

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 4.4.2

Date: 2023-03-22

MECCA config (*.ini) file: example.ini

Integrator: rosenbrock_posdef

Gas equation file: gas.eqn

Replacement file:

Selected reactions:

“Tr and (G or (Aa or Mb1)) and not I and not Hg”

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase: 671

Aqueous phase: 462

All species: 1133

Number of reactions in selected mechanism:
Gas phase (Gnn): 1741

Aqueous phase (Annn): 385

Henry (Hnnn): 713

Photolysis (Jnnn): 348

Aqueous phase photolysis (PHnnn): 26

Heterogeneous (HETnnn): 0

Equilibria (EQnn): 112

Isotope exchange (IEXnnn): 0

Tagging equations (TAGnnn): 0

Dummy (Dnn): 1

All equations: 3326

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)
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)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	$1.7E-12*EXP(-940./temp)$	Burkholder et al. (2015)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	$2.8E-12*EXP(-1800./temp)$	Burkholder et al. (2015)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2 O_2$	$1.E-14*EXP(-490./temp)$	Burkholder et al. (2015)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8E-11*EXP(250./temp)$	Burkholder et al. (2015)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Burkholder et al. (2015)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$1.63E-10*EXP(60./temp)$	Burkholder et al. (2015)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Burkholder et al. (2015)
G2117	UpStTrG	$H_2O + H_2O \rightarrow (H_2O)_2$	$6.521E-26*temp*EXP(1851.09/temp)$ *EXP(-5.10485E-3*temp)	Scribano et al. (2006)*
G2118	UpStTrG	$(H_2O)_2 \rightarrow H_2O + H_2O$	1.E0	see note*
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$2.15E-11*EXP(110./temp)$	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.0E-12*EXP(-1500./temp)$	Burkholder et al. (2015)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Burkholder et al. (2015)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Burkholder et al. (2015)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_N03_N02	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_N03_N02/(5.8E-27*EXP(10840./$ $temp))$	Burkholder et al. (2015)*
G3200	TrGN	$NO + OH \rightarrow HONO$	$k_3rd(temp, cair, 7.0E-31, 2.6,$ $3.6E-11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	$3.3E-12*EXP(270./temp)$	Burkholder et al. (2015)
G3202a	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	$(1.-alpha_H00N0) * k_N02_OH$	Amedro et al. (2020)
G3202b	UpStTrGN	$NO_2 + OH \rightarrow HOONO$	$alpha_H00N0 * k_N02_OH$	Amedro et al. (2020)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_N02_HO2	Burkholder et al. (2015)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Burkholder et al. (2015)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	$1.8E-11*EXP(-390./temp)$	Burkholder et al. (2015)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HN03_OH	Dulitz et al. (2018)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k_N02_HO2/(2.1E-27*EXP(10900./$ $temp))$	Burkholder et al. (2015)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	$1.3E-12*EXP(380./temp)$	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E}-12 \cdot \text{EXP}(-710./\text{temp})$	Kohlmann and Poppe (1999)
G3210	TrGN	$\text{NH}_2 + \text{O}_3 \rightarrow \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E}-12 \cdot \text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E}-07 \cdot \text{EXP}(-628./\text{temp}) \cdot (\text{temp})^{**(-1.32)}$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E}-09 \cdot \text{EXP}(-356./\text{temp}) \cdot (\text{temp})^{**(-1.12)}$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E}-12 \cdot ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E}-11 \cdot ((\text{temp}/298.)^{**(-1.5)})$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E}-11 \cdot ((\text{temp}/298.)^{**(-2.0)})$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E}-11 \cdot ((\text{temp}/298.)^{**(-2.0)})$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{NH}_2 + \text{O}_2$	$1.2\text{E}-14$	Kohlmann and Poppe (1999)
G3218	TrGN	$\text{NH}_2\text{O} \rightarrow \text{NHOH}$	$1.3\text{E}3$	Kohlmann and Poppe (1999)
G3219	TrGN	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	$8.0\text{E}-11 \cdot \text{EXP}(-500./\text{temp})$	Kohlmann and Poppe (1999)
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E}-12 \cdot \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$	$1.0\text{E}-12 \cdot \text{EXP}(-1000./\text{temp})$	Kohlmann and Poppe (1999)
G3222	TrGN	$\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$	$1.66\text{E}-12$	Kohlmann and Poppe (1999)
G3223	TrGN	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E}-11 \cdot \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E}-14 \cdot \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G3227	UpStTrGN	$\text{HOONO} \rightarrow \text{NO}_2 + \text{OH}$	$(\text{alpha_HOONO} \cdot \text{k_NO2_OH}) / (3.5\text{E}-27 \cdot \text{EXP}(10135./\text{temp}))$	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)*
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)*

