

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

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

G40206: SAR-estimated rate constant, $(k_{\text{ads}} + k_{\text{adt}}) \cdot \text{acoch}_3 = 6.46\text{E-}11$ 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: ROO6R1OOH is produced but no sink for it.

G40262: RO6R1OOH 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 RO6R1NO₃ in G4085.

G40276: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G40282a: Products from Vereecken and Peeters (2012).

G40282b: Products from Vereecken and Peeters (2012).

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

G40284: Products from Rickard and Pascoe (2009).

G40285a: Products from Vereecken and Peeters (2012).

G40285b: Products from Vereecken and Peeters (2012).

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

G40287: Products from Rickard and Pascoe (2009).

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

G40401: Same products as for toluene.

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

G6204: At low temperatures, there may be a minor reaction channel leading to $O_3 + HCl$. 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 and Cl atoms. 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 and Cl atoms. The fate of the carbon atom is currently not considered.

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

G8102: Consistent with O'Dowd and Hoffmann (2005), it is assumed that the reaction produces new particles.

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

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

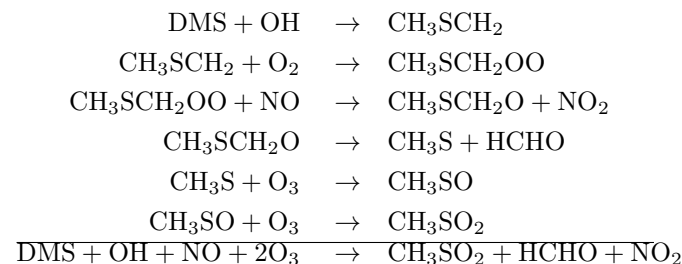
G8305: The rate coefficient is defined as backward reaction (Atkinson et al., 2007) divided by equilibrium constant (van den Bergh and Troe, 1976).

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).

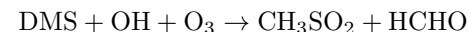
G8402: The products are from Nakano et al. (2005).

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: $k_{DMS_OH} = 1.0E-39 * EXP(5820./temp) * C(ind_02) / (1.+5.0E-30 * EXP(6280./temp) * C(ind_02))$.

G9402: Products and yields are not from Hynes and Wine (1996).

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

G10201: Upper limit.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
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	$NO_2 + h\nu \rightarrow NO + O(^3P)$	$jx(ip_N02)$	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow N + O(^3P)$	$jx(ip_N0)$	Sander et al. (2014)
J3102b	UpGJN	$NO + h\nu \rightarrow NO^+ + e^-$	$jx(ip_N0p)$	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	$jx(ip_N020)$	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	$jx(ip_N002)$	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	$jx(ip_N205)$	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow NO + OH$	$jx(ip_H0N0)$	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	$jx(ip_HN03)$	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	$jx(ip_HN04)$	Sander et al. (2014)
J41000	StTrGJ	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	$jx(ip_CH300H)$	Sander et al. (2014)
J41001a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	$jx(ip_COH2)$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41001b	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H} + \text{CO} + \text{HO}_2$	jx(ip_CH0H)	Sander et al. (2014)
J41002	StGJ	$\text{CO}_2 + h\nu \rightarrow \text{CO} + \text{O}(^3\text{P})$	jx(ip_CO2)	Sander et al. (2014)
J41003	StGJ	$\text{CH}_4 + h\nu \rightarrow .42 \text{ CH}_3 + .42 \text{ H} + .6912 \text{ H}_2 + .0864 \text{ HCHO} + .0864 \text{ O}(^3\text{P}) + .1584 \text{ OH} + .1584 \text{ HO}_2 + .2112 \text{ CO}_2 + .1824 \text{ CO} + .024 \text{ H}_2\text{O} + .10 \text{ L CARBON}$	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_CH3O2NO2)	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_CH3O2NO2)	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	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHOH}$	$\text{jx(ip_CH3CHO2VINY)}$	Clubb et al. (2012)
J42002	TrGJC	$\text{CH}_3\text{C(O)OOH} + h\nu \rightarrow \text{CH}_3 + \text{OH} + \text{CO}_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J42004	TrGJCN	$\text{PAN} + h\nu \rightarrow .7 \text{ CH}_3\text{C(O)} + .7 \text{ NO}_2 + .3 \text{ CH}_3 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	Sander et al. (2014)*
J42005a	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{HCHO} + 2 \text{ HO}_2 + \text{CO}$	$\text{jx(ip_HOCH2CHO)*0.83}$	Sander et al. (2014)*
J42005b	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCOCH}_2\text{O}_2$	$\text{jx(ip_HOCH2CHO)*0.07}$	Sander et al. (2014)*
J42005c	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{CH}_3\text{OH} + \text{CO}$	$\text{jx(ip_HOCH2CHO)*0.10}$	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	$\text{HCOCO}_3\text{H} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J42011	TrGJC	$\text{HYETHO2H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	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_IC3H7NO3	Rickard and Pascoe (2009)
J42013	TrGJC	$\text{HOOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	$2 * \text{jx(ip_CH300H)}$	Sander et al. (2019)
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)	Sander et al. (2019)
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	Sander et al. (2019)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42016	TrGC	$\text{CH}_3\text{CHOHOOH} + h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J42017	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	$(\text{jx}(\text{ip_C2H5N03}) + \text{jx}(\text{ip_CH3CHO}))$ $\ast(\text{jx}(\text{ip_NOA}) + 1\text{E-}10) / (0.59 \ast \text{j_}$ $\text{IC3H7N03} + \text{jx}(\text{ip_CH3COCH}_3) + 1\text{E-}10)$	Sander et al. (2019)*
J42018	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)
J42019	TrGJCN	$\text{C}_2\text{H}_5\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{jx}(\text{ip_C2H5N03})$	Sander et al. (2019)
J42020	TrGJCN	$\text{NO}_3\text{CH}_2\text{CHO} + h\nu \rightarrow .7 \text{ NO}_3\text{CH}_2\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ HCHO} +$ $.3 \text{ NO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2019)*
J42021	StTrGJCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + h\nu \rightarrow .667 \text{ NO}_2 + .667 \text{ C}_2\text{H}_5\text{O}_2 + .333 \text{ NO}_3 +$ $.333 \text{ CH}_3\text{CHO} + .333 \text{ HO}_2$	$\text{jx}(\text{ip_CH302N02})$	Sander et al. (2019)*
J42022	TrGJC	$\text{HOCCOOH} + h\nu \rightarrow \text{CO}_2 + .72 \text{ HCOOH} + .28 \text{ CO} + .28 \text{ H}_2\text{O}$	$\text{jx}(\text{ip_H00CC00H})$	Yamamoto and Back (1985)
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	$\text{CH}_3\text{COCH}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CH}_3$	$\text{jx}(\text{ip_CH3COCH}_3)$	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	$\text{HOCH}_2\text{COCH}_2\text{OOH} + h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{j_ACETOL}$	Sander et al. (2019)
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	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{j_ACETOL}$	Sander et al. (2019)
J43013	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J43014	TrGJTerC	$\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) \ast 2.$	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	$\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$	$2 \ast \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J43018	TrGJC	$\text{CH}_3\text{COCO}_2\text{H} + h\nu \rightarrow .32 \text{ CH}_3\text{CHO} + .16 \text{ CH}_2\text{CHOH} + .54 \text{ CO}_2$ $+ .38 \text{ CH}_3\text{C}(\text{O}) + .38 \text{ HO}_2 + .38 \text{ CO}_2 + .07 \text{ CH}_3\text{COOH} + .07$ $\text{CO} + .05 \text{ CH}_3\text{C}(\text{O}) + .05 \text{ CO} + .05 \text{ OH}$	$\text{jx}(\text{ip_CH3COCOC}_2\text{H})$	Sander et al. (2019)*
J43019	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_CH300H})$	Sander et al. (2019)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43020	TrGC	$\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{j_ketene} \cdot 0.36 \cdot 2.$	Sander et al. (2019)
J43021	TrGCN	$\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	j_IC3H7NO_3	Sander et al. (2019)
J43022	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$	$\text{jx}(\text{ip_CH302NO}_2) + \text{jx}(\text{ip_CH3COCH}_3)$	Sander et al. (2019)
J43023	TrGJC	$\text{C}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43024	TrGJCN	$\text{C}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{NO}_2 + \text{HO}_2$	$0.59 \cdot \text{j_IC3H7NO}_3$	see note*
J43025a	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_C2H5CHO2HCO})$	see note*
J43025b	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$	$\text{jx}(\text{ip_C2H5CHO2ENOL})$	Andrews et al. (2012), Sander et al. (2019)*
J43026	TrGJCN	$\text{PPN} + h\nu \rightarrow .7 \text{ C}_2\text{H}_5\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ C}_2\text{H}_5\text{O}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2014)
J43027	TrGJC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)
J43028a	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J43028b	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J43200	TrGJTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J43400	TrGJAroC	$\text{C3DIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) \cdot 2. + \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J43401	TrGJAroC	$\text{C32OH13CO} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) \cdot 2.$	Rickard and Pascoe (2009)
J43402	TrGJAroC	$\text{HCOCOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J44000a	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) \cdot (\text{k_p}/(\text{k_p} + \text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2019)
J44000b	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip_CH300H}) \cdot (\text{k_s}/(\text{k_p} + \text{k_s}))$	Rickard and Pascoe (2009), Sander et al. (2019)
J44001	TrGJC	$\text{MVK} + h\nu \rightarrow .5 \text{ C}_3\text{H}_6 + .5 \text{ CH}_3\text{C}(\text{O}) + .5 \text{ HCHO} + \text{CO} + .5 \text{ HO}_2$	$\text{jx}(\text{ip_MVK})$	Sander et al. (2014)
J44002	TrGJC	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$	$0.42 \cdot \text{jx}(\text{ip_CHOH})$	von Kuhlmann et al. (2003)
J44003	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow .62 \text{ CH}_3\text{C}(\text{O}) + .62 \text{ CH}_3\text{CHO} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 0.42 \cdot \text{jx}(\text{ip_CHOH})$	Sander et al. (2019)
J44004	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{ CH}_3\text{C}(\text{O})$	$2.15 \cdot \text{jx}(\text{ip_MGLYOX})$	see note*
J44005a	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{j_IC3H7NO}_3 \cdot (\text{k_p}/(\text{k_p} + \text{k_s}))$	see note*
J44005b	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$	$\text{j_IC3H7NO}_3 \cdot (\text{k_s}/(\text{k_p} + \text{k_s}))$	see note*
J44006	TrGJCN	$\text{MPAN} + h\nu \rightarrow .7 \text{ MACO}_3 + .7 \text{ NO}_2 + .3 \text{ MACO}_2 + .3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	see note*
J44007a	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44007b	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HO}_2 + \text{HCOCO}_3\text{H}$	j_ACETOL	Rickard and Pascoe (2009)
J44008	TrGJC	$\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$	jx(ip_MACR)	Sander et al. (2014)
J44009	TrGJC	$\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)	Sander et al. (2019)*
J44010	TrGJC	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	2.77*jx(ip_HOCH2CHO)	see note*
J44011	TrGJC	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$	jx(ip_CH300H)	Sander et al. (2019)
J44012	TrGJC	$\text{LHMKABOOH} + h\nu \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{CH}_3\text{C}(\text{O}) + .88 \text{HOCH}_2\text{CHO} + .12 \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Sander et al. (2019)
J44013	TrGJC	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	jx(ip_HOCH2CHO)+j_ACETOL	Sander et al. (2019)
J44014	TrGJC	$\text{HO}_2\text{CO}_3\text{C}_4 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{HO}_2$	j_ACETOL	Rickard and Pascoe (2009)
J44015	TrGJC	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	2.15*jx(ip_MGLYOX)	see note*
J44016	TrGC	$\text{HCOCCH}_3\text{CO} + h\nu \rightarrow .5 \text{OH} + .5 \text{CH}_3\text{CHO} + \text{CO} + .5 \text{CH}_3\text{CHCO} + .5 \text{CO}$	j_ketene	Sander et al. (2019)
J44017a	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{CH}_3\text{COCO}_2\text{H} + .1848 \text{H}_2\text{O}_2 + .2208 \text{MGLYOX} + .36 \text{OH} + .36 \text{CO} + .56 \text{CH}_3\text{C}(\text{O}) + .2 \text{CH}_3\text{CHO} + .2 \text{CO}_2 + .2 \text{HCHO} + .2 \text{HO}_2 + \text{CO}$	j_ketene*0.5	Sander et al. (2019), Rickard and Pascoe (2009)*
J44017b	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$	j_ketene*0.5	Sander et al. (2019)
J44018a	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Sander et al. (2019)
J44018b	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$	2.15*jx(ip_MGLYOX)	Sander et al. (2019)
J44019	TrGJC	$\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$	3.15*jx(ip_MGLYOX)	Sander et al. (2019)
J44020a	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$	jx(ip_CH300H)+j_ACETOL	Rickard and Pascoe (2009)
J44020b	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44021	TrGJTerC	$\text{C}_4\text{OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J44022	TrGJTerC	$\text{C}_4\text{OOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+jx(ip_HOCH2CHO)+j_ACETOL	Rickard and Pascoe (2009)
J44023a	TrGJTerC	$\text{C}_4\text{CODIAL} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44023b	TrGJTerC	$\text{C}_4\text{CODIAL} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44024	TrGJTerC	$\text{C}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44025	TrGJCN	$\text{LMEKNO}_3 + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	jx(ip_MEKNO3)	Barnes et al. (1993), Sander et al. (2019)*
J44026	TrGJCN	$\text{MVKNO}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{NO}_2$	jx(ip_MEKNO3)	Barnes et al. (1993), Sander et al. (2019)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44027	TrGJCN	$\text{MACRNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$(2.84*j_IC3H7N03+jx(ip_CH3CHO))$ $*(jx(ip_MEKN03)+1E-10)/(j_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)$	Müller et al. (2014), Sander et al. (2019)*
J44028	TrGJCN	$\text{TC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{NO}_2$	$2.84*j_IC3H7N03$	Sander et al. (2019)
J44029	TrGJC	$\text{TC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44030	TrGJCN	$\text{IBUTOLBNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84*j_IC3H7N03$	Sander et al. (2019)
J44031	TrGJC	$\text{IBUTOLBOOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44032	TrGJC	$\text{LBUT1ENOOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44033	TrGJCN	$\text{LBUT1ENNO}_3 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$j_IC3H7N03$	Sander et al. (2019)
J44034	TrGJC	$\text{BUT2OLOOH} + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44035	TrGJCN	$\text{BUT2OLNO}_3 + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$j_IC3H7N03$	Sander et al. (2019)
J44036	TrGJC	$\text{BUT2OLO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	j_ACETOL	Sander et al. (2019)
J44037a	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$jx(ip_C3H7CHO2HCO)$	Sander et al. (2019)
J44037b	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{CHOH}$	$jx(ip_C3H7CHO2VINYL)$	Sander et al. (2019)*
J44038	TrGJC	$\text{IPRCHO} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$jx(ip_IPRCHO2HCO)$	Sander et al. (2019)
J44039	TrGJCN	$\text{IC}_4\text{H}_9\text{NO}_3 + h\nu \rightarrow \text{IPRCHO} + \text{NO}_2$	$j_IC3H7N03$	Sander et al. (2019)
J44040	TrGJC	$\text{IC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{IPRCHO} + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44041	TrGJC	$\text{PERIBUACID} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	$jx(ip_CH300H)$	Sander et al. (2019)
J44042	TrGJCN	$\text{PIPN} + h\nu \rightarrow .7 \text{IPRCO}_3 + .7 \text{NO}_2 + .3 \text{iC}_3\text{H}_7\text{O}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	$jx(ip_PAN)$	Sander et al. (2019), Sander et al. (2014)
J44043	TrGJC	$\text{HVMK} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + 2 \text{OH}$	$jx(ip_PeDIONE24)$	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	$\text{HMAC} + h\nu \rightarrow \text{HCOCCH}_3\text{CO} + 2 \text{OH}$	$jx(ip_PeDIONE24)$	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$jx(ip_C2H5CHO2HCO)$	Rickard and Pascoe (2009)
J44045b	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$	$jx(ip_C2H5CHO2ENOL)$	Andrews et al. (2012), Sander et al. (2019)
J44046a	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$jx(ip_C2H5CHO2HCO)*2.$	see note*
J44046b	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$	$jx(ip_C2H5CHO2ENOL)*2.$	Andrews et al. (2012), Sander et al. (2019)
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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44201	TrGJTerC	$\text{IPRHOCO3H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J44400a	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{C32OH13CO} + \text{CO} + \text{OH} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard and Pascoe (2009)
J44400b	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44401	TrGJAroC	$\text{BZFUOOH} + h\nu \rightarrow \text{CO14O3CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44402	TrGJAroC	$\text{HOCOC4DIAL} + h\nu \rightarrow \text{HCOCO3H} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44403	TrGJAroCN	$\text{NBZFUOOH} + h\nu \rightarrow .5 \text{ CO14O3CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	$\text{MALDALCO3H} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard and Pascoe (2009)
J44404b	TrGJAroC	$\text{MALDALCO3H} + h\nu \rightarrow .6 \text{ MALANHY} + \text{HO}_2 + .4 \text{ GLYOX} + .4 \text{ CO} + .4 \text{ CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44405	TrGJAroC	$\text{EPXDLCO2H} + h\nu \rightarrow \text{C3DIALO2} + \text{CO}_2 + \text{HO}_2$	$2.77 * \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44406	TrGJAroC	$\text{MALDIAL} + h\nu \rightarrow .4 \text{ BZFUONE} + .6 \text{ MALDIALCO3} + .6 \text{ HO}_2$	$\text{jx}(\text{ip_NO2}) * 0.14$	Rickard and Pascoe (2009)
J44407	TrGJAroC	$\text{MALANHYOOH} + h\nu \rightarrow \text{HCOCO3H} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J44408	TrGJAroC	$\text{EPXDLCO3H} + h\nu \rightarrow \text{C3DIALO2} + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H}) + 2.77 * \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J44409	TrGJAroC	$\text{CO2C4DIAL} + h\nu \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{HO}_2 + \text{CO} + \text{CO}$	$\text{jx}(\text{ip_MGLYOX}) * 2.$	Rickard and Pascoe (2009)
J44410	TrGJAroC	$\text{MALDALCO2H} + h\nu \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard and Pascoe (2009)
J44411	TrGJAroC	$\text{EPXC4DIAL} + h\nu \rightarrow \text{C3DIALO2} + \text{CO} + \text{HO}_2$	$2.77 * \text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard and Pascoe (2009)
J44412	TrGJAroC	$\text{CO14O3CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J44414	TrGJAroC	$\text{MECOACEOOH} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
J45002	TrGJC	$\text{LISOPACOOH} + h\nu \rightarrow \text{LISOPACO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45003	TrGJCN	$\text{LISOPACNO3} + h\nu \rightarrow \text{LISOPACO} + \text{NO}_2$	$0.59 * \text{j_IC3H7N03}$	see note*
J45004	TrGJC	$\text{ISOPBOOH} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45005	TrGJCN	$\text{ISOPBNO3} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{j_IC3H7N03}$	see note*
J45006	TrGJC	$\text{ISOPDOOH} + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45007	TrGJCN	$\text{ISOPDNO3} + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	j_IC3H7N03	see note*
J45008	TrGJCN	$\text{NISOPOOH} + h\nu \rightarrow \text{NC4CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J45009	TrGJCN	$\text{NC4CHO} + h\nu \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	$(.59 * \text{j_IC3H7N03} + \text{jx}(\text{ip_MACR})) * (\text{jx}(\text{ip_MEKN03}) + 1\text{E-10}) / (\text{j_IC3H7N03} + 0.42 * \text{jx}(\text{ip_CHOH}) + 1\text{E-10})$	Müller et al. (2014), Sander et al. (2019)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45010	TrGJCN	$\text{LNISOOH} + h\nu \rightarrow \text{NOA} + \text{OH} + .5 \text{HOCHCHO} + .5 \text{CO} + .5 \text{HO}_2 + .5 \text{CO}_2$	$\text{jx}(\text{ip_CH300H})$	Taraborrelli et al. (2009), Sander et al. (2019)
J45011	TrGJC	$\text{LHC4ACCHO} + h\nu \rightarrow .5 \text{LHC4ACCO3} + .5 \text{HO}_2 + .5 \text{CO} + .5 \text{OH} + .25 \text{MACRO2} + .25 \text{LHMKABO2}$	$\text{jx}(\text{ip_MACR})$	Sander et al. (2019)
J45012	TrGJC	$\text{LC578OOH} + h\nu \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)
J45013	TrGJC	$\text{LHC4ACCO3H} + h\nu \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{OH} + \text{CO}_2$	j_HPALD	Sander et al. (2019)
J45014	TrGJCN	$\text{LC5PAN1719} + h\nu \rightarrow .7 \text{LHC4ACCO3} + .7 \text{NO}_2 + .15 \text{MACRO2} + .15 \text{LHMKABO2} + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2019)
J45015	TrGJC	$\text{HCOC5} + h\nu \rightarrow .65 \text{CH}_3 + .65 \text{CO} + .65 \text{HCHO} + .35 \text{OH} + .35 \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HOCH}_2\text{CO}$	$0.5 * \text{jx}(\text{ip_MVK})$	Sander et al. (2019)*
J45016	TrGJC	$\text{C59OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{OH}$	$\text{j_ACETOL} + \text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J45017	TrGJTerC	$\text{C511OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCH}_2\text{CHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J45018a	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J45018b	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCH}_2\text{CO}_3$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
J45019	TrGJTerC	$\text{CO23C4CO3H} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J45020	TrGJTerC	$\text{C512OOH} + h\nu \rightarrow \text{C513O}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J45021	TrGJTerC	$\text{CO13C4CHO} + h\nu \rightarrow \text{CHOC3COO}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard and Pascoe (2009)
J45022	TrGJTerC	$\text{C513OOH} + h\nu \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO})$	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	$\text{C514OOH} + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard and Pascoe (2009)
J45025	TrGJTerCN	$\text{C514NO}_3 + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	$\text{j_IC3H7NO}_3 + \text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard and Pascoe (2009)
J45026a	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HVMK} + \text{OH}$	$\text{j_HPALD} * 0.6 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO}$	$\text{j_HPALD} * 0.6 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HMAC} + \text{OH}$	$\text{j_HPALD} * 0.4 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2$	$\text{j_HPALD} * 0.4 * 0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45027	TrGJC	$\text{LZCO}_3\text{HC}_2\text{3DBCOD} + h\nu \rightarrow .62 \text{EZCH}_3\text{CO}_2\text{CHCHO} + .38 \text{EZCHOCCH}_3\text{CHO}_2 + \text{OH} + \text{CO}_2$	j_HPALD	Sander et al. (2019)
J45028a	TrGJC	$\text{C1OOHC}_2\text{OOHC}_4\text{OD} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} + 2 \text{CO} + \text{HO}_2$	$2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)
J45028b	TrGJC	$\text{C1OOHC}_2\text{OOHC}_4\text{OD} + h\nu \rightarrow .5 \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + .5 \text{HOCHCHO} + .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{HCHO} + 1.5 \text{OH}$	$2 * \text{jx}(\text{ip_CH}_3\text{OOH})$	Sander et al. (2019)
J45029	TrGC	$\text{DB1OOH} + h\nu \rightarrow \text{DB1O}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH})$	Sander et al. (2019)
J45030	TrGC	$\text{DB2OOH} + h\nu \rightarrow .48 \text{CH}_3\text{COCH}_2\text{OH} + .52 \text{HOCH}_2\text{CHO} + .52 \text{MGLYOX} + .48 \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH})$	Sander et al. (2019)
J45031a	TrGJC	$\text{C1ODC}_2\text{OOHC}_4\text{OD} + h\nu \rightarrow \text{MGLYOX} + \text{HOCHCHO} + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH})$	Sander et al. (2019)
J45031b	TrGJC	$\text{C1ODC}_2\text{OOHC}_4\text{OD} + h\nu \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$2 * 2.77 * \text{jx}(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)
J45032	TrGJC	$\text{C4MDIAL} + h\nu \rightarrow .5 \text{CH}_3\text{COCHCO} + .5 \text{HCOCCH}_3\text{CO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_N02}) * 0.1 * 0.5$	Sander et al. (2019)*
J45033	TrGCN	$\text{DB1NO}_3 + h\nu \rightarrow \text{DB1O}_2 + \text{NO}_2$	j_IC3H7N03	Sander et al. (2019)
J45034	TrGJTerC	$\text{CHOC}_3\text{COOOH} + h\nu \rightarrow \text{CHOC}_3\text{COO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH}) + \text{jx}(\text{ip_HOCH}_2\text{CHO}) + \text{j_ACETOL}$	Rickard and Pascoe (2009)
J45200a	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH}) * .67$	Rickard and Pascoe (2009), Sander et al. (2019)
J45200b	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH}) * .33$	Rickard and Pascoe (2009), Sander et al. (2019)
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	$\text{LNMBOABOOH} + h\nu \rightarrow \text{NO}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH}) * .65$	Rickard and Pascoe (2009), Sander et al. (2019)
J45203b	TrGJTerCN	$\text{LNMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH}) * .35$	Rickard and Pascoe (2009), Sander et al. (2019)
J45204	TrGJTerCN	$\text{NC}_4\text{OHCO}_3\text{H} + h\nu \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH}_3\text{OOH})$	Rickard and Pascoe (2009)
J45400	TrGJAroC	$\text{C}_5\text{4CO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{CO} + \text{CO} + \text{CH}_3\text{C(O)}$	$\text{jx}(\text{ip_MGLYOX}) + 2.15 * \text{jx}(\text{ip_MGLYOX}) * 2.$	Rickard and Pascoe (2009)
J45401	TrGJAroC	$\text{C}_5\text{134CO}_2\text{OH} + h\nu \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) + 2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45402	TrGJAroC	$\text{C5DIALOOH} + h\nu \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_MACR)}$	Rickard and Pascoe (2009)*
J45406	TrGJAroC	$\text{C5CO14OH} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO}$	jx(ip_MVK)	Rickard and Pascoe (2009)
J45407	TrGJAroC	$\text{C5DICARB} + h\nu \rightarrow .6 \text{ C5CO14O2} + .6 \text{ HO}_2 + .4 \text{ TLFUONE}$	$\text{jx(ip_N02)} * 0.2$	Rickard and Pascoe (2009)*
J45408	TrGJAroC	$\text{MC3ODBCO2H} + h\nu \rightarrow \text{CH}_3\text{COCO}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	jx(ip_MACR)	Rickard and Pascoe (2009)
J45409	TrGJAroC	$\text{ACCOMMECHO} + h\nu \rightarrow \text{MECOACETO2} + \text{HO}_2 + \text{CO}$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45410	TrGJAroC	$\text{MMALNHOOH} + h\nu \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45411	TrGJAroC	$\text{C5DICAROOH} + h\nu \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)} + \text{j_ACETOL}$	Rickard and Pascoe (2009)*
J45412	TrGJAroCN	$\text{NTLFUOOH} + h\nu \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45414	TrGJAroC	$\text{C5CO14OOH} + h\nu \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45415	TrGJAroC	$\text{TLFUOOH} + h\nu \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45417	TrGJAroC	$\text{ACCOMECO3H} + h\nu \rightarrow \text{MECOACETO2} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45418	TrGJAroC	$\text{C5DIALCO} + h\nu \rightarrow \text{MALDIALCO3} + \text{CO} + \text{HO}_2$	$\text{jx(ip_MGLYOX)} + \text{jx(ip_MACR)}$	Rickard and Pascoe (2009)
J46200	TrGJTerCN	$\text{C614NO3} + h\nu \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.15 * \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J46201	TrGJTerC	$\text{C614OOH} + h\nu \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + 2.15 * \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J46202	TrGJTerC	$\text{CO235C5CHO} + h\nu \rightarrow \text{CO23C4CO3} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46203	TrGJTerC	$\text{CO235C6OOH} + h\nu \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$	$\text{jx(ip_CH300H)} + 2.15 * \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J46400	TrGJAroC	$\text{PHENOOH} + h\nu \rightarrow .71 \text{ MALDALCO2H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46401	TrGJAroC	$\text{C6CO4DB} + h\nu \rightarrow \text{C4CO2DBCO3} + \text{HO}_2 + \text{CO}$	$\text{jx(ip_MGLYOX)} * 2.$	Rickard and Pascoe (2009)
J46402	TrGJAroC	$\text{C5CO2DCO3H} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J46403	TrGJAroCN	$\text{NDNPHENOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	$\text{BZBIPERNO3} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{NO}_2$	j_IC3H7N03	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	$\text{HOC6H4NO2} + h\nu \rightarrow \text{HONO} + \text{CPDKETENE}$	jx(ip_HOC6H4N02)	Chen et al. (2011)*
J46406	TrGJAroC	$\text{CPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{ HO}_2 + \text{MALDIAL}$	j_ketene	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46407	TrGJAroC	$\text{C5COOHCO3H} + h\nu \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46408	TrGJAroC	$\text{BZEPOXMUC} + h\nu \rightarrow .5 \text{ C5DIALO2} + 1.5 \text{ HO}_2 + 1.5 \text{ CO} + .5 \text{ MALDIAL}$	$4.\text{E3}*\text{jx(ip_MVK)}*0.1$	Rickard and Pascoe (2009)
J46409	TrGJAroCN	$\text{NPHEN1OOH} + h\nu \rightarrow \text{NPHEN1O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46410	TrGJAroC	$\text{BZEMUCCO} + h\nu \rightarrow \text{HCOCO2HCO3} + \text{C3DIALO2}$	$\text{jx(ip_HOCH2CHO)}*2.+ \text{j_ACETOL}$	Rickard and Pascoe (2009)
J46411	TrGJAroC	$\text{BZEMUCCO2H} + h\nu \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{HO}_2$	jx(ip_MACR)	Rickard and Pascoe (2009)
J46412	TrGJAroCN	$\text{NNCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46413	TrGJAroC	$\text{C615CO2OOH} + h\nu \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip_MVK)}+\text{jx(ip_CH300H)}$	Rickard and Pascoe (2009)
J46414	TrGJAroCN	$\text{NPHENOOH} + h\nu \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{OH} + \text{NO}_2$	$\text{j_IC3H7N03} + \text{jx(ip_CH300H)}$	Rickard and Pascoe (2009)
J46415	TrGJAroCN	$\text{NCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46416	TrGJAroC	$\text{PBZQOOH} + h\nu \rightarrow \text{C5CO2OHCO3} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46417	TrGJAroC	$\text{BZOBIPEROH} + h\nu \rightarrow \text{MALDIALCO3} + \text{GLYOX} + \text{HO}_2$	j_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	$\text{BZBIPEROOH} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	$\text{NBZQOOH} + h\nu \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46420	TrGJAroC	$\text{CATEC1OOH} + h\nu \rightarrow \text{CATEC1O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46421	TrGJAroC	$\text{C6125CO} + h\nu \rightarrow \text{C5CO14O2} + \text{CO} + \text{HO}_2$	$\text{jx(ip_MGLYOX)}+\text{jx(ip_MVK)}$	Rickard and Pascoe (2009)
J46422	TrGJAroCN	$\text{DNPHENOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J46423	TrGJAroC	$\text{BZEMUCCO3H} + h\nu \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)}+\text{jx(ip_MACR)}$	Rickard and Pascoe (2009)
J46424	TrGJAroC	$\text{C6H5OOH} + h\nu \rightarrow \text{C6H5O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46425	TrGJAroC	$\text{BZEMUCOOH} + h\nu \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{OH}$	$\text{jx(ip_CH300H)}+\text{jx(ip_HOCH2CHO)}*2.$	Rickard and Pascoe (2009)*
J46427	TrGJAroCN	$\text{BZEMUCNO3} + h\nu \rightarrow \text{EPXC4DIAL} + \text{NO}_2 + \text{GLYOX} + \text{HO}_2$	$2.77*\text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J46428	TrGJAroCN	$\text{DNPHEN} + h\nu \rightarrow \text{HONO} + \text{NCPDKETENE}$	jx(ip_HOC6H4N02)	Sander et al. (2019)
J46429	TrGJAroCN	$\text{NCPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{ HO}_2 + \text{NC4DCO2H}$	j_ketene	see note*
J47200	TrGJTerC	$\text{CO235C6CHO} + h\nu \rightarrow \text{CHOC3COCO3} + \text{CH}_3\text{C(O)}$	$2.15*\text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J47201	TrGJTerC	$\text{C235C6CO3H} + h\nu \rightarrow \text{CO235C6O2} + \text{CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)}+2.15*\text{jx(ip_MGLYOX)}$	Rickard and Pascoe (2009)
J47202	TrGJTerC	$\text{C716OOH} + h\nu \rightarrow \text{CO13C4CHO} + \text{CH}_3\text{C(O)} + \text{OH}$	$\text{jx(ip_CH300H)}+\text{jx(ip_HOCH2CHO)}$	Rickard and Pascoe (2009)
J47203	TrGJTerC	$\text{C721OOH} + h\nu \rightarrow \text{C722O2} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47204	TrGJTerC	$C722OOH + h\nu \rightarrow CH_3COCH_3 + C44O2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J47400	TrGJAroC	$TLEPOXMUC + h\nu \rightarrow .5 C615CO2O2 + HO_2 + CO + .5 EPXC4DIAL + .5 CH_3C(O)$	$4.E3*jx(ip_MVK)*0.1$	Rickard and Pascoe (2009)
J47401	TrGJAroC	$C6H5CH2OOH + h\nu \rightarrow BENZAL + HO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J47402	TrGJAroCN	$C6H5CH2NO3 + h\nu \rightarrow BENZAL + HO_2 + NO_2$	$0.59*j_IC3H7N03$	Rickard and Pascoe (2009)*
J47403	TrGJAroC	$BENZAL + h\nu \rightarrow HO_2 + CO + C6H5O2$	$jx(ip_BENZAL)$	Wallington et al. (2018)
J47404	TrGJAroC	$TLBIPEROOH + h\nu \rightarrow .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J47405	TrGJAroCN	$TLBIPERNO3 + h\nu \rightarrow .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO_2$	$j_IC3H7N03$	Rickard and Pascoe (2009)*
J47406	TrGJAroC	$TLOBIPEROH + h\nu \rightarrow C5CO14O2 + GLYOX + HO_2$	j_ACETOL	Rickard and Pascoe (2009)
J47407	TrGJAroC	$CRESOOH + h\nu \rightarrow .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J47408a	TrGJAroCN	$NCRESOOH + h\nu \rightarrow .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH + NO_2$	$j_IC3H7N03$	Rickard and Pascoe (2009)*
J47408b	TrGJAroCN	$NCRESOOH + h\nu \rightarrow C5CO14OH + GLYOX + NO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	$TOL1OHNO2 + h\nu \rightarrow HONO + MCPDKETENE$	$jx(ip_HOPh3Me2N02)$	see note*
J47410	TrGJAroC	$TLEMUCCO2H + h\nu \rightarrow C615CO2O2 + CO_2 + HO_2$	$jx(ip_MACR)$	Rickard and Pascoe (2009)
J47411	TrGJAroC	$TLEMUCCO3H + h\nu \rightarrow C615CO2O2 + CO_2 + OH$	$jx(ip_CH300H)+jx(ip_MACR)$	Rickard and Pascoe (2009)
J47412	TrGJAroC	$TLEMUCOOH + h\nu \rightarrow .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH$	$jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)+j_ACETOL$	Rickard and Pascoe (2009)*
J47413	TrGJAroCN	$TLEMUCNO3 + h\nu \rightarrow EPXC4DIAL + NO_2 + CH_3C(O) + CO + HO_2$	$2.77*jx(ip_HOCH2CHO)+j_ACETOL$	Rickard and Pascoe (2009)
J47414	TrGJAroC	$TLEMUCCO + h\nu \rightarrow CH_3C(O) + EPXC4DIAL + CO + HO_2$	$2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)$	Rickard and Pascoe (2009)
J47415	TrGJAroC	$C6H5CO3H + h\nu \rightarrow C6H5O2 + CO_2 + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J47416	TrGJAroC	$OXYL1OOH + h\nu \rightarrow TOL1O + OH$	$jx(ip_CH300H)$	Rickard and Pascoe (2009)
J47417	TrGJAroCN	$MNCATECH + h\nu \rightarrow HONO + MCPDKETENE$	$jx(ip_HOPh3Me2N02)$	see note*
J47418	TrGJAroC	$MCPDKETENE + h\nu \rightarrow CO_2 + CO + 2 HO_2 + C4MDIAL$	j_ketene	see note*
J47419	TrGJAroCN	$DNCRES + h\nu \rightarrow HONO + MNCPDKETENE$	$jx(ip_HOPh3Me2N02)$	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47420	TrGJAroCN	MNCPDKETENE + $h\nu$ → CO ₂ + CO + 2 HO ₂ + NC4MDCO2HN	j_ketene	see note*
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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J49202	TrGJTerC	$\text{C98OOH} + h\nu \rightarrow \text{C614O2} + \text{CH}_3\text{COCH}_3 + \text{OH}$	$(\text{jx}(\text{ip_CH300H}) + 2.15 * \text{jx}(\text{ip_MGLYOX}))$	Rickard and Pascoe (2009)
J49203a	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{C85O2} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_PINAL2HCO})$	Rickard and Pascoe (2009), Sander et al. (2019)
J49203b	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{NORPINENOL}$	$\text{jx}(\text{ip_PINAL2ENOL})$	Sander et al. (2019), Andrews et al. (2012)
J49204	TrGJTerC	$\text{C85CO3H} + h\nu \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{j_ACETOL}$	Rickard and Pascoe (2009)
J49205	TrGJTerC	$\text{C89CO2H} + h\nu \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{HO}_2$	$\text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J49206	TrGJTerC	$\text{C89CO3H} + h\nu \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J49207	TrGJTerC	$\text{C811CO3H} + h\nu \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J49208	TrGJTerC	$\text{NOPINDOOH} + h\nu \rightarrow \text{C89CO3} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J40200	TrGJTerC	$\text{LAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J40201	TrGJTerC	$\text{MENTHEN6ONE} + h\nu \rightarrow \text{RO6R1O2} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Vereecken et al. (2007)
J40202	TrGJTerC	$2\text{OHMENTHEN6ONE} + h\nu \rightarrow 10 \text{ LCARBON} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Vereecken et al. (2007)
J40203a	TrGJTerC	$\text{PINAL} + h\nu \rightarrow \text{C96O2} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_PINAL2HCO})$	Rickard and Pascoe (2009)
J40203b	TrGJTerC	$\text{PINAL} + h\nu \rightarrow \text{PINEOL}$	$\text{jx}(\text{ip_PINAL2ENOL})$	Sander et al. (2019), Andrews et al. (2012)*
J40204	TrGJTerC	$\text{PERPINONIC} + h\nu \rightarrow \text{C96O2} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{j_ACETOL}$	Rickard and Pascoe (2009)
J40205	TrGJTerC	$\text{PINALOOH} + h\nu \rightarrow \text{C106O2} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40206	TrGJTerCN	$\text{PINALNO3} + h\nu \rightarrow \text{C106O2} + \text{NO}_2$	$\text{j_IC3H7N03} + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40207	TrGJTerC	$\text{C106OOH} + h\nu \rightarrow \text{C716O2} + \text{CH}_3\text{COCH}_3 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40208	TrGJTerCN	$\text{C106NO3} + h\nu \rightarrow \text{C716O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$\text{j_IC3H7N03} + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40209	TrGJTerC	$\text{C109OOH} + h\nu \rightarrow \text{C89CO3} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40210	TrGJTerC	$\text{C109CO} + h\nu \rightarrow \text{C89CO3} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard and Pascoe (2009)
J40211	TrGJTerCN	$\text{LNAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J40212	TrGJTerC	$\text{BPINAOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J40213	TrGJTerCN	$\text{LNBPINABOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
J40214	TrGJTerCN	$\text{ROO6R1NO3} + h\nu \rightarrow \text{ROO6R3O2} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$2.84 * \text{j_IC3H7N03} + \text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J40215	TrGJTerCN	$\text{RO6R1NO3} + h\nu \rightarrow 9 \text{ LCARBON} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{j_IC3H7N03}$	Sander et al. (2019)
J6000	StTrGJCl	$\text{Cl}_2 + h\nu \rightarrow \text{Cl} + \text{Cl}$	$\text{jx}(\text{ip_Cl2})$	Sander et al. (2014)
J6100	StTrGJCl	$\text{Cl}_2\text{O}_2 + h\nu \rightarrow 2 \text{ Cl}$	$\text{jx}(\text{ip_Cl2O2})$	Sander et al. (2014)
J6101	StTrGJCl	$\text{OClO} + h\nu \rightarrow \text{ClO} + \text{O}(^3\text{P})$	$\text{jx}(\text{ip_OC10})$	Sander et al. (2014)
J6200	StGJCl	$\text{HCl} + h\nu \rightarrow \text{Cl} + \text{H}$	$\text{jx}(\text{ip_HCl})$	Sander et al. (2014)
J6201	StTrGJCl	$\text{HOCl} + h\nu \rightarrow \text{OH} + \text{Cl}$	$\text{jx}(\text{ip_HOC1})$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6300	TrGJCIN	$\text{ClNO}_2 + h\nu \rightarrow \text{Cl} + \text{NO}_2$	jx(ip_ClNO2)	Sander et al. (2014)
J6301a	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{Cl} + \text{NO}_3$	jx(ip_ClNO3)	Sander et al. (2014)
J6301b	StTrGJCIN	$\text{ClNO}_3 + h\nu \rightarrow \text{ClO} + \text{NO}_2$	jx(ip_ClON02)	Sander et al. (2014)
J6400	StGJCl	$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3$	jx(ip_CH3Cl)	Sander et al. (2014)
J6401	StGJCl	$\text{CCl}_4 + h\nu \rightarrow \text{LCARBON} + 4 \text{ Cl}$	jx(ip_CCl4)	Sander et al. (2014)
J6402	StGJCCl	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 2 \text{ LCARBON} + 3 \text{ Cl}$	jx(ip_CH3CCl3)	Sander et al. (2014)
J6500	StGJCIF	$\text{CFCl}_3 + h\nu \rightarrow \text{LCARBON} + \text{LFLUORINE} + 3 \text{ Cl}$	jx(ip_CFC13)	Sander et al. (2014)*
J6501	StGJCIF	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ LFLUORINE} + 2 \text{ Cl}$	jx(ip_CF2Cl2)	Sander et al. (2014)*
J7000	StTrGJBr	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	jx(ip_Br2)	Sander et al. (2014)
J7100	StTrGJBr	$\text{BrO} + h\nu \rightarrow \text{Br} + \text{O}(^3\text{P})$	jx(ip_BrO)	Sander et al. (2014)
J7200	StTrGJBr	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	jx(ip_HOBr)	Sander et al. (2014)
J7300	TrGJBrN	$\text{BrNO}_2 + h\nu \rightarrow \text{Br} + \text{NO}_2$	jx(ip_BrNO2)	Sander et al. (2014)
J7301	StTrGJBrN	$\text{BrNO}_3 + h\nu \rightarrow .85 \text{ Br} + .85 \text{ NO}_3 + .15 \text{ BrO} + .15 \text{ NO}_2$	jx(ip_BrNO3)	Sander et al. (2014)*
J7400	StGJBr	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3$	jx(ip_CH3Br)	Sander et al. (2014)
J7401	TrGJBr	$\text{CH}_2\text{Br}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br}$	jx(ip_CH2Br2)	Sander et al. (2014)
J7402	TrGJBr	$\text{CHBr}_3 + h\nu \rightarrow \text{LCARBON} + 3 \text{ Br}$	jx(ip_CHBr3)	Sander et al. (2014)
J7500	StGJBrF	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{LCARBON} + 3 \text{ LFLUORINE} + \text{Br}$	jx(ip_CF3Br)	Sander et al. (2014)
J7600	StTrGJBrCl	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	jx(ip_BrCl)	Sander et al. (2014)
J7601	StGJBrClF	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + 2 \text{ LFLUORINE} + \text{Br} + \text{Cl}$	jx(ip_CF2ClBr)	Sander et al. (2014)
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + \text{Br} + \text{Cl}$	jx(ip_CH2ClBr)	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{LCARBON} + \text{Br} + 2 \text{ Cl}$	jx(ip_CHCl2Br)	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{ Br} + \text{Cl}$	jx(ip_CHClBr2)	Sander et al. (2014)
J8000	TrGJI	$\text{I}_2 + h\nu \rightarrow \text{I} + \text{I}$	jx(ip_I2)	Sander et al. (2014)
J8100	TrGJI	$\text{IO} + h\nu \rightarrow \text{I} + \text{O}(^3\text{P})$	jx(ip_IO)	Sander et al. (2014)
J8200	TrGJI	$\text{HOI} + h\nu \rightarrow \text{I} + \text{OH}$	jx(ip_HOI)	Sander et al. (2014)
J8300	TrGJIN	$\text{INO}_2 + h\nu \rightarrow \text{I} + \text{NO}_2$	jx(ip_INO2)	Sander et al. (2014)
J8301	TrGJIN	$\text{INO}_3 + h\nu \rightarrow \text{I} + \text{NO}_3$	jx(ip_INO3)	Sander et al. (2014)
J8400	TrGJI	$\text{CH}_2\text{I}_2 + h\nu \rightarrow 2 \text{ I} + 2 \text{ HO}_2 + \text{CO}$	jx(ip_CH2I2)	Sander et al. (2014)
J8401	TrGJI	$\text{CH}_3\text{I} + h\nu \rightarrow \text{I} + \text{CH}_3$	jx(ip_CH3I)	Sander et al. (2014)
J8402	TrGJCI	$\text{CH}_3\text{CHICH}_3 + h\nu \rightarrow 2 \text{ LCARBON} + \text{I} + \text{CH}_3$	jx(ip_C3H7I)	Sander et al. (2014)
J8403	TrGJCII	$\text{CH}_2\text{CI} + h\nu \rightarrow \text{I} + \text{Cl} + 2 \text{ HO}_2 + \text{CO}$	jx(ip_CH2ClI)	Sander et al. (2014)
J8600	TrGJCII	$\text{ICl} + h\nu \rightarrow \text{I} + \text{Cl}$	jx(ip_ICl)	Sander et al. (2014)
J8700	TrGJBrI	$\text{IBr} + h\nu \rightarrow \text{I} + \text{Br}$	jx(ip_IBr)	Sander et al. (2014)
PH (aqueous)				

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH2100_a01	TrAa01ScJ	$\text{H}_2\text{O}_2(\text{aq}) + h\nu \rightarrow 2 \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_H2O2})$	see note*
PH3200_a01	TrAa01JN	$\text{NO}_3^-(\text{aq}) + h\nu \rightarrow \text{NO}_2(\text{aq}) + \text{OH}(\text{aq}) + \text{OH}^-(\text{aq})$	$\text{xaer}(01) * \text{jx}(\text{ip_NO2}) * 1.4\text{E-}4$	see note*
PH4100_a01	TrAa01J	$\text{HOCH}_2\text{OOH}(\text{aq}) + h\nu \rightarrow \text{HCOOH}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	Sander et al. (2014)
PH4101_a01	TrAa01J	$\text{CH}_3\text{OOH}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	Sander et al. (2014)
PH4200_a01	TrAa01JC	$\text{C}_2\text{H}_5\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{CHO}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)*
PH4201_a01	TrAa01JC	$\text{HOCH}_2\text{CO}_2\text{H}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{CO}_2(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)*
PH4202_a01	TrAa01JC	$\text{CH}_2\text{OOHCO}_2^-(\text{aq}) + h\nu \rightarrow \text{CHOHOOC}_2^-(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	see note*
PH4203_a01	TrAa01JC	$\text{CH}_3\text{C}(\text{O})\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OO}(\text{aq}) + \text{CO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH3C03H})$	Sander et al. (2014)
PH4204_a01	TrAa01JC	$\text{HOCH}_2\text{CO}_3\text{H}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{CO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	Rickard and Pascoe (2009)
PH4205_a01	TrAa01JC	$\text{CH}_3\text{CHO}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OO}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH3CHO})$	Sander et al. (2014)
PH4206_a01	TrAa01JC	$\text{CH}_2\text{OOHCHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{CO}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * (\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO}))$	Sander et al. (2019)
PH4207a_a01	TrAa01JC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_HOCH2CHO}) * 0.83$	Sander et al. (2014)*
PH4207b_a01	TrAa01JC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + .6 \text{HCHO}(\text{aq}) + .6 \text{CO}(\text{aq}) + .6 \text{HO}_2(\text{aq}) + .2 \text{GLYOX}(\text{aq}) + .2 \text{CH}_2\text{OHCHO}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_HOCH2CHO}) * 0.07$	Sander et al. (2014)*
PH4207c_a01	TrAa01JC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OH}(\text{aq}) + \text{CO}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_HOCH2CHO}) * 0.10$	Sander et al. (2014)*
PH4208_a01	TrAa01JC	$\text{CHOCOOH}(\text{aq}) + h\nu \rightarrow 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq}) + \text{CO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_MGLYOX})$	Rickard and Pascoe (2009)
PH4209_a01	TrAa01JC	$\text{GLYOX}(\text{aq}) + h\nu \rightarrow 2 \text{CO}(\text{aq}) + 2 \text{HO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_GLYOX})$	Sander et al. (2014)
PH4210a_a01	TrAa01JC	$\text{HOCCOOH}(\text{aq}) + h\nu \rightarrow \text{CO}_2(\text{aq}) + \text{HCOOH}(\text{aq})$	$2.33 * \text{xaer}(01) * 0.72 * \text{jx}(\text{ip_HOCCOOH})$	Yamamoto and Back (1985)
PH4210b_a01	TrAa01JC	$\text{HOCCOOH}(\text{aq}) + h\nu \rightarrow \text{CO}_2(\text{aq}) + \text{CO}(\text{aq}) + \text{H}_2\text{O}(\text{aq})$	$2.33 * \text{xaer}(01) * 0.28 * \text{jx}(\text{ip_HOCCOOH})$	Yamamoto and Back (1985)
PH4211_a01	TrAa01JC	$\text{CHOCHOHOH}(\text{aq}) + h\nu \rightarrow \text{HCOOH}(\text{aq}) + 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_HOCH2CHO})$	Sander et al. (2014)*
PH4300_a01	TrAa01JC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{COOO}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * (\text{jx}(\text{ip_CH300H}) + 0.65 * 0.11 * \text{jx}(\text{ip_CHOH}))$	see note*
PH4301_a01	TrAa01JC	$\text{iC}_3\text{H}_7\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{COCH}_3(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_CH300H})$	see note*
PH4302_a01	TrAa01JC	$\text{CH}_3\text{COCH}_2\text{OH}(\text{aq}) + h\nu \rightarrow .5 \text{OH}(\text{aq}) + .5 \text{HCHO}(\text{aq}) + .5 \text{CO}(\text{aq}) + .5 \text{HCHO}(\text{aq}) + .5 \text{HO}_2(\text{aq}) + .5 \text{CH}_2\text{OHCO}_3(\text{aq}) + .5 \text{CH}_3\text{OO}(\text{aq})$	$2.33 * \text{xaer}(01) * 0.65 * 0.11 * \text{jx}(\text{ip_CHOH})$	Sander et al. (2014)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH4303_a01	TrAa01JJC	$\text{CH}_3\text{C}(\text{O})\text{CHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{CO}(\text{aq}) + \text{CO}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33 * \text{xaer}(01) * \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2014)*
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*
PH11200_a01	TrAa01JFe	$\text{FeOH}^{2+}(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{OH}(\text{aq})$	$\text{xaer}(01) * 4.51\text{E}-3 * 0.312$	Herrmann et al. (2000)
PH11201_a01	TrAa01JFe	$\text{Fe}(\text{OH})_2^+(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{OH}(\text{aq}) + \text{OH}^-(\text{aq})$	$\text{xaer}(01) * 5.77\text{E}-3 * 0.255$	Herrmann et al. (2000)
PH11800_a01	TrAa01JFeS	$\text{FeSO}_4^+(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{SO}_4^-(\text{aq})$	$\text{xaer}(01) * 6.43\text{E}-3 * 7.9\text{E}-3$	Herrmann et al. (2000)

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:

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

Specific notes

J41003: CH_3 - and CH_2 -channels are considered only and with their branching ratios being 0.42 and 0.48,

respectively (Gans et al., 2011). CH -production is neglected. CH_2 is assumed to react only with O_2 yielding $1.44 \text{ H}_2 + 0.18 \text{ HCHO} + 0.18 \text{ O}(^3\text{P}) + 0.33 \text{ OH} + 0.33 \text{ HO}_2 + 0.44 \text{ CO}_2 + 0.38 \text{ CO} + 0.05 \text{ H}_2\text{O}$ as assumed in the WACCM model by J. Orlando (Doug Kinnison, pers. comm. with D. Taraborrelli).

J41006: product distribution as for HNO_4

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 $J(\text{PHAN})$ is the same as $J(\text{PAN})$.

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

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

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

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

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

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

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

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

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

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

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

J44005a: It is assumed that $J(\text{LC4H9NO}_3)$ is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J44005b: It is assumed that $J(\text{LC4H9NO}_3)$ is the same as $J(\text{iC}_3\text{H}_7\text{ONO}_2)$.

J44006: It is assumed that $J(\text{MPAN})$ is the same as $J(\text{PAN})$.

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 → GLYOX + GLYOX + HO₂

J44401: KDEC BZFUO → CO₁₄O₃CHO + HO₂

J44403: KDEC NBZFUO → 0.5 CO₁₄O₃CHO + 0.5 NO₂ + 0.5 NBZFUONE + 0.5 HO₂

J44404b: KDEC MALDIALCO₂ → 0.6 MALANHY + HO₂ + 0.4 GLYOX + 0.4 CO

J44407: KDEC MALANHYO → HCOCOHCO₃

J44414: KDEC MECOACETO → CH₃CO₃ + HCHO

J45003: It is assumed that J(LISOPACNO₃) = 0.59 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that J(ISOPBNO₃) = 2.84 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that J(ISOPDNO₃) is the same as J(iC₃H₇ONO₂).

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

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

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

J45402: KDEC C₅DIALO → MALDIAL + CO + HO₂

J45407: KDEC TLFUONE → 0.6 C₅CO₁₄O₂ + 0.6 HO₂ + 0.4 TLFUONE

J45410: KDEC MMALANHYO → CO₂H₃CO₃

J45411: KDEC C₅DICARBO → MGLYOX + GLYOX + HO₂

J45412: KDEC NTLFUO → ACCOMECHO + NO₂

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

J45415: KDEC TLFUO → ACCOMECHO + HO₂

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

J46403: KDEC NDNPHENO → NC₄DCO₂H + HNO₃ + CO + CO + NO₂

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

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO → NC₄DCO₂H + HCOCO₂H + NO₂

J46415: KDEC NCATECO → NC₄DCO₂H + HCOCO₂H + HO₂

J46416: KDEC PBZQO → C₅CO₂OHCO₃

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

J46419: KDEC NBZQO → C₆CO₄DB + NO₂

J46422: KDEC DNPHEO → NC₄DCO₂H + HCOCO₂H + NO₂

J46425: KDEC BZEMUCO → 0.5 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 → 0.6 GLYOX + 0.4 MGLYOX + HO₂ + 0.2 C₄MDIAL + 0.2 C₅DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47405: KDEC TLBIPERO \rightarrow 0.6 GLYOX + 0.4 MG-LYOX + HO₂ + 0.2 C4MDIAL + 0.2 C5DICARB + 0.2 TLFUONE + 0.2 BZFUONE + 0.2 MALDIAL

J47407: KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO₂ + 0.32 PTLQONE

J47408a: KDEC CRESO \rightarrow 0.68 C5CO14OH + 0.68 GLYOX + HO₂ + 0.32 PTLQONE

J47408b: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO₂

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

J47412: KDEC TLEMUCO \rightarrow 0.5 C3DIALO₂ + 0.5 CO₂H₃CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO₂

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

J47418: new channel

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

J47420: new channel

J47422: KDEC NPTLQO \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-ZAL

J40203b: Substituted vinyl alcohol in analogy to CH₃CHO photolysis.

J6500: Even though the elementary reaction produces only 1 Cl atom (Felder and Demuth, 1993), it is assumed here that eventually all Cl atoms are released in secondary reactions.

J6501: Even though the elementary reaction probably produces only 1 Cl atom (as for CFC₁₃), it is assumed here that eventually all Cl atoms are released in secondary reactions.

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

PH2100_a01: 2.33 times the gas-phase value

PH3200_a01: Scaled to J(NO₂) so that its lifetime is about 10.5 days, as suggested by Zellner et al. (1990).

PH4200_a01: CH₃CHOHO₂ is assumed to directly decompose into CH₃CHO + HO₂

PH4201_a01: COOHOO is not formed but directly dissociates into CO₂ + HO₂

PH4202_a01: assumed to be the same as C₂H₅OOH + hv

PH4207a_a01: Quantum yields from Burkholder et al. (2015).

PH4207b_a01: Quantum yields from Burkholder et al. (2015). HCOCH₂O₂ decomposes directly to .6 HCHO + .6 CO + .6 HO₂ + .2 GLYOX + .2 HOCH₂CHO

PH4207c_a01: Quantum yields from Burkholder et al. (2015).

PH4211_a01: Assumed in analogy to the main channel for *j*(HOCH₂CHO).

PH4300_a01: 2.33* *k* from the gas-phase reaction, CH₃CO directly reacts with O₂ to form CH₃CO₃

PH4301_a01: 2.33 * *k* from the gas-phase reaction,

PH4302_a01: Following von Kuhlmann et al. (2003), we use $j(\text{CH}_3\text{COCH}_2\text{OH}) = 0.11 * j_{\text{x}}(\text{ip_CHOH})$. As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a). CH₃CO reacts with O₂ to form OH + HCHO + CO. HOCH₂CO reacts with O₂ to form HOCH₂CO₃