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

#	labels	reaction	rate coefficient	reference
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	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$(\text{k_CH302} - 7.4\text{E-}13 \cdot \text{EXP}(-520./\text{temp})) \cdot \text{R02} \cdot 2.$	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_CH300H_OH	Wallington et al. (2018)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E-}18 \cdot \text{EXP}(2.03 \cdot \text{LOG}(\text{temp}) + 636./\text{temp})$	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	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$2.94\text{E-}14 \cdot \text{exp}(786./\text{temp}) + 9.85\text{E-}13 \cdot \text{EXP}(-1036./\text{temp})$	Paulot et al. (2011)
G4114	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	k_N02_CH302	Burkholder et al. (2015)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$\text{k_N02_CH302} / (9.5\text{E-}29 \cdot \text{EXP}(11234./\text{temp}))$	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	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E-}14 \cdot \text{exp}(-663./\text{temp}) \cdot \text{c}(\text{ind_02})$	Chai et al. (2014)
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.1\text{E-}29, 4.5, 2.1\text{E-}11, 0., 0.44)$	Atkinson et al. (2006)
G4119b	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$	$9.6\text{E-}12 \cdot \text{EXP}(-1150./\text{temp})$	Atkinson et al. (2006)
G4120a	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 2.6\text{E-}29, 2.8, 3.3\text{E-}11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/900.), \text{SP}))$	Atkinson et al. (2006)
G4120b	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$	$2.3\text{E-}12 \cdot (\text{temp}/300.)^{**}(0.7)$	Atkinson et al. (2006)
G4121	StTrG	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E-}16 \cdot \text{exp}(-1000./\text{temp})$	Burkholder et al. (2015)
G4122	StTrGN	$\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$	$1\text{E-}10 \cdot \text{exp}(-1764./\text{temp})$	Nielsen et al. (1991)
G4123	StTrG	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$9.7\text{E-}15 \cdot \text{EXP}(625./\text{temp})$	Atkinson et al. (2006)
G4124	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.4\text{E}12 \cdot \text{EXP}(-7000./\text{temp})$	Atkinson et al. (2006)
G4125	StTrG	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2 \text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$	$5.6\text{E-}15 \cdot \text{EXP}(2300./\text{temp})$	Atkinson et al. (2006)
G4126	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$0.7275 \cdot 2.3\text{E-}12 \cdot \text{EXP}(360./\text{temp})$	Atkinson et al. (2006)*
G4127	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	1.2E-12	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(\text{k_CH302} \cdot 5.5\text{E-}12)^{**}(0.5) \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(\text{k_CH302} \cdot 5.7\text{E-}14 \cdot \text{EXP}(750./\text{temp}))^{**}(0.5) \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$k_{\text{ROOHR O}}$	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{ROHR O}} + k_{\text{s*f_sOOH*f_sOH}}$	Taraborrelli (2010)*
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$2.*k_{\text{ROHR O}} + k_{\text{s*f_sOH*f_sOH}}$	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)
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	$1.\text{E}-12$	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	$6.\text{E}-11$	Buras et al. (2014)
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	$k_{\text{N02_CH302}}$	see note*
G4149	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$	$k_{\text{N02_CH302}}/(9.5\text{E}-29*\text{EXP}(11234./\text{temp}))$	Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13*\text{EXP}(-650./\text{temp})*f_{\text{sOH}}$	see note*
G4151	StTrG	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 7.0\text{E}-31, 3., 1.8\text{E}-12, -1.1, 0.33)$	Atkinson et al. (2006)
G4152	StTrG	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{HCHO} + .956 \text{H} + .044 \text{CH}_3\text{O} + \text{O}_2$	$5.1\text{E}-12*\text{exp}(-210./\text{temp})$	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{HCHO} + .83 \text{H} + .17 \text{CO} + .17 \text{H}_2 + .17 \text{H}$	$1.3\text{E}-10$	Atkinson et al. (2006)
G4154	StTrG	$\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$	$2.53\text{E}-14$	Albaladejo et al. (2002)*
G4155	StTrG	$\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{CH}_3 + .75 \text{O}_2 + .25 \text{HCHO} + .25 \text{OH}$	$2.5\text{E}-11$	Baulch et al. (2005)
G4156	StTrG	$\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$	$4.3\text{E}-11$	Zellner et al. (1988)
G4157	StTrG	$\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{OH} + .7 \text{CO} + .3 \text{H} + .3 \text{CO}_2 + \text{HO}_2$	$3.4\text{E}-11*\text{EXP}(-1600./\text{temp})$	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
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	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	$\text{k_3rd}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$	Kleinböhl et al. (2006)
G4160a	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{HCN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.15 * \text{EXP}(200./\text{temp})$	Strekowski et al. (2010)
G4160b	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{NCO}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.68/2.$	Strekowski et al. (2010)*
G4160c	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{CN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * (1. - (0.68/2. + 0.15 * \text{EXP}(200./\text{temp})))$	Strekowski et al. (2010)*
G4161	TrGN	$\text{HCN} + \text{O}(^3\text{P}) \rightarrow \text{H} + \text{NCO}$	$1.0\text{E-}11 * \text{EXP}(-4000./\text{temp})$	Burkholder et al. (2015)*
G4162	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}(^3\text{P})$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.75$	Baulch et al. (2005)
G4163	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{CO} + \text{NO}$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.25$	Baulch et al. (2005)
G4164	TrGN	$\text{NCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{NO}$	$7.\text{E-}15$	Becker et al. (2000)*
G42000	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(-499./\text{temp})$	Atkinson et al. (2006)
G42001	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{OO}^*$	$9.1\text{E-}15 * \text{EXP}(-2580./\text{temp})$	Atkinson et al. (2006)*
G42002	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$\text{k_3rd_iupac}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$	Atkinson et al. (2006), Rickard (2022)
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_sOOH	Sander et al. (2019)
G42008a	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.95$	Atkinson et al. (2006)
G42008b	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.05$	Atkinson et al. (2006)
G42009	TrGCN	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HNO}_3$	KN03AL	Rickard (2022)
G42010	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$	k_CH3CO2H_OH	Atkinson et al. (2006)*
G42011a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.61$	Groß et al. (2014)
G42011b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.23$	Groß et al. (2014)

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

#	labels	reaction	rate coefficient	reference
G42011c	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$5.20\text{E}-13 \cdot \text{EXP}(980./\text{temp}) \cdot 1.507 \cdot 0.16$	Groß et al. (2014)
G42012	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E}-12 \cdot \text{EXP}(270./\text{temp})$	Tyndall et al. (2001a)
G42013	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3C03_N02	Burkholder et al. (2015)*
G42014	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G42017a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3 + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2019)
G42017b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOH}$	k1_R02RC03*0.1	Sander et al. (2019)
G42018	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	k_R00HRO	Rickard (2022)*
G42020	TrGCN	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	3.00E-14	Rickard (2022)
G42021	TrGCN	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Burkholder et al. (2015)*
G42022a	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.71	Burkholder et al. (2015)*
G42022b	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$	k_3rd(temp, cair, 5.5e-30, 0.0, 8.3e-13, -2., 0.6)*0.29	Burkholder et al. (2015)*
G42023a	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$	8.00E-12*0.80	Atkinson et al. (2006)
G42023b	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$	8.00E-12*0.20	Atkinson et al. (2006)
G42024a	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$	$5.1\text{E}-12 \cdot (1 - 1./ (1 + 1.85\text{E}-18 \cdot \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42024b	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	$5.1\text{E}-12 \cdot 1./ (1 + 1.85\text{E}-18 \cdot \text{cair})$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
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 (2022)
G42027a	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*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*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 (2022)
G42030	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$	k_CH3C03_N02	Rickard (2022)
G42031	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KR02N03*1.74	Rickard (2022)
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*f_sOH*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)