PH4303_a01: CH₃CO reacts with O₂ to form OH + HCHO + CO

PH10200_a01: Scaled to J(NO₂) so that it produces 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*
H10001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{O3})$	see general notes*
H10001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(01, \text{ind}_{O3})$	see general notes*
H21000f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	$k_{\text{exf}}(01, \text{ind}_{OH})$	see general notes*
H21000b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	$k_{\text{exb}}(01, \text{ind}_{OH})$	see general notes*
H21001f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{HO2})$	see general notes*
H21001b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	$k_{\text{exb}}(01, \text{ind}_{HO2})$	see general notes*
H21002f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{H2O2})$	see general notes*
H21002b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(01, \text{ind}_{H2O2})$	see general notes*
H31000f_a01	TrAa01ScN	$NO \rightarrow NO(aq)$	$k_{\text{exf}}(01, \text{ind}_{NO})$	see general notes*
H31000b_a01	TrAa01ScN	$NO(aq) \rightarrow NO$	$k_{\text{exb}}(01, \text{ind}_{NO})$	see general notes*
H31001f_a01	TrAa01ScN	$NO_2 \rightarrow NO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{NO2})$	see general notes*
H31001b_a01	TrAa01ScN	$NO_2(aq) \rightarrow NO_2$	$k_{\text{exb}}(01, \text{ind}_{NO2})$	see general notes*
H31002f_a01	TrAa01ScN	$NO_3 \rightarrow NO_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{NO3})$	see general notes*
H31002b_a01	TrAa01ScN	$NO_3(aq) \rightarrow NO_3$	$k_{\text{exb}}(01, \text{ind}_{NO3})$	see general notes*
H32000f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{NH3})$	see general notes*
H32000b_a01	TrAa01MblScScmN	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(01, \text{ind}_{NH3})$	see general notes*
H32001_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf_N205}}(01) * C(\text{ind}_{H2O_a01})$	Behnke et al. (1994), Behnke et al. (1997)
H32002f_a01	TrAa01ScN	$HONO \rightarrow HONO(aq)$	$k_{\text{exf}}(01, \text{ind}_{HONO})$	see general notes*
H32002b_a01	TrAa01ScN	$HONO(aq) \rightarrow HONO$	$k_{\text{exb}}(01, \text{ind}_{HONO})$	see general notes*
H32003f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(01, \text{ind}_{HNO3})$	see general notes*
H32003b_a01	TrAa01MblScScmN	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(01, \text{ind}_{HNO3})$	see general notes*
H32004f_a01	TrAa01ScN	$HNO_4 \rightarrow HNO_4(aq)$	$k_{\text{exf}}(01, \text{ind}_{HNO4})$	see general notes*
H32004b_a01	TrAa01ScN	$HNO_4(aq) \rightarrow HNO_4$	$k_{\text{exb}}(01, \text{ind}_{HNO4})$	see general notes*
H41000f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(01, \text{ind}_{CO2})$	see general notes*
H41000b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(01, \text{ind}_{CO2})$	see general notes*
H41001f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCHO})$	see general notes*
H41001b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	$k_{\text{exb}}(01, \text{ind}_{HCHO})$	see general notes*
H41002f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	$k_{\text{exf}}(01, \text{ind}_{CH3O2})$	see general notes*
H41002b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	$k_{\text{exb}}(01, \text{ind}_{CH3O2})$	see general notes*
H41003f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{HCOOH})$	see general notes*
H41003b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	$k_{\text{exb}}(01, \text{ind}_{HCOOH})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H41004f_a01	TrAa01ScScm	$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CH300H})$	see general notes*
H41004b_a01	TrAa01ScScm	$\text{CH}_3\text{OOH(aq)} \rightarrow \text{CH}_3\text{OOH}$	$k_{\text{exb}}(01, \text{ind_CH300H})$	see general notes*
H41005f_a01	TrAa01Sc	$\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OH(aq)}$	$k_{\text{exf}}(01, \text{ind_CH30H})$	see general notes*
H41005b_a01	TrAa01Sc	$\text{CH}_3\text{OH(aq)} \rightarrow \text{CH}_3\text{OH}$	$k_{\text{exb}}(01, \text{ind_CH30H})$	see general notes*
H41006f_a01	TrAa01	$\text{HOCH}_2\text{OH} \rightarrow \text{HOCH}_2\text{OH(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCH20H})$	see general notes*
H41006b_a01	TrAa01	$\text{HOCH}_2\text{OH(aq)} \rightarrow \text{HOCH}_2\text{OH}$	$k_{\text{exb}}(01, \text{ind_HOCH20H})$	see general notes*
H41007f_a01	TrAa01	$\text{HOCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCH200H})$	see general notes*
H41007b_a01	TrAa01	$\text{HOCH}_2\text{OOH(aq)} \rightarrow \text{HOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_HOCH200H})$	see general notes*
H41008f_a01	TrAa01	$\text{CO} \rightarrow \text{CO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO})$	see general notes*
H41008b_a01	TrAa01	$\text{CO(aq)} \rightarrow \text{CO}$	$k_{\text{exb}}(01, \text{ind_CO})$	see general notes*
H42000f_a01	TrAa01ScScmC	$\text{CH}_3\text{COOH} \rightarrow \text{CH}_3\text{COOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3C02H})$	see general notes*
H42000b_a01	TrAa01ScScmC	$\text{CH}_3\text{COOH(aq)} \rightarrow \text{CH}_3\text{COOH}$	$k_{\text{exb}}(01, \text{ind_CH3C02H})$	see general notes*
H42001f_a01	TrAa01ScC	$\text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3CHO})$	see general notes*
H42001b_a01	TrAa01ScC	$\text{CH}_3\text{CHO(aq)} \rightarrow \text{CH}_3\text{CHO}$	$k_{\text{exb}}(01, \text{ind_CH3CHO})$	see general notes*
H42002f_a01	TrAa01ScCN	$\text{PAN} \rightarrow \text{PAN(aq)}$	$k_{\text{exf}}(01, \text{ind_PAN})$	see general notes*
H42002b_a01	TrAa01ScCN	$\text{PAN(aq)} \rightarrow \text{PAN}$	$k_{\text{exb}}(01, \text{ind_PAN})$	see general notes*
H42003f_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{OH(aq)}$	$k_{\text{exf}}(01, \text{ind_C2H50H})$	see general notes*
H42003b_a01	TrAa01C	$\text{CH}_3\text{CH}_2\text{OH(aq)} \rightarrow \text{C}_2\text{H}_5\text{OH}$	$k_{\text{exb}}(01, \text{ind_C2H50H})$	see general notes*
H42004f_a01	TrAa01C	$\text{ETHGLY} \rightarrow \text{ETHGLY(aq)}$	$k_{\text{exf}}(01, \text{ind_ETHGLY})$	see general notes*
H42004b_a01	TrAa01C	$\text{ETHGLY(aq)} \rightarrow \text{ETHGLY}$	$k_{\text{exb}}(01, \text{ind_ETHGLY})$	see general notes*
H42006f_a01	TrAa01C	$\text{CH}_3\text{C(O)OO} \rightarrow \text{CH}_3\text{COOO(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3C03})$	see general notes*
H42006b_a01	TrAa01C	$\text{CH}_3\text{COOO(aq)} \rightarrow \text{CH}_3\text{C(O)OO}$	$k_{\text{exb}}(01, \text{ind_CH3C03})$	see general notes*
H42007f_a01	TrAa01C	$\text{HOCH}_2\text{CHO} \rightarrow \text{CH}_2\text{OHCHO(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCH2CH0})$	see general notes*
H42007b_a01	TrAa01C	$\text{CH}_2\text{OHCHO(aq)} \rightarrow \text{HOCH}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HOCH2CH0})$	see general notes*
H42008f_a01	TrAa01C	$\text{GLYOX} \rightarrow \text{GLYOX(aq)}$	$k_{\text{exf}}(01, \text{ind_GLYOX})$	see general notes*
H42008b_a01	TrAa01C	$\text{GLYOX(aq)} \rightarrow \text{GLYOX}$	$k_{\text{exb}}(01, \text{ind_GLYOX})$	see general notes*
H42009f_a01	TrAa01C	$\text{CH}_3\text{C(O)OOH} \rightarrow \text{CH}_3\text{C(O)OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3C03H})$	see general notes*
H42009b_a01	TrAa01C	$\text{CH}_3\text{C(O)OOH(aq)} \rightarrow \text{CH}_3\text{C(O)OOH}$	$k_{\text{exb}}(01, \text{ind_CH3C03H})$	see general notes*
H42010f_a01	TrAa01C	$\text{HOCH}_2\text{CO}_3\text{H} \rightarrow \text{HOCH}_2\text{CO}_3\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCH2C03H})$	see general notes*
H42010b_a01	TrAa01C	$\text{HOCH}_2\text{CO}_3\text{H(aq)} \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOCH2C03H})$	see general notes*
H42011f_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C2H500H})$	see general notes*
H42011b_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OOH(aq)} \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$k_{\text{exb}}(01, \text{ind_C2H500H})$	see general notes*
H42012f_a01	TrAa01C	$\text{HOCCOOH} \rightarrow \text{HOCCOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCC00H})$	see general notes*
H42012b_a01	TrAa01C	$\text{HOCCOOH(aq)} \rightarrow \text{HOCCOOH}$	$k_{\text{exb}}(01, \text{ind_HOCC00H})$	see general notes*
H42013f_a01	TrAa01C	$\text{HOOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOOCH}_2\text{CO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HOOCH2C02H})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H42013b_a01	TrAa01C	$\text{HOOCH}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOOCH}_2\text{CO}_2\text{H})$	see general notes*
H42014f_a01	TrAa01C	$\text{HOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOCH}_2\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	see general notes*
H42014b_a01	TrAa01C	$\text{HOCH}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	see general notes*
H42015f_a01	TrAa01C	$\text{HCOCO}_2\text{H} \rightarrow \text{CHOCOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCO}_2\text{H})$	see general notes*
H42015b_a01	TrAa01C	$\text{CHOCOOH}(\text{aq}) \rightarrow \text{HCOCO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CHOCOOH})$	see general notes*
H42017f_a01	TrAa01CN	$\text{C}_2\text{H}_5\text{ONO}_2 \rightarrow \text{C}_2\text{H}_5\text{ONO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_2\text{H}_5\text{NO}_3)$	see general notes*
H42017b_a01	TrAa01CN	$\text{C}_2\text{H}_5\text{ONO}_2(\text{aq}) \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$k_{\text{exb}}(01, \text{ind_C}_2\text{H}_5\text{NO}_3)$	see general notes*
H42018f_a01	TrAa01CN	$\text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CN})$	see general notes*
H42018b_a01	TrAa01CN	$\text{CH}_3\text{CN}(\text{aq}) \rightarrow \text{CH}_3\text{CN}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CN})$	see general notes*
H42019f_a01	TrAa01C	$\text{HOCH}_2\text{CHOHOH} \rightarrow \text{CH}_2\text{OHCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{CHOHOH})$	see general notes*
H42019b_a01	TrAa01C	$\text{CH}_2\text{OHCHOHOH}(\text{aq}) \rightarrow \text{HOCH}_2\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{CHOHOH})$	see general notes*
H42020f_a01	TrAa01C	$\text{CH}_3\text{CHOHOH} \rightarrow \text{CH}_3\text{CHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHOHOH})$	see general notes*
H42020b_a01	TrAa01C	$\text{CH}_3\text{CHOHOH}(\text{aq}) \rightarrow \text{CH}_3\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHOHOH})$	see general notes*
H42021f_a01	TrAa01C	$\text{CHOHOHCOOH} \rightarrow \text{CHOOHOHCOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOHOHCOOH})$	see general notes*
H42021b_a01	TrAa01C	$\text{CHOOHOHCOOH}(\text{aq}) \rightarrow \text{CHOHOHCOOH}$	$k_{\text{exb}}(01, \text{ind_CHOOHOHCOOH})$	see general notes*
H42022f_a01	TrAa01C	$\text{CHOHOHCHOHOH} \rightarrow \text{CHOHOHCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOHOHCHOHOH})$	see general notes*
H42022b_a01	TrAa01C	$\text{CHOHOHCHOHOH}(\text{aq}) \rightarrow \text{CHOHOHCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CHOHOHCHOHOH})$	see general notes*
H42023f_a01	TrAa01C	$\text{HOOCH}_2\text{CHO} \rightarrow \text{CH}_2\text{OOHCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOCH}_2\text{CHO})$	see general notes*
H42023b_a01	TrAa01C	$\text{CH}_2\text{OOHCHO}(\text{aq}) \rightarrow \text{HOOCH}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HOOCH}_2\text{CHO})$	see general notes*
H42024f_a01	TrAa01C	$\text{CHOCHOHOH} \rightarrow \text{CHOCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOCHOHOH})$	see general notes*
H42024b_a01	TrAa01C	$\text{CHOCHOHOH}(\text{aq}) \rightarrow \text{CHOCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CHOCHOHOH})$	see general notes*
H42025f_a01	TrAa01C	$\text{HOOCH}_2\text{CHOHOH} \rightarrow \text{HOOCH}_2\text{CHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOCH}_2\text{CHOHOH})$	see general notes*
H42025b_a01	TrAa01C	$\text{HOOCH}_2\text{CHOHOH}(\text{aq}) \rightarrow \text{HOOCH}_2\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_HOOCH}_2\text{CHOHOH})$	see general notes*
H42026f_a01	TrAa01C	$\text{CH}_2\text{CO} \rightarrow \text{CH}_2\text{CO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_2\text{CO})$	see general notes*
H42026b_a01	TrAa01C	$\text{CH}_2\text{CO}(\text{aq}) \rightarrow \text{CH}_2\text{CO}$	$k_{\text{exb}}(01, \text{ind_CH}_2\text{CO})$	see general notes*
H42027f_a01	TrAa01C	$\text{CH}_3\text{CHOHOOH} \rightarrow \text{CH}_3\text{CHOHOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHOHOOH})$	see general notes*
H42027b_a01	TrAa01C	$\text{CH}_3\text{CHOHOOH}(\text{aq}) \rightarrow \text{CH}_3\text{CHOHOOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHOHOOH})$	see general notes*
H42028f_a01	TrAa01CN	$\text{ETHOHNO}_3 \rightarrow \text{ETHOHNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ETHOHNO}_3)$	see general notes*
H42028b_a01	TrAa01CN	$\text{ETHOHNO}_3(\text{aq}) \rightarrow \text{ETHOHNO}_3$	$k_{\text{exb}}(01, \text{ind_ETHOHNO}_3)$	see general notes*
H42029f_a01	TrAa01C	$\text{HCOCO}_3\text{H} \rightarrow \text{HCOCO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCO}_3\text{H})$	see general notes*
H42029b_a01	TrAa01C	$\text{HCOCO}_3\text{H}(\text{aq}) \rightarrow \text{HCOCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCO}_3\text{H})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H42030f_a01	TrAa01C	$\text{HOOCH}_2\text{CO}_3\text{H} \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOCH}_2\text{CO}_3\text{H})$	see general notes*
H42030b_a01	TrAa01C	$\text{HOOCH}_2\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOOCH}_2\text{CO}_3\text{H})$	see general notes*
H42031f_a01	TrAa01C	$\text{HYETHO}_2\text{H} \rightarrow \text{HYETHO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HYETHO}_2\text{H})$	see general notes*
H42031b_a01	TrAa01C	$\text{HYETHO}_2\text{H}(\text{aq}) \rightarrow \text{HYETHO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYETHO}_2\text{H})$	see general notes*
H42032f_a01	TrAa01CN	$\text{PHAN} \rightarrow \text{PHAN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_PHAN})$	see general notes*
H42032b_a01	TrAa01CN	$\text{PHAN}(\text{aq}) \rightarrow \text{PHAN}$	$k_{\text{exb}}(01, \text{ind_PHAN})$	see general notes*
H43000f_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_3 \rightarrow \text{CH}_3\text{COCH}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCH}_3)$	see general notes*
H43000b_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_3(\text{aq}) \rightarrow \text{CH}_3\text{COCH}_3$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCH}_3)$	see general notes*
H43001f_a01	TrAa01C	$\text{MGLYOX} \rightarrow \text{CH}_3\text{C}(\text{O})\text{CHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_MGLYOX})$	see general notes*
H43001b_a01	TrAa01C	$\text{CH}_3\text{C}(\text{O})\text{CHO}(\text{aq}) \rightarrow \text{MGLYOX}$	$k_{\text{exb}}(01, \text{ind_MGLYOX})$	see general notes*
H43002f_a01	TrAa01C	$\text{CH}_3\text{COCO}_2\text{H} \rightarrow \text{CH}_3\text{COCO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCO}_2\text{H})$	see general notes*
H43002b_a01	TrAa01C	$\text{CH}_3\text{COCO}_2\text{H}(\text{aq}) \rightarrow \text{CH}_3\text{COCO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCO}_2\text{H})$	see general notes*
H43003f_a01	TrAa01C	$\text{CH}_3\text{COCHOHOH} \rightarrow \text{CH}_3\text{COCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCHOHOH})$	see general notes*
H43003b_a01	TrAa01C	$\text{CH}_3\text{COCHOHOH}(\text{aq}) \rightarrow \text{CH}_3\text{COCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCHOHOH})$	see general notes*
H43005f_a01	TrAa01C	$\text{IPROPOL} \rightarrow \text{IPROPOL}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_IPROPOL})$	see general notes*
H43005b_a01	TrAa01C	$\text{IPROPOL}(\text{aq}) \rightarrow \text{IPROPOL}$	$k_{\text{exb}}(01, \text{ind_IPROPOL})$	see general notes*
H43006f_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HYPERACET})$	see general notes*
H43006b_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H}(\text{aq}) \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYPERACET})$	see general notes*
H43007f_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{OOH} \rightarrow \text{iC}_3\text{H}_7\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_IC}_3\text{H}_7\text{OOH})$	see general notes*
H43007b_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{OOH}(\text{aq}) \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$k_{\text{exb}}(01, \text{ind_IC}_3\text{H}_7\text{OOH})$	see general notes*
H43008f_a01	TrAa01C	$\text{HCOCOCH}_2\text{OOH} \rightarrow \text{HCOCOCH}_2\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ALCOCH}_2\text{OOH})$	see general notes*
H43008b_a01	TrAa01C	$\text{HCOCOCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_ALCOCH}_2\text{OOH})$	see general notes*
H43009f_a01	TrAa01C	$\text{C}_3\text{OH13CO} \rightarrow \text{C}_3\text{OH13CO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_3\text{OH13CO})$	see general notes*
H43009b_a01	TrAa01C	$\text{C}_3\text{OH13CO}(\text{aq}) \rightarrow \text{C}_3\text{OH13CO}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{OH13CO})$	see general notes*
H43010f_a01	TrAa01C	$\text{HCOCOCHO} \rightarrow \text{HCOCOCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_3\text{CO})$	see general notes*
H43010b_a01	TrAa01C	$\text{HCOCOCHO}(\text{aq}) \rightarrow \text{HCOCOCHO}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{CO})$	see general notes*
H43011f_a01	TrAa01C	$\text{C}_3\text{DIALOOH} \rightarrow \text{C}_3\text{DIALOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_3\text{DIALOOH})$	see general notes*
H43011b_a01	TrAa01C	$\text{C}_3\text{DIALOOH}(\text{aq}) \rightarrow \text{C}_3\text{DIALOOH}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{DIALOOH})$	see general notes*
H43012f_a01	TrAa01CN	$\text{C}_3\text{PAN1} \rightarrow \text{C}_3\text{PAN1}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_3\text{PAN1})$	see general notes*
H43012b_a01	TrAa01CN	$\text{C}_3\text{PAN1}(\text{aq}) \rightarrow \text{C}_3\text{PAN1}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{PAN1})$	see general notes*
H43013f_a01	TrAa01CN	$\text{C}_3\text{PAN2} \rightarrow \text{C}_3\text{PAN2}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_3\text{PAN2})$	see general notes*
H43013b_a01	TrAa01CN	$\text{C}_3\text{PAN2}(\text{aq}) \rightarrow \text{C}_3\text{PAN2}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{PAN2})$	see general notes*
H43014f_a01	TrAa01C	$\text{CH}_3\text{CHCO} \rightarrow \text{CH}_3\text{CHCO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHCO})$	see general notes*
H43014b_a01	TrAa01C	$\text{CH}_3\text{CHCO}(\text{aq}) \rightarrow \text{CH}_3\text{CHCO}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHCO})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H43015f_a01	TrAa01CN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2(\text{aq})$	$\rightarrow k_{\text{exf}}(01, \text{ind_CH3COCH2O2N02})$	see general notes*
H43015b_a01	TrAa01CN	$\text{CH}_3\text{COCH}_2\text{OONO}_2(\text{aq}) \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$\rightarrow k_{\text{exb}}(01, \text{ind_CH3COCH2O2N02})$	see general notes*
H43016f_a01	TrAa01C	$\text{CH}_3\text{COCO}_3\text{H} \rightarrow \text{CH}_3\text{COCO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3COC03H})$	see general notes*
H43016b_a01	TrAa01C	$\text{CH}_3\text{COCO}_3\text{H}(\text{aq}) \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_CH3COC03H})$	see general notes*
H43017f_a01	TrAa01C	$\text{HCOCH}_2\text{CHO} \rightarrow \text{HCOCH}_2\text{CHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH2CHO})$	see general notes*
H43017b_a01	TrAa01C	$\text{HCOCH}_2\text{CHO}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HCOCH2CHO})$	see general notes*
H43018f_a01	TrAa01C	$\text{HCOCH}_2\text{CO}_2\text{H} \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH2CO2H})$	see general notes*
H43018b_a01	TrAa01C	$\text{HCOCH}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCH2CO2H})$	see general notes*
H43019f_a01	TrAa01C	$\text{HCOCH}_2\text{CO}_3\text{H} \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH2CO3H})$	see general notes*
H43019b_a01	TrAa01C	$\text{HCOCH}_2\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCH2CO3H})$	see general notes*
H43020f_a01	TrAa01C	$\text{HCOCOCH}_2\text{OOH} \rightarrow \text{HCOCOCH}_2\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOCH2OOH})$	see general notes*
H43020b_a01	TrAa01C	$\text{HCOCOCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_HCOCOCH2OOH})$	see general notes*
H43021f_a01	TrAa01C	$\text{HCOCOCHCO}_3\text{H} \rightarrow \text{HCOCOCHCO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOCHCO3H})$	see general notes*
H43021b_a01	TrAa01C	$\text{HCOCOCHCO}_3\text{H}(\text{aq}) \rightarrow \text{HCOCOCHCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCOCHCO3H})$	see general notes*
H43022f_a01	TrAa01CN	$\text{HCOCOHPAN} \rightarrow \text{HCOCOHPAN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOHPAN})$	see general notes*
H43022b_a01	TrAa01CN	$\text{HCOCOHPAN}(\text{aq}) \rightarrow \text{HCOCOHPAN}$	$k_{\text{exb}}(01, \text{ind_HCOCOHPAN})$	see general notes*
H43023f_a01	TrAa01C	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOC2H4CO2H})$	see general notes*
H43023b_a01	TrAa01C	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOC2H4CO2H})$	see general notes*
H43024f_a01	TrAa01C	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOC2H4CO3H})$	see general notes*
H43024b_a01	TrAa01C	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOC2H4CO3H})$	see general notes*
H43025f_a01	TrAa01C	$\text{HOCH}_2\text{COCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}(\text{aq})$	$\rightarrow k_{\text{exf}}(01, \text{ind_HOCH2COCH2OOH})$	see general notes*
H43025b_a01	TrAa01C	$\text{HOCH}_2\text{COCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$\rightarrow k_{\text{exb}}(01, \text{ind_HOCH2COCH2OOH})$	see general notes*
H43026f_a01	TrAa01C	$\text{HOCH}_2\text{COCHO} \rightarrow \text{HOCH}_2\text{COCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH2COCHO})$	see general notes*
H43026b_a01	TrAa01C	$\text{HOCH}_2\text{COCHO}(\text{aq}) \rightarrow \text{HOCH}_2\text{COCHO}$	$k_{\text{exb}}(01, \text{ind_HOCH2COCHO})$	see general notes*
H43027f_a01	TrAa01C	$\text{HYPROPO}_2\text{H} \rightarrow \text{HYPROPO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HYPROPO2H})$	see general notes*
H43027b_a01	TrAa01C	$\text{HYPROPO}_2\text{H}(\text{aq}) \rightarrow \text{HYPROPO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYPROPO2H})$	see general notes*
H43028f_a01	TrAa01C	$\text{METACETHO} \rightarrow \text{METACETHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_METACETHO})$	see general notes*
H43028b_a01	TrAa01C	$\text{METACETHO}(\text{aq}) \rightarrow \text{METACETHO}$	$k_{\text{exb}}(01, \text{ind_METACETHO})$	see general notes*
H43029f_a01	TrAa01CN	$\text{NOA} \rightarrow \text{NOA}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_NOA})$	see general notes*
H43029b_a01	TrAa01CN	$\text{NOA}(\text{aq}) \rightarrow \text{NOA}$	$k_{\text{exb}}(01, \text{ind_NOA})$	see general notes*
H43030f_a01	TrAa01CN	$\text{PR}_2\text{O}_2\text{HNO}_3 \rightarrow \text{PR}_2\text{O}_2\text{HNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_PR2O2HNO3})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H43030b_a01	TrAa01CN	$\text{PR2O2HNO3(aq)} \rightarrow \text{PR2O2HNO3}$	$k_{\text{exb}}(01, \text{ind_PR2O2HNO3})$	see general notes*
H43031f_a01	TrAa01CN	$\text{PROPOLNO3} \rightarrow \text{PROPOLNO3(aq)}$	$k_{\text{exf}}(01, \text{ind_PROPOLNO3})$	see general notes*
H43031b_a01	TrAa01CN	$\text{PROPOLNO3(aq)} \rightarrow \text{PROPOLNO3}$	$k_{\text{exb}}(01, \text{ind_PROPOLNO3})$	see general notes*
H43032f_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH(aq)}$	$k_{\text{exf}}(01, \text{ind_ACETOL})$	see general notes*
H43032b_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{OH(aq)} \rightarrow \text{CH}_3\text{COCH}_2\text{OH}$	$k_{\text{exb}}(01, \text{ind_ACETOL})$	see general notes*
H44000f_a01	TrAa01C	$\text{MACR} \rightarrow \text{MACR(aq)}$	$k_{\text{exf}}(01, \text{ind_MACR})$	see general notes*
H44000b_a01	TrAa01C	$\text{MACR(aq)} \rightarrow \text{MACR}$	$k_{\text{exb}}(01, \text{ind_MACR})$	see general notes*
H44001f_a01	TrAa01C	$\text{MVK} \rightarrow \text{MVK(aq)}$	$k_{\text{exf}}(01, \text{ind_MVK})$	see general notes*
H44001b_a01	TrAa01C	$\text{MVK(aq)} \rightarrow \text{MVK}$	$k_{\text{exb}}(01, \text{ind_MVK})$	see general notes*
H44002f_a01	TrAa01C	$\text{CH}_3\text{COCOCH}_2\text{O}_2 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_BIACETO2})$	see general notes*
H44002b_a01	TrAa01C	$\text{CH}_3\text{COCOCH}_2\text{O}_2(\text{aq}) \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2$	$k_{\text{exb}}(01, \text{ind_BIACETO2})$	see general notes*
H44003f_a01	TrAa01C	$\text{BIACETOH} \rightarrow \text{BIACETOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BIACETOH})$	see general notes*
H44003b_a01	TrAa01C	$\text{BIACETOH(aq)} \rightarrow \text{BIACETOH}$	$k_{\text{exb}}(01, \text{ind_BIACETOH})$	see general notes*
H44004f_a01	TrAa01C	$\text{CH}_3\text{COCOCH}_2\text{OOH} \rightarrow \text{CH}_3\text{COCOCH}_2\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BIACETO0H})$	see general notes*
H44004b_a01	TrAa01C	$\text{CH}_3\text{COCOCH}_2\text{OOH(aq)} \rightarrow \text{CH}_3\text{COCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_BIACETO0H})$	see general notes*
H44005f_a01	TrAa01C	$\text{BUT2OLO} \rightarrow \text{BUT2OLO(aq)}$	$k_{\text{exf}}(01, \text{ind_BUT2OLO})$	see general notes*
H44005b_a01	TrAa01C	$\text{BUT2OLO(aq)} \rightarrow \text{BUT2OLO}$	$k_{\text{exb}}(01, \text{ind_BUT2OLO})$	see general notes*
H44006f_a01	TrAa01C	$\text{BUT2OLOOH} \rightarrow \text{BUT2OLOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BUT2OLOOH})$	see general notes*
H44006b_a01	TrAa01C	$\text{BUT2OLOOH(aq)} \rightarrow \text{BUT2OLOOH}$	$k_{\text{exb}}(01, \text{ind_BUT2OLOOH})$	see general notes*
H44007f_a01	TrAa01C	$\text{BZFUCO} \rightarrow \text{BZFUCO(aq)}$	$k_{\text{exf}}(01, \text{ind_BZFUCO})$	see general notes*
H44007b_a01	TrAa01C	$\text{BZFUCO(aq)} \rightarrow \text{BZFUCO}$	$k_{\text{exb}}(01, \text{ind_BZFUCO})$	see general notes*
H44008f_a01	TrAa01C	$\text{BZFUOOH} \rightarrow \text{BZFUOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BZFUOOH})$	see general notes*
H44008b_a01	TrAa01C	$\text{BZFUOOH(aq)} \rightarrow \text{BZFUOOH}$	$k_{\text{exb}}(01, \text{ind_BZFUOOH})$	see general notes*
H44009f_a01	TrAa01C	$\text{C312COCO3H} \rightarrow \text{C312COCO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_C312COCO3H})$	see general notes*
H44009b_a01	TrAa01C	$\text{C312COCO3H(aq)} \rightarrow \text{C312COCO3H}$	$k_{\text{exb}}(01, \text{ind_C312COCO3H})$	see general notes*
H44010f_a01	TrAa01CN	$\text{C312COPAN} \rightarrow \text{C312COPAN(aq)}$	$k_{\text{exf}}(01, \text{ind_C312COPAN})$	see general notes*
H44010b_a01	TrAa01CN	$\text{C312COPAN(aq)} \rightarrow \text{C312COPAN}$	$k_{\text{exb}}(01, \text{ind_C312COPAN})$	see general notes*
H44011f_a01	TrAa01C	$\text{C413COOOH} \rightarrow \text{C413COOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C413COOOH})$	see general notes*
H44011b_a01	TrAa01C	$\text{C413COOOH(aq)} \rightarrow \text{C413COOOH}$	$k_{\text{exb}}(01, \text{ind_C413COOOH})$	see general notes*
H44012f_a01	TrAa01C	$\text{C44OOH} \rightarrow \text{C44OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C44OOH})$	see general notes*
H44012b_a01	TrAa01C	$\text{C44OOH(aq)} \rightarrow \text{C44OOH}$	$k_{\text{exb}}(01, \text{ind_C44OOH})$	see general notes*
H44013f_a01	TrAa01C	$\text{C4CODIAL} \rightarrow \text{C4CODIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_C4CODIAL})$	see general notes*
H44013b_a01	TrAa01C	$\text{C4CODIAL(aq)} \rightarrow \text{C4CODIAL}$	$k_{\text{exb}}(01, \text{ind_C4CODIAL})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H44014f_a01	TrAa01CN	$\text{C4PAN5} \rightarrow \text{C4PAN5(aq)}$	$k_{\text{exf}}(01, \text{ind_C4PAN5})$	see general notes*
H44014b_a01	TrAa01CN	$\text{C4PAN5(aq)} \rightarrow \text{C4PAN5}$	$k_{\text{exb}}(01, \text{ind_C4PAN5})$	see general notes*
H44015f_a01	TrAa01C	$\text{CH}_3\text{COCHCO} \rightarrow \text{CH}_3\text{COCHCO(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3COCHCO})$	see general notes*
H44015b_a01	TrAa01C	$\text{CH}_3\text{COCHCO(aq)} \rightarrow \text{CH}_3\text{COCHCO}$	$k_{\text{exb}}(01, \text{ind_CH3COCHCO})$	see general notes*
H44016f_a01	TrAa01C	$\text{CH}_3\text{COCOCO}_2\text{H} \rightarrow \text{CH}_3\text{COCOCO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3COCOCO}_2\text{H})$	see general notes*
H44016b_a01	TrAa01C	$\text{CH}_3\text{COCOCO}_2\text{H(aq)} \rightarrow \text{CH}_3\text{COCOCO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CH3COCOCO}_2\text{H})$	see general notes*
H44017f_a01	TrAa01C	$\text{CH}_3\text{COOHCHCHO} \rightarrow \text{CH}_3\text{COOHCHCHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CH3COOHCHCHO})$	see general notes*
H44017b_a01	TrAa01C	$\text{CH}_3\text{COOHCHCHO(aq)} \rightarrow \text{CH}_3\text{COOHCHCHO}$	$k_{\text{exb}}(01, \text{ind_CH3COOHCHCHO})$	see general notes*
H44018f_a01	TrAa01C	$\text{CHOC3COO}_2 \rightarrow \text{CHOC3COO}_2\text{(aq)}$	$k_{\text{exf}}(01, \text{ind_CHOC3COO}_2)$	see general notes*
H44018b_a01	TrAa01C	$\text{CHOC3COO}_2\text{(aq)} \rightarrow \text{CHOC3COO}_2$	$k_{\text{exb}}(01, \text{ind_CHOC3COO}_2)$	see general notes*
H44019f_a01	TrAa01C	$\text{CO14O3CHO} \rightarrow \text{CO14O3CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO14O3CHO})$	see general notes*
H44019b_a01	TrAa01C	$\text{CO14O3CHO(aq)} \rightarrow \text{CO14O3CHO}$	$k_{\text{exb}}(01, \text{ind_CO14O3CHO})$	see general notes*
H44020f_a01	TrAa01C	$\text{CO14O3CO}_2\text{H} \rightarrow \text{CO14O3CO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_CO14O3CO}_2\text{H})$	see general notes*
H44020b_a01	TrAa01C	$\text{CO14O3CO}_2\text{H(aq)} \rightarrow \text{CO14O3CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CO14O3CO}_2\text{H})$	see general notes*
H44021f_a01	TrAa01C	$\text{CH}_3\text{COCOCHO} \rightarrow \text{CH}_3\text{COCOCHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO23C3CHO})$	see general notes*
H44021b_a01	TrAa01C	$\text{CH}_3\text{COCOCHO(aq)} \rightarrow \text{CH}_3\text{COCOCHO}$	$k_{\text{exb}}(01, \text{ind_CO23C3CHO})$	see general notes*
H44022f_a01	TrAa01C	$\text{CO}_2\text{C3CHO} \rightarrow \text{CO}_2\text{C3CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO}_2\text{C3CHO})$	see general notes*
H44022b_a01	TrAa01C	$\text{CO}_2\text{C3CHO(aq)} \rightarrow \text{CO}_2\text{C3CHO}$	$k_{\text{exb}}(01, \text{ind_CO}_2\text{C3CHO})$	see general notes*
H44023f_a01	TrAa01C	$\text{CO}_2\text{C4DIAL} \rightarrow \text{CO}_2\text{C4DIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_CO}_2\text{C4DIAL})$	see general notes*
H44023b_a01	TrAa01C	$\text{CO}_2\text{C4DIAL(aq)} \rightarrow \text{CO}_2\text{C4DIAL}$	$k_{\text{exb}}(01, \text{ind_CO}_2\text{C4DIAL})$	see general notes*
H44024f_a01	TrAa01C	$\text{CO}_2\text{H3CHO} \rightarrow \text{CO}_2\text{H3CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO}_2\text{H3CHO})$	see general notes*
H44024b_a01	TrAa01C	$\text{CO}_2\text{H3CHO(aq)} \rightarrow \text{CO}_2\text{H3CHO}$	$k_{\text{exb}}(01, \text{ind_CO}_2\text{H3CHO})$	see general notes*
H44025f_a01	TrAa01C	$\text{CO}_2\text{H3CO}_2\text{H} \rightarrow \text{CO}_2\text{H3CO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_CO}_2\text{H3CO}_2\text{H})$	see general notes*
H44025b_a01	TrAa01C	$\text{CO}_2\text{H3CO}_2\text{H(aq)} \rightarrow \text{CO}_2\text{H3CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CO}_2\text{H3CO}_2\text{H})$	see general notes*
H44026f_a01	TrAa01C	$\text{CO}_2\text{H3CO}_3\text{H} \rightarrow \text{CO}_2\text{H3CO}_3\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_CO}_2\text{H3CO}_3\text{H})$	see general notes*
H44026b_a01	TrAa01C	$\text{CO}_2\text{H3CO}_3\text{H(aq)} \rightarrow \text{CO}_2\text{H3CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_CO}_2\text{H3CO}_3\text{H})$	see general notes*
H44027f_a01	TrAa01C	$\text{EPXC4DIAL} \rightarrow \text{EPXC4DIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_EPXC4DIAL})$	see general notes*
H44027b_a01	TrAa01C	$\text{EPXC4DIAL(aq)} \rightarrow \text{EPXC4DIAL}$	$k_{\text{exb}}(01, \text{ind_EPXC4DIAL})$	see general notes*
H44028f_a01	TrAa01C	$\text{EPXDLCO}_2\text{H} \rightarrow \text{EPXDLCO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_EPXDLCO}_2\text{H})$	see general notes*
H44028b_a01	TrAa01C	$\text{EPXDLCO}_2\text{H(aq)} \rightarrow \text{EPXDLCO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_EPXDLCO}_2\text{H})$	see general notes*
H44029f_a01	TrAa01C	$\text{EPXDLCO}_3\text{H} \rightarrow \text{EPXDLCO}_3\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_EPXDLCO}_3\text{H})$	see general notes*
H44029b_a01	TrAa01C	$\text{EPXDLCO}_3\text{H(aq)} \rightarrow \text{EPXDLCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_EPXDLCO}_3\text{H})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H44030f_a01	TrAa01C	$\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCCH}_3\text{CHOOH(aq)}$	$\rightarrow k_{\text{exf}}(01, \text{ind_HCOCCH}_3\text{CHOOH})$	see general notes*
H44030b_a01	TrAa01C	$\text{HCOCCH}_3\text{CHOOH(aq)} \rightarrow \text{HCOCCH}_3\text{CHOOH}$	$\rightarrow k_{\text{exb}}(01, \text{ind_HCOCCH}_3\text{CHOOH})$	see general notes*
H44031f_a01	TrAa01C	$\text{HCOCCH}_3\text{CO} \rightarrow \text{HCOCCH}_3\text{CO(aq)}$	$k_{\text{exf}}(01, \text{ind_HCOCCH}_3\text{CO})$	see general notes*
H44031b_a01	TrAa01C	$\text{HCOCCH}_3\text{CO(aq)} \rightarrow \text{HCOCCH}_3\text{CO}$	$k_{\text{exb}}(01, \text{ind_HCOCCH}_3\text{CO})$	see general notes*
H44032f_a01	TrAa01C	$\text{HMAC} \rightarrow \text{HMAC(aq)}$	$k_{\text{exf}}(01, \text{ind_HMAC})$	see general notes*
H44032b_a01	TrAa01C	$\text{HMAC(aq)} \rightarrow \text{HMAC}$	$k_{\text{exb}}(01, \text{ind_HMAC})$	see general notes*
H44033f_a01	TrAa01C	$\text{HO12CO3C4} \rightarrow \text{HO12CO3C4(aq)}$	$k_{\text{exf}}(01, \text{ind_HO12CO3C4})$	see general notes*
H44033b_a01	TrAa01C	$\text{HO12CO3C4(aq)} \rightarrow \text{HO12CO3C4}$	$k_{\text{exb}}(01, \text{ind_HO12CO3C4})$	see general notes*
H44034f_a01	TrAa01C	$\text{HOCOC4DIAL} \rightarrow \text{HOCOC4DIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_HOCOC4DIAL})$	see general notes*
H44034b_a01	TrAa01C	$\text{HOCOC4DIAL(aq)} \rightarrow \text{HOCOC4DIAL}$	$k_{\text{exb}}(01, \text{ind_HOCOC4DIAL})$	see general notes*
H44035f_a01	TrAa01C	$\text{HVMK} \rightarrow \text{HVMK(aq)}$	$k_{\text{exf}}(01, \text{ind_HVMK})$	see general notes*
H44035b_a01	TrAa01C	$\text{HVMK(aq)} \rightarrow \text{HVMK}$	$k_{\text{exb}}(01, \text{ind_HVMK})$	see general notes*
H44036f_a01	TrAa01C	$\text{IBUTALOH} \rightarrow \text{IBUTALOH(aq)}$	$k_{\text{exf}}(01, \text{ind_IBUTALOH})$	see general notes*
H44036b_a01	TrAa01C	$\text{IBUTALOH(aq)} \rightarrow \text{IBUTALOH}$	$k_{\text{exb}}(01, \text{ind_IBUTALOH})$	see general notes*
H44037f_a01	TrAa01C	$\text{IBUTDIAL} \rightarrow \text{IBUTDIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_IBUTDIAL})$	see general notes*
H44037b_a01	TrAa01C	$\text{IBUTDIAL(aq)} \rightarrow \text{IBUTDIAL}$	$k_{\text{exb}}(01, \text{ind_IBUTDIAL})$	see general notes*
H44038f_a01	TrAa01C	$\text{IBUTOLBOOH} \rightarrow \text{IBUTOLBOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_IBUTOLBOOH})$	see general notes*
H44038b_a01	TrAa01C	$\text{IBUTOLBOOH(aq)} \rightarrow \text{IBUTOLBOOH}$	$k_{\text{exb}}(01, \text{ind_IBUTOLBOOH})$	see general notes*
H44039f_a01	TrAa01C	$\text{IPRHOCO2H} \rightarrow \text{IPRHOCO2H(aq)}$	$k_{\text{exf}}(01, \text{ind_IPRHOCO2H})$	see general notes*
H44039b_a01	TrAa01C	$\text{IPRHOCO2H(aq)} \rightarrow \text{IPRHOCO2H}$	$k_{\text{exb}}(01, \text{ind_IPRHOCO2H})$	see general notes*
H44040f_a01	TrAa01C	$\text{IPRHOCO3H} \rightarrow \text{IPRHOCO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_IPRHOCO3H})$	see general notes*
H44040b_a01	TrAa01C	$\text{IPRHOCO3H(aq)} \rightarrow \text{IPRHOCO3H}$	$k_{\text{exb}}(01, \text{ind_IPRHOCO3H})$	see general notes*
H44041f_a01	TrAa01C	$\text{LBUT1ENOOH} \rightarrow \text{LBUT1ENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_LBUT1ENOOH})$	see general notes*
H44041b_a01	TrAa01C	$\text{LBUT1ENOOH(aq)} \rightarrow \text{LBUT1ENOOH}$	$k_{\text{exb}}(01, \text{ind_LBUT1ENOOH})$	see general notes*
H44042f_a01	TrAa01C	$\text{LHMKABOOH} \rightarrow \text{LHMKABOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_LHMKABOOH})$	see general notes*
H44042b_a01	TrAa01C	$\text{LHMKABOOH(aq)} \rightarrow \text{LHMKABOOH}$	$k_{\text{exb}}(01, \text{ind_LHMKABOOH})$	see general notes*
H44043f_a01	TrAa01C	$\text{LMEKOOH} \rightarrow \text{LMEKOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_LMEKOOH})$	see general notes*
H44043b_a01	TrAa01C	$\text{LMEKOOH(aq)} \rightarrow \text{LMEKOOH}$	$k_{\text{exb}}(01, \text{ind_LMEKOOH})$	see general notes*
H44044f_a01	TrAa01C	$\text{MACO2H} \rightarrow \text{MACO2H(aq)}$	$k_{\text{exf}}(01, \text{ind_MACO2H})$	see general notes*
H44044b_a01	TrAa01C	$\text{MACO2H(aq)} \rightarrow \text{MACO2H}$	$k_{\text{exb}}(01, \text{ind_MACO2H})$	see general notes*
H44045f_a01	TrAa01C	$\text{MACO3H} \rightarrow \text{MACO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_MACO3H})$	see general notes*
H44045b_a01	TrAa01C	$\text{MACO3H(aq)} \rightarrow \text{MACO3H}$	$k_{\text{exb}}(01, \text{ind_MACO3H})$	see general notes*
H44046f_a01	TrAa01C	$\text{MACROH} \rightarrow \text{MACROH(aq)}$	$k_{\text{exf}}(01, \text{ind_MACROH})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H44046b_a01	TrAa01C	MACROH(aq) \rightarrow MACROH	$k_{\text{exb}}(01, \text{ind_MACROH})$	see general notes*
H44047f_a01	TrAa01C	MACROOH \rightarrow MACROOH(aq)	$k_{\text{exf}}(01, \text{ind_MACROOH})$	see general notes*
H44047b_a01	TrAa01C	MACROOH(aq) \rightarrow MACROOH	$k_{\text{exb}}(01, \text{ind_MACROOH})$	see general notes*
H44048f_a01	TrAa01C	MALANHYOOH \rightarrow MALANHYOOH(aq)	$k_{\text{exf}}(01, \text{ind_MALANHYOOH})$	see general notes*
H44048b_a01	TrAa01C	MALANHYOOH(aq) \rightarrow MALANHYOOH	$k_{\text{exb}}(01, \text{ind_MALANHYOOH})$	see general notes*
H44049f_a01	TrAa01C	MALDALCO2H \rightarrow MALDALCO2H(aq)	$k_{\text{exf}}(01, \text{ind_MALDALCO2H})$	see general notes*
H44049b_a01	TrAa01C	MALDALCO2H(aq) \rightarrow MALDALCO2H	$k_{\text{exb}}(01, \text{ind_MALDALCO2H})$	see general notes*
H44050f_a01	TrAa01C	MALDALCO3H \rightarrow MALDALCO3H(aq)	$k_{\text{exf}}(01, \text{ind_MALDALCO3H})$	see general notes*
H44050b_a01	TrAa01C	MALDALCO3H(aq) \rightarrow MALDALCO3H	$k_{\text{exb}}(01, \text{ind_MALDALCO3H})$	see general notes*
H44051f_a01	TrAa01C	MALDIAL \rightarrow MALDIAL(aq)	$k_{\text{exf}}(01, \text{ind_MALDIAL})$	see general notes*
H44051b_a01	TrAa01C	MALDIAL(aq) \rightarrow MALDIAL	$k_{\text{exb}}(01, \text{ind_MALDIAL})$	see general notes*
H44052f_a01	TrAa01C	MALDIALOOH \rightarrow MALDIALOOH(aq)	$k_{\text{exf}}(01, \text{ind_MALDIALOOH})$	see general notes*
H44052b_a01	TrAa01C	MALDIALOOH(aq) \rightarrow MALDIALOOH	$k_{\text{exb}}(01, \text{ind_MALDIALOOH})$	see general notes*
H44053f_a01	TrAa01C	MALNHYOHCO \rightarrow MALNHYOHCO(aq)	$k_{\text{exf}}(01, \text{ind_MALNHYOHCO})$	see general notes*
H44053b_a01	TrAa01C	MALNHYOHCO(aq) \rightarrow MALNHYOHCO	$k_{\text{exb}}(01, \text{ind_MALNHYOHCO})$	see general notes*
H44054f_a01	TrAa01C	MECOACEOOH \rightarrow MECOACEOOH(aq)	$k_{\text{exf}}(01, \text{ind_MECOACEOOH})$	see general notes*
H44054b_a01	TrAa01C	MECOACEOOH(aq) \rightarrow MECOACEOOH	$k_{\text{exb}}(01, \text{ind_MECOACEOOH})$	see general notes*
H44055f_a01	TrAa01CN	MVKNO3 \rightarrow MVKNO3(aq)	$k_{\text{exf}}(01, \text{ind_MVKNO3})$	see general notes*
H44055b_a01	TrAa01CN	MVKNO3(aq) \rightarrow MVKNO3	$k_{\text{exb}}(01, \text{ind_MVKNO3})$	see general notes*
H44056f_a01	TrAa01CN	NBZFUOOH \rightarrow NBZFUOOH(aq)	$k_{\text{exf}}(01, \text{ind_NBZFUOOH})$	see general notes*
H44056b_a01	TrAa01CN	NBZFUOOH(aq) \rightarrow NBZFUOOH	$k_{\text{exb}}(01, \text{ind_NBZFUOOH})$	see general notes*
H44057f_a01	TrAa01CN	NC4DCO2H \rightarrow NC4DCO2H(aq)	$k_{\text{exf}}(01, \text{ind_NC4DCO2H})$	see general notes*
H44057b_a01	TrAa01CN	NC4DCO2H(aq) \rightarrow NC4DCO2H	$k_{\text{exb}}(01, \text{ind_NC4DCO2H})$	see general notes*
H45000f_a01	TrAa01C	ACCOMMECHO \rightarrow ACCOMMECHO(aq)	$k_{\text{exf}}(01, \text{ind_ACCOMMECHO})$	see general notes*
H45000b_a01	TrAa01C	ACCOMMECHO(aq) \rightarrow ACCOMMECHO	$k_{\text{exb}}(01, \text{ind_ACCOMMECHO})$	see general notes*
H45001f_a01	TrAa01C	ACCOMMECO3H \rightarrow ACCOMMECO3H(aq)	$k_{\text{exf}}(01, \text{ind_ACCOMMECO3H})$	see general notes*
H45001b_a01	TrAa01C	ACCOMMECO3H(aq) \rightarrow ACCOMMECO3H	$k_{\text{exb}}(01, \text{ind_ACCOMMECO3H})$	see general notes*
H45002f_a01	TrAa01C	C10DC2O2C4OOH \rightarrow C10DC2O2C4OOH(aq)	$k_{\text{exf}}(01, \text{ind_C10DC2O2C4OOH})$	see general notes*
H45002b_a01	TrAa01C	C10DC2O2C4OOH(aq) \rightarrow C10DC2O2C4OOH	$k_{\text{exb}}(01, \text{ind_C10DC2O2C4OOH})$	see general notes*
H45003f_a01	TrAa01C	C10DC2OOHC4OD \rightarrow C10DC2OOHC4OD(aq)	$k_{\text{exf}}(01, \text{ind_C10DC2OOHC4OD})$	see general notes*
H45003b_a01	TrAa01C	C10DC2OOHC4OD(aq) \rightarrow C10DC2OOHC4OD	$k_{\text{exb}}(01, \text{ind_C10DC2OOHC4OD})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45004f_a01	TrAa01C	C10DC3O2C4OOH C10DC3O2C4OOH(aq)	→ k_exf(01, ind_C10DC3O2C4OOH)	see general notes*
H45004b_a01	TrAa01C	C10DC3O2C4OOH(aq) C10DC3O2C4OOH	→ k_exb(01, ind_C10DC3O2C4OOH)	see general notes*
H45005f_a01	TrAa01C	C10OHC2OOHC4OD C10OHC2OOHC4OD(aq)	→ k_exf(01, ind_C10OHC2OOHC4OD)	see general notes*
H45005b_a01	TrAa01C	C10OHC2OOHC4OD(aq) C10OHC2OOHC4OD	→ k_exb(01, ind_C10OHC2OOHC4OD)	see general notes*
H45006f_a01	TrAa01C	C24O3CCO2H → C24O3CCO2H(aq)	k_exf(01, ind_C24O3CCO2H)	see general notes*
H45006b_a01	TrAa01C	C24O3CCO2H(aq) → C24O3CCO2H	k_exb(01, ind_C24O3CCO2H)	see general notes*
H45007f_a01	TrAa01C	C4CO2DBC03 → C4CO2DBC03(aq)	k_exf(01, ind_C4CO2DBC03)	see general notes*
H45007b_a01	TrAa01C	C4CO2DBC03(aq) → C4CO2DBC03	k_exb(01, ind_C4CO2DBC03)	see general notes*
H45008f_a01	TrAa01CN	C4CO2DBPAN → C4CO2DBPAN(aq)	k_exf(01, ind_C4CO2DBPAN)	see general notes*
H45008b_a01	TrAa01CN	C4CO2DBPAN(aq) → C4CO2DBPAN	k_exb(01, ind_C4CO2DBPAN)	see general notes*
H45009f_a01	TrAa01C	C4CO2DCO3H → C4CO2DCO3H(aq)	k_exf(01, ind_C4CO2DCO3H)	see general notes*
H45009b_a01	TrAa01C	C4CO2DCO3H(aq) → C4CO2DCO3H	k_exb(01, ind_C4CO2DCO3H)	see general notes*
H45010f_a01	TrAa01CN	C4MCONO3OH → C4MCONO3OH(aq)	k_exf(01, ind_C4MCONO3OH)	see general notes*
H45010b_a01	TrAa01CN	C4MCONO3OH(aq) → C4MCONO3OH	k_exb(01, ind_C4MCONO3OH)	see general notes*
H45011f_a01	TrAa01C	C511OOH → C511OOH(aq)	k_exf(01, ind_C511OOH)	see general notes*
H45011b_a01	TrAa01C	C511OOH(aq) → C511OOH	k_exb(01, ind_C511OOH)	see general notes*
H45012f_a01	TrAa01C	C512OOH → C512OOH(aq)	k_exf(01, ind_C512OOH)	see general notes*
H45012b_a01	TrAa01C	C512OOH(aq) → C512OOH	k_exb(01, ind_C512OOH)	see general notes*
H45013f_a01	TrAa01C	C5134CO2OH → C5134CO2OH(aq)	k_exf(01, ind_C5134CO2OH)	see general notes*
H45013b_a01	TrAa01C	C5134CO2OH(aq) → C5134CO2OH	k_exb(01, ind_C5134CO2OH)	see general notes*
H45014f_a01	TrAa01C	C513CO → C513CO(aq)	k_exf(01, ind_C513CO)	see general notes*
H45014b_a01	TrAa01C	C513CO(aq) → C513CO	k_exb(01, ind_C513CO)	see general notes*
H45015f_a01	TrAa01C	C513OOH → C513OOH(aq)	k_exf(01, ind_C513OOH)	see general notes*
H45015b_a01	TrAa01C	C513OOH(aq) → C513OOH	k_exb(01, ind_C513OOH)	see general notes*
H45016f_a01	TrAa01CN	C514NO3 → C514NO3(aq)	k_exf(01, ind_C514NO3)	see general notes*
H45016b_a01	TrAa01CN	C514NO3(aq) → C514NO3	k_exb(01, ind_C514NO3)	see general notes*
H45017f_a01	TrAa01C	C514OOH → C514OOH(aq)	k_exf(01, ind_C514OOH)	see general notes*
H45017b_a01	TrAa01C	C514OOH(aq) → C514OOH	k_exb(01, ind_C514OOH)	see general notes*
H45018f_a01	TrAa01C	C54CO → C54CO(aq)	k_exf(01, ind_C54CO)	see general notes*
H45018b_a01	TrAa01C	C54CO(aq) → C54CO	k_exb(01, ind_C54CO)	see general notes*
H45019f_a01	TrAa01C	C59OOH → C59OOH(aq)	k_exf(01, ind_C59OOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45019b_a01	TrAa01C	$\text{C59OOH(aq)} \rightarrow \text{C59OOH}$	$k_{\text{exb}}(01, \text{ind_C59OOH})$	see general notes*
H45020f_a01	TrAa01C	$\text{C5CO14OH} \rightarrow \text{C5CO14OH(aq)}$	$k_{\text{exf}}(01, \text{ind_C5CO14OH})$	see general notes*
H45020b_a01	TrAa01C	$\text{C5CO14OH(aq)} \rightarrow \text{C5CO14OH}$	$k_{\text{exb}}(01, \text{ind_C5CO14OH})$	see general notes*
H45021f_a01	TrAa01C	$\text{C5CO14OOH} \rightarrow \text{C5CO14OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C5CO14OOH})$	see general notes*
H45021b_a01	TrAa01C	$\text{C5CO14OOH(aq)} \rightarrow \text{C5CO14OOH}$	$k_{\text{exb}}(01, \text{ind_C5CO14OOH})$	see general notes*
H45022f_a01	TrAa01C	$\text{C5DIALCO} \rightarrow \text{C5DIALCO(aq)}$	$k_{\text{exf}}(01, \text{ind_C5DIALCO})$	see general notes*
H45022b_a01	TrAa01C	$\text{C5DIALCO(aq)} \rightarrow \text{C5DIALCO}$	$k_{\text{exb}}(01, \text{ind_C5DIALCO})$	see general notes*
H45023f_a01	TrAa01C	$\text{C5DIALOOH} \rightarrow \text{C5DIALOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C5DIALOOH})$	see general notes*
H45023b_a01	TrAa01C	$\text{C5DIALOOH(aq)} \rightarrow \text{C5DIALOOH}$	$k_{\text{exb}}(01, \text{ind_C5DIALOOH})$	see general notes*
H45024f_a01	TrAa01C	$\text{C5DICARB} \rightarrow \text{C5DICARB(aq)}$	$k_{\text{exf}}(01, \text{ind_C5DICARB})$	see general notes*
H45024b_a01	TrAa01C	$\text{C5DICARB(aq)} \rightarrow \text{C5DICARB}$	$k_{\text{exb}}(01, \text{ind_C5DICARB})$	see general notes*
H45025f_a01	TrAa01C	$\text{C5DICAROOH} \rightarrow \text{C5DICAROOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C5DICAROOH})$	see general notes*
H45025b_a01	TrAa01C	$\text{C5DICAROOH(aq)} \rightarrow \text{C5DICAROOH}$	$k_{\text{exb}}(01, \text{ind_C5DICAROOH})$	see general notes*
H45026f_a01	TrAa01CN	$\text{C5PAN9} \rightarrow \text{C5PAN9(aq)}$	$k_{\text{exf}}(01, \text{ind_C5PAN9})$	see general notes*
H45026b_a01	TrAa01CN	$\text{C5PAN9(aq)} \rightarrow \text{C5PAN9}$	$k_{\text{exb}}(01, \text{ind_C5PAN9})$	see general notes*
H45027f_a01	TrAa01C	$\text{CHOC3COOOH} \rightarrow \text{CHOC3COOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CHOC3COOOH})$	see general notes*
H45027b_a01	TrAa01C	$\text{CHOC3COOOH(aq)} \rightarrow \text{CHOC3COOOH}$	$k_{\text{exb}}(01, \text{ind_CHOC3COOOH})$	see general notes*
H45028f_a01	TrAa01CN	$\text{CHOC3COPAN} \rightarrow \text{CHOC3COPAN(aq)}$	$k_{\text{exf}}(01, \text{ind_CHOC3COPAN})$	see general notes*
H45028b_a01	TrAa01CN	$\text{CHOC3COPAN(aq)} \rightarrow \text{CHOC3COPAN}$	$k_{\text{exb}}(01, \text{ind_CHOC3COPAN})$	see general notes*
H45029f_a01	TrAa01C	$\text{CO13C4CHO} \rightarrow \text{CO13C4CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO13C4CHO})$	see general notes*
H45029b_a01	TrAa01C	$\text{CO13C4CHO(aq)} \rightarrow \text{CO13C4CHO}$	$k_{\text{exb}}(01, \text{ind_CO13C4CHO})$	see general notes*
H45030f_a01	TrAa01C	$\text{CO23C4CHO} \rightarrow \text{CO23C4CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO23C4CHO})$	see general notes*
H45030b_a01	TrAa01C	$\text{CO23C4CHO(aq)} \rightarrow \text{CO23C4CHO}$	$k_{\text{exb}}(01, \text{ind_CO23C4CHO})$	see general notes*
H45031f_a01	TrAa01C	$\text{CO23C4CO3H} \rightarrow \text{CO23C4CO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_CO23C4CO3H})$	see general notes*
H45031b_a01	TrAa01C	$\text{CO23C4CO3H(aq)} \rightarrow \text{CO23C4CO3H}$	$k_{\text{exb}}(01, \text{ind_CO23C4CO3H})$	see general notes*
H45032f_a01	TrAa01CN	$\text{DB1NO3} \rightarrow \text{DB1NO3(aq)}$	$k_{\text{exf}}(01, \text{ind_DB1NO3})$	see general notes*
H45032b_a01	TrAa01CN	$\text{DB1NO3(aq)} \rightarrow \text{DB1NO3}$	$k_{\text{exb}}(01, \text{ind_DB1NO3})$	see general notes*
H45033f_a01	TrAa01C	$\text{DB1OOH} \rightarrow \text{DB1OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_DB1OOH})$	see general notes*
H45033b_a01	TrAa01C	$\text{DB1OOH(aq)} \rightarrow \text{DB1OOH}$	$k_{\text{exb}}(01, \text{ind_DB1OOH})$	see general notes*
H45034f_a01	TrAa01C	$\text{DB2OOH} \rightarrow \text{DB2OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_DB2OOH})$	see general notes*
H45034b_a01	TrAa01C	$\text{DB2OOH(aq)} \rightarrow \text{DB2OOH}$	$k_{\text{exb}}(01, \text{ind_DB2OOH})$	see general notes*
H45035f_a01	TrAa01C	$\text{ISOPA OH} \rightarrow \text{ISOPA OH(aq)}$	$k_{\text{exf}}(01, \text{ind_ISOPA OH})$	see general notes*
H45035b_a01	TrAa01C	$\text{ISOPA OH(aq)} \rightarrow \text{ISOPA OH}$	$k_{\text{exb}}(01, \text{ind_ISOPA OH})$	see general notes*
H45036f_a01	TrAa01CN	$\text{ISOPBNO3} \rightarrow \text{ISOPBNO3(aq)}$	$k_{\text{exf}}(01, \text{ind_ISOPBNO3})$	see general notes*
H45036b_a01	TrAa01CN	$\text{ISOPBNO3(aq)} \rightarrow \text{ISOPBNO3}$	$k_{\text{exb}}(01, \text{ind_ISOPBNO3})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45037f_a01	TrAa01C	ISOPBOH \rightarrow ISOPBOH(aq)	k_exf(01, ind_ISOPBOH)	see general notes*
H45037b_a01	TrAa01C	ISOPBOH(aq) \rightarrow ISOPBOH	k_exb(01, ind_ISOPBOH)	see general notes*
H45038f_a01	TrAa01C	ISOPBOOH \rightarrow ISOPBOOH(aq)	k_exf(01, ind_ISOPBOOH)	see general notes*
H45038b_a01	TrAa01C	ISOPBOOH(aq) \rightarrow ISOPBOOH	k_exb(01, ind_ISOPBOOH)	see general notes*
H45039f_a01	TrAa01CN	ISOPDNO3 \rightarrow ISOPDNO3(aq)	k_exf(01, ind_ISOPDNO3)	see general notes*
H45039b_a01	TrAa01CN	ISOPDNO3(aq) \rightarrow ISOPDNO3	k_exb(01, ind_ISOPDNO3)	see general notes*
H45040f_a01	TrAa01C	ISOPDOH \rightarrow ISOPDOH(aq)	k_exf(01, ind_ISOPDOH)	see general notes*
H45040b_a01	TrAa01C	ISOPDOH(aq) \rightarrow ISOPDOH	k_exb(01, ind_ISOPDOH)	see general notes*
H45041f_a01	TrAa01C	ISOPDOOH \rightarrow ISOPDOOH(aq)	k_exf(01, ind_ISOPDOOH)	see general notes*
H45041b_a01	TrAa01C	ISOPDOOH(aq) \rightarrow ISOPDOOH	k_exb(01, ind_ISOPDOOH)	see general notes*
H45042f_a01	TrAa01C	LC578OOH \rightarrow LC578OOH(aq)	k_exf(01, ind_LC578OOH)	see general notes*
H45042b_a01	TrAa01C	LC578OOH(aq) \rightarrow LC578OOH	k_exb(01, ind_LC578OOH)	see general notes*
H45043f_a01	TrAa01CN	LC5PAN1719 \rightarrow LC5PAN1719(aq)	k_exf(01, ind_LC5PAN1719)	see general notes*
H45043b_a01	TrAa01CN	LC5PAN1719(aq) \rightarrow LC5PAN1719	k_exb(01, ind_LC5PAN1719)	see general notes*
H45044f_a01	TrAa01C	LHC4ACCHO \rightarrow LHC4ACCHO(aq)	k_exf(01, ind_LHC4ACCHO)	see general notes*
H45044b_a01	TrAa01C	LHC4ACCHO(aq) \rightarrow LHC4ACCHO	k_exb(01, ind_LHC4ACCHO)	see general notes*
H45045f_a01	TrAa01C	LHC4ACCO2H \rightarrow LHC4ACCO2H(aq)	k_exf(01, ind_LHC4ACCO2H)	see general notes*
H45045b_a01	TrAa01C	LHC4ACCO2H(aq) \rightarrow LHC4ACCO2H	k_exb(01, ind_LHC4ACCO2H)	see general notes*
H45046f_a01	TrAa01C	LHC4ACCO3H \rightarrow LHC4ACCO3H(aq)	k_exf(01, ind_LHC4ACCO3H)	see general notes*
H45046b_a01	TrAa01C	LHC4ACCO3H(aq) \rightarrow LHC4ACCO3H	k_exb(01, ind_LHC4ACCO3H)	see general notes*
H45047f_a01	TrAa01C	LIEPOX \rightarrow LIEPOX(aq)	k_exf(01, ind_LIEPOX)	see general notes*
H45047b_a01	TrAa01C	LIEPOX(aq) \rightarrow LIEPOX	k_exb(01, ind_LIEPOX)	see general notes*
H45048f_a01	TrAa01CN	LISOPACNO3 \rightarrow LISOPACNO3(aq)	k_exf(01, ind_LISOPACNO3)	see general notes*
H45048b_a01	TrAa01CN	LISOPACNO3(aq) \rightarrow LISOPACNO3	k_exb(01, ind_LISOPACNO3)	see general notes*
H45049f_a01	TrAa01C	LISOPACOOH \rightarrow LISOPACOOH(aq)	k_exf(01, ind_LISOPACOOH)	see general notes*
H45049b_a01	TrAa01C	LISOPACOOH(aq) \rightarrow LISOPACOOH	k_exb(01, ind_LISOPACOOH)	see general notes*
H45050f_a01	TrAa01CN	LMBOABNO3 \rightarrow LMBOABNO3(aq)	k_exf(01, ind_LMBOABNO3)	see general notes*
H45050b_a01	TrAa01CN	LMBOABNO3(aq) \rightarrow LMBOABNO3	k_exb(01, ind_LMBOABNO3)	see general notes*
H45051f_a01	TrAa01C	LMBOABOOH \rightarrow LMBOABOOH(aq)	k_exf(01, ind_LMBOABOOH)	see general notes*
H45051b_a01	TrAa01C	LMBOABOOH(aq) \rightarrow LMBOABOOH	k_exb(01, ind_LMBOABOOH)	see general notes*
H45052f_a01	TrAa01CN	LNMBABOOH \rightarrow LNMBABOOH(aq)	k_exf(01, ind_LNMBABOOH)	see general notes*
H45052b_a01	TrAa01CN	LNMBABOOH(aq) \rightarrow LNMBABOOH	k_exb(01, ind_LNMBABOOH)	see general notes*
H45053f_a01	TrAa01C	MBO \rightarrow MBO(aq)	k_exf(01, ind_MBO)	see general notes*
H45053b_a01	TrAa01C	MBO(aq) \rightarrow MBO	k_exb(01, ind_MBO)	see general notes*
H45054f_a01	TrAa01C	MBOACO \rightarrow MBOACO(aq)	k_exf(01, ind_MBOACO)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45054b_a01	TrAa01C	MBOACO(aq) \rightarrow MBOACO	k_exb(01, ind_MBOACO)	see general notes*
H45055f_a01	TrAa01C	MBOCOCO \rightarrow MBOCOCO(aq)	k_exf(01, ind_MBOCOCO)	see general notes*
H45055b_a01	TrAa01C	MBOCOCO(aq) \rightarrow MBOCOCO	k_exb(01, ind_MBOCOCO)	see general notes*
H45056f_a01	TrAa01C	MC3ODBCO2H \rightarrow MC3ODBCO2H(aq)	k_exf(01, ind_MC3ODBCO2H)	see general notes*
H45056b_a01	TrAa01C	MC3ODBCO2H(aq) \rightarrow MC3ODBCO2H	k_exb(01, ind_MC3ODBCO2H)	see general notes*
H45057f_a01	TrAa01C	3METHYLFURAN \rightarrow 3METHYLFURAN(aq)	k_exf(01, ind_ME3FURAN)	see general notes*
H45057b_a01	TrAa01C	3METHYLFURAN(aq) \rightarrow 3METHYLFURAN	k_exb(01, ind_ME3FURAN)	see general notes*
H45058f_a01	TrAa01C	MMALNHOOH \rightarrow MMALNHOOH(aq)	k_exf(01, ind_MMALNHOOH)	see general notes*
H45058b_a01	TrAa01C	MMALNHOOH(aq) \rightarrow MMALNHOOH	k_exb(01, ind_MMALNHOOH)	see general notes*
H45059f_a01	TrAa01CN	NC4MDCO2HN \rightarrow NC4MDCO2HN(aq)	k_exf(01, ind_NC4MDCO2H)	see general notes*
H45059b_a01	TrAa01CN	NC4MDCO2HN(aq) \rightarrow NC4MDCO2HN	k_exb(01, ind_NC4MDCO2H)	see general notes*
H45060f_a01	TrAa01CN	NC4OHCO3H \rightarrow NC4OHCO3H(aq)	k_exf(01, ind_NC4OHCO3H)	see general notes*
H45060b_a01	TrAa01CN	NC4OHCO3H(aq) \rightarrow NC4OHCO3H	k_exb(01, ind_NC4OHCO3H)	see general notes*
H45061f_a01	TrAa01CN	NC4OHCPAN \rightarrow NC4OHCPAN(aq)	k_exf(01, ind_NC4OHCPAN)	see general notes*
H45061b_a01	TrAa01CN	NC4OHCPAN(aq) \rightarrow NC4OHCPAN	k_exb(01, ind_NC4OHCPAN)	see general notes*
H45062f_a01	TrAa01CN	NISOPPOOH \rightarrow NISOPPOOH(aq)	k_exf(01, ind_NISOPPOOH)	see general notes*
H45062b_a01	TrAa01CN	NISOPPOOH(aq) \rightarrow NISOPPOOH	k_exb(01, ind_NISOPPOOH)	see general notes*
H45063f_a01	TrAa01CN	NMBOBCO \rightarrow NMBOBCO(aq)	k_exf(01, ind_NMBOBCO)	see general notes*
H45063b_a01	TrAa01CN	NMBOBCO(aq) \rightarrow NMBOBCO	k_exb(01, ind_NMBOBCO)	see general notes*
H45064f_a01	TrAa01CN	NTLFUOOH \rightarrow NTLFUOOH(aq)	k_exf(01, ind_NTLFUOOH)	see general notes*
H45064b_a01	TrAa01CN	NTLFUOOH(aq) \rightarrow NTLFUOOH	k_exb(01, ind_NTLFUOOH)	see general notes*
H45065f_a01	TrAa01C	TLFUOOH \rightarrow TLFUOOH(aq)	k_exf(01, ind_TLFUOOH)	see general notes*
H45065b_a01	TrAa01C	TLFUOOH(aq) \rightarrow TLFUOOH	k_exb(01, ind_TLFUOOH)	see general notes*
H45066f_a01	TrAa01C	LZCO3HC23DBCOD \rightarrow LZCO3HC23DBCOD(aq)	k_exf(01, ind_LZCO3HC23DBCOD)	see general notes*
H45066b_a01	TrAa01C	LZCO3HC23DBCOD(aq) \rightarrow LZCO3HC23DBCOD	k_exb(01, ind_LZCO3HC23DBCOD)	see general notes*
H45067f_a01	TrAa01C	C4MDIAL \rightarrow C4MDIAL(aq)	k_exf(01, ind_C4MDIAL)	see general notes*
H45067b_a01	TrAa01C	C4MDIAL(aq) \rightarrow C4MDIAL	k_exb(01, ind_C4MDIAL)	see general notes*
H46000f_a01	TrAa01CN	BZBIPERNO3 \rightarrow BZBIPERNO3(aq)	k_exf(01, ind_BZBIPERNO3)	see general notes*
H46000b_a01	TrAa01CN	BZBIPERNO3(aq) \rightarrow BZBIPERNO3	k_exb(01, ind_BZBIPERNO3)	see general notes*
H46001f_a01	TrAa01C	BZBIPEROOH \rightarrow BZBIPEROOH(aq)	k_exf(01, ind_BZBIPEROOH)	see general notes*
H46001b_a01	TrAa01C	BZBIPEROOH(aq) \rightarrow BZBIPEROOH	k_exb(01, ind_BZBIPEROOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H46002f_a01	TrAa01C	BZEMUCCO \rightarrow BZEMUCCO(aq)	k_exf(01, ind_BZEMUCCO)	see general notes*
H46002b_a01	TrAa01C	BZEMUCCO(aq) \rightarrow BZEMUCCO	k_exb(01, ind_BZEMUCCO)	see general notes*
H46003f_a01	TrAa01C	BZEMUCCO2H \rightarrow BZEMUCCO2H(aq)	k_exf(01, ind_BZEMUCCO2H)	see general notes*
H46003b_a01	TrAa01C	BZEMUCCO2H(aq) \rightarrow BZEMUCCO2H	k_exb(01, ind_BZEMUCCO2H)	see general notes*
H46004f_a01	TrAa01C	BZEMUCCO3H \rightarrow BZEMUCCO3H(aq)	k_exf(01, ind_BZEMUCCO3H)	see general notes*
H46004b_a01	TrAa01C	BZEMUCCO3H(aq) \rightarrow BZEMUCCO3H	k_exb(01, ind_BZEMUCCO3H)	see general notes*
H46005f_a01	TrAa01CN	BZEMUCNO3 \rightarrow BZEMUCNO3(aq)	k_exf(01, ind_BZEMUCNO3)	see general notes*
H46005b_a01	TrAa01CN	BZEMUCNO3(aq) \rightarrow BZEMUCNO3	k_exb(01, ind_BZEMUCNO3)	see general notes*
H46006f_a01	TrAa01C	BZEMUCOOH \rightarrow BZEMUCOOH(aq)	k_exf(01, ind_BZEMUCOOH)	see general notes*
H46006b_a01	TrAa01C	BZEMUCOOH(aq) \rightarrow BZEMUCOOH	k_exb(01, ind_BZEMUCOOH)	see general notes*
H46007f_a01	TrAa01C	BZEPOXMUC \rightarrow BZEPOXMUC(aq)	k_exf(01, ind_BZEPOXMUC)	see general notes*
H46007b_a01	TrAa01C	BZEPOXMUC(aq) \rightarrow BZEPOXMUC	k_exb(01, ind_BZEPOXMUC)	see general notes*
H46008f_a01	TrAa01C	BZOBIPEROH \rightarrow BZOBIPEROH(aq)	k_exf(01, ind_BZOBIPEROH)	see general notes*
H46008b_a01	TrAa01C	BZOBIPEROH(aq) \rightarrow BZOBIPEROH	k_exb(01, ind_BZOBIPEROH)	see general notes*
H46009f_a01	TrAa01CN	C5CO2DBPAN \rightarrow C5CO2DBPAN(aq)	k_exf(01, ind_C5CO2DBPAN)	see general notes*
H46009b_a01	TrAa01CN	C5CO2DBPAN(aq) \rightarrow C5CO2DBPAN	k_exb(01, ind_C5CO2DBPAN)	see general notes*
H46010f_a01	TrAa01C	C5CO2DCO3H \rightarrow C5CO2DCO3H(aq)	k_exf(01, ind_C5CO2DCO3H)	see general notes*
H46010b_a01	TrAa01C	C5CO2DCO3H(aq) \rightarrow C5CO2DCO3H	k_exb(01, ind_C5CO2DCO3H)	see general notes*
H46011f_a01	TrAa01CN	C5CO2OHPAN \rightarrow C5CO2OHPAN(aq)	k_exf(01, ind_C5CO2OHPAN)	see general notes*
H46011b_a01	TrAa01CN	C5CO2OHPAN(aq) \rightarrow C5CO2OHPAN	k_exb(01, ind_C5CO2OHPAN)	see general notes*
H46012f_a01	TrAa01C	C5COOHCO3H \rightarrow C5COOHCO3H(aq)	k_exf(01, ind_C5COOHCO3H)	see general notes*
H46012b_a01	TrAa01C	C5COOHCO3H(aq) \rightarrow C5COOHCO3H	k_exb(01, ind_C5COOHCO3H)	see general notes*
H46013f_a01	TrAa01C	C6125CO \rightarrow C6125CO(aq)	k_exf(01, ind_C6125CO)	see general notes*
H46013b_a01	TrAa01C	C6125CO(aq) \rightarrow C6125CO	k_exb(01, ind_C6125CO)	see general notes*
H46014f_a01	TrAa01C	C614CO \rightarrow C614CO(aq)	k_exf(01, ind_C614CO)	see general notes*
H46014b_a01	TrAa01C	C614CO(aq) \rightarrow C614CO	k_exb(01, ind_C614CO)	see general notes*
H46015f_a01	TrAa01CN	C614NO3 \rightarrow C614NO3(aq)	k_exf(01, ind_C614NO3)	see general notes*
H46015b_a01	TrAa01CN	C614NO3(aq) \rightarrow C614NO3	k_exb(01, ind_C614NO3)	see general notes*
H46016f_a01	TrAa01C	C614OOH \rightarrow C614OOH(aq)	k_exf(01, ind_C614OOH)	see general notes*
H46016b_a01	TrAa01C	C614OOH(aq) \rightarrow C614OOH	k_exb(01, ind_C614OOH)	see general notes*
H46017f_a01	TrAa01C	C615CO2OOH \rightarrow C615CO2OOH(aq)	k_exf(01, ind_C615CO2OOH)	see general notes*
H46017b_a01	TrAa01C	C615CO2OOH(aq) \rightarrow C615CO2OOH	k_exb(01, ind_C615CO2OOH)	see general notes*
H46018f_a01	TrAa01C	C6CO4DB \rightarrow C6CO4DB(aq)	k_exf(01, ind_C6CO4DB)	see general notes*
H46018b_a01	TrAa01C	C6CO4DB(aq) \rightarrow C6CO4DB	k_exb(01, ind_C6CO4DB)	see general notes*
H46019f_a01	TrAa01C	C6H5O \rightarrow C6H5O(aq)	k_exf(01, ind_C6H5O)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H46019b_a01	TrAa01C	$\text{C6H5O(aq)} \rightarrow \text{C6H5O}$	$k_{\text{exb}}(01, \text{ind_C6H5O})$	see general notes*
H46020f_a01	TrAa01C	$\text{C6H5OOH} \rightarrow \text{C6H5OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C6H5OOH})$	see general notes*