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

#	labels	reaction	rate coefficient	reference
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	$k_{\text{s*f_sOH*f_CO2H}}$	Sander et al. (2019)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G42035	TrGCN	$\text{PHAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f_sOH*f_cpan+k_ROHRO}}$	Sander et al. (2019)
G42036	TrGC	$\text{GLYOX} + \text{OH} \rightarrow \text{HCOCO} + \text{H}_2\text{O}$	$3.1\text{E-}12*\text{EXP}(340./\text{temp})$	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 (2022)
G42038a	TrGC	$\text{HCOCO} \rightarrow \text{CO} + \text{CO} + \text{HO}_2$	$7.\text{E}11*\text{EXP}(-3160./\text{temp})$ $+5.\text{E-}12*c(\text{ind_02})$	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard (2022)
G42037b	TrGC	$\text{HCOCO} \rightarrow \text{HCOCO}_3$	$5.\text{E-}12*c(\text{ind_02})*3.2*\text{exp}(-550./\text{temp})$	Lockhart et al. (2013), Rickard (2022)
G42037c	TrGC	$\text{HCOCO} \rightarrow \text{OH} + \text{CO} + \text{CO}_2$	$5.\text{E-}12*c(\text{ind_02})$ $*(1.-3.2*\text{exp}(-550./\text{temp}))$	Lockhart et al. (2013), Rickard (2022)
G42039a	TrGC	$\text{HCOCO}_3 \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2$	$k1_{\text{R02RC03}*0.9}$	Sander et al. (2019)
G42039b	TrGC	$\text{HCOCO}_3 \rightarrow \text{HCOCO}_2\text{H}$	$k1_{\text{R02RC03}*0.1}$	Sander et al. (2019)
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 (2022)
G42042	TrGCN	$\text{HCOCO}_3 + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_2 + \text{CO}_2$	$\text{KR02NO3}*1.74$	Rickard (2022)
G42043	TrGCN	$\text{HCOCO}_3 + \text{NO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{NO}_3 + \text{CO}_2$	$k_{\text{CH3CO3_NO2}}$	Orlando and Tyndall (2001), Sander et al. (2019)
G42044	TrGC	$\text{HCOCO}_2\text{H} + \text{OH} \rightarrow \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$k_{\text{CO2H+k_t*f_0*f_CO2H}}$	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	$\text{HCOCO}_3\text{H} + \text{OH} \rightarrow \text{CO} + \text{CO}_2 + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t*f_0*f_CO2H}}$	Sander et al. (2019)
G42046	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 \rightarrow .6 \text{HOCH}_2\text{CH}_2\text{O} + .2 \text{HOCH}_2\text{CHO} + .2 \text{ETHGLY}$	$2.*(7.8\text{E-}14*\text{EXP}(1000./\text{temp})$ $*k_{\text{CH302}})**(.5)*\text{R02}$	Atkinson et al. (2006), Rickard (2022)
G42047	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow .25 \text{HO}_2 + .5 \text{HCHO} + .75 \text{HOCH}_2\text{CH}_2\text{O} + \text{NO}_2$	$\text{KR02NO}*(1.-\alpha_{\text{AN}}(3,1,0,0,0, \text{temp}, \text{cair}))$	Rickard (2022)*
G42048	TrGCN	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{ETHOHNO}_3$	$\text{KR02NO}*\alpha_{\text{AN}}(3,1,0,0,0, \text{temp}, \text{cair})$	Sander et al. (2019)
G42049a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HYETHO}_2\text{H}$	$1.53\text{E-}13*\text{EXP}(1300./\text{temp})$ $*(1.-r_{\text{CHOHCH202_OH}})$	Rickard (2022)
G42049b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	$1.53\text{E-}13*\text{EXP}(1300./\text{temp})$ $*r_{\text{CHOHCH202_OH}}$	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G42050	TrGCN	ETHOHNO ₃ + OH → .93 NO ₃ CH ₂ CHO + .93 HO ₂ + .07 HOCH ₂ CHO + .07 NO ₂ + H ₂ O	k_s*(f_sOH*f_CH2ON02+f_ON02*f_pCH2OH)+k_ROHRO	Sander et al. (2019)
G42051a	TrGC	HYETHO ₂ H + OH → HOCH ₂ CH ₂ O ₂ + H ₂ O	k_ROOHR0	Rickard (2022)*
G42051b	TrGC	HYETHO ₂ H + OH → HOCH ₂ CHO + OH + H ₂ O	k_s*f_s00H*f_pCH2OH	Sander et al. (2019)
G42051c	TrGC	HYETHO ₂ H + OH → HOOCH ₂ CHO + HO ₂ + H ₂ O	k_s*f_sOH*f_pCH2OH+k_ROHRO	Sander et al. (2019)
G42052a	TrGC	HOCH ₂ CH ₂ O → HO ₂ + HOCH ₂ CHO	6.00E-14*EXP(-550./temp) *C(ind_02)	Rickard (2022)
G42052b	TrGC	HOCH ₂ CH ₂ O → HO ₂ + HCHO + HCHO	9.50E13*EXP(-5988./temp)	Rickard (2022)
G42053	TrGC	ETHGLY + OH → HOCH ₂ CHO + HO ₂ + H ₂ O	2.*k_s*f_sOH*f_pCH2OH+2.*k_ROHRO	Sander et al. (2019)
G42054	TrGC	HCOCH ₂ O ₂ → .6 HCHO + .6 CO + .6 HO ₂ + .2 GLYOX + .2 HOCH ₂ CHO	k1_R02p0R02	Sander et al. (2019)
G42055a	TrGC	HCOCH ₂ O ₂ + HO ₂ → HOOCH ₂ CHO	k_R02_H02(temp,2)*r_COCH202_00H	Sander et al. (2019)
G42055b	TrGC	HCOCH ₂ O ₂ + HO ₂ → HCHO + CO + HO ₂ + OH	k_R02_H02(temp,2)*r_COCH202_0H	Sander et al. (2019)
G42056a	TrGCN	HCOCH ₂ O ₂ + NO → NO ₂ + HCHO + CO + HO ₂	KR02N0*(1.-alpha_AN(3,1,1,0,0, temp, cair))	Sander et al. (2019)