H46020b_a01	TrAa01C	$\text{C6H5OOH(aq)} \rightarrow \text{C6H5OOH}$	$k_{\text{exb}}(01, \text{ind_C6H5OOH})$	see general notes*
H46021f_a01	TrAa01C	$\text{CATEC1O} \rightarrow \text{CATEC1O(aq)}$	$k_{\text{exf}}(01, \text{ind_CATEC1O})$	see general notes*
H46021b_a01	TrAa01C	$\text{CATEC1O(aq)} \rightarrow \text{CATEC1O}$	$k_{\text{exb}}(01, \text{ind_CATEC1O})$	see general notes*
H46022f_a01	TrAa01C	$\text{CATEC1OOH} \rightarrow \text{CATEC1OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CATEC1OOH})$	see general notes*
H46022b_a01	TrAa01C	$\text{CATEC1OOH(aq)} \rightarrow \text{CATEC1OOH}$	$k_{\text{exb}}(01, \text{ind_CATEC1OOH})$	see general notes*
H46023f_a01	TrAa01C	$\text{CATECHOL} \rightarrow \text{CATECHOL(aq)}$	$k_{\text{exf}}(01, \text{ind_CATECHOL})$	see general notes*
H46023b_a01	TrAa01C	$\text{CATECHOL(aq)} \rightarrow \text{CATECHOL}$	$k_{\text{exb}}(01, \text{ind_CATECHOL})$	see general notes*
H46024f_a01	TrAa01C	$\text{CO235C5CHO} \rightarrow \text{CO235C5CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO235C5CHO})$	see general notes*
H46024b_a01	TrAa01C	$\text{CO235C5CHO(aq)} \rightarrow \text{CO235C5CHO}$	$k_{\text{exb}}(01, \text{ind_CO235C5CHO})$	see general notes*
H46025f_a01	TrAa01C	$\text{CO235C6OOH} \rightarrow \text{CO235C6OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CO235C6OOH})$	see general notes*
H46025b_a01	TrAa01C	$\text{CO235C6OOH(aq)} \rightarrow \text{CO235C6OOH}$	$k_{\text{exb}}(01, \text{ind_CO235C6OOH})$	see general notes*
H46026f_a01	TrAa01CN	$\text{DNPHEN} \rightarrow \text{DNPHEN(aq)}$	$k_{\text{exf}}(01, \text{ind_DNPHEN})$	see general notes*
H46026b_a01	TrAa01CN	$\text{DNPHEN(aq)} \rightarrow \text{DNPHEN}$	$k_{\text{exb}}(01, \text{ind_DNPHEN})$	see general notes*
H46027f_a01	TrAa01CN	$\text{DNPHENOOH} \rightarrow \text{DNPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_DNPHENOOH})$	see general notes*
H46027b_a01	TrAa01CN	$\text{DNPHENOOH(aq)} \rightarrow \text{DNPHENOOH}$	$k_{\text{exb}}(01, \text{ind_DNPHENOOH})$	see general notes*
H46028f_a01	TrAa01CN	$\text{NBZQOOH} \rightarrow \text{NBZQOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NBZQOOH})$	see general notes*
H46028b_a01	TrAa01CN	$\text{NBZQOOH(aq)} \rightarrow \text{NBZQOOH}$	$k_{\text{exb}}(01, \text{ind_NBZQOOH})$	see general notes*
H46029f_a01	TrAa01CN	$\text{NCATECHOL} \rightarrow \text{NCATECHOL(aq)}$	$k_{\text{exf}}(01, \text{ind_NCATECHOL})$	see general notes*
H46029b_a01	TrAa01CN	$\text{NCATECHOL(aq)} \rightarrow \text{NCATECHOL}$	$k_{\text{exb}}(01, \text{ind_NCATECHOL})$	see general notes*
H46030f_a01	TrAa01CN	$\text{NCATECOOH} \rightarrow \text{NCATECOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NCATECOOH})$	see general notes*
H46030b_a01	TrAa01CN	$\text{NCATECOOH(aq)} \rightarrow \text{NCATECOOH}$	$k_{\text{exb}}(01, \text{ind_NCATECOOH})$	see general notes*
H46031f_a01	TrAa01CN	$\text{NDNPHENOOH} \rightarrow \text{NDNPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NDNPHENOOH})$	see general notes*
H46031b_a01	TrAa01CN	$\text{NDNPHENOOH(aq)} \rightarrow \text{NDNPHENOOH}$	$k_{\text{exb}}(01, \text{ind_NDNPHENOOH})$	see general notes*
H46032f_a01	TrAa01CN	$\text{NNCATECOOH} \rightarrow \text{NNCATECOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NNCATECOOH})$	see general notes*
H46032b_a01	TrAa01CN	$\text{NNCATECOOH(aq)} \rightarrow \text{NNCATECOOH}$	$k_{\text{exb}}(01, \text{ind_NNCATECOOH})$	see general notes*
H46033f_a01	TrAa01CN	$\text{NPHENOOH} \rightarrow \text{NPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NPHENOOH})$	see general notes*
H46033b_a01	TrAa01CN	$\text{NPHENOOH(aq)} \rightarrow \text{NPHENOOH}$	$k_{\text{exb}}(01, \text{ind_NPHENOOH})$	see general notes*
H46034f_a01	TrAa01C	$\text{PBZQCO} \rightarrow \text{PBZQCO(aq)}$	$k_{\text{exf}}(01, \text{ind_PBZQCO})$	see general notes*
H46034b_a01	TrAa01C	$\text{PBZQCO(aq)} \rightarrow \text{PBZQCO}$	$k_{\text{exb}}(01, \text{ind_PBZQCO})$	see general notes*
H46035f_a01	TrAa01C	$\text{PBZQOOH} \rightarrow \text{PBZQOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_PBZQOOH})$	see general notes*
H46035b_a01	TrAa01C	$\text{PBZQOOH(aq)} \rightarrow \text{PBZQOOH}$	$k_{\text{exb}}(01, \text{ind_PBZQOOH})$	see general notes*
H46036f_a01	TrAa01C	$\text{PHENOL} \rightarrow \text{PHENOL(aq)}$	$k_{\text{exf}}(01, \text{ind_PHENOL})$	see general notes*
H46036b_a01	TrAa01C	$\text{PHENOL(aq)} \rightarrow \text{PHENOL}$	$k_{\text{exb}}(01, \text{ind_PHENOL})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H46037f_a01	TrAa01C	PHENOOH \rightarrow PHENOOH(aq)	k_exf(01, ind_PHENOOH)	see general notes*
H46037b_a01	TrAa01C	PHENOOH(aq) \rightarrow PHENOOH	k_exb(01, ind_PHENOOH)	see general notes*
H47000f_a01	TrAa01C	C235C6CO3H \rightarrow C235C6CO3H(aq)	k_exf(01, ind_C235C6CO3H)	see general notes*
H47000b_a01	TrAa01C	C235C6CO3H(aq) \rightarrow C235C6CO3H	k_exb(01, ind_C235C6CO3H)	see general notes*
H47001f_a01	TrAa01CN	C6CO2OHPAN \rightarrow C6CO2OHPAN(aq)	k_exf(01, ind_C6CO2OHPAN)	see general notes*
H47001b_a01	TrAa01CN	C6CO2OHPAN(aq) \rightarrow C6CO2OHPAN	k_exb(01, ind_C6CO2OHPAN)	see general notes*
H47002f_a01	TrAa01C	C6COOHCO3H \rightarrow C6COOHCO3H(aq)	k_exf(01, ind_C6COOHCO3H)	see general notes*
H47002b_a01	TrAa01C	C6COOHCO3H(aq) \rightarrow C6COOHCO3H	k_exb(01, ind_C6COOHCO3H)	see general notes*
H47003f_a01	TrAa01C	C6H5CH2OOH \rightarrow C6H5CH2OOH(aq)	k_exf(01, ind_C6H5CH2OOH)	see general notes*
H47003b_a01	TrAa01C	C6H5CH2OOH(aq) \rightarrow C6H5CH2OOH	k_exb(01, ind_C6H5CH2OOH)	see general notes*
H47004f_a01	TrAa01C	C6H5CO3H \rightarrow C6H5CO3H(aq)	k_exf(01, ind_C6H5CO3H)	see general notes*
H47004b_a01	TrAa01C	C6H5CO3H(aq) \rightarrow C6H5CO3H	k_exb(01, ind_C6H5CO3H)	see general notes*
H47005f_a01	TrAa01C	C716OOH \rightarrow C716OOH(aq)	k_exf(01, ind_C716OOH)	see general notes*
H47005b_a01	TrAa01C	C716OOH(aq) \rightarrow C716OOH	k_exb(01, ind_C716OOH)	see general notes*
H47006f_a01	TrAa01C	C721OOH \rightarrow C721OOH(aq)	k_exf(01, ind_C721OOH)	see general notes*
H47006b_a01	TrAa01C	C721OOH(aq) \rightarrow C721OOH	k_exb(01, ind_C721OOH)	see general notes*
H47007f_a01	TrAa01C	C722OOH \rightarrow C722OOH(aq)	k_exf(01, ind_C722OOH)	see general notes*
H47007b_a01	TrAa01C	C722OOH(aq) \rightarrow C722OOH	k_exb(01, ind_C722OOH)	see general notes*
H47008f_a01	TrAa01C	C7CO4DB \rightarrow C7CO4DB(aq)	k_exf(01, ind_C7CO4DB)	see general notes*
H47008b_a01	TrAa01C	C7CO4DB(aq) \rightarrow C7CO4DB	k_exb(01, ind_C7CO4DB)	see general notes*
H47009f_a01	TrAa01CN	C7PAN3 \rightarrow C7PAN3(aq)	k_exf(01, ind_C7PAN3)	see general notes*
H47009b_a01	TrAa01CN	C7PAN3(aq) \rightarrow C7PAN3	k_exb(01, ind_C7PAN3)	see general notes*
H47010f_a01	TrAa01C	CO235C6CHO \rightarrow CO235C6CHO(aq)	k_exf(01, ind_CO235C6CHO)	see general notes*
H47010b_a01	TrAa01C	CO235C6CHO(aq) \rightarrow CO235C6CHO	k_exb(01, ind_CO235C6CHO)	see general notes*
H47011f_a01	TrAa01C	CRESOL \rightarrow CRESOL(aq)	k_exf(01, ind_CRESOL)	see general notes*
H47011b_a01	TrAa01C	CRESOL(aq) \rightarrow CRESOL	k_exb(01, ind_CRESOL)	see general notes*
H47012f_a01	TrAa01C	CRESOOH \rightarrow CRESOOH(aq)	k_exf(01, ind_CRESOOH)	see general notes*
H47012b_a01	TrAa01C	CRESOOH(aq) \rightarrow CRESOOH	k_exb(01, ind_CRESOOH)	see general notes*
H47013f_a01	TrAa01CN	DNCRES \rightarrow DNCRES(aq)	k_exf(01, ind_DNCRES)	see general notes*
H47013b_a01	TrAa01CN	DNCRES(aq) \rightarrow DNCRES	k_exb(01, ind_DNCRES)	see general notes*
H47014f_a01	TrAa01CN	DNCRESOOH \rightarrow DNCRESOOH(aq)	k_exf(01, ind_DNCRESOOH)	see general notes*
H47014b_a01	TrAa01CN	DNCRESOOH(aq) \rightarrow DNCRESOOH	k_exb(01, ind_DNCRESOOH)	see general notes*
H47015f_a01	TrAa01C	MCATEC1O \rightarrow MCATEC1O(aq)	k_exf(01, ind_MCATEC1O)	see general notes*
H47015b_a01	TrAa01C	MCATEC1O(aq) \rightarrow MCATEC1O	k_exb(01, ind_MCATEC1O)	see general notes*
H47016f_a01	TrAa01C	MCATEC1OOH \rightarrow MCATEC1OOH(aq)	k_exf(01, ind_MCATEC1OOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H47016b_a01	TrAa01C	MCATEC1OOH(aq) \rightarrow MCATEC1OOH	k_exb(01,ind_MCATEC1OOH)	see general notes*
H47017f_a01	TrAa01C	MCATECHOL \rightarrow MCATECHOL(aq)	k_exf(01,ind_MCATECHOL)	see general notes*
H47017b_a01	TrAa01C	MCATECHOL(aq) \rightarrow MCATECHOL	k_exb(01,ind_MCATECHOL)	see general notes*
H47018f_a01	TrAa01CN	MNCATECH \rightarrow MNCATECH(aq)	k_exf(01,ind_MNCATECH)	see general notes*
H47018b_a01	TrAa01CN	MNCATECH(aq) \rightarrow MNCATECH	k_exb(01,ind_MNCATECH)	see general notes*
H47019f_a01	TrAa01CN	MNCATECOOH \rightarrow MNCATECOOH(aq)	k_exf(01,ind_MNCATECOOH)	see general notes*
H47019b_a01	TrAa01CN	MNCATECOOH(aq) \rightarrow MNCATECOOH	k_exb(01,ind_MNCATECOOH)	see general notes*
H47020f_a01	TrAa01CN	MNNCATCOOH \rightarrow MNNCATCOOH(aq)	k_exf(01,ind_MNNCATCOOH)	see general notes*
H47020b_a01	TrAa01CN	MNNCATCOOH(aq) \rightarrow MNNCATCOOH	k_exb(01,ind_MNNCATCOOH)	see general notes*
H47021f_a01	TrAa01CN	NCRESOOH \rightarrow NCRESOOH(aq)	k_exf(01,ind_NCRESOOH)	see general notes*
H47021b_a01	TrAa01CN	NCRESOOH(aq) \rightarrow NCRESOOH	k_exb(01,ind_NCRESOOH)	see general notes*
H47022f_a01	TrAa01CN	NDNCRESOOH \rightarrow NDNCRESOOH(aq)	k_exf(01,ind_NDNCRESOOH)	see general notes*
H47022b_a01	TrAa01CN	NDNCRESOOH(aq) \rightarrow NDNCRESOOH	k_exb(01,ind_NDNCRESOOH)	see general notes*
H47023f_a01	TrAa01C	OXYL1OOH \rightarrow OXYL1OOH(aq)	k_exf(01,ind_OXYL1OOH)	see general notes*
H47023b_a01	TrAa01C	OXYL1OOH(aq) \rightarrow OXYL1OOH	k_exb(01,ind_OXYL1OOH)	see general notes*
H47024f_a01	TrAa01C	PHCOOH \rightarrow PHCOOH(aq)	k_exf(01,ind_PHCOOH)	see general notes*
H47024b_a01	TrAa01C	PHCOOH(aq) \rightarrow PHCOOH	k_exb(01,ind_PHCOOH)	see general notes*
H47025f_a01	TrAa01C	TLBIPEROOH \rightarrow TLBIPEROOH(aq)	k_exf(01,ind_TLBIPEROOH)	see general notes*
H47025b_a01	TrAa01C	TLBIPEROOH(aq) \rightarrow TLBIPEROOH	k_exb(01,ind_TLBIPEROOH)	see general notes*
H47026f_a01	TrAa01C	TLEMUCCO \rightarrow TLEMUCCO(aq)	k_exf(01,ind_TLEMUCCO)	see general notes*
H47026b_a01	TrAa01C	TLEMUCCO(aq) \rightarrow TLEMUCCO	k_exb(01,ind_TLEMUCCO)	see general notes*
H47027f_a01	TrAa01C	TLEMUCCO2H \rightarrow TLEMUCCO2H(aq)	k_exf(01,ind_TLEMUCCO2H)	see general notes*
H47027b_a01	TrAa01C	TLEMUCCO2H(aq) \rightarrow TLEMUCCO2H	k_exb(01,ind_TLEMUCCO2H)	see general notes*
H47028f_a01	TrAa01C	TLEMUCCO3H \rightarrow TLEMUCCO3H(aq)	k_exf(01,ind_TLEMUCCO3H)	see general notes*
H47028b_a01	TrAa01C	TLEMUCCO3H(aq) \rightarrow TLEMUCCO3H	k_exb(01,ind_TLEMUCCO3H)	see general notes*
H47029f_a01	TrAa01CN	TLEMUCNO3 \rightarrow TLEMUCNO3(aq)	k_exf(01,ind_TLEMUCNO3)	see general notes*
H47029b_a01	TrAa01CN	TLEMUCNO3(aq) \rightarrow TLEMUCNO3	k_exb(01,ind_TLEMUCNO3)	see general notes*
H47030f_a01	TrAa01C	TLEMUCOOH \rightarrow TLEMUCOOH(aq)	k_exf(01,ind_TLEMUCOOH)	see general notes*
H47030b_a01	TrAa01C	TLEMUCOOH(aq) \rightarrow TLEMUCOOH	k_exb(01,ind_TLEMUCOOH)	see general notes*
H47031f_a01	TrAa01C	TLOBIPEROH \rightarrow TLOBIPEROH(aq)	k_exf(01,ind_TLOBIPEROH)	see general notes*
H47031b_a01	TrAa01C	TLOBIPEROH(aq) \rightarrow TLOBIPEROH	k_exb(01,ind_TLOBIPEROH)	see general notes*
H47032f_a01	TrAa01C	TOL1O \rightarrow TOL1O(aq)	k_exf(01,ind_TOL1O)	see general notes*
H47032b_a01	TrAa01C	TOL1O(aq) \rightarrow TOL1O	k_exb(01,ind_TOL1O)	see general notes*
H48000f_a01	TrAa01C	C721CHO \rightarrow C721CHO(aq)	k_exf(01,ind_C721CHO)	see general notes*
H48000b_a01	TrAa01C	C721CHO(aq) \rightarrow C721CHO	k_exb(01,ind_C721CHO)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H48001f_a01	TrAa01C	$C721CO3H \rightarrow C721CO3H(aq)$	$k_{\text{exf}}(01, \text{ind}_{C721CO3H})$	see general notes*
H48001b_a01	TrAa01C	$C721CO3H(aq) \rightarrow C721CO3H$	$k_{\text{exb}}(01, \text{ind}_{C721CO3H})$	see general notes*
H48002f_a01	TrAa01CN	$C721PAN \rightarrow C721PAN(aq)$	$k_{\text{exf}}(01, \text{ind}_{C721PAN})$	see general notes*
H48002b_a01	TrAa01CN	$C721PAN(aq) \rightarrow C721PAN$	$k_{\text{exb}}(01, \text{ind}_{C721PAN})$	see general notes*
H48003f_a01	TrAa01CN	$C810NO3 \rightarrow C810NO3(aq)$	$k_{\text{exf}}(01, \text{ind}_{C810NO3})$	see general notes*
H48003b_a01	TrAa01CN	$C810NO3(aq) \rightarrow C810NO3$	$k_{\text{exb}}(01, \text{ind}_{C810NO3})$	see general notes*
H48004f_a01	TrAa01C	$C810OOH \rightarrow C810OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C810OOH})$	see general notes*
H48004b_a01	TrAa01C	$C810OOH(aq) \rightarrow C810OOH$	$k_{\text{exb}}(01, \text{ind}_{C810OOH})$	see general notes*
H48005f_a01	TrAa01C	$C812OOH \rightarrow C812OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C812OOH})$	see general notes*
H48005b_a01	TrAa01C	$C812OOH(aq) \rightarrow C812OOH$	$k_{\text{exb}}(01, \text{ind}_{C812OOH})$	see general notes*
H48006f_a01	TrAa01C	$C813OOH \rightarrow C813OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C813OOH})$	see general notes*
H48006b_a01	TrAa01C	$C813OOH(aq) \rightarrow C813OOH$	$k_{\text{exb}}(01, \text{ind}_{C813OOH})$	see general notes*
H48007f_a01	TrAa01C	$C85OOH \rightarrow C85OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C85OOH})$	see general notes*
H48007b_a01	TrAa01C	$C85OOH(aq) \rightarrow C85OOH$	$k_{\text{exb}}(01, \text{ind}_{C85OOH})$	see general notes*
H48008f_a01	TrAa01C	$C86OOH \rightarrow C86OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C86OOH})$	see general notes*
H48008b_a01	TrAa01C	$C86OOH(aq) \rightarrow C86OOH$	$k_{\text{exb}}(01, \text{ind}_{C86OOH})$	see general notes*
H48009f_a01	TrAa01CN	$C89NO3 \rightarrow C89NO3(aq)$	$k_{\text{exf}}(01, \text{ind}_{C89NO3})$	see general notes*
H48009b_a01	TrAa01CN	$C89NO3(aq) \rightarrow C89NO3$	$k_{\text{exb}}(01, \text{ind}_{C89NO3})$	see general notes*
H48010f_a01	TrAa01C	$C89OOH \rightarrow C89OOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C89OOH})$	see general notes*
H48010b_a01	TrAa01C	$C89OOH(aq) \rightarrow C89OOH$	$k_{\text{exb}}(01, \text{ind}_{C89OOH})$	see general notes*
H48011f_a01	TrAa01C	$C8BC \rightarrow C8BC(aq)$	$k_{\text{exf}}(01, \text{ind}_{C8BC})$	see general notes*
H48011b_a01	TrAa01C	$C8BC(aq) \rightarrow C8BC$	$k_{\text{exb}}(01, \text{ind}_{C8BC})$	see general notes*
H48012f_a01	TrAa01C	$C8BCCO \rightarrow C8BCCO(aq)$	$k_{\text{exf}}(01, \text{ind}_{C8BCCO})$	see general notes*
H48012b_a01	TrAa01C	$C8BCCO(aq) \rightarrow C8BCCO$	$k_{\text{exb}}(01, \text{ind}_{C8BCCO})$	see general notes*
H48013f_a01	TrAa01CN	$C8BCNO3 \rightarrow C8BCNO3(aq)$	$k_{\text{exf}}(01, \text{ind}_{C8BCNO3})$	see general notes*
H48013b_a01	TrAa01CN	$C8BCNO3(aq) \rightarrow C8BCNO3$	$k_{\text{exb}}(01, \text{ind}_{C8BCNO3})$	see general notes*
H48014f_a01	TrAa01C	$C8BCOOH \rightarrow C8BCOOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{C8BCOOH})$	see general notes*
H48014b_a01	TrAa01C	$C8BCOOH(aq) \rightarrow C8BCOOH$	$k_{\text{exb}}(01, \text{ind}_{C8BCOOH})$	see general notes*
H48015f_a01	TrAa01C	$NORPINIC \rightarrow NORPINIC(aq)$	$k_{\text{exf}}(01, \text{ind}_{NORPINIC})$	see general notes*
H48015b_a01	TrAa01C	$NORPINIC(aq) \rightarrow NORPINIC$	$k_{\text{exb}}(01, \text{ind}_{NORPINIC})$	see general notes*
H48016f_a01	TrAa01C	$STYRENOOH \rightarrow STYRENOOH(aq)$	$k_{\text{exf}}(01, \text{ind}_{STYRENOOH})$	see general notes*
H48016b_a01	TrAa01C	$STYRENOOH(aq) \rightarrow STYRENOOH$	$k_{\text{exb}}(01, \text{ind}_{STYRENOOH})$	see general notes*
H49000f_a01	TrAa01C	$C811CO3H \rightarrow C811CO3H(aq)$	$k_{\text{exf}}(01, \text{ind}_{C811CO3H})$	see general notes*
H49000b_a01	TrAa01C	$C811CO3H(aq) \rightarrow C811CO3H$	$k_{\text{exb}}(01, \text{ind}_{C811CO3H})$	see general notes*
H49001f_a01	TrAa01CN	$C811PAN \rightarrow C811PAN(aq)$	$k_{\text{exf}}(01, \text{ind}_{C811PAN})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H49001b_a01	TrAa01CN	C811PAN(aq) \rightarrow C811PAN	k_exb(01, ind_C811PAN)	see general notes*
H49002f_a01	TrAa01C	C85CO3H \rightarrow C85CO3H(aq)	k_exf(01, ind_C85CO3H)	see general notes*
H49002b_a01	TrAa01C	C85CO3H(aq) \rightarrow C85CO3H	k_exb(01, ind_C85CO3H)	see general notes*
H49003f_a01	TrAa01C	C89CO2H \rightarrow C89CO2H(aq)	k_exf(01, ind_C89CO2H)	see general notes*
H49003b_a01	TrAa01C	C89CO2H(aq) \rightarrow C89CO2H	k_exb(01, ind_C89CO2H)	see general notes*
H49004f_a01	TrAa01C	C89CO3H \rightarrow C89CO3H(aq)	k_exf(01, ind_C89CO3H)	see general notes*
H49004b_a01	TrAa01C	C89CO3H(aq) \rightarrow C89CO3H	k_exb(01, ind_C89CO3H)	see general notes*
H49005f_a01	TrAa01CN	C89PAN \rightarrow C89PAN(aq)	k_exf(01, ind_C89PAN)	see general notes*
H49005b_a01	TrAa01CN	C89PAN(aq) \rightarrow C89PAN	k_exb(01, ind_C89PAN)	see general notes*
H49006f_a01	TrAa01CN	C96NO3 \rightarrow C96NO3(aq)	k_exf(01, ind_C96NO3)	see general notes*
H49006b_a01	TrAa01CN	C96NO3(aq) \rightarrow C96NO3	k_exb(01, ind_C96NO3)	see general notes*
H49007f_a01	TrAa01C	C96OOH \rightarrow C96OOH(aq)	k_exf(01, ind_C96OOH)	see general notes*
H49007b_a01	TrAa01C	C96OOH(aq) \rightarrow C96OOH	k_exb(01, ind_C96OOH)	see general notes*
H49008f_a01	TrAa01C	C97OOH \rightarrow C97OOH(aq)	k_exf(01, ind_C97OOH)	see general notes*
H49008b_a01	TrAa01C	C97OOH(aq) \rightarrow C97OOH	k_exb(01, ind_C97OOH)	see general notes*
H49009f_a01	TrAa01C	C98OOH \rightarrow C98OOH(aq)	k_exf(01, ind_C98OOH)	see general notes*
H49009b_a01	TrAa01C	C98OOH(aq) \rightarrow C98OOH	k_exb(01, ind_C98OOH)	see general notes*
H49010f_a01	TrAa01CN	C9PAN2 \rightarrow C9PAN2(aq)	k_exf(01, ind_C9PAN2)	see general notes*
H49010b_a01	TrAa01CN	C9PAN2(aq) \rightarrow C9PAN2	k_exb(01, ind_C9PAN2)	see general notes*
H49011f_a01	TrAa01C	NOPINDCO \rightarrow NOPINDCO(aq)	k_exf(01, ind_NOPINDCO)	see general notes*
H49011b_a01	TrAa01C	NOPINDCO(aq) \rightarrow NOPINDCO	k_exb(01, ind_NOPINDCO)	see general notes*
H49012f_a01	TrAa01C	NOPINDOOH \rightarrow NOPINDOOH(aq)	k_exf(01, ind_NOPINDOOH)	see general notes*
H49012b_a01	TrAa01C	NOPINDOOH(aq) \rightarrow NOPINDOOH	k_exb(01, ind_NOPINDOOH)	see general notes*
H49013f_a01	TrAa01C	NOPINONE \rightarrow NOPINONE(aq)	k_exf(01, ind_NOPINONE)	see general notes*
H49013b_a01	TrAa01C	NOPINONE(aq) \rightarrow NOPINONE	k_exb(01, ind_NOPINONE)	see general notes*
H49014f_a01	TrAa01C	NOPINOO \rightarrow NOPINOO(aq)	k_exf(01, ind_NOPINOO)	see general notes*
H49014b_a01	TrAa01C	NOPINOO(aq) \rightarrow NOPINOO	k_exb(01, ind_NOPINOO)	see general notes*
H49015f_a01	TrAa01C	NORPINAL \rightarrow NORPINAL(aq)	k_exf(01, ind_NORPINAL)	see general notes*
H49015b_a01	TrAa01C	NORPINAL(aq) \rightarrow NORPINAL	k_exb(01, ind_NORPINAL)	see general notes*
H49016f_a01	TrAa01C	NORPINENOL \rightarrow NORPINENOL(aq)	k_exf(01, ind_NORPINENOL)	see general notes*
H49016b_a01	TrAa01C	NORPINENOL(aq) \rightarrow NORPINENOL	k_exb(01, ind_NORPINENOL)	see general notes*
H49017f_a01	TrAa01C	PINIC \rightarrow PINIC(aq)	k_exf(01, ind_PINIC)	see general notes*
H49017b_a01	TrAa01C	PINIC(aq) \rightarrow PINIC	k_exb(01, ind_PINIC)	see general notes*
H410000f_a01	TrAa01CN	BPINANO3 \rightarrow BPINANO3(aq)	k_exf(01, ind_BPINANO3)	see general notes*
H410000b_a01	TrAa01CN	BPINANO3(aq) \rightarrow BPINANO3	k_exb(01, ind_BPINANO3)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410001f_a01	TrAa01C	BPINAOOH \rightarrow BPINAOOH(aq)	k_exf(01, ind_BPINAOOH)	see general notes*
H410001b_a01	TrAa01C	BPINAOOH(aq) \rightarrow BPINAOOH	k_exb(01, ind_BPINAOOH)	see general notes*
H410002f_a01	TrAa01CN	C106NO3 \rightarrow C106NO3(aq)	k_exf(01, ind_C106NO3)	see general notes*
H410002b_a01	TrAa01CN	C106NO3(aq) \rightarrow C106NO3	k_exb(01, ind_C106NO3)	see general notes*
H410003f_a01	TrAa01C	C106OOH \rightarrow C106OOH(aq)	k_exf(01, ind_C106OOH)	see general notes*
H410003b_a01	TrAa01C	C106OOH(aq) \rightarrow C106OOH	k_exb(01, ind_C106OOH)	see general notes*
H410004f_a01	TrAa01C	C109CO \rightarrow C109CO(aq)	k_exf(01, ind_C109CO)	see general notes*
H410004b_a01	TrAa01C	C109CO(aq) \rightarrow C109CO	k_exb(01, ind_C109CO)	see general notes*
H410005f_a01	TrAa01C	C109OOH \rightarrow C109OOH(aq)	k_exf(01, ind_C109OOH)	see general notes*
H410005b_a01	TrAa01C	C109OOH(aq) \rightarrow C109OOH	k_exb(01, ind_C109OOH)	see general notes*
H410006f_a01	TrAa01CN	C10PAN2 \rightarrow C10PAN2(aq)	k_exf(01, ind_C10PAN2)	see general notes*
H410006b_a01	TrAa01CN	C10PAN2(aq) \rightarrow C10PAN2	k_exb(01, ind_C10PAN2)	see general notes*
H410007f_a01	TrAa01CN	LAPINABNO3 \rightarrow LAPINABNO3(aq)	k_exf(01, ind_LAPINABNO3)	see general notes*
H410007b_a01	TrAa01CN	LAPINABNO3(aq) \rightarrow LAPINABNO3	k_exb(01, ind_LAPINABNO3)	see general notes*
H410008f_a01	TrAa01C	LAPINABOOH \rightarrow LAPINABOOH(aq)	k_exf(01, ind_LAPINABOOH)	see general notes*
H410008b_a01	TrAa01C	LAPINABOOH(aq) \rightarrow LAPINABOOH	k_exb(01, ind_LAPINABOOH)	see general notes*
H410009f_a01	TrAa01CN	LNAPINABOOH \rightarrow LNAPINABOOH(aq)	k_exf(01, ind_LNAPINABOOH)	see general notes*
H410009b_a01	TrAa01CN	LNAPINABOOH(aq) \rightarrow LNAPINABOOH	k_exb(01, ind_LNAPINABOOH)	see general notes*
H410010f_a01	TrAa01CN	LNBPINABOOH \rightarrow LNBPINABOOH(aq)	k_exf(01, ind_LNBPINABOOH)	see general notes*
H410010b_a01	TrAa01CN	LNBPINABOOH(aq) \rightarrow LNBPINABOOH	k_exb(01, ind_LNBPINABOOH)	see general notes*
H410011f_a01	TrAa01C	MENTHEN6ONE \rightarrow MENTHEN6ONE(aq)	k_exf(01, ind_MENTHEN6ONE)	see general notes*
H410011b_a01	TrAa01C	MENTHEN6ONE(aq) \rightarrow MENTHEN6ONE	k_exb(01, ind_MENTHEN6ONE)	see general notes*
H410012f_a01	TrAa01C	2OHMENTHEN6ONE \rightarrow 2OHMENTHEN6ONE(aq)	k_exf(01, ind_OH2MENTHEN6ONE)	see general notes*
H410012b_a01	TrAa01C	2OHMENTHEN6ONE(aq) \rightarrow 2OHMENTHEN6ONE	k_exb(01, ind_OH2MENTHEN6ONE)	see general notes*
H410013f_a01	TrAa01C	PERPINONIC \rightarrow PERPINONIC(aq)	k_exf(01, ind_PERPINONIC)	see general notes*
H410013b_a01	TrAa01C	PERPINONIC(aq) \rightarrow PERPINONIC	k_exb(01, ind_PERPINONIC)	see general notes*
H410014f_a01	TrAa01C	PINAL \rightarrow PINAL(aq)	k_exf(01, ind_PINAL)	see general notes*
H410014b_a01	TrAa01C	PINAL(aq) \rightarrow PINAL	k_exb(01, ind_PINAL)	see general notes*
H410015f_a01	TrAa01CN	PINALNO3 \rightarrow PINALNO3(aq)	k_exf(01, ind_PINALNO3)	see general notes*
H410015b_a01	TrAa01CN	PINALNO3(aq) \rightarrow PINALNO3	k_exb(01, ind_PINALNO3)	see general notes*
H410016f_a01	TrAa01C	PINALOOH \rightarrow PINALOOH(aq)	k_exf(01, ind_PINALOOH)	see general notes*
H410016b_a01	TrAa01C	PINALOOH(aq) \rightarrow PINALOOH	k_exb(01, ind_PINALOOH)	see general notes*
H410017f_a01	TrAa01C	PINEOL \rightarrow PINEOL(aq)	k_exf(01, ind_PINENOL)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410017b_a01	TrAa01C	PINEOL(aq) \rightarrow PINEOL	k_exb(01,ind_PINENOL)	see general notes*
H410018f_a01	TrAa01C	PINONIC \rightarrow PINONIC(aq)	k_exf(01,ind_PINONIC)	see general notes*
H410018b_a01	TrAa01C	PINONIC(aq) \rightarrow PINONIC	k_exb(01,ind_PINONIC)	see general notes*
H410019f_a01	TrAa01CN	RO6R1NO3 \rightarrow RO6R1NO3(aq)	k_exf(01,ind_RO6R1NO3)	see general notes*
H410019b_a01	TrAa01CN	RO6R1NO3(aq) \rightarrow RO6R1NO3	k_exb(01,ind_RO6R1NO3)	see general notes*
H410020f_a01	TrAa01CN	ROO6R1NO3 \rightarrow ROO6R1NO3(aq)	k_exf(01,ind_ROO6R1NO3)	see general notes*
H410020b_a01	TrAa01CN	ROO6R1NO3(aq) \rightarrow ROO6R1NO3	k_exb(01,ind_ROO6R1NO3)	see general notes*
H60000f_a01	TrAa01MblScCl	Cl ₂ \rightarrow Cl ₂ (aq)	k_exf(01,ind_Cl2)	see general notes*
H60000b_a01	TrAa01MblScCl	Cl ₂ (aq) \rightarrow Cl ₂	k_exb(01,ind_Cl2)	see general notes*
H62000f_a01	TrAa01MblScScmCl	HCl \rightarrow HCl(aq)	k_exf(01,ind_HCl)	see general notes*
H62000b_a01	TrAa01MblScScmCl	HCl(aq) \rightarrow HCl	k_exb(01,ind_HCl)	see general notes*
H62001f_a01	TrAa01MblScCl	HOCl \rightarrow HOCl(aq)	k_exf(01,ind_HOCl)	see general notes*
H62001b_a01	TrAa01MblScCl	HOCl(aq) \rightarrow HOCl	k_exb(01,ind_HOCl)	see general notes*
H63000_a01	TrAa01MblClN	N ₂ O ₅ + Cl ⁻ (aq) \rightarrow ClNO ₂ + NO ₃ ⁻ (aq)	k_exf_N205(01) * 5.E2	Behnke et al. (1994), Behnke et al. (1997)
H63001_a01	TrAa01MblClN	ClNO ₃ \rightarrow HOCl(aq) + HNO ₃ (aq)	k_exf_ClN03(01) * C(ind_H2O_a01)	see general notes*
H63002_a01	TrAa01MblClN	ClNO ₃ + Cl ⁻ (aq) \rightarrow Cl ₂ (aq) + NO ₃ ⁻ (aq)	k_exf_ClN03(01) * 5.E2	see general notes*
H70000f_a01	TrAa01MblScBr	Br ₂ \rightarrow Br ₂ (aq)	k_exf(01,ind_Br2)	see general notes*
H70000b_a01	TrAa01MblScBr	Br ₂ (aq) \rightarrow Br ₂	k_exb(01,ind_Br2)	see general notes*
H72000f_a01	TrAa01MblScScmBr	HBr \rightarrow HBr(aq)	k_exf(01,ind_HBr)	see general notes*
H72000b_a01	TrAa01MblScScmBr	HBr(aq) \rightarrow HBr	k_exb(01,ind_HBr)	see general notes*
H72001f_a01	TrAa01MblScBr	HOBr \rightarrow HOBr(aq)	k_exf(01,ind_HOBr)	see general notes*
H72001b_a01	TrAa01MblScBr	HOBr(aq) \rightarrow HOBr	k_exb(01,ind_HOBr)	see general notes*
H73000_a01	TrAa01MblBrN	N ₂ O ₅ + Br ⁻ (aq) \rightarrow BrNO ₂ + NO ₃ ⁻ (aq)	k_exf_N205(01) * 3.E5	Behnke et al. (1994), Behnke et al. (1997)
H73001_a01	TrAa01MblBrN	BrNO ₃ \rightarrow HOBr(aq) + HNO ₃ (aq)	k_exf_BrN03(01) * C(ind_H2O_a01)	see general notes*
H73002_a01	TrAa01MblBrN	BrNO ₃ + Br ⁻ (aq) \rightarrow Br ₂ (aq) + NO ₃ ⁻ (aq)	k_exf_BrN03(01) * 3.E5	see general notes*
H76000f_a01	TrAa01MblScBrCl	BrCl \rightarrow BrCl(aq)	k_exf(01,ind_BrCl)	see general notes*
H76000b_a01	TrAa01MblScBrCl	BrCl(aq) \rightarrow BrCl	k_exb(01,ind_BrCl)	see general notes*
H76001_a01	TrAa01MblBrClN	ClNO ₃ + Br ⁻ (aq) \rightarrow BrCl(aq) + NO ₃ ⁻ (aq)	k_exf_ClN03(01) * 3.E5	see general notes*
H76002_a01	TrAa01MblBrClN	BrNO ₃ + Cl ⁻ (aq) \rightarrow BrCl(aq) + NO ₃ ⁻ (aq)	k_exf_BrN03(01) * 5.E2	see general notes*
H80000f_a01	TrAa01ScI	I ₂ \rightarrow I ₂ (aq)	k_exf(01,ind_I2)	see general notes*
H80000b_a01	TrAa01ScI	I ₂ (aq) \rightarrow I ₂	k_exb(01,ind_I2)	see general notes*
H81000f_a01	TrAa01MblScI	IO \rightarrow IO(aq)	k_exf(01,ind_IO)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H81000b_a01	TrAa01MblScI	$\text{IO(aq)} \rightarrow \text{IO}$	$k_{\text{exb}}(01, \text{ind_IO})$	see general notes*
H81001_a01	TrAa01I	$\text{OIO} \rightarrow \text{HOI(aq)} + \text{HO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_OIO})$	see general notes*
H81002_a01	TrAa01I	$\text{I}_2\text{O}_2 \rightarrow \text{HOI(aq)} + \text{H}^+(\text{aq}) + \text{IO}_2^-(\text{aq})$	$k_{\text{exf}}(01, \text{ind_I2O2})$	see general notes*
H82000f_a01	TrAa01MblScI	$\text{HOI} \rightarrow \text{HOI(aq)}$	$k_{\text{exf}}(01, \text{ind_HOI})$	see general notes*
H82000b_a01	TrAa01MblScI	$\text{HOI(aq)} \rightarrow \text{HOI}$	$k_{\text{exb}}(01, \text{ind_HOI})$	see general notes*
H82001_a01	TrAa01MblScI	$\text{HI} \rightarrow \text{H}^+(\text{aq}) + \text{I}^-(\text{aq})$	$k_{\text{mt}}(\text{HI}) \cdot lwc$	see general notes*
H82002_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*
H83000_a01	TrAa01IN	$\text{INO}_2 \rightarrow \text{HOI(aq)} + \text{HONO(aq)}$	$k_{\text{exf}}(01, \text{ind_INO2})$	see general notes*
H83001_a01	TrAa01MblIN	$\text{INO}_3 \rightarrow \text{HOI(aq)} + \text{HNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_INO3})$	see general notes*
H86000f_a01	TrAa01MblScClI	$\text{ICl} \rightarrow \text{ICl(aq)}$	$k_{\text{exf}}(01, \text{ind_ICl})$	see general notes*
H86000b_a01	TrAa01MblScClI	$\text{ICl(aq)} \rightarrow \text{ICl}$	$k_{\text{exb}}(01, \text{ind_ICl})$	see general notes*
H87000f_a01	TrAa01MblScBrI	$\text{IBr} \rightarrow \text{IBr(aq)}$	$k_{\text{exf}}(01, \text{ind_IBr})$	see general notes*
H87000b_a01	TrAa01MblScBrI	$\text{IBr(aq)} \rightarrow \text{IBr}$	$k_{\text{exb}}(01, \text{ind_IBr})$	see general notes*
H91000f_a01	TrAa01MblScScmS	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_SO2})$	see general notes*
H91000b_a01	TrAa01MblScScmS	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(01, \text{ind_SO2})$	see general notes*
H92000_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$xnom7sulf * k_{\text{exf}}(01, \text{ind_H2SO4})$	see general notes*
H94000f_a01	TrAa01CS	$\text{DMSO} \rightarrow \text{DMSO(aq)}$	$k_{\text{exf}}(01, \text{ind_DMSO})$	see general notes*
H94000b_a01	TrAa01CS	$\text{DMSO(aq)} \rightarrow \text{DMSO}$	$k_{\text{exb}}(01, \text{ind_DMSO})$	see general notes*
H94001_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*
H94002f_a01	TrAa01CS	$\text{DMS} \rightarrow \text{DMS(aq)}$	$k_{\text{exf}}(01, \text{ind_DMS})$	see general notes*
H94002b_a01	TrAa01CS	$\text{DMS(aq)} \rightarrow \text{DMS}$	$k_{\text{exb}}(01, \text{ind_DMS})$	see general notes*
H100000f_a01	TrAa01Hg	$\text{Hg} \rightarrow \text{Hg(aq)}$	$k_{\text{exf}}(01, \text{ind_Hg})$	see general notes*
H100000b_a01	TrAa01Hg	$\text{Hg(aq)} \rightarrow \text{Hg}$	$k_{\text{exb}}(01, \text{ind_Hg})$	see general notes*
H100100f_a01	TrAa01Hg	$\text{HgO} \rightarrow \text{HgO(aq)}$	$k_{\text{exf}}(01, \text{ind_HgO})$	see general notes*
H100100b_a01	TrAa01Hg	$\text{HgO(aq)} \rightarrow \text{HgO}$	$k_{\text{exb}}(01, \text{ind_HgO})$	see general notes*
H100600f_a01	TrAa01ClHg	$\text{HgCl}_2 \rightarrow \text{HgCl}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HgCl2})$	see general notes*
H100600b_a01	TrAa01ClHg	$\text{HgCl}_2(\text{aq}) \rightarrow \text{HgCl}_2$	$k_{\text{exb}}(01, \text{ind_HgCl2})$	see general notes*
H100700f_a01	TrAa01BrHg	$\text{HgBr}_2 \rightarrow \text{HgBr}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HgBr2})$	see general notes*
H100700b_a01	TrAa01BrHg	$\text{HgBr}_2(\text{aq}) \rightarrow \text{HgBr}_2$	$k_{\text{exb}}(01, \text{ind_HgBr2})$	see general notes*
H100701f_a01	TrAa01BrClHg	$\text{ClHgBr} \rightarrow \text{ClHgBr(aq)}$	$k_{\text{exf}}(01, \text{ind_ClHgBr})$	see general notes*
H100701b_a01	TrAa01BrClHg	$\text{ClHgBr(aq)} \rightarrow \text{ClHgBr}$	$k_{\text{exb}}(01, \text{ind_ClHgBr})$	see general notes*
H100702f_a01	TrAa01BrHg	$\text{BrHgOBr} \rightarrow \text{BrHgOBr(aq)}$	$k_{\text{exf}}(01, \text{ind_BrHgOBr})$	see general notes*
H100702b_a01	TrAa01BrHg	$\text{BrHgOBr(aq)} \rightarrow \text{BrHgOBr}$	$k_{\text{exb}}(01, \text{ind_BrHgOBr})$	see general notes*
H100703f_a01	TrAa01BrClHg	$\text{ClHgOBr} \rightarrow \text{ClHgOBr(aq)}$	$k_{\text{exf}}(01, \text{ind_ClHgOBr})$	see general notes*
H100703b_a01	TrAa01BrClHg	$\text{ClHgOBr(aq)} \rightarrow \text{ClHgOBr}$	$k_{\text{exb}}(01, \text{ind_ClHgOBr})$	see general notes*