G42056b	TrGCN	HCOCH ₂ O ₂ + NO → NO ₃ CH ₂ CHO	KR02N0*alpha_AN(3,1,1,0,0,temp, cair)	Sander et al. (2019)
G42057	TrGCN	HCOCH ₂ O ₂ + NO ₃ → HCHO + CO + HO ₂ + NO ₂	KR02N03	Sander et al. (2019)
G42058a	TrGC	HOOCH ₂ CHO + OH → HCOCH ₂ O ₂	k_ROOHR0	Sander et al. (2019)
G42058b	TrGC	HOOCH ₂ CHO + OH → HCHO + CO + OH	0.8*8.E-12	Sander et al. (2019)*
G42058c	TrGC	HOOCH ₂ CHO + OH → GLYOX + OH	k_s*f_s00H*f_CHO	Sander et al. (2019)
G42059	TrGCN	HOOCH ₂ CHO + NO ₃ → OH + HCHO + CO + HNO ₃	KN03AL	Rickard (2022)
G42060	TrGCN	HOOCH ₂ CO ₃ + NO → NO ₂ + OH + HCHO + CO ₂	KAPN0	Sander et al. (2019)
G42061	TrGCN	HOOCH ₂ CO ₃ + NO ₃ → NO ₂ + OH + HCHO + CO ₂	KR02N03*1.74	Sander et al. (2019)
G42062a	TrGC	HOOCH ₂ CO ₃ + HO ₂ → 2 OH + HCHO + CO ₂	KAPH02*r_C03_0H	Sander et al. (2019)
G42062b	TrGC	HOOCH ₂ CO ₃ + HO ₂ → HOOCH ₂ CO ₃ H	KAPH02*r_C03_00H	Sander et al. (2019)
G42062c	TrGC	HOOCH ₂ CO ₃ + HO ₂ → HOOCH ₂ CO ₂ H + O ₃	KAPH02*r_C03_03	Sander et al. (2019)
G42063a	TrGC	HOOCH ₂ CO ₃ → OH + HCHO + CO ₂	k1_R02RC03*0.9	Sander et al. (2019)
G42063b	TrGC	HOOCH ₂ CO ₃ → HOOCH ₂ CO ₂ H	k1_R02RC03*0.1	Sander et al. (2019)
G42064a	TrGC	HOOCH ₂ CO ₃ H + OH → HOOCH ₂ CO ₃ + H ₂ O	2.*k_ROOHR0	Sander et al. (2019)
G42064b	TrGC	HOOCH ₂ CO ₃ H + OH → HCOCO ₃ H + OH + H ₂ O	k_s*f_s00H*f_C02H	Sander et al. (2019)
G42065	TrGC	HOOCH ₂ CO ₂ H + OH → HCOCO ₂ H + OH + H ₂ O	k_s*f_s00H*f_C02H+k_C02H	Sander et al. (2019)
G42066	TrGC	CH ₂ CO + OH → .6 HCHO + .6 HO ₂ + .6 CO + .4 HOOCH ₂ CO ₂ H	2.8E-12*exp(510./temp)	Baulch et al. (2005), Sander et al. (2019)
G42067a	TrGC	CH ₃ CHOHOOH + OH → CH ₃ COOH + OH	(k_t*f_t00H*f_t0H + k_ROHRO)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G42067b	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$	k_R00HR0	Sander et al. (2019)
G42068	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$3.46\text{E}12 \cdot \text{EXP}(-12500./ (1.98 \cdot \text{temp}))$	Hermans et al. (2005), Sander et al. (2019)
G42069	TrGC	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$	$3.46\text{E}12 \cdot \text{EXP}(-12500./ (1.98 \cdot \text{temp})) / (6.34\text{E}26 \cdot \text{EXP}(-14700./ (1.98 \cdot \text{temp})))$	Hermans et al. (2005), Sander et al. (2019)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{ CH}_3\text{CHOHOOH} + .3 \text{ CH}_3\text{COOH} + .2 \text{ CH}_3 + .2 \text{ HCOOH} + .2 \text{ OH}$	$5.6\text{E}-15 \cdot \text{EXP}(2300./ \text{temp})$	Sander et al. (2019)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	k1_R02s0R02	Sander et al. (2019)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KR02NO	Sander et al. (2019)
G42073	TrGCN	$\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$	$6.7\text{E}-13 \cdot \text{EXP}(-395./ \text{temp})$	Atkinson et al. (2006)
G42074a	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{NO}_2 + \text{H}_2\text{O}$	k_s*f_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)*
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 (2022)*
G42076	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
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 (2022)
G42078	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$	k1_R02RC03	Rickard (2022)*
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 (2022)
G42080	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2\text{NO}_2$	k_3rd_iupac(temp, cair, 1.3E-29, 6.2, 8.8E-12, 0.0, 0.31)	Atkinson et al. (2006)
G42081	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$	k_3rd_iupac(temp, cair, REAL(4.8E-4*EXP(-9285./temp), SP), 0.0, REAL(8.8E15*EXP(-10440./temp), SP), 0.0, 0.31)	Atkinson et al. (2006)
G42082	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./ \text{temp})$	Sander et al. (2019)*
G42083a	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$5.1\text{E}-12 \cdot (1. - 1./ (1. + 9.4\text{E}-18 \cdot \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42083b	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$	$5.1\text{E}-12 \cdot 1./ (1. + 9.4\text{E}-18 \cdot \text{cair})$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{ C}_2\text{H}_5\text{O}_2 + .95 \text{ HO}_2 + .05 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$3.0\text{E}-12 \cdot \text{EXP}(20./ \text{temp})$	Sander et al. (2019), Atkinson et al. (2006)
G42085a	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$	$8.1\text{E}-13 \cdot \text{EXP}(-1080./ \text{temp}) \cdot 0.40$	Atkinson et al. (2006), Tyndall et al. (2001b)*

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

#	labels	reaction	rate coefficient	reference
G42085b	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$	$8.1\text{E}-13 \cdot \text{EXP}(-1080./\text{temp}) \cdot (1.-0.40)$	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$	$2.54\text{E}-10 \cdot \text{EXP}(-24./\text{temp}) \cdot 0.0269 \cdot \text{EXP}(137./\text{temp})$	Strekowski et al. (2010)
G42086b	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{H} + \text{CO} + \text{HCN}$	$2.54\text{E}-10 \cdot \text{EXP}(-24./\text{temp}) \cdot 0.16$	Strekowski et al. (2010)*
G42086c	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{CH}_3 + .5 \text{NCO} + .5 \text{NCCH}_2\text{O}_2 + .5 \text{OH}$	$2.54\text{E}-10 \cdot \text{EXP}(-24./\text{temp}) \cdot (1. - (0.16 + 0.0269 \cdot \text{EXP}(137./\text{temp})))$	Strekowski et al. (2010)*
G42087	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N0	see note*
G42088	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$	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)*
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*

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

#	labels	reaction	rate coefficient	reference
G42098b	TrGC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$2.0 * k_{\text{rohro}}$	see note*
G42098c	TrGC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{CHOCHOHOH} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f_pch2oh*f_sooh}}$	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	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	$2.*k_{\text{p}}$	Sander et al. (2019)
G43001a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{ CH}_3\text{CHOHOOH} + .50 \text{ OH} + .50 \text{ HCOCH}_2\text{O}_2 + .05 \text{ CH}_2\text{CO} + .09 \text{ CH}_3\text{OH} + .09 \text{ CO} + .2 \text{ CH}_4 + .2 \text{ CO}_2$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.57$	Atkinson et al. (2006)*
G43001b	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{OO}^*$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.43$	Atkinson et al. (2006)*
G43002	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO}_2$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 8.6\text{E-}27, 3.5, 3.\text{E-}11, 1., 0.5)$	Atkinson et al. (2006), Rickard (2022)
G43003	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO}_3\text{BO}_2$	$4.6\text{E-}13*\text{EXP}(-1155./\text{temp})$	Wallington et al. (2018)
G43004	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$1.9\text{E-}13*\text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43005a	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Wallington et al. (2018)
G43005b	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{ONO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair})$	Wallington et al. (2018)
G43006	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{ CH}_3\text{COCH}_3 + .2 \text{ IPROPOL} + .6 \text{ HO}_2$	$2.*(1.6\text{E-}12*\text{EXP}(-2200./\text{temp})*k_{\text{CH302}})**(.5)*\text{R02}$	Rickard (2022), Atkinson et al. (2006)
G43007a	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_{R00HRO}	Sander et al. (2019)
G43007b	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t*f_t00H}}$	Sander et al. (2019)
G43008	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	$1.9\text{E-}13*\text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43009a	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Wallington et al. (2018)
G43009b	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_3\text{H}_7\text{ONO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*\alpha_{\text{AN}}(3, 1, 0, 0, 0, \text{temp}, \text{cair})$	Wallington et al. (2018)
G43010	TrGC	$\text{C}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{ CH}_3\text{COCH}_3 + .2 \text{ NPROPOL} + .6 \text{ HO}_2$	$2.*(k_{\text{CH302}}*3.\text{E-}13)**(.5)*\text{R02}$	Rickard (2022), Atkinson et al. (2006)
G43011	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$(8.8\text{E-}12*\text{EXP}(-1320./\text{temp}) + 1.7\text{E-}14*\text{EXP}(423./\text{temp}))$	Atkinson et al. (2006)*
G43012a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E-}13*\text{EXP}(700./\text{temp})*r_{\text{C0CH202_00H}}$	Tyndall et al. (2001a), Sander et al. (2019)
G43012b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{HCHO}$	$8.6\text{E-}13*\text{EXP}(700./\text{temp})*r_{\text{C0CH202_0H}}$	Tyndall et al. (2001a), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G43013a	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12 \cdot \text{EXP}(300./\text{temp}) \cdot (1.-\alpha_{\text{AN}}(4,1,1,0,0,\text{temp},\text{cair}))$	Burkholder et al. (2015)
G43013b	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NOA}$	$2.9\text{E}-12 \cdot \text{EXP}(300./\text{temp}) \cdot \alpha_{\text{AN}}(4,1,1,0,0,\text{temp},\text{cair})$	Burkholder et al. (2015)
G43014	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .3 \text{CH}_3\text{C}(\text{O}) + .3 \text{HCHO} + .5 \text{MGLYOX} + .2 \text{CH}_3\text{COCH}_2\text{OH}$	k1_R02p0R02	Orlando and Tyndall (2012)
G43015a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	k_R00HRO	see note*
G43015b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	k_s*f_s00H*f_CO	Sander et al. (2019)
G43016	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$1.6\text{E}-12 \cdot \text{EXP}(305./\text{temp})$	Atkinson et al. (2006)
G43017	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{CH}_3 + .6 \text{CH}_3\text{C}(\text{O}) + 1.4 \text{CO} + \text{H}_2\text{O}$	$1.9\text{E}-12 \cdot \text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E}-13 \cdot \text{EXP}(-230./\text{temp})$	Wallington et al. (2018)