General notes

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

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

subsequent reaction with H_2O , Cl^- , and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\text{exf}}(\text{X}) = \frac{k_{\text{mt}}(\text{X}) \times \text{LWC}}{[\text{H}_2\text{O}] + 5 \times 10^2 [\text{Cl}^-] + 3 \times 10^5 [\text{Br}^-]}$$

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt} . The factors only affect

the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[\text{Cl}^-] > 0.1 \text{ M}$ (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\text{H}_2\text{O}]/[\text{Cl}^-]$ is less than 5×10^2 . The ratio $5 \times 10^2 / 3 \times 10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N_2O_5 . Here, they are also used for ClNO_3 and BrNO_3 .

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET300	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*
HET301	TrHetN	$\text{N}_2\text{O}_5 \rightarrow 2 \text{NO}_3^-(\text{cs}) + 2 \text{H}^+(\text{cs})$	<code>khet_Tr(iht_N2O5)</code>	see general notes*
HET610	StHetCl	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HCl)</code>	see general notes*
HET620	StHetClN	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HCl)</code>	see general notes*
HET621	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*
HET622	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*
HET710	StHetBr	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	<code>khet_St(ihs_HOBr_HBr)</code>	see general notes*
HET720	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*
HET740	StHetBrClN	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_ClNO3_HBr)</code>	see general notes*
HET741	StHetBrClN	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	<code>khet_St(ihs_BrNO3_HCl)</code>	see general notes*
HET742	StHetBrCl	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	<code>khet_St(ihs_HOCl_HBr)</code>	see general notes*
HET743	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	$\text{Hg} \rightarrow \text{Hg}(\text{cs})$	<code>khet_Tr(iht_Hg) + khet_St(ihs_Hg)</code>	see general notes*
HET1002	StTrHetHg	$\text{HgO} \rightarrow \text{Hg}(\text{cs})$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1003	StTrHetClHg	$\text{HgCl} \rightarrow \text{Hg}(\text{cs}) + \text{LCHLORINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1004	StTrHetClHg	$\text{HgCl}_2 \rightarrow \text{Hg}(\text{cs}) + 2 \text{LCHLORINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1005	StTrHetBrHg	$\text{HgBr} \rightarrow \text{Hg}(\text{cs}) + \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1006	StTrHetBrHg	$\text{HgBr}_2 \rightarrow \text{Hg}(\text{cs}) + 2 \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1007	StTrHetBrClHg	$\text{ClHgBr} \rightarrow \text{Hg}(\text{cs}) + \text{LCHLORINE} + \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1008	StTrHetBrHg	$\text{BrHgOBr} \rightarrow \text{Hg}(\text{cs}) + 2 \text{LBROMINE}$	<code>khet_Tr(iht_RGM) + khet_St(ihs_RGM)</code>	see general notes*
HET1009	StTrHetBrClHg	$\text{ClHgOBr} \rightarrow \text{Hg}(\text{cs}) + \text{LCHLORINE} + \text{LBROMINE}$	<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
EQ2100_a01	TrAa01Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ2101_a01	TrAa01MblScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716	Chameides (1984)
EQ2102_a01	TrAa01Sc	$\text{HO}_3 \rightleftharpoons \text{O}_3^- + \text{H}^+$	4.4E-9		Staehelin et al. (1984)
EQ3200_a01	TrAa01MblScScmN	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391	Chameides (1984)
EQ3201_a01	TrAa01ScN	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ3202_a01	TrAa01MblScScmN	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700	Davis and de Bruin (1964)
EQ3203_a01	TrAa01ScN	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5		Warneck (1999)
EQ4100_a01	TrAa01MblScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913	Chameides (1984)*
EQ4101_a01	TrAa01ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4		Weast (1980)
EQ4150_a01	TrAa01Sc	$\text{HCHO} \rightleftharpoons \text{HOCH}_2\text{OH}$	4.11E-3	-3769	see note*
EQ4151_a01	TrAa01Sc	$\text{HCO}_3 \rightleftharpoons \text{HCOHOHO}_2$	1.08E1	-2936	see note*
EQ4200_a01	TrAa01ScScmC	$\text{CH}_3\text{COOH} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COO}^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4201_a01	TrAa01C	$\text{CH}_3\text{C(O)OOH} \rightleftharpoons \text{CH}_3\text{COOO}^- + \text{H}^+$	6.3E-9		Schuchmann and von Sonntag (1988)
EQ4202_a01	TrAa01C	$\text{HOCH}_2\text{CO}_3\text{H} \rightleftharpoons \text{CH}_2\text{OHCO}_2\text{O}^- + \text{H}^+$	6.3E-9		Schuchmann and von Sonntag (1988)*
EQ4203_a01	TrAa01C	$\text{HOCCOOH} \rightleftharpoons \text{H}^+ + \text{HOCCOO}^-$	5.6E-2		Martell (1977)
EQ4204_a01	TrAa01C	$\text{HOCCOO}^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	5.4E-5		Martell (1977)
EQ4205_a01	TrAa01C	$\text{HOCH}_2\text{CO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OOHCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4206_a01	TrAa01C	$\text{CH}_2\text{OOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OOCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4207_a01	TrAa01C	$\text{CHOOHOOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CHOOHOOCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4208_a01	TrAa01C	$\text{HOCH}_2\text{CO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OHCO}_2^-$	1.5E-4		Rumble (2020)
EQ4209_a01	TrAa01C	$\text{CHOHOOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CHOHOOCO}_2^-$	1.5E-4		Rumble (2020)*
EQ4210_a01	TrAa01C	$\text{CHOCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CHOCO}_2^-$	1.754E-5		Fisher and Barnes (1972)
EQ4211_a01	TrAa01C	$\text{COOHCO}_3 \rightleftharpoons \text{H}^+ + \text{CO}_2^- \text{CO}_3$	1.754E-5		Fisher and Barnes (1972)
EQ4250_a01	TrAa01ScC	$\text{CH}_3\text{CHO} \rightleftharpoons \text{CH}_3\text{CHOHOH}$	1.22		Tur'yan (2000)
EQ4251_a01	TrAa01C	$\text{CHOHOOCO}_2\text{H} \rightleftharpoons \text{CHOHOOCO}_2^- + \text{H}^+$	1.57E1		see note*
EQ4252_a01	TrAa01C	$\text{CH}_2\text{OHCHO} \rightleftharpoons \text{CH}_2\text{OHCHOHOH}$	1.56E1		Doussin and Monod (2013)
EQ4253_a01	TrAa01C	$\text{GLYOX} \rightleftharpoons \text{CHOCHOHOH}$	3.5E2		Ervens and Volkamer (2010)
EQ4254_a01	TrAa01C	$\text{CHOCHOHOH} \rightleftharpoons \text{CHOHOHCHOHOH}$	2.0E2		Ervens and Volkamer (2010)
EQ4255_a01	TrAa01C	$\text{CHOCO}_2\text{H} \rightleftharpoons \text{CHOOHOHCO}_2\text{H}$	1.1E3		Doussin and Monod (2013)
EQ4256_a01	TrAa01C	$\text{CHOCO}_2^- \rightleftharpoons \text{CHOHOHCO}_2^-$	6.6E1		Doussin and Monod (2013)
EQ4257_a01	TrAa01C	$\text{CO}_2^- \text{CO}_3 \rightleftharpoons \text{CO}_2^- \text{COHOHO}_2$	6.6E1		see note*
EQ4258_a01	TrAa01C	$\text{CH}_2\text{OOHCHO} \rightleftharpoons \text{HOCH}_2\text{CHOHOH}$	1.56E1		see note*
EQ4300_a01	TrAa01C	$\text{CH}_3\text{COCO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COCO}_2^-$	4.1E-3		Rumble (2020)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ4350_a01	TrAa01C	$\text{CH}_3\text{C}(\text{O})\text{CHO} \rightleftharpoons \text{CH}_3\text{COCHOHOH}$	1.98E3		Doussin and Monod (2013)
EQ6000_a01	TrAa01Cl	$\text{Cl}_2^- \rightleftharpoons \text{Cl} + \text{Cl}^-$	7.3E-6		Yu (2004)
EQ6200_a01	TrAa01MblScScmCl	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ6201_a01	TrAa01ScCl	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8		Lax (1969)
EQ7000_a01	TrAa01Br	$\text{Br}_2^- \rightleftharpoons \text{Br} + \text{Br}^-$	2.54E-6	-2256	Liu et al. (2002)
EQ7200_a01	TrAa01MblScScmBr	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9		Lax (1969)
EQ7201_a01	TrAa01ScBr	$\text{HOBr} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ7600_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Cl}^- \rightleftharpoons \text{BrCl}_2^-$	3.8	1191	Wang et al. (1994)
EQ7601_a01	TrAa01MblBrCl	$\text{BrCl} + \text{Br}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.8E4	7457	Wang et al. (1994)
EQ7602_a01	TrAa01MblBrCl	$\text{Br}_2 + \text{Cl}^- \rightleftharpoons \text{Br}_2\text{Cl}^-$	1.3	0	Wang et al. (1994)
EQ7603_a01	TrAa01MblBrCl	$\text{Br}^- + \text{Cl}_2 \rightleftharpoons \text{BrCl}_2^-$	4.2E6	14072	Wang et al. (1994)
EQ8600_a01	TrAa01MblScClI	$\text{ICl} + \text{Cl}^- \rightleftharpoons \text{ICl}_2^-$	7.7E1		Wang et al. (1989)
EQ8700_a01	TrAa01MblScBrI	$\text{IBr} + \text{Br}^- \rightleftharpoons \text{IBr}_2^-$	2.9E2		Troy and Margerum (1991)
EQ8701_a01	TrAa01MblScBrClI	$\text{ICl} + \text{Br}^- \rightleftharpoons \text{IBr} + \text{Cl}^-$	3.3E2		see note*
EQ9200_a01	TrAa01MblScScmS	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090	Chameides (1984)
EQ9201_a01	TrAa01MblScScmS	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ9202_a01	TrAa01MblScScmS	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ9203_a01	TrAa01MblScScmS	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ10200_a01	TrAa01Hg	$\text{Hg}^{2+} + \text{OH}^- \rightleftharpoons \text{HgOH}^+$	4.0E10		Ammann and Pöschl (2007)
EQ10201_a01	TrAa01Hg	$\text{HgOH}^+ + \text{OH}^- \rightleftharpoons \text{Hg}(\text{OH})_2$	1.58E11		Ammann and Pöschl (2007)
EQ10600_a01	TrAa01ClHg	$\text{Hg}^{2+} + \text{Cl}^- \rightleftharpoons \text{HgCl}^+$	5.8E6		Ammann and Pöschl (2007)
EQ10601_a01	TrAa01ClHg	$\text{HgCl}^+ + \text{Cl}^- \rightleftharpoons \text{HgCl}_2$	2.5E6		Ammann and Pöschl (2007)
EQ10602_a01	TrAa01ClHg	$\text{HgOH}^+ + \text{Cl}^- \rightleftharpoons \text{Hg}(\text{OH})\text{Cl}$	2.69E7		Ammann and Pöschl (2007)
EQ10700_a01	TrAa01BrHg	$\text{Hg}^{2+} + \text{Br}^- \rightleftharpoons \text{HgBr}^+$	1.1E9		Raofie and Ariya (2004)
EQ10701_a01	TrAa01BrHg	$\text{HgBr}^+ + \text{Br}^- \rightleftharpoons \text{HgBr}_2$	2.5E8		Raofie and Ariya (2004)
EQ10800_a01	TrAa01HgS	$\text{Hg}^{2+} + \text{SO}_3^{2-} \rightleftharpoons \text{HgSO}_3$	2.E13		van Loon et al. (2001)
EQ10801_a01	TrAa01HgS	$\text{HgSO}_3 + \text{SO}_3^{2-} \rightleftharpoons \text{Hg}(\text{SO}_3)_2^{2-}$	1.E10		van Loon et al. (2001)
EQ11200_a01	TrAa01Fe	$\text{Fe}^{3+} \rightleftharpoons \text{FeOH}^{2+} + \text{H}^+$	2.34E-3		de Laat and Le (2006)*
EQ11201_a01	TrAa01Fe	$\text{FeOH}^{2+} \rightleftharpoons \text{Fe}(\text{OH})_2^+ + \text{H}^+$	2E-4		de Laat and Le (2006)*
EQ11202_a01	TrAa01Fe	$\text{Fe}^{3+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{FeHO}_2^{2+} + \text{H}^+$	3.1E-3		de Laat and Le (2006)
EQ11203_a01	TrAa01Fe	$\text{FeOH}^{2+} + \text{H}_2\text{O}_2 \rightleftharpoons \text{Fe}(\text{OH})(\text{HO}_2)^+ + \text{H}^+$	2E-4		de Laat and Le (2006)
EQ11600_a01	TrAa01ClFe	$\text{Fe}^{3+} + \text{Cl}^- \rightleftharpoons \text{FeCl}^{2+}$	6.61		de Laat and Le (2006)*
EQ11601_a01	TrAa01ClFe	$\text{FeCl}^{2+} + \text{Cl}^- \rightleftharpoons \text{FeCl}_2^+$	1.6		de Laat and Le (2006)*
EQ11800_a01	TrAa01FeS	$\text{Fe}^{3+} + \text{SO}_4^{2-} \rightleftharpoons \text{FeSO}_4^+$	120		Brand and van Eldik (1995)*

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ11801_a01	TrAa01FeS	$\text{FeOH}^{2+} + \text{HSO}_3^- \rightleftharpoons \text{FeSO}_3^+$	8.25E2		Warneck (2018)*
EQ11802_a01	TrAa01FeS	$\text{Fe}^{2+} + \text{SO}_3^- \rightleftharpoons \text{FeSO}_3^+$	1.6E7		Warneck (2018)

Specific notes

EQ4100_a01: For $pK_a(\text{CO}_2)$, see also Dickson and Millero (1987).

EQ4150_a01: Hydration from Winkelman et al. (2000) and dehydration from Winkelman et al. (2002). Bell and Evans (1966) found that acid catalysis is negligible.

EQ4151_a01: Assumed to be the same as for HCHO.

EQ4200_a01: The pK_A has a minimum near 298 K, the temperature dependence is therefore small.

EQ4202_a01: Same as for $\text{CH}_3\text{CO}_3\text{H}$.

EQ4205_a01: Same as for $\text{CH}_3\text{CO}_2\text{H}$.

EQ4206_a01: Same as for $\text{CH}_3\text{CO}_2\text{H}$.

EQ4207_a01: Same as for $\text{CH}_3\text{CO}_2\text{H}$.

EQ4209_a01: Same as $\text{HOCH}_2\text{CO}_2\text{H}$.

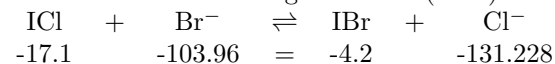
EQ4251_a01: Calculated as $K_{\text{eq}} * k(\text{dehydration})$ where dehydration is assumed to be the same as for acetaldehyde.

EQ4257_a01: Assumed to be equal to CHOCO_2m .

EQ4258_a01: Same as for HOCH_2CHO .

EQ7201_a01: For $pK_a(\text{HOBr})$, see also Keller-Rudek et al. (1992).

EQ8701_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.

EQ11200_a01: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11201_a01: Equilibrium calculated from K_1 and K_2 in Tab. 1 of de Laat and Le (2006). k for back reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11600_a01: See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11601_a01: Equilibrium calculated from K_{29} and K_{30} in Tab. 2 of de Laat and Le (2006). k for forward reaction assumed. See also K values listed in Tab. 2.5 of Brand and van Eldik (1995).

EQ11800_a01: Equilibrium at $I = 1$ M. k for back reaction assumed.

EQ11801_a01: Rate of equilibration assumed.