G43021	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	KR02NO3	Rickard (2022)
G43022	TrGC	$\text{HYPROPO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	k1_R02s0R02	Rickard (2022)
G43023a	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{HYPROPO}_2\text{H}$	$k_{\text{R02_HO2}}(\text{temp},3) \cdot (1.-r_{\text{CHOHCH2O2_OH}})$	Rickard (2022)
G43023b	TrGC	$\text{HYPROPO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp},3) \cdot r_{\text{CHOHCH2O2_OH}}$	Rickard (2022)
G43024a	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02NO} \cdot (1.-\alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair}))$	Rickard (2022)
G43024b	TrGCN	$\text{HYPROPO}_2 + \text{NO} \rightarrow \text{PROPOLNO}_3$	$\text{KR02NO} \cdot \alpha_{\text{AN}}(4,1,0,0,0,\text{temp},\text{cair})$	Rickard (2022)
G43025	TrGCN	$\text{HYPROPO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Rickard (2022)
G43026a	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{HYPROPO}_2$	k_R00HRO	Rickard (2022)
G43026b	TrGC	$\text{HYPROPO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{\text{s*f_s0H*f_pCH2OH}} + k_{\text{t*f_t00H*f_pCH2OH}})$	Sander et al. (2019)
G43027	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{HO}_2 \rightarrow \text{PR}_2\text{O}_2\text{HNO}_3$	$k_{\text{R02_HO2}}(\text{temp},3)$	Rickard (2022)
G43028	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02NO	Rickard (2022)*
G43029	TrGCN	$\text{PRONO}_3\text{BO}_2 + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	KR02NO3	Rickard (2022)
G43030a	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{PRONO}_3\text{BO}_2$	k_R00HRO	Rickard (2022)
G43030b	TrGCN	$\text{PR}_2\text{O}_2\text{HNO}_3 + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{\text{t*f_t00H*f_CH2ON02}}$	Sander et al. (2019)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HNO}_3$	$\text{KN03AL} \cdot 2.4$	Rickard (2022)
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	$\text{HOCH}_2\text{COCHO} + \text{OH} \rightarrow .8609 \text{HOCH}_2\text{CO} + .8609 \text{CO} + .1391 \text{HCOCOCHO} + .1391 \text{HO}_2$	$(1.9\text{E}-12 \cdot \text{EXP}(575./\text{temp}) + k_{\text{s*f_s0H*f_CO}})$	Sander et al. (2019)
G43034	TrGCN	$\text{HOCH}_2\text{COCHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL} \cdot 2.4$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E}-14 \cdot \text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Sander et al. (2019)
G43036	TrGC	$\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{ HCOCO} + .6 \text{ HCHO} + .2 \text{ HCOCOCHO} + .2 \text{ HOCH}_2\text{COCHO}$	$k_{1_R02p0R02}$	Sander et al. (2019)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{_R02_H02}(\text{temp}, 3) \cdot r_{_COCH202_00H}$	Sander et al. (2019)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$k_{_R02_H02}(\text{temp}, 3) \cdot r_{_COCH202_0H}$	Sander et al. (2019)
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{_t \cdot f_CO \cdot f_0}$	Sander et al. (2019)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{_s \cdot f_s00H \cdot f_CO}$	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	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	$\text{KN03AL} \cdot 2.4$	Sander et al. (2019)
G43042	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO}$	$k_{1_R02p0R02}$	Sander et al. (2019)
G43043a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$k_{_R02_H02}(\text{temp}, 3) \cdot r_{_COCH202_00H}$	Sander et al. (2019)
G43043b	TrGC	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{OH}$	$k_{_R02_H02}(\text{temp}, 3) \cdot r_{_COCH202_0H}$	Sander et al. (2019)
G43044	TrGCN	$\text{HOCH}_2\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{HOCH}_2\text{CO} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G43045a	TrGC	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{COCHO} + \text{OH}$	$k_{_s \cdot f_s00H \cdot f_CO}$	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	$\text{HOCH}_2\text{COCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E}-12 \cdot \text{EXP}(305./\text{temp})$	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	$\text{PROPOLNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{_t \cdot f_ON02 \cdot f_pCH20H} + k_{_s \cdot f_s0H \cdot f_CH20N02}$	Sander et al. (2019)
G43048	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(300./\text{temp})$	Tyndall et al. (2001a)*
G43049	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2$	$1.9\text{E}16 \cdot \text{EXP}(-10830./\text{temp})$	Sehested et al. (1998)*
G43050	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp}) \cdot f_{_CO}$	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	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{_s \cdot f_s00H}$	Sander et al. (2019)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{_s \cdot f_pCH20H}$	Sander et al. (2019)*
G43052	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$4.9\text{E}-12 \cdot \text{EXP}(405./\text{temp})$	Atkinson et al. (2006)*
G43053	TrGCN	$\text{C}_2\text{H}_5\text{CHO} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HNO}_3$	$6.3\text{E}-15$	Atkinson et al. (2006)
G43054a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	$k_{1_R02RC03} \cdot 0.9$	Sander et al. (2019)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	$k_{1_R02RC03} \cdot 0.1$	Sander et al. (2019)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot r_{_C03_0H}$	Sander et al. (2019), Groß et al. (2014)

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

#	labels	reaction	rate coefficient	reference
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_00H	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_03	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 (2022)
G43057	TrGCN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	k_CH3C03_N02	Rickard (2022)
G43058	TrGCN	$\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard (2022)
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_C02H+k_p+k_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_s*f_C02H+k_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_s*f_cpan+k_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	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Sander et al. (2019)
G43063b	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	KAPH02*(r_C03_00H+r_C03_03)	Sander et al. (2019)
G43064	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_2$	KAPNO	Sander et al. (2019)
G43065	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2 + \text{NO}_3$	k_CH3C03_N02	Sander et al. (2019)*
G43066	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Sander et al. (2019)
G43067	TrGC	$\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}_2$	k1_R02RC03	Sander et al. (2019)
G43068	TrGC	$\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{CO} + \text{HO}_2$	2.*k_t*f_CO*f_0	Sander et al. (2019)
G43069	TrGC	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$	2.6E-12*EXP(200./temp)	Atkinson et al. (2006)
G43070a	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	4.6E-12*EXP(70./temp)*(k_s*f_sOH/(k_p+k_s*f_pCH2OH+k_s*f_sOH))	Atkinson et al. (2006), Sander et al. (2019)*
G43070b	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO}_2 + \text{H}_2\text{O}$	4.6E-12*EXP(70./temp)*((k_p+k_s*f_pCH2OH)/(k_p+k_s*f_pCH2OH+k_s*f_sOH))	Atkinson et al. (2006), Sander et al. (2019)*
G43071a	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$	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	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$	k_s*f_s00H*f_CO+k_R00HRO	Sander et al. (2019)*
G43075a	TrGC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOOH} + \text{H}_2\text{O}$	2.0 * k_rohro	see note*
G43075b	TrGC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_2\text{H} + \text{H}_2\text{O}$	k_t*f_toh*f_toh*f_co	see note*
G43202	TrGTerC	$\text{HCOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{CO}_3$	4.29E-11	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G43203	TrGTerCN	$\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$	$2.*\text{KN03AL}*2.4$	Rickard (2022)
G43204a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{k1_R02RC03}*0.9$	Sander et al. (2019)
G43204b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$\text{k1_R02RC03}*0.1$	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 (2022)
G43206	TrGTerCN	$\text{HCOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN}_2$	k_CH3C03_N02	Rickard (2022)
G43207a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02}*r_C03_00\text{H}$	Rickard (2022)
G43207b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02}*r_C03_03$	Rickard (2022)
G43207c	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_C03_0\text{H}$	Rickard (2022)
G43210	TrGTerCN	$\text{C}_3\text{PAN}_2 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard (2022)
G43211	TrGTerCN	$\text{C}_3\text{PAN}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	$2.10\text{E}-11$	Rickard (2022)
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 (2022)
G43213a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$\text{k1_R02RC03}*0.9$	Sander et al. (2019)
G43213b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$\text{k1_R02RC03}*0.1$	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 (2022)
G43215a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$\text{KAPH02}*r_C03_00\text{H}$	Rickard (2022)
G43215b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_C03_0\text{H}$	Rickard (2022)
G43215c	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02}*r_C03_03$	Rickard (2022)
G43218	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN}_1$	k_CH3C03_N02	Rickard (2022)
G43219	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$1.39\text{E}-11$	Rickard (2022)
G43220	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3$	$1.73\text{E}-11$	Rickard (2022)
G43221	TrGTerCN	$\text{C}_3\text{PAN}_1 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard (2022)
G43222	TrGTerCN	$\text{C}_3\text{PAN}_1 + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{CO} + \text{NO}_2$	$4.51\text{E}-12$	Rickard (2022)
G43223	TrGTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$2.49\text{E}-11$	Rickard (2022)*
G43415	TrGAroC	$\text{C3DIALOOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{OH}$	$1.44\text{E}-10$	Rickard (2022)
G43418a	TrGAroC	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{C3DIALOOH}$	$\text{k_R02_H02}(\text{temp}, 3) * (\text{r_C03_00H} + \text{r_C03_03})$	Rickard (2022)
G43418b	TrGAroC	$\text{C3DIALO}_2 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{k_R02_H02}(\text{temp}, 3) * \text{r_C03_0H}$	Rickard (2022)
G43419	TrGAroCN	$\text{C3DIALO}_2 + \text{NO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G43420	TrGAroCN	$\text{C3DIALO}_2 + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*
G43421	TrGAroC	$\text{C3DIALO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard (2022)*
G43422a	TrGAroC	$\text{HCOCOHHCO}_3 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$\text{KAPH02}*r_C03_0\text{H}$	Rickard (2022)
G43422b	TrGAroC	$\text{HCOCOHHCO}_3 + \text{HO}_2 \rightarrow \text{HCOCOHHCO}_3\text{H}$	$\text{KAPH02} * (\text{r_C03_00H} + \text{r_C03_03})$	Rickard (2022)
G43424	TrGAroCN	$\text{HCOCOHHCO}_3 + \text{NO} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G43425	TrGAroCN	$\text{HCOCOHHCO}_3 + \text{NO}_2 \rightarrow \text{HCOCOHPAN}$	k_CH3C03_N02	Rickard (2022)
G43426	TrGAroCN	$\text{HCOCOHHCO}_3 + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03}*1.74$	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G43427	TrGAroC	$\text{HCOCOHCO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03	Rickard (2022)
G43428	TrGAroC	$\text{METACETHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO}_2$	9.82E-11	Rickard (2022)
G43442	TrGAroCN	$\text{HCOCOH PAN} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	6.97E-11	Rickard (2022)
G43443	TrGAroCN	$\text{HCOCOH PAN} \rightarrow \text{HCOCOHCO}_3 + \text{NO}_2$	k_PAN_M	Rickard (2022)
G43444	TrGAroC	$\text{C}_3\text{OH}_2\text{CO} + \text{OH} \rightarrow \text{HCOCOHCO}_3$	1.36E-10	Rickard (2022)
G43446	TrGAroC	$\text{HCOCOHCO}_3\text{H} + \text{OH} \rightarrow \text{HCOCOHCO}_3$	7.33E-11	Rickard (2022)
G44000	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$2.03\text{E}-17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(78./\text{temp})$	Atkinson et al. (2006)*