Table 6: Aqueous phase reactions

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A10000_a01	TrAa01Sc	$O_3 + O_2^- \rightarrow O_3^- + O_2$	1.50E9		Staehelin et al. (1984)
A21000_a01	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A21001_a01	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A21002_a01	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A21003_a01	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A21004_a01	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A21005_a01	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A21006_a01	TrAa01Sc	$O_3 + OH \rightarrow HO_4$	1.10E8		Staehelin et al. (1984)
A21007_a01	TrAa01Sc	$O_3 + OH^- \rightarrow HO_2 + O_2^-$	7.00E1		Staehelin et al. (1984)
A21008_a01	TrAa01Sc	$HO_3 \rightarrow OH + O_2$	1.10E5		Staehelin et al. (1984)
A21009_a01	TrAa01Sc	$HO_4 \rightarrow HO_2 + O_2$	2.80E4		Staehelin et al. (1984)
A21010_a01	TrAa01Sc	$HO_4 + HO_4 \rightarrow H_2O_2 + 2 O_3$	5.00E9		Staehelin et al. (1984)
A21011_a01	TrAa01Sc	$HO_4 + HO_3 \rightarrow H_2O_2 + O_3 + O_2$	5.00E9		Staehelin et al. (1984)
A31000_a01	TrAa01ScN	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A31001_a01	TrAa01ScN	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A31002_a01	TrAa01ScN	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A32000_a01	TrAa01ScN	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A32001_a01	TrAa01ScN	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A32002_a01	TrAa01ScN	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A32003_a01	TrAa01ScN	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A32004_a01	TrAa01ScN	$HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$	4.6E3	-6800	Damschen and Martin (1983)
A41000_a01	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A41001_a01	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A41002_a01	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2 HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A41003_a01	TrAa01Sc	$HCOO^- + OH \rightarrow O_2^- + H_2O + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A41004_a01	TrAa01ScN	$HCOO^- + NO_3 \rightarrow NO_3^- + H^+ + O_2^- + CO_2$	5.1E7	-2200	Exner et al. (1994)*
A41005_a01	TrAa01Sc	$HCOO^- + O_3 \rightarrow OH + O_2^- + CO_2$	1.00E2		Hoigné and Bader (1983)
A41006_a01	TrAa01Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6		Ross et al. (1992)
A41007_a01	TrAa01Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020	Chin and Wine (1994)
A41008_a01	TrAa01Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991	Chin and Wine (1994)
A41009_a01	TrAa01ScN	$HCOOH + NO_3 \rightarrow NO_3^- + H^+ + HO_2 + CO_2$	3.8E5	-3400	Exner et al. (1994)*
A41010_a01	TrAa01Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5		Jacob (1986)
A41011_a01	TrAa01Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7		Jacob (1986)
A41012a_a01	TrAa01Sc	$CH_3OO + CH_3OO \rightarrow 2 HCHO + H_2O_2$	$0.20 \times 1.96E8$	-2165	Herrmann et al. (1999b)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A41012b_a01	TrAa01Sc	$CH_3OO + CH_3OO \rightarrow 2 HOCH_2O_2$	$0.80 \times 1.96E8$	-2165	Herrmann et al. (1999b)*
A41013a_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HOCH_2O_2 + H_2O$	$0.93 \times 9.70E8$	-600	Elliot and McCracken (1989)*
A41013b_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2 + H_2O$	$0.07 \times 9.70E8$	-600	Elliot and McCracken (1989)
A41014_a01	TrAa01ScN	$CH_3OH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$	5.40E5	-4300	Ervens et al. (2003a)
A41015_a01	TrAa01Sc	$CH_3OH + CO_3^- \rightarrow HOCH_2O_2 + HCO_3^-$	5.8E3	-3079	Clifton and Huie (1993)
A41016a_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow CH_3OO + H_2O$	$0.25 \times 6.30E8$		Monod et al. (2007)*
A41016b_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH + H_2O$	$0.75 \times 6.30E8$		Monod et al. (2007)*
A41017a_a01	TrAa01ScN	$CH_3OOH + NO_3 \rightarrow CH_3OO + NO_3^- + H^+$	$0.25 \times 4.90E6$	-2000	see note*
A41017b_a01	TrAa01ScN	$CH_3OOH + NO_3 \rightarrow HCHO + HO_2 + NO_3^- + H^+$	$0.75 \times 4.90E6$	-2000	see note*
A41018a_a01	TrAa01Sc	$CH_3OOH + CO_3^- \rightarrow CH_3OO + HCO_3^-$	$0.25 \times 4.30E5$		see note*
A41018b_a01	TrAa01Sc	$CH_3OOH + CO_3^- \rightarrow HCHO + HO_2 + HCO_3^-$	$0.75 \times 4.30E5$		see note*
A41019a_a01	TrAa01	$HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$	$0.25 \times 6.30E8$		see note*
A41019b_a01	TrAa01	$HOCH_2OOH + OH \rightarrow CHOOOH + HO_2 + H_2O$	$0.75 \times 6.30E8$		see note*
A41020a_a01	TrAa01N	$HOCH_2OOH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$	$0.25 \times 4.90E6$	-2000	see note*
A41020b_a01	TrAa01N	$HOCH_2OOH + NO_3 \rightarrow CHOOOH + HO_2 + NO_3^- + H^+$	$0.75 \times 4.90E6$	-2000	see note*
A41021_a01	TrAa01Sc	$HOCH_2O_2 \rightarrow HCHO + HO_2$	1.00E1		see note*
A41022_a01	TrAa01Sc	$HOCH_2O_2 + HO_2 \rightarrow HOCH_2OOH + O_2$	9.7E5	-2500	see note*
A41023_a01	TrAa01Sc	$HOCH_2O_2 + O_2^- \rightarrow HOCH_2OOH + O_2 + OH^-$	1.0E8	-900	see note*
A41024_a01	TrAa01Sc	$HOCH_2O_2 + HOCH_2O_2 \rightarrow 2 HCOOH + H_2O_2$	7.4E8	-1395	Huie and Clifton (1993)
A41025_a01	TrAa01Sc	$HCOOH + H_2O_2 + H^+ \rightarrow CHOOOH + H_2O + H^+$	3.1E-4	-5235	De Filippis et al. (2009)
A41026a_a01	TrAa01Sc	$CHOOOH + H^+ \rightarrow HCOOH + H_2O_2 + H^+$	3.8E-4	-5235	De Filippis et al. (2009)
A41026b_a01	TrAa01Sc	$CHOOOH + H^+ \rightarrow CO_2 + H_2O + H^+$	1.2E-3	-8735	De Filippis et al. (2009)
A41027_a01	TrAa01Sc	$HOCH_2OH + OH \rightarrow HCOHOHO_2 + H_2O$	7.70E8	-1000	Chin and Wine (1994)
A41028_a01	TrAa01Sc	$HOCH_2OH + CO_3^- \rightarrow HCO_3^- + HCOHOHO_2$	1.30E4		Zellner et al. (1996)
A41029_a01	TrAa01ScN	$HOCH_2OH + NO_3 \rightarrow NO_3^- + H^+ + HCOHOHO_2$	1.0E6	-4500	Exner et al. (1993)
A41030_a01	TrAa01Sc	$HCOHOHO_2 \rightarrow HCOOH + HO_2$	1.00E6		see note*
A42000a_a01	TrAa01C	$CH_3CH_2OH + OH \rightarrow CH_3CHO + HO_2 + H_2O$	$0.90 \times 2.1E9$	-830	Monod et al. (2005)*
A42000b_a01	TrAa01C	$CH_3CH_2OH + OH \rightarrow CH_2OHCH_2OO + H_2O$	$0.10 \times 2.1E9$	-830	Monod et al. (2005)
A42001a_a01	TrAa01CN	$CH_3CH_2OH + NO_3 \rightarrow CH_3CHO + HO_2 + NO_3^- + H^+$	$0.90 \times 2.2E6$	-3300	Ervens et al. (2003a)*
A42001b_a01	TrAa01CN	$CH_3CH_2OH + NO_3 \rightarrow CH_2OHCH_2OO + NO_3^- + H^+$	$0.10 \times 2.2E6$	-3300	Ervens et al. (2003a)
A42002a_a01	TrAa01C	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow CH_2OHCHO + CH_2OHCHO + H_2O_2$	$0.50 \times 1.00E8$		Piesiak et al. (1984)

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A42002b_a01	TrAa01C	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow CH_2OHCHO + ETHGLY$	$0.33 \times 1.00E8$		Piesiak et al. (1984)
A42002c_a01	TrAa01C	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow 2 HOCH_2O_2 + 2 HCHO$	$0.17 \times 1.00E8$		Piesiak et al. (1984)
A42003_a01	TrAa01C	$CH_2OHCH_2OO + O_2^- \rightarrow HYETHO2H + OH^-$	1.0E8	-900	see note*
A42004_a01	TrAa01C	$CH_2OHCH_2OO + HO_2 \rightarrow HYETHO2H$	9.7E5	-2500	see note*
A42005_a01	TrAa01C	$HYETHO2H + OH \rightarrow CH_2OHCHO$	1.10E9		see note*
A42006_a01	TrAa01C	$ETHGLY + OH \rightarrow CH_2OHCHO + HO_2 + H_2O$	1.7E9	-1191	Hoffmann et al. (2009)*
A42007_a01	TrAa01CN	$ETHGLY + NO_3 \rightarrow CH_2OHCHO + HO_2 + NO_3^- + H^+$	5.8E6	-2117	Hoffmann et al. (2009)*
A42008_a01	TrAa01C	$CH_3CHO + OH \rightarrow CH_3COOO + H_2O$	3.60E9		Schuchmann and von Sonntag (1988)
A42009_a01	TrAa01CN	$CH_3CHO + NO_3 \rightarrow CH_3COOO + NO_3^- + H^+$	3.10E6		Rousse and George (2004)
A42010_a01	TrAa01C	$CH_3COOO + CH_3COOO \rightarrow CH_3OO + CH_3OO + CO_2 + CO_2$	1.9E8	1563	see note*
A42011_a01	TrAa01C	$CH_3COOO + O_2^- \rightarrow CH_3COOO^- + O_2$	1.00E9		Schuchmann and von Sonntag (1988)
A42012_a01	TrAa01C	$CH_3CHOHOH + OH \rightarrow CH_3COHOHOHOO + H_2O$	1.20E9		Schuchmann and von Sonntag (1988)
A42013_a01	TrAa01CN	$CH_3CHOHOH + NO_3 \rightarrow CH_3COHOHOHOO + NO_3^- + H^+$	1.10E6		Rousse and George (2004)
A42014_a01	TrAa01C	$CH_3COHOHOHOO \rightarrow CH_3COOH + HO_2$	1.00E6		see note*
A42015a_a01	TrAa01C	$CH_2OHCHO + OH \rightarrow CH_2OHCO_3 + H_2O$	$0.77 \times 1.40E9$		Doussin and Monod (2013)
A42015b_a01	TrAa01C	$CH_2OHCHO + OH \rightarrow CHOHOOCOCHO + H_2O$	$0.23 \times 1.40E9$		Doussin and Monod (2013)
A42016a_a01	TrAa01CN	$CH_2OHCHO + NO_3 \rightarrow CH_2OHCO_3 + NO_3^- + H^+$	$0.77 \times 3.10E6$		see note*
A42016b_a01	TrAa01CN	$CH_2OHCHO + NO_3 \rightarrow CHOHOOCOCHO + NO_3^- + H^+$	$0.23 \times 3.10E6$		see note*
A42017_a01	TrAa01C	$CH_2OHCO_3 + O_2^- \rightarrow CH_2OHCO_2O^-$	1.00E9		see note*
A42018_a01	TrAa01C	$CH_2OHCOHOHO_2 \rightarrow HOCH_2CO_2H + HO_2$	1.00E6		see note*
A42019_a01	TrAa01C	$CHOHOOCOCHO \rightarrow GLYOX + HO_2$	1.90E2		see note*
A42020_a01	TrAa01C	$CHOHOOCOHOHOH \rightarrow CHOCHOHOH + HO_2$	1.90E2		see note*
A42021a_a01	TrAa01C	$CH_2OHCHOHOH + OH \rightarrow CH_2OHCOHOHO_2 + H_2O$	$0.33 \times 1.10E9$		Doussin and Monod (2013)
A42021b_a01	TrAa01C	$CH_2OHCHOHOH + OH \rightarrow CHOHOOCOHOHOH + H_2O$	$0.28 \times 1.10E9$		Doussin and Monod (2013)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42021c_a01	TrAa01C	$\text{CH}_2\text{OHCHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.39 \times 1.10\text{E9}$		Doussin and Monod (2013)
A42022a_a01	TrAa01CN	$\text{CH}_2\text{OHCHOHOH} + \text{NO}_3 \rightarrow \text{CH}_2\text{OHCOHOHO}_2 + \text{NO}_3^- + \text{H}^+$	$0.33 \times 1.10\text{E6}$		see note*
A42022b_a01	TrAa01CN	$\text{CH}_2\text{OHCHOHOH} + \text{NO}_3 \rightarrow \text{CHOHOOCOHOHOH} + \text{NO}_3^- + \text{H}^+$	$0.28 \times 1.10\text{E6}$		see note*
A42022c_a01	TrAa01CN	$\text{CH}_2\text{OHCHOHOH} + \text{NO}_3 \rightarrow \text{HCOOH} + \text{HOCH}_2\text{O}_2 + \text{NO}_3^- + \text{H}^+$	$0.39 \times 1.10\text{E6}$		see note*
A42023a_a01	TrAa01C	$\text{CHOHOHCHOHOH} + \text{OH} \rightarrow \text{CHOHOHCOHOHO}_2 + \text{H}_2\text{O}$	$0.27 \times 1.1\text{E9}$	-1516	Buxton et al. (1997)
A42023b_a01	TrAa01C	$\text{CHOHOHCHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HCOHOHO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$0.73 \times 1.1\text{E9}$	-1516	Buxton et al. (1997)*
A42024a_a01	TrAa01CN	$\text{CHOHOHCHOHOH} + \text{NO}_3 \rightarrow \text{CHOHOHCOHOHO}_2 + \text{NO}_3^- + \text{H}^+$	$0.27 \times 1.00\text{E6}$		see note*
A42024b_a01	TrAa01CN	$\text{CHOHOHCHOHOH} + \text{NO}_3 \rightarrow \text{HCOOH} + \text{HCOHOHO}_2 + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	$0.73 \times 1.00\text{E6}$		see note*
A42025_a01	TrAa01C	$\text{CHOHOHCOHOHO}_2 \rightarrow \text{CHOOHOHCOOH} + \text{HO}_2$	$0.77 \times 1.00\text{E6}$		see note*
A42026_a01	TrAa01C	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_2\text{OOCOOH} + \text{H}_2\text{O}$	1.50E7	-1330	Chin and Wine (1994)
A42027_a01	TrAa01CN	$\text{CH}_3\text{COOH} + \text{NO}_3 \rightarrow \text{CH}_2\text{OOCOOH} + \text{NO}_3^- + \text{H}^+$	1.4E4	-3800	Exner et al. (1994)*
A42028_a01	TrAa01C	$\text{CH}_3\text{COO}^- + \text{OH} \rightarrow \text{CH}_2\text{OOCO}_2^- + \text{H}_2\text{O}$	1.00E8	-1800	Fisher and Hamill (1973)
A42029_a01	TrAa01CN	$\text{CH}_3\text{COO}^- + \text{NO}_3 \rightarrow \text{CH}_2\text{OOCO}_2^- + \text{NO}_3^- + \text{H}^+$	2.9E6	-3800	Exner et al. (1994)*
A42030a_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{OO} + \text{H}_2\text{O}$	$0.80 \times 5.80\text{E8}$		Monod et al. (2007)
A42030b_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{HO}_2 + \text{H}_2\text{O}$	$0.20 \times 5.80\text{E8}$		Monod et al. (2007)*
A42031a_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OO} + \text{C}_2\text{H}_5\text{OO} \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CHO} + \text{H}_2\text{O}_2$	$0.20 \times 1.9\text{E8}$	1563	Herrmann et al. (1999b)*
A42031b_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OO} + \text{C}_2\text{H}_5\text{OO} \rightarrow 2 \text{CH}_3\text{CHO} + 2 \text{HO}_2$	$0.80 \times 1.9\text{E8}$	1563	Herrmann et al. (1999b)*
A42032_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OO} + \text{O}_2^- \rightarrow \text{C}_2\text{H}_5\text{OOH} + \text{OH}^-$	1.0E8	-900	see note*
A42033_a01	TrAa01C	$\text{C}_2\text{H}_5\text{OO} + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	9.7E5	-2500	see note*
A42034_a01	TrAa01C	$\text{CH}_2\text{OOCOOH} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	9.7E5	-2500	see note*
A42035_a01	TrAa01C	$\text{CH}_2\text{OOCOOH} + \text{O}_2^- + \text{H}^+ \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	1.0E8	-900	see note*
A42036a_a01	TrAa01C	$\text{CH}_2\text{OOCOOH} + \text{CH}_2\text{OOCOOH} \rightarrow \text{CHOCOOH} + \text{CHOCOOH} + \text{H}_2\text{O}_2$	$0.30 \times 7.50\text{E7}$		Schuchmann et al. (1985)
A42036b_a01	TrAa01C	$\text{CH}_2\text{OOCOOH} + \text{CH}_2\text{OOCOOH} \rightarrow 2 \text{HCHO} + 2 \text{CO}_2 + \text{H}_2\text{O}_2$	$0.30 \times 7.50\text{E7}$		Schuchmann et al. (1985)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42036c_a01	TrAa01C	$CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOCOOH + HOCH_2CO_2H$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42036d_a01	TrAa01C	$CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOHOOCOOH + CHOHOOCOOH$	$0.10 \times 7.50E7$		Schuchmann et al. (1985)
A42037_a01	TrAa01C	$CH_2OOCO_2^- + HO_2 \rightarrow CH_2OOHCO_2^- + O_2$	9.7E5	-2500	see note*
A42038_a01	TrAa01C	$CH_2OOCO_2^- + O_2^- + H^+ \rightarrow CH_2OOHCO_2^-$	1.0E8	-900	see note*
A42039a_a01	TrAa01C	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CHOCOO^- + H_2O_2$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039b_a01	TrAa01C	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2 HCHO + 2 CO_2 + H_2O_2 + 2 OH^-$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039c_a01	TrAa01C	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CH_2OHCO_2^-$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039d_a01	TrAa01C	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2 CHOHOOCOO_2^-$	$0.10 \times 7.50E7$		Schuchmann et al. (1985)
A42040_a01	TrAa01C	$CH_2OOCO_2^- + O_3 \rightarrow O_3^- + HOCH_2OOH + CO_2$	2.00E9		Sehested et al. (1984)
A42141_a01	TrAa01C	$HOCCOO^- + OH \rightarrow C_2O_4^- + H_2O$	2.3E8	-2766	Ervens et al. (2003b)*
A42142_a01	TrAa01C	$C_2O_4^{2-} + OH \rightarrow C_2O_4^- + OH^-$	2.25E8	-4330	Ervens et al. (2003b)*
A42143_a01	TrAa01C	$C_2O_4^- + O_2 \rightarrow 2 CO_2 + O_2^-$	2.40E9		Hislop and Bolton (1999)
A42144a_a01	TrAa01C	$HOCH_2CO_2H + OH \rightarrow CH_2OOCOOH + H_2O$	$0.80 \times 5.80E8$		see note*
A42144b_a01	TrAa01C	$HOCH_2CO_2H + OH \rightarrow CHOOHOOCOOH + H_2O$	$0.20 \times 5.80E8$		see note*
A42145a_a01	TrAa01CN	$HOCH_2CO_2H + NO_3 \rightarrow CH_2OOCOOH + NO_3^- + H^+$	$0.80 \times 1.70E6$		Herrmann et al. (2005)
A42145b_a01	TrAa01CN	$HOCH_2CO_2H + NO_3 \rightarrow CHOOHOOCOOH + NO_3^- + H^+$	$0.20 \times 1.70E6$		Herrmann et al. (2005)
A42146a_a01	TrAa01C	$CH_2OOHCO_2^- + OH \rightarrow CH_2OOCO_2^- + H_2O$	$0.80 \times 5.80E8$		see note*
A42146b_a01	TrAa01C	$CH_2OOHCO_2^- + OH \rightarrow CHOOHOOCO_2^- + H_2O$	$0.20 \times 5.80E8$		see note*
A42147a_a01	TrAa01CN	$CH_2OOHCO_2^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$	$0.80 \times 7.10E6$		Herrmann et al. (2005)
A42147b_a01	TrAa01CN	$CH_2OOHCO_2^- + NO_3 \rightarrow CHOOHOOCO_2^- + NO_3^- + H^+$	$0.20 \times 7.10E6$		Herrmann et al. (2005)
A42148_a01	TrAa01C	$CHOOHOOCOOH \rightarrow HOCCOOH + HO_2$	1.90E2		see note*
A42149_a01	TrAa01C	$CHOOHOOCO_2^- \rightarrow HOCCOO^- + HO_2$	1.90E2		see note*
A42150a_a01	TrAa01C	$HOCH_2CO_2H + OH \rightarrow CHOHOOCOOH + H_2O$	$0.62 \times 6.00E8$		see note*
A42150b_a01	TrAa01C	$HOCH_2CO_2H + OH \rightarrow HCHO + CO_2 + HO_2 + H_2O$	$0.38 \times 6.00E8$		see note*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42151a_a01	TrAa01CN	$\text{HOCH}_2\text{CO}_2\text{H} + \text{NO}_3 \rightarrow \text{CHOHOOCOOH} + \text{NO}_3^- + \text{H}^+$	$0.62 \times 7.4\text{E}5$	-3969	Gaillard de Sémainville et al. (2007)*
A42151b_a01	TrAa01CN	$\text{HOCH}_2\text{CO}_2\text{H} + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	$0.38 \times 7.4\text{E}5$	-3969	Gaillard de Sémainville et al. (2007)*
A42152_a01	TrAa01C	$\text{CHOHOOCOOH} \rightarrow \text{CHOCOOH} + \text{HO}_2$	1.90E2		von Sonntag (1987)
A42153a_a01	TrAa01C	$\text{CH}_2\text{OHCO}_2^- + \text{OH} \rightarrow \text{CHOHOOCOO}_2^- + \text{H}_2\text{O}$	$0.60 \times 8.60\text{E}8$		Buxton et al. (1988)
A42153b_a01	TrAa01C	$\text{CH}_2\text{OHCO}_2^- + \text{OH} \rightarrow \text{HCHO} + \text{CO}_2 + \text{O}_2^- + \text{H}_2\text{O}$	$0.19 \times 8.60\text{E}8$		Buxton et al. (1988)
A42153c_a01	TrAa01C	$\text{CH}_2\text{OHCO}_2^- + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}^-$	$0.21 \times 8.60\text{E}8$		Buxton et al. (1988)
A42154a_a01	TrAa01CN	$\text{CH}_2\text{OHCO}_2^- + \text{NO}_3 \rightarrow \text{CHOHOOCOO}_2^- + \text{NO}_3^- + \text{H}^+$	$0.76 \times 7.5\text{E}6$	-3007	Gaillard de Sémainville et al. (2007)*
A42154b_a01	TrAa01CN	$\text{CH}_2\text{OHCO}_2^- + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{O}_2^- + \text{NO}_3^- + \text{H}^+$	$0.24 \times 7.5\text{E}6$	-3007	Gaillard de Sémainville et al. (2007)*
A42155_a01	TrAa01C	$\text{CHOHOOCOO}_2^- \rightarrow \text{CHOCOO}^- + \text{HO}_2$	1.90E2		von Sonntag (1987)
A42156a_a01	TrAa01C	$\text{CHOOHOHCOOH} + \text{OH} \rightarrow \text{COOHCOHOHO}_2 + \text{H}_2\text{O}$	$0.15 \times 3.2\text{E}8$	-962	Ervens et al. (2003b)*
A42156b_a01	TrAa01C	$\text{CHOOHOHCOOH} + \text{OH} \rightarrow \text{HCOOH} + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$0.85 \times 3.2\text{E}8$	-962	Ervens et al. (2003b)*
A42157a_a01	TrAa01CN	$\text{CHOOHOHCOOH} + \text{NO}_3 \rightarrow \text{COOHCOHOHO}_2 + \text{NO}_3^- + \text{H}^+$	$0.15 \times 1.00\text{E}6$		see note*
A42157b_a01	TrAa01CN	$\text{CHOOHOHCOOH} + \text{NO}_3 \rightarrow \text{HCOOH} + \text{CO}_2 + \text{HO}_2 + \text{NO}_3^- + \text{H}^+$	$0.85 \times 1.00\text{E}6$		see note*
A42158a_a01	TrAa01C	$\text{CHOHOHCO}_2^- + \text{OH} \rightarrow \text{CO}_2^- \text{COHOHO}_2 + \text{H}_2\text{O}$	$0.26 \times 2.9\text{E}9$	-4330	Ervens et al. (2003b)*
A42158b_a01	TrAa01C	$\text{CHOHOHCO}_2^- + \text{OH} \rightarrow \text{HCOOH} + \text{CO}_2 + \text{O}_2^- + \text{H}_2\text{O}$	$0.74 \times 2.9\text{E}9$	-4330	Ervens et al. (2003b)*
A42159a_a01	TrAa01CN	$\text{CHOHOHCO}_2^- + \text{NO}_3 \rightarrow \text{CO}_2^- \text{COHOHO}_2 + \text{NO}_3^- + \text{H}^+$	$0.26 \times 1.80\text{E}5$		Herrmann et al. (2005)
A42159b_a01	TrAa01CN	$\text{CHOHOHCO}_2^- + \text{NO}_3 \rightarrow \text{HCOOH} + \text{CO}_2 + \text{O}_2^- + \text{NO}_3^- + \text{H}^+$	$0.74 \times 1.80\text{E}5$		Herrmann et al. (2005)
A42160_a01	TrAa01C	$\text{CHOHOHCO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{HCOO}^- + \text{CO}_2 + \text{H}_2\text{O} + \text{H}_2\text{O}$	1.10E-1		Schöne and Herrmann (2014)
A42161_a01	TrAa01C	$\text{COOHCOHOHO}_2 \rightarrow \text{HOCCOOH} + \text{HO}_2$	1.00E6		see note*
A42162_a01	TrAa01C	$\text{CO}_2^- \text{COHOHO}_2 \rightarrow \text{HOCCOO}^- + \text{HO}_2$	1.00E6		see note*
A42163a_a01	TrAa01C	$\text{CH}_2\text{OOHCHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH} + \text{H}_2\text{O}$	$0.77 \times 1.40\text{E}9$		see note*
A42163b_a01	TrAa01C	$\text{CH}_2\text{OOHCHO} + \text{OH} \rightarrow \text{GLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$0.23 \times 1.40\text{E}9$		see note*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42164a_a01	TrAa01CN	$CH_2OOHCHO + NO_3 \rightarrow HCHO + CO + NO_3 + H_2O$	$0.77 \times 3.10E6$		see note*
A42164b_a01	TrAa01CN	$CH_2OOHCHO + NO_3 \rightarrow GLYOX + NO_3^- + H_2O + H^+$	$0.23 \times 3.10E6$		see note*
A42165a_a01	TrAa01C	$HOOCH_2CHOHOH + OH \rightarrow HOOCH_2CO_2H + HO_2 + H_2O$	$0.33 \times 1.10E9$		see note*
A42165b_a01	TrAa01C	$HOOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + OH + H_2O$	$0.28 \times 1.10E9$		see note*
A42165c_a01	TrAa01C	$HOOCH_2CHOHOH + OH \rightarrow HCOOH + HCHO + OH + H_2O$	$0.39 \times 1.10E9$		see note*
A42166a_a01	TrAa01CN	$HOOCH_2CHOHOH + NO_3 \rightarrow HOOCH_2CO_2H + NO_3^- + H_2O + H^+$	$0.33 \times 1.10E6$		see note*
A42166b_a01	TrAa01CN	$HOOCH_2CHOHOH + NO_3 \rightarrow CHOCHOHOH + NO_3 + H_2O$	$0.28 \times 1.10E6$		see note*
A42166c_a01	TrAa01CN	$HOOCH_2CHOHOH + NO_3 \rightarrow HCOOH + HCHO + NO_3 + H_2O$	$0.39 \times 1.10E6$		see note*
A42167_a01	TrAa01ScC	$HOCH_2OH + HOCH_2OH \rightarrow MG2 + H_2O$	see note	see note	Hahnenstein et al. (1995)*
A42168_a01	TrAa01C	$MG2 + H_2O \rightarrow HOCH_2OH + HOCH_2OH$	see note	see note	Hahnenstein et al. (1995)
A42169_a01	TrAa01C	$MG2 + OH \rightarrow HMF + HO_2$	1.54E9	-1000	see note*
A42470_a01	TrAa01C	$CH_3COOO + H_2O \rightarrow CH_3COOH + HO_2$	7.0E5		Villalta et al. (1996)
A42471_a01	TrAa01C	$CH_2OHCO_3 + H_2O \rightarrow HOCH_2CO_2H + HO_2$	7.0E5		see note*
A42472_a01	TrAa01C	$CHOCO_3 + H_2O \rightarrow CHOCO_2H + HO_2$	7.0E5		see note*
A42473_a01	TrAa01C	$COOHCO_3 + H_2O \rightarrow HOCCOOH + HO_2$	7.0E5		see note*
A43000a_a01	TrAa01C	$CH_3COCHOHOH + OH \rightarrow CH_3COCO_2H + HO_2$	$0.29 \times 9.2E8$	-1235	Schaefer et al. (2015)*
A43000b_a01	TrAa01C	$CH_3COCHOHOH + OH \rightarrow HCOOH + CH_3COOO$	$0.71 \times 9.2E8$	-1235	Schaefer et al. (2015)
A43001_a01	TrAa01CN	$CH_3COCHOHOH + NO_3 \rightarrow CH_3COCO_2H + NO_3^- + H^+$	4.5E6	-4213	Schaefer et al. (2015)*
A43002_a01	TrAa01C	$CH_3COCO_2H + OH \rightarrow CH_3COOH + HO_2 + CO_2$	2.6E8	-1804	Schaefer et al. (2012)*
A43003_a01	TrAa01CN	$CH_3COCO_2H + NO_3 \rightarrow CH_3COOH + NO_3^- + CO_2 + H^+$	2.8E6	-1804	Gaillard de Sémainville et al. (2007)*
A43004_a01	TrAa01C	$CH_3COCO_2^- + OH \rightarrow CH_3COO^- + HO_2 + CO_2$	6.2E8	-3007	Schaefer et al. (2012)*
A43005_a01	TrAa01CN	$CH_3COCO_2^- + NO_3 \rightarrow CH_3COO^- + NO_3^- + CO_2 + H^+$	2.3E7	-2887	Gaillard de Sémainville et al. (2007)*
A43006_a01	TrAa01C	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2$	1.80E8		Gligorovski et al. (2009)
A43007_a01	TrAa01CN	$CH_3COCH_3 + NO_3 \rightarrow CH_3COCH_2O_2 + NO_3^- + H^+$	4.4E3	-4332	Herrmann et al. (1994)*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A43008a_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CH}_3\text{C}(\text{O})\text{CHO}$	$0.20 \times 4.00\text{E}8$		Zegota et al. (1986)
A43008b_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow 2.0 \text{ CH}_3\text{C}(\text{O})\text{CHO} + \text{H}_2\text{O}_2$	$0.45 \times 4.00\text{E}8$		Zegota et al. (1986)
A43009c_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow 2.0 \text{ HCHO} + 2.0 \text{ CH}_3\text{COOO}$	$0.15 \times 4.00\text{E}8$		Zegota et al. (1986)
A43009d_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow 2.0 \text{ CH}_3\text{C}(\text{O})\text{CHO} + 2.0 \text{ HO}_2$	$0.20 \times 4.00\text{E}8$		Zegota et al. (1986)
A43010a_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{CH}_3\text{COCHOHO}_2$	$0.85 \times 5.10\text{E}8$		Doussin and Monod (2013)*
A43010b_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{CH}_3\text{COOO}$	$0.15 \times 5.10\text{E}8$		Doussin and Monod (2013)
A43011_a01	TrAa01CN	$\text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHOHO}_2 + \text{NO}_3^- + \text{H}^+$	2.1E7	-1564	Gaillard de Sémerville et al. (2007)*
A43012_a01	TrAa01C	$\text{CH}_3\text{COCHOHO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{CHO} + \text{HO}_2$	1.90E2		von Sonntag (1987)
A43013_a01	TrAa01C	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2$	1.90E9		see note*
A43014_a01	TrAa01CN	$\text{IPROPOL} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_3^- + \text{H}^+ + \text{HO}_2$	3.70E6		see note*
A43015a_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{CHO} + \text{OH}$	1.80E8		see note*
A43015b_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2$	4.70E8		see note*
A43016_a01	TrAa01CN	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3^- + \text{H}^+$	4.50E6		see note*
A43017_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	4.30E5		see note*
A43018_a01	TrAa01C	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{O}_2^- \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{O}_2 + \text{OH}^-$	5.00E7		see note*
A43019a_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{OH}$	9.90E8		see note*
A43019b_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2$	1.80E8		see note*
A43020_a01	TrAa01CN	$\text{iC}_3\text{H}_7\text{OOH} + \text{NO}_3 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{NO}_3^- + \text{H}^+$	4.50E6		see note*
A43021_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	4.30E5		see note*
A43022_a01	TrAa01C	$\text{iC}_3\text{H}_7\text{O}_2 + \text{O}_2^- \rightarrow \text{iC}_3\text{H}_7\text{OOH} + \text{O}_2 + \text{OH}^-$	5.00E7		see note*
A43023_a01	TrAa01C	$\text{HOCH}_2\text{OH} + \text{MG2} \rightarrow \text{MG3} + \text{H}_2\text{O}$	see note	see note	Hahnenstein et al. (1995)*
A43024_a01	TrAa01C	$\text{MG3} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OH} + \text{MG2}$	see note	see note	Hahnenstein et al. (1995)
A43025_a01	TrAa01C	$\text{MG3} + \text{OH} \rightarrow \text{HM2F} + \text{HO}_2$	1.54E9	-1000	see note*
A44000_a01	TrAa01ScC	$\text{MACR} + \text{OH} \rightarrow \text{CH}_2\text{OHCO}_2\text{CH}_3\text{CHO}$	9.9E9	-1203	Schöne et al. (2014)*
A44001_a01	TrAa01ScC	$\text{CH}_2\text{OHCO}_2\text{CH}_3\text{CHO} + \text{CH}_2\text{OHCO}_2\text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{CHO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{O}_2 + \text{HCOHOHO}_2$	4.00E8		see note*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A44002_a01	TrAa01ScC	$MVK + OH \rightarrow CH_3COCHO_2CH_2OH$	7.1E9	-1443	Schöne et al. (2014)*
A44003_a01	TrAa01ScC	$CH_3COCHO_2CH_2OH + CH_3COCHO_2CH_2OH \rightarrow$ 1.1 BIACETOH + .8 LCARBON + .35 CH_2OHCHO + .35 $CH_3C(O)CHO$ + .35 $HOCH_2O_2$ + .35 CH_3COOO + .45 H_2O_2	4.00E8		see note*
A44004_a01	TrAa01C	$GLYOX + CHOCHOHOH \rightarrow GOLIG1 + H_2O$	1.00E2		Ervens and Volkamer (2010)
A44005_a01	TrAa01C	$GOLIG1 + H_2O \rightarrow GLYOX + CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44006_a01	TrAa01C	$CHOCHOHOH + CHOCHOHOH \rightarrow GOLIG2 +$ H_2O	1.00E2		Ervens and Volkamer (2010)
A44007_a01	TrAa01C	$GOLIG2 + H_2O \rightarrow CHOCHOHOH +$ $CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44008_a01	TrAa01C	$CHOHOHCHOHOH + CHOCHOHOH \rightarrow GOLIG3$ + H_2O	1.00E2		Ervens and Volkamer (2010)
A44009_a01	TrAa01C	$GOLIG3 + H_2O \rightarrow CHOHOHCHOHOH +$ $CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44010_a01	TrAa01C	$GOLIG1 + OH \rightarrow GOLIGO1 + HO_2$	2.2E9	-1516	see note*
A44011_a01	TrAa01C	$GOLIG2 + OH \rightarrow GOLIGO2 + HO_2$	2.2E9	-1516	see note*
A44012_a01	TrAa01C	$GOLIG3 + OH \rightarrow GOLIGO3 + HO_2$	2.2E9	-1516	see note*
A46000_a01	TrAa01C	$CH_3C(O)CHO + CH_3COCHOHOH \rightarrow$ $CH_3COCHOHOCHOHCOCH_3 + H_2O$	1.00E2		Ervens and Volkamer (2010)*
A46001_a01	TrAa01C	$CH_3COCHOHOCHOHCOCH_3 + H_2O \rightarrow$ $CH_3COCHOHOH + CH_3C(O)CHO$	1.00E-1		Ervens and Volkamer (2010)*
A46002_a01	TrAa01C	$CH_3COCHOHOCHOHCOCH_3 + OH \rightarrow$ $CH_3COCOHOCHOHCOCH_3 + HO_2$	1.84E9	-1235	see note*
A46003_a01	TrAa01C	$CH_3COCHOHOH + CH_3COCHOHOH \rightarrow$ $CH_3COCHOHOCOHC_3CHOHOH + H_2O$	1.00E2		Ervens and Volkamer (2010)*
A46004_a01	TrAa01C	$CH_3COCHOHOCOHC_3CHOHOH + H_2O \rightarrow 2$ $CH_3COCHOHOH$	1.00E-1		Ervens and Volkamer (2010)*
A46005_a01	TrAa01C	$CH_3COCHOHOCOHC_3CHOHOH + OH \rightarrow$ $CH_3COCOHOCHOHC_3COHOH + HO_2$	1.84E9	-1235	see note*
A60000_a01	TrAa01Cl	$Cl + Cl \rightarrow Cl_2$	8.8E7		Wu et al. (1980)
A60001_a01	TrAa01Cl	$Cl_2 + Cl_2^- \rightarrow Cl_2 + 2 Cl^-$	3.5E9		Yu (2004)
A61000_a01	TrAa01Cl	$Cl^- + O_3 \rightarrow ClO^-$	3.0E-3		Hoigné et al. (1985)
A61001_a01	TrAa01Cl	$Cl_2 + O_2^- \rightarrow Cl_2^-$	1.0E9		Bjergbakke et al. (1981)
A61002_a01	TrAa01Cl	$Cl_2^- + O_2^- \rightarrow 2 Cl^-$	1.0E9		Jacobi (1996)*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A62000_a01	TrAa01Cl	$Cl \rightarrow H^+ + ClOH^-$	1.8E5		Yu (2004)
A62001_a01	TrAa01Cl	$Cl + H_2O_2 \rightarrow HO_2 + Cl^- + H^+$	2.7E7	-1684	Christensen et al. (1982)
A62002_a01	TrAa01Cl	$Cl^- + OH \rightarrow ClOH^-$	4.2E9		Yu (2004)
A62003_a01	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A62004_a01	TrAa01MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A62005_a01	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2 Cl^- + H^+$	1.3E10		Jacobi (1996)
A62006_a01	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A62007_a01	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A62008_a01	TrAa01MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A62009_a01	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH$	6.0E9		Yu (2004)
A62010_a01	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A63000_a01	TrAa01ClN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A63001_a01	TrAa01ClN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A63002_a01	TrAa01ClN	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A64000_a01	TrAa01ScCl	$Cl_2^- + CH_3OOH \rightarrow 2 Cl^- + H^+ + CH_3OO$	6.20E5		see note*
A70000_a01	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2 Br^- + Br_2$	1.9E9		Ross et al. (1992)
A71000_a01	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A71001_a01	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A71002_a01	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2 Br^-$	1.7E8		Wagner and Strehlow (1987)
A72000_a01	TrAa01Br	$Br^- + OH \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)
A72001_a01	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A72002_a01	TrAa01MblBr	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A72003_a01	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A72004_a01	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2 Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A72005_a01	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A72006_a01	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999a)
A72007_a01	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A72008_a01	TrAa01MblBr	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A72009a_a01	TrAa01Br	$BrOH^- \rightarrow Br^- + OH$	3.3E7		Zehavi and Rabani (1972)
A72009b_a01	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A72010_a01	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A73000_a01	TrAa01BrN	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A73001_a01	TrAa01BrN	$Br_2^- + NO_2^- \rightarrow 2 Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A74000_a01	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2 Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A76001_a01	TrAa01BrCl	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A76002_a01	TrAa01MblBrCl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A76003_a01	TrAa01MblBrCl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		Liu and Margerum (2001)*
A76004_a01	TrAa01MblBrCl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A81000_a01	TrAa01MblI	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A81001_a01	TrAa01MblI	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A82000_a01	TrAa01MblI	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A82001_a01	TrAa01I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
A82002_a01	TrAa01MblI	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A82003_a01	TrAa01MblI	$IO_2^- + I^- + H^+ \rightarrow 2 HOI + OH^-$	2.0E10		Edblom et al. (1987)
A86000_a01	TrAa01MblClI	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A86001_a01	TrAa01MblClI	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A86002_a01	TrAa01ClI	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A86003_a01	TrAa01MblClI	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A86004_a01	TrAa01ClI	$HOI + Cl_2 \rightarrow IO_2^- + 2 Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A86005_a01	TrAa01ClI	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2 H^+$	5.0E5		Citri and Epstein (1988)
A86006_a01	TrAa01ClI	$ICl + I^- \rightarrow I_2 + Cl^-$	1.1E9		Margerum et al. (1986)
A87000_a01	TrAa01MblBrI	$IBr \rightarrow HOI + H^+ + Br^-$	8.0E5		Troy et al. (1991)
A87001_a01	TrAa01MblBrI	$I^- + HOBr \rightarrow IBr + OH^-$	5.0E9		Troy and Margerum (1991)
A87002_a01	TrAa01BrI	$IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$	1.0E6		Chinake and Simoyi (1996)
A87003_a01	TrAa01MblBrI	$HOI + Br^- + H^+ \rightarrow IBr$	3.3E12		Troy et al. (1991)
A87004_a01	TrAa01BrI	$HOI + HOBr \rightarrow IO_2^- + Br^- + 2 H^+$	1.0E6		Chinake and Simoyi (1996)
A87005_a01	TrAa01BrI	$IBr + I^- \rightarrow I_2 + Br^-$	2.0E9		Faria et al. (1993)
A91000_a01	TrAa01ScS	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A91001_a01	TrAa01MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A91002_a01	TrAa01ScS	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A91003_a01	TrAa01ScS	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A91004_a01	TrAa01ScS	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A91005_a01	TrAa01S	$SO_5^- + SO_3^{2-} \rightarrow .72 SO_4^- + .72 SO_4^{2-} + .28 SO_3^- + .28 HSO_5^- + .28 OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A91006_a01	TrAa01S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + LSULFUR$	1.0E8		Ross et al. (1992)*
A92000_a01	TrAa01ScS	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A92001_a01	TrAa01ScS	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A92002_a01	TrAa01ScS	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A92003_a01	TrAa01ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A92004_a01	TrAa01ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A92005_a01	TrAa01ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note*
A92006_a01	TrAa01MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A92007_a01	TrAa01ScS	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A92008_a01	TrAa01ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note*
A92009_a01	TrAa01MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A92010_a01	TrAa01ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A92011_a01	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75 SO_4^- + .75 SO_4^{2-} + .75 H^+ + .25 SO_3^- + .25 HSO_5^-$	1.0E5		Huie and Neta (1987)
A92012_a01	TrAa01ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2 HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A93001_a01	TrAa01ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A93002_a01	TrAa01ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Løgager et al. (1993)
A93004_a01	TrAa01ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A93005_a01	TrAa01ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A94100_a01	TrAa01ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OH SO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)*
A94101_a01	TrAa01ScS	$SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A94102_a01	TrAa01ScS	$HSO_3^- + HCHO \rightarrow CH_2OH SO_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A94103_a01	TrAa01ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A94104_a01	TrAa01ScS	$HSO_3^- + CH_3OO \rightarrow SO_3^- + CH_3OOH$	5.00E5		Herrmann et al. (1999b)
A94105_a01	TrAa01ScS	$SO_4^- + HCOO^- \rightarrow SO_4^{2-} + CO_2 + HO_2$	1.7E8	-1500	Jacob (1986)
A94106_a01	TrAa01ScS	$SO_4^- + HCOOH \rightarrow SO_4^{2-} + CO_2 + H^+ + HO_2$	1.7E8	-1500	Jacob (1986)
A94107_a01	TrAa01ScS	$SO_4^- + CH_3OH \rightarrow SO_4^{2-} + HOCH_2O_2 + H^+$	9.0E6	-2190	Clifton and Huie (1989)
A94108a_a01	TrAa01ScS	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + CH_3OO + H^+$	$0.25 \times 1.20E7$		see note*
A94108b_a01	TrAa01ScS	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + HCHO + HO_2 + H^+$	$0.75 \times 1.20E7$		see note*
A94109_a01	TrAa01ScS	$SO_4^- + HOCH_2OH \rightarrow SO_4^{2-} + HCOHOHO_2 + H^+$	1.40E7	-1300	Buxton et al. (1990)
A94110_a01	TrAa01ScS	$SO_5^- + HCOO^- \rightarrow HSO_5^- + CO_2 + O_2^-$	1.4E4	-4000	Jacob (1986)
A94111_a01	TrAa01ScS	$CH_2OH SO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A94200_a01	TrAa01ScCS	$HSO_3^- + CH_2OOCOOH \rightarrow SO_3^- + HOOCH_2CO_2H$	5.00E5		see note*
A94201_a01	TrAa01ScCS	$HSO_3^- + CH_2OOCO_2^- \rightarrow SO_3^- + CH_2OOHCO_2^-$	5.00E5		see note*
A94202a_a01	TrAa01ScCS	$SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_3CHO + HO_2 + H^+$	$0.90 \times 4.1E7$	-1750	Clifton and Huie (1989)*
A94202b_a01	TrAa01ScCS	$SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_2OHCH_2OO + H^+$	$0.10 \times 4.1E7$	-1750	Clifton and Huie (1989)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A94203a_a01	TrAa01ScCS	$SO_4^- + \text{CHOHOHCHOHOH} \rightarrow SO_4^{2-} + \text{CHOHOHCHOHOH}_2 + H^+$	$0.27 \times 2.40E7$		George et al. (2001)
A94203b_a01	TrAa01ScCS	$SO_4^- + \text{CHOHOHCHOHOH} \rightarrow SO_4^{2-} + \text{HCOHOHO}_2 + \text{HCOOH} + \text{HO}_2 + H^+$	$0.73 \times 2.40E7$		George et al. (2001)*
A94204_a01	TrAa01ScCS	$SO_4^- + \text{CH}_3\text{COO}^- \rightarrow SO_4^{2-} + \text{CH}_2\text{OOCO}_2^- + H^+$	5.10E6		Huie and Clifton (1990)
A94205_a01	TrAa01ScCS	$SO_4^- + \text{HOCCOO}^- \rightarrow SO_4^{2-} + \text{C}_2\text{O}_4^- + H^+$	1.70E6		Grgić et al. (2007)
A94206_a01	TrAa01ScCS	$SO_4^- + \text{C}_2\text{O}_4^{2-} \rightarrow SO_4^{2-} + \text{C}_2\text{O}_4^-$	1.30E7		Grgić et al. (2007)
A96000_a01	TrAa01ClS	$SO_3^{2-} + \text{Cl}_2 \rightarrow SO_3^- + 2 \text{Cl}^-$	6.2E7		Jacobi et al. (1996)
A96001_a01	TrAa01MblClS	$SO_3^{2-} + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^-$	7.6E8		Fogelman et al. (1989)
A96002_a01	TrAa01ClS	$SO_4^- + \text{Cl}^- \rightarrow SO_4^{2-} + \text{Cl}$	2.5E8		Buxton et al. (1999a)
A96003_a01	TrAa01ClS	$SO_4^{2-} + \text{Cl} \rightarrow SO_4^- + \text{Cl}^-$	2.1E8		Buxton et al. (1999a)
A96004_a01	TrAa01ClS	$\text{HSO}_3^- + \text{Cl}_2 \rightarrow \text{SO}_3^- + 2 \text{Cl}^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A96005_a01	TrAa01MblClS	$\text{HSO}_3^- + \text{HOCl} \rightarrow \text{Cl}^- + \text{HSO}_4^- + H^+$	7.6E8		see note*
A96006_a01	TrAa01ClS	$\text{HSO}_5^- + \text{Cl}^- \rightarrow \text{HOCl} + \text{SO}_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A97000_a01	TrAa01BrS	$SO_3^{2-} + \text{Br}_2 \rightarrow 2 \text{Br}^- + \text{SO}_3^-$	2.2E8	-649	Shoute et al. (1991)
A97001_a01	TrAa01BrS	$SO_3^{2-} + \text{BrO}^- \rightarrow \text{Br}^- + \text{SO}_4^{2-}$	1.0E8		Troy and Margerum (1991)
A97002_a01	TrAa01MblBrS	$SO_3^{2-} + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^-$	5.0E9		Troy and Margerum (1991)
A97003_a01	TrAa01BrS	$SO_4^- + \text{Br}^- \rightarrow \text{Br} + \text{SO}_4^{2-}$	2.1E9		Jacobi (1996)
A97004_a01	TrAa01BrS	$\text{HSO}_3^- + \text{Br}_2 \rightarrow 2 \text{Br}^- + H^+ + \text{SO}_3^-$	6.3E7	-782	Shoute et al. (1991)
A97005_a01	TrAa01MblBrS	$\text{HSO}_3^- + \text{HOBr} \rightarrow \text{Br}^- + \text{HSO}_4^- + H^+$	5.0E9		see note*
A97006_a01	TrAa01BrS	$\text{HSO}_5^- + \text{Br}^- \rightarrow \text{HOBr} + \text{SO}_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)
A98000_a01	TrAa01IS	$\text{HSO}_3^- + \text{I}_2 \rightarrow 2 \text{I}^- + \text{HSO}_4^- + 2 \text{H}^+$	1.7E9		Yiin and Margerum (1990)
A101000_a01	TrAa01Hg	$\text{Hg} + \text{O}_3 \rightarrow \text{HgO} + \text{O}_2$	4.7E7		Munthe (1992)
A102000_a01	TrAa01Hg	$\text{HgO} + \text{H}^+ \rightarrow \text{Hg}^{2+} + \text{OH}^-$	1.0E10		Pleijel and Munthe (1995)
A102001_a01	TrAa01Hg	$\text{Hg} + \text{OH} \rightarrow \text{Hg}^+ + \text{OH}^-$	2.0E9		Lin and Pehkonen (1997)
A102002_a01	TrAa01Hg	$\text{Hg}^+ + \text{OH} \rightarrow \text{Hg}^{2+} + \text{OH}^-$	1.0E10		Lin and Pehkonen (1997)
A102003_a01	TrAa01Hg	$\text{Hg}^{2+} + \text{HO}_2 \rightarrow \text{Hg}^+ + \text{O}_2 + \text{H}^+$	1.7E4		Enami et al. (2007)
A102004_a01	TrAa01Hg	$\text{Hg}^+ + \text{HO}_2 \rightarrow \text{Hg} + \text{O}_2 + \text{H}^+$	1.0E10		Lin and Pehkonen (1997)
A106000_a01	TrAa01ClHg	$\text{Hg} + \text{HOCl} \rightarrow \text{Hg}^{2+} + \text{Cl}^- + \text{OH}^-$	2.09E6		Lin and Pehkonen (1998)
A106001_a01	TrAa01ClHg	$\text{Hg} + \text{ClO}^- \rightarrow \text{Hg}^{2+} + \text{Cl}^- + 2 \text{OH}^-$	1.99E6		Lin and Pehkonen (1998)
A107000_a01	TrAa01BrHg	$\text{Hg} + \text{HOBr} \rightarrow \text{Hg}^{2+} + \text{Br}^- + \text{OH}^-$	0.279		Wang and Pehkonen (2004)
A107001_a01	TrAa01BrHg	$\text{Hg} + \text{BrO}^- \rightarrow \text{Hg}^{2+} + \text{Br}^- + 2 \text{OH}^-$	0.273		Wang and Pehkonen (2004)
A107002_a01	TrAa01BrHg	$\text{Hg} + \text{Br}_2 \rightarrow \text{Hg}^{2+} + 2 \text{Br}^-$	0.196		Wang and Pehkonen (2004)
A109000_a01	TrAa01HgS	$\text{HgSO}_3 \rightarrow \text{Hg} + \text{HSO}_4^- + \text{H}^+$	0.0106		van Loon et al. (2000)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A111001_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A111002_a01	TrAa01Fe	$Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$	5E7		de Laat and Le (2006)
A111003_a01	TrAa01Fe	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	8.2E5		Løgager et al. (1992)
A112001a_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$	2.7E8		de Laat and Le (2006)
A112001b_a01	TrAa01Fe	$FeOH^+ + OH \rightarrow Fe^{3+} + 2 OH^-$	2.7E8		de Laat and Le (2006)
A112002a_a01	TrAa01Fe	$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$	5.5E1		de Laat and Le (2006)
A112002b_a01	TrAa01Fe	$FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2 OH^-$	5.9E6		de Laat and Le (2006)
A112003_a01	TrAa01Fe	$FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$	2.3E-3		de Laat and Le (2006)
A112004_a01	TrAa01Fe	$Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$	2.3E-3		de Laat and Le (2006)
A112006_a01	TrAa01Fe	$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO_2^-$	1.2E6		de Laat and Le (2006)
A112008a_a01	TrAa01Fe	$FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$	1.5E8		Rush and Bielski (1985)
A112008b_a01	TrAa01Fe	$Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2 OH^-$	1.5E8		Rush and Bielski (1985)
A112009_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2 OH^-$	1.0E7		Rush and Bielski (1985)
A112010_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow FeOH^{2+}$	4.3E8		Christensen and Sehested (1981)
A112011_a01	TrAa01Fe	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	9.5E3		Løgager et al. (1992)
A112012_a01	TrAa01Fe	$FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$	1.3E-2		Løgager et al. (1992)
A112013_a01	TrAa01Fe	$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	2.0E6		Løgager et al. (1992)
A112014_a01	TrAa01Fe	$FeO^{2+} + OH \rightarrow Fe^{3+} + HO_2^-$	1.0E7		Løgager et al. (1992)
A112015_a01	TrAa01Fe	$FeO^{2+} + Fe^{2+} \rightarrow 2 Fe^{3+} + 2 OH^-$	1.4E5		Løgager et al. (1992)
A112016_a01	TrAa01Fe	$FeO^{2+} + Fe^{2+} \rightarrow Fe(OH)_2Fe^{4+}$	1.8E4		Jacobsen et al. (1997)
A112017_a01	TrAa01Fe	$Fe(OH)_2Fe^{4+} + H^+ \rightarrow 2 Fe^{3+} + OH^-$	2.0		Jacobsen et al. (1997)
A112018_a01	TrAa01Fe	$Fe(OH)_2Fe^{4+} \rightarrow 2 Fe^{3+} + 2 OH^-$	0.49		Jacobsen et al. (1997)
A113001_a01	TrAa01FeN	$FeO^{2+} + HONO \rightarrow Fe^{3+} + NO_2 + OH^-$	1.1E4		Jacobsen et al. (1998)
A113002_a01	TrAa01FeN	$Fe^{2+} + NO_3 \rightarrow Fe^{3+} + NO_3^-$	8.0E6		Herrmann et al. (2000)
A116001_a01	TrAa01ClFe	$Fe^{2+} + Cl \rightarrow Fe^{3+} + Cl^-$	5.9E9		Jayson et al. (1973)
A116002a_a01	TrAa01ClFe	$Fe^{2+} + Cl_2^- \rightarrow Fe^{3+} + 2 Cl^-$	1E7		Thornton and Laurence (1973)
A116002b_a01	TrAa01ClFe	$Fe^{2+} + Cl_2^- \rightarrow FeCl^{2+} + Cl^-$	4E6		Thornton and Laurence (1973)
A116003a_a01	TrAa01ClFe	$FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO_2^-$	1.2E6		de Laat and Le (2006)
A116003b_a01	TrAa01ClFe	$FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO_2^- + OH^-$	1E7		de Laat and Le (2006)
A116004a_a01	TrAa01ClFe	$FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A116004b_a01	TrAa01ClFe	$FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2 Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A116004c_a01	TrAa01ClFe	$FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$	5E7		de Laat and Le (2006)
A116004d_a01	TrAa01ClFe	$FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2 Cl^- + O_2$	5E7		de Laat and Le (2006)
A116005_a01	TrAa01ClFe	$FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2 OH^-$	1E2		Jacobsen et al. (1998)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A117001_a01	TrAa01BrFe	$Fe^{2+} + Br_2^- \rightarrow Fe^{3+} + 2 Br^-$	3.6E6		Thornton and Laurence (1973)
A119001_a01	TrAa01FeS	$FeO^{2+} + SO_2 \rightarrow Fe^{3+} + SO_3^-$	4.5E5		Jacobsen et al. (1998)*
A119002_a01	TrAa01FeS	$FeO^{2+} + HSO_3^- \rightarrow Fe^{3+} + SO_3^- + OH^-$	2.5E5		Jacobsen et al. (1998)*
A119003_a01	TrAa01FeS	$FeOH^{2+} + HSO_3^- \rightarrow Fe^{2+} + SO_3^- + H_2O$	30		Ziajka et al. (1994)
A119004_a01	TrAa01FeS	$Fe^{2+} + SO_5^- \rightarrow FeOH^{2+} + HSO_5^-$	8E5		Ziajka et al. (1994)*
A119005_a01	TrAa01FeS	$Fe^{2+} + HSO_5^- \rightarrow FeOH^{2+} + SO_4^-$	3.0E4		Gilbert and Stell (1990)
A119006_a01	TrAa01FeS	$Fe^{2+} + SO_4^- \rightarrow FeSO_4^+$	3.6E7		McElroy and Waygood (1990)*
A119007_a01	TrAa01FeS	$FeOH^{2+} + SO_3^- \rightarrow Fe^{2+} + HSO_4^-$	3E7		Warneck (2018)
A119008_a01	TrAa01FeS	$FeSO_3^+ + SO_3^- \rightarrow Fe^{2+} + SO_4^{2-} + SO_2$	2.16E6		Warneck (2018)*

Specific notes

A41004_a01: We use the values A and E_A from $k_2(T)$ of Exner et al. (1994), which is different from k at 298 K listed in Table II of the same study.

A41009_a01: We use the values A and E_A from $k_1(T)$ of Exner et al. (1994), which is different from k at 298 K listed in Table I of the same study.

A41012a_a01: We use the values A and E_A from Table 1 of Herrmann et al. (1999b), which is different from k at 298 K listed in the same table.

A41012b_a01: See branch a.

A41013a_a01: Branching ratios taken from Asmus et al. (1973)

A41016a_a01: Branching ratio explaining the HCOOH-yield by Monod et al. (2007) who originally assigned it to the channel for the methylic H-abstraction. However, Monod et al. (2007), differently from Herrmann et al. (1999b), assumed that the self-reaction of CH_3O_2 would only produce 2 CH_3O radicals and thus HCHO + HO_2 . Instead, the latter reaction has a 0.8 yield of $HOCH_2O_2$, which is a precursor of hydroxymethyl hydroperoxide and thus HCOOH.

A41016b_a01: The CH_2OOH radical has a lifetime of 10^{-9} s in the gas phase decomposing to HCHO and OH. O_2 -addition in the aqueous-phase seems unlikely. It is hard to imagine how the $HOOHCH_2O_2$ radical would decompose into HCOOH and HO_2 .

A41017a_a01: $k(H_2O_2+NO_3)$, branching ratio as for $CH_3OOH + OH$

A41017b_a01: See branch a.

A41018a_a01: $k(H_2O_2+CO_3^-)$, branching ratio as for $CH_3OOH + OH$

A41018b_a01: See branch a.

A41019a_a01: Branching ratio as for $CH_3OOH + OH$

A41019b_a01: $HOCHOOHO_2$ is assumed to directly decompose into $CHOOOH$ and HO_2

A41020a_a01: $k(H_2O_2+NO_3)$, branching ratio as for $CH_3OOH + OH$

A41020b_a01: $HOCHOOHO_2$ is assumed to directly decompose into $CHOOOH$ and HO_2

A41021_a01: HO_2 elimination

A41022_a01: $k(HO_2+HO_2)$

A41023_a01: $k(HO_2+O_2^-)$

A41030_a01: HO_2 elimination

A42000a_a01: CH_3CHOHO_2 is assumed to directly decompose into $CH_3CHO + HO_2$

A42001a_a01: CH_3CHOHO_2 is assumed to directly decompose into $CH_3CHO + HO_2$

A42003_a01: $k(HO_2+O_2^-)$

A42004_a01: $k(HO_2+HO_2)$

A42005_a01: k approximated from $(k(CH_3OOH+OH)/k(CH_3OH+OH))$

A42006_a01: $CH_2OHCHOHO_2$ is assumed to directly decompose into $HOCH_2CHO + HO_2$

A42007_a01: We use the values A and E_A from Table 3 of Hoffmann et al. (2009), which is different from k at 298 K listed in Tables 1 and 2 of the same study. $CH_2OHCHOHO_2$ is assumed to directly decompose into $HOCH_2CHO + HO_2$.

A42010_a01: k based on Monod et al. (2005): $k=k(2CH_3CH_2(OO))$

A42014_a01: HO_2 elimination

A42016a_a01: k assumed to be the same as for $CH_3CHO + NO_3$

A42016b_a01: See branch a.	A42037_a01: $k(\text{HO}_2 + \text{HO}_2)$	k at 298 K listed in the abstract and Table 10 of the same study.
A42017_a01: $k(\text{CH}_3\text{CHOHOH} + \text{O}_2^-)$	A42038_a01: $k(\text{HO}_2 + \text{O}_2^-)$	
A42018_a01: HO_2 elimination	A42141_a01: We use the values A and E_A from the abstract of Ervens et al. (2003b), which is different from k at 298 K listed in abstract and Table 11 of the same study.	A42156b_a01: See branch a. COOHOO is not formed but directly dissociates into $\text{CO}_2 + \text{HO}_2$.
A42019_a01: k based on von Sonntag (1987)		A42157a_a01: $k(\text{CHOHOHCHOHOH} + \text{NO}_3)$
A42020_a01: k based on von Sonntag (1987)		A42157b_a01: COOHOO is not formed but directly dissociates into $\text{CO}_2 + \text{HO}_2$
A42022a_a01: $k(\text{CH}_3\text{CHOHOH} + \text{NO}_3)$	A42142_a01: We use the values A and E_A from the abstract of Ervens et al. (2003b), which is different from k at 298 K listed in the abstract and Table 11 of the same study.	A42158a_a01: We use the values A and E_A from the abstract of Ervens et al. (2003b), which is different from k at 298 K listed in the abstract and Table 10 of the same study.
A42022b_a01: See branch a.	A42144a_a01: k assumed to be the same as $\text{C}_2\text{H}_5\text{OOH} + \text{OH}$ based on Monod et al. (2007)	A42158b_a01: See branch a.
A42022c_a01: See branch a.	A42144b_a01: See branch a.	A42161_a01: HO_2 elimination
A42023b_a01: CHOHOHO_2 directly decomposes into $\text{HCOOH} + \text{HO}_2$	A42146a_a01: k assumed to be the same as $\text{C}_2\text{H}_5\text{OOH} + \text{OH}$ based on Monod et al. (2007)	A42162_a01: HO_2 elimination
A42024a_a01: k based on Neta and Huie (1986)	A42146b_a01: See branch a.	A42163a_a01: $k(\text{HOCH}_2\text{CHO} + \text{OH})$
A42024b_a01: CHOHOHO_2 directly decomposes into $\text{HCOOH} + \text{HO}_2$	A42148_a01: HO_2 elimination	A42163b_a01: See branch a.
A42025_a01: HO_2 elimination	A42149_a01: HO_2 elimination	A42164a_a01: $k(\text{HOCH}_2\text{CHO} + \text{NO}_3)$
A42027_a01: We use the values A and E_A from $k_3(T)$ of Exner et al. (1994), which is different from k at 298 K listed in Table IV of the same study.	A42150a_a01: COOHOO is not formed but directly dissociates into $\text{CO}_2 + \text{HO}_2$. Rate coefficient based on Buxton et al. (1988)	A42164b_a01: See branch a.
A42029_a01: We use the values A and E_A from $k_4(T)$ of Exner et al. (1994), which is different from k at 298 K listed in Table V of the same study.	A42150b_a01: See branch a.	A42165a_a01: $k(\text{HOCH}_2\text{CHOHOH} + \text{OH})$
A42030b_a01: $\text{CH}_3\text{CHOOHO}_2$ is assumed to directly decompose into $\text{CH}_3\text{CO}_2\text{H}$ and HO_2	A42151a_a01: We use the values A and E_A from Table 2 of Gaillard de Sémainville et al. (2007), which is different from k at 298 K listed in the same Table. COOHOO is not formed but directly dissociates into $\text{CO}_2 + \text{HO}_2$.	A42165b_a01: See branch a.
A42031a_a01: We use the values A and E_A from Table 1 of Herrmann et al. (1999b), which is different from k at 298 K listed in the same table.	A42151b_a01: See branch a.	A42165c_a01: See branch a.
A42031b_a01: See branch a. $\text{CH}_3\text{CHOHO}_2$ is assumed to directly decompose into $\text{CH}_3\text{CHO} + \text{HO}_2$.	A42154a_a01: We use the values A and E_A from Table 2 of Gaillard de Sémainville et al. (2007), which is different from k at 298 K listed in the same table.	A42166a_a01: $k(\text{HOCH}_2\text{CHOHOH} + \text{NO}_3)$
A42032_a01: $k(\text{HO}_2 + \text{O}_2^-)$	A42154b_a01: See branch a.	A42166b_a01: See branch a.
A42033_a01: $k(\text{HO}_2 + \text{HO}_2)$		A42166c_a01: See branch a.
A42034_a01: $k(\text{HO}_2 + \text{HO}_2)$	A42156a_a01: We use the values A and E_A from the abstract of Ervens et al. (2003b), which is different from	A42167_a01: pH-dependent
A42035_a01: $k(\text{HO}_2 + \text{O}_2^-)$		A42169_a01: $k = 2 \times k(\text{HOCH}_2\text{OH} + \text{OH})$
		A42471_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)
		A42472_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)
		A42473_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)

A43000a_a01: Intermediate reaction with O_2^- and $CH(OH)_2COCH_2O_2$ neglected

A43001_a01: $CH(OH)_2COCH_2O_2$ neglected

A43002_a01: We use the values A and E_A from Table 3 of Schaefer et al. (2012), which is different from k at 298 K listed in the same table. CO_2 added for mass balance intermediate reactions neglected.

A43003_a01: We use the values A and E_A from $k_{pyruvic\ acid}(T)$ (Reaction 11) of Gaillard de Sémainville et al. (2007), which is different from k at 298 K listed in Table 2 in the same study.

A43004_a01: We use the values A and E_A from Table 3 of Schaefer et al. (2012), which is different from k at 298 K listed in the same table. CO_2 added for mass balance intermediate reactions neglected.

A43005_a01: We use the values A and E_A from Table 2 of Gaillard de Sémainville et al. (2007), which is different from k at 298 K listed in the same table.

A43007_a01: Temperature dependence from Herrmann et al. (2005)

A43010a_a01: $CH_2(OH)COCH_2O_2$ was neglected with a branching ratio 0.16 added to $CH_3COCHOHO_2$

A43011_a01: We use the values A and E_A from Table 2 of Gaillard de Sémainville et al. (2007), which is different from k at 298 K listed in the same table.

A43013_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Monod et al., 2005)

A43014_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Herrmann et al., 1994)

A43015a_a01: k calculated comparing the rates $(CH_3OH + OH/CH_3OOH + OH)$ and $(ACETOL + OH/HYPERACET + OH)$

A43015b_a01: k from $CH_3OOH + OH \rightarrow HCHO$.

A43016_a01: k taken from the reaction of the hydrated form of MGLYOX and NO_3

A43017_a01: k from $CH_3O_2 + HO_2$

A43018_a01: k from $CH_3O_2 + O_2^-$

A43019a_a01: k calculated comparing $CH_3OH + OH / CH_3OOH + OH$ with $IPROPL + OH$

A43019b_a01: k calculated comparing $CH_3OH + OH / CH_3OOH + OH$ with $ACETOL + OH / HYPERCET + OH$

A43020_a01: k taken from the reaction of the hydrated form of MGLYOX and NO_3

A43021_a01: k from $CH_3O_2 + HO_2$

A43022_a01: k from $CH_3O_2 + O_2^-$

A43023_a01: pH-dependent

A43025_a01: $k = 2 \times k(HOCH_2OH + OH)$

A44000_a01: We use the values A and E_A from Table 3 of Schöne et al. (2014), which is different from k at 298 K listed in Table 2 of the same study.

A44001_a01: $k = k(2\ CH_3COCH_2O_2)$

A44002_a01: We use the values A and E_A from Table 3 of Schöne et al. (2014), which is different from k at 298 K listed in Table 2 of the same study.

A44003_a01: $k = k(2\ CH_3COCH_2O_2)$. Originally, $.2\ CH_2OHCHOHCOCH_3$ is produced by this reaction. However, the oxidation or the phase-transfer of $CH_2OHCHOHCOCH_3$ is not represented. Thus, lumped carbon (.8 LCARBON) is used to represent $.2\ CH_2OHCHOHCOCH_3$.

A44010_a01: $k = 2 \times k(CHOHOHCHOHOH + OH)$

A44011_a01: $k = 2 \times k(CHOHOHCHOHOH + OH)$

A44012_a01: $k = 2 \times k(CHOHOHCHOHOH + OH)$

A46000_a01: Assumed to be the same as for glyoxal

A46001_a01: Assumed to be the same as for glyoxal

A46002_a01: $k = 2 \times k(CH_3COCHOHOH + OH)$

A46003_a01: Assumed to be the same as for glyoxal

A46004_a01: Assumed to be the same as for glyoxal

A46005_a01: $k = 2 \times k(CH_3COCHOHOH + OH)$

A61002_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.

A63001_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.

A64000_a01: k taken from $H_2O_2 + Cl_2^-$ (Yu, 2004).

A74000_a01: Assumed to be the same as for $Br_2^- + H_2O_2$.

A76003_a01: The rate coefficient is defined as backward reaction divided by equilibrium constant.

A91005_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).

A91006_a01: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^{2-} , it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ 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.

A92005_a01: D. Sedlak, pers. comm. (1993).

A92008_a01: D. Sedlak, pers. comm. (1993).

A94100_a01: $2.48 \times 10^7 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.

A94102_a01: $790 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.

A94108a_a01: $k(H_2O_2 + SO_4^-)$, branching ratio as for $CH_3OOH + OH$

A94108b_a01: See branch a.	A96005_a01: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOCl}$.	A119004_a01: Assumed. Note that CAPRAM 2.4 lists $k=4.3\text{E}7$ from Herrmann Air Pollution Research Report 57 and it also lists $k=2.65\text{E}7$ from Williams PhD 1996 http://lib.leeds.ac.uk/record=b1835184~S5 . Brand and van Eldik (1995) also list $k=3.56\text{E}4$ from Waygood EUROTRAC 1992 report.
A94200_a01: $k(\text{CH}_3\text{OO}+\text{HSO}_3^-)$	A97005_a01: Assumed to be the same as for $\text{SO}_3^{2-} + \text{HOBr}$.	A119006_a01: $3\text{E}8*6500/(48000+6500)$
A94201_a01: $k(\text{CH}_3\text{OO}+\text{HSO}_3^-)$	A116005_a01: products assumed	A119008_a01: Assuming that the intermediate $\text{S}_2\text{O}_6^{2-}$ dissociates quickly.
A94202a_a01: $\text{CH}_3\text{CHOHO}_2$ is assumed to directly decompose into $\text{CH}_3\text{CHO} + \text{HO}_2$	A119001_a01: products assumed	
A94203b_a01: CHOHOHO_2 directly decomposes into $\text{HCOOH} + \text{HO}_2$	A119002_a01: products assumed	

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