G44001a	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$(k1_R02pR02 \cdot 0.1273 + k1_R02sR02 \cdot 0.8727) \cdot 0.1273$	Rickard (2022), Sander et al. (2019)
G44001b	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$(k1_R02pR02 \cdot 0.1273 + k1_R02sR02 \cdot 0.8727) \cdot 0.8727$	Rickard (2022), 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 (2022)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N0} \cdot (1 - (0.1273 \cdot \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 \cdot \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) \cdot 0.1273$	Rickard (2022), Sander et al. (2019)
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N0} \cdot (1 - (0.1273 \cdot \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 \cdot \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) \cdot 0.8727$	Rickard (2022), Sander et al. (2019)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC}_4\text{H}_9\text{NO}_3$	$\text{KR02N0} \cdot (0.1273 \cdot \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 \cdot \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard (2022)*
G44004a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N03} \cdot 0.1273$	Rickard (2022), Sander et al. (2019)
G44004b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N03} \cdot 0.8727$	Rickard (2022), 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_R00HR0	Sander et al. (2019)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_s \cdot f_t00H \cdot f_alk \cdot (k_p / (k_p + k_s))$	Sander et al. (2019)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_t \cdot f_t00H \cdot f_alk \cdot (k_s / (k_p + k_s))$	Sander et al. (2019)
G44006a	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp}) \cdot k_t / (3 \cdot k_p + k_t)$	Atkinson (2003)
G44006b	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E}-17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp}) \cdot 3 \cdot k_p / (3 \cdot k_p + k_t)$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	k1_R02tR02	Rickard (2022), 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_R02_H02(temp, 4)	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G44009a	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(4,3,0,0,0,\text{temp},\text{cair}))$	Rickard (2022), Sander et al. (2019)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC4H9NO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(4,3,0,0,0,\text{temp},\text{cair})$	Rickard (2022)
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	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k1_{\text{R02sR02}}$	Rickard (2022), 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 (2022)
G44014a	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair}))$	Rickard (2022), Sander et al. (2019)
G44014b	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC4H9NO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(4,2,0,0,0,\text{temp},\text{cair})$	Rickard (2022)
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)
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{sOOH}}+2.*k_{\text{s}}+k_{\text{t}}*f_{\text{pCH2OH}}$	Sander et al. (2019)*
G44016	TrGCN	$\text{IC4H9NO3} + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}}*f_{\text{ON02}}+2.*k_{\text{p}}+k_{\text{t}}*f_{\text{CH2ON02}}$	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	$\text{MVK} + \text{OH} \rightarrow \text{LHMKABO2}$	$2.6\text{E-}12*\text{EXP}(610./\text{temp})$	Sander et al. (2019), Atkinson et al. (2006)*
G44019	TrGC	$\text{MEK} + \text{OH} \rightarrow \text{LMEKO2} + \text{H}_2\text{O}$	$1.5\text{E-}12*\text{EXP}(-90./\text{temp})$	Atkinson et al. (2006), Sander et al. (2019)*
G44020	TrGC	$\text{LMEKO2} + \text{HO}_2 \rightarrow \text{LMEKOOH}$	$k_{\text{R02_H02}}(\text{temp},4)$	Sander et al. (2019)
G44021a	TrGCN	$\text{LMEKO2} + \text{NO} \rightarrow .62 \text{ CH}_3\text{CHO} + .62 \text{ CH}_3\text{C(O)} + .38 \text{ HCHO} + .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-(.62*\alpha_{\text{AN}}(4,2,1,0,0,\text{temp},\text{cair})+.38*\alpha_{\text{AN}}(4,1,0,1,0,\text{temp},\text{cair})))$	Sander et al. (2019)*
G44021b	TrGCN	$\text{LMEKO2} + \text{NO} \rightarrow \text{LMEKNO3}$	$\text{KR02N0}*(.62*\alpha_{\text{AN}}(4,2,1,0,0,\text{temp},\text{cair})+.38*\alpha_{\text{AN}}(4,1,0,1,0,\text{temp},\text{cair}))$	Sander et al. (2019)
G44022a	TrGC	$\text{LMEKOOH} + \text{OH} \rightarrow \text{LMEKO2} + \text{H}_2\text{O}$	k_{ROOHR0}	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
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	$\text{LC4H9NO}_3 + \text{OH} \rightarrow \text{MEK} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{t}}*f_{\text{ON02}}*f_{\text{alk}}+k_{\text{p}}*f_{\text{alk}}+k_{\text{s}}*f_{\text{CH2ON02}}+k_{\text{p}})*(k_{\text{s}}/(k_{\text{p}}+k_{\text{s}}))$	Sander et al. (2019)*
G44023b	TrGCN	$\text{LC4H9NO}_3 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{NO}_2 + \text{H}_2\text{O}$	$(k_{\text{p}}+k_{\text{s}}*(1.+f_{\text{CH2ON02}}+f_{\text{ON02}})*f_{\text{alk}})*(k_{\text{p}}/(k_{\text{p}}+k_{\text{s}}))$	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	$\text{LMEKO}_2 \rightarrow .538 \text{ HCHO} + .538 \text{ CO}_2 + .459 \text{ HOCH}_2\text{CH}_2\text{O}_2 + .079 \text{ C}_2\text{H}_5\text{O}_2 + .462 \text{ CH}_3\text{C(O)} + .462 \text{ CH}_3\text{CHO}$	$(.62*k_{\text{1_R02s0R02}}+.38*k_{\text{1_R02p0R02}})$	Rickard (2022)*
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)
G44029	TrGCN	$\text{MACR} + \text{NO}_3 \rightarrow \text{MACO}_3 + \text{HNO}_3$	$\text{KN03AL}*2.0$	Rickard (2022)
G44030a	TrGC	$\text{MACO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{CO}_2$	$k_{\text{1_R02RC03}}*0.9$	Sander et al. (2019)
G44030b	TrGC	$\text{MACO}_3 \rightarrow \text{MACO}_2\text{H}$	$k_{\text{1_R02RC03}}*0.1$	Sander et al. (2019)
G44031a	TrGC	$\text{MACO}_3 + \text{HO}_2 \rightarrow \text{MACO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{C03_OH}}$	Sander et al. (2019)
G44031b	TrGC	$\text{MACO}_3 + \text{HO}_2 \rightarrow \text{MACO}_3\text{H}$	$\text{KAPH02}*r_{\text{C03_00H}}$	Sander et al. (2019)
G44031c	TrGC	$\text{MACO}_3 + \text{HO}_2 \rightarrow \text{MACO}_2\text{H} + \text{O}_3$	$\text{KAPH02}*r_{\text{C03_03}}$	Sander et al. (2019)
G44032	TrGCN	$\text{MACO}_3 + \text{NO} \rightarrow \text{MACO}_2 + \text{NO}_2$	$8.70\text{E}-12*\text{EXP}(290./\text{temp})$	Sander et al. (2019)
G44033	TrGCN	$\text{MACO}_3 + \text{NO}_2 \rightarrow \text{MPAN}$	$k_{\text{CH3C03_N02}}$	Rickard (2022)
G44034	TrGCN	$\text{MACO}_3 + \text{NO}_3 \rightarrow \text{MACO}_2 + \text{NO}_2$	$\text{KR02N03}*1.74$	Sander et al. (2019)
G44035	TrGC	$\text{MACRO}_2 \rightarrow .7 \text{ CH}_3\text{COCH}_2\text{OH} + .7 \text{ HCHO} + .7 \text{ HO}_2 + .3 \text{ MACROH}$	$k_{\text{1_R02t0R02}}$	Rickard (2022)*
G44036a	TrGC	$\text{MACRO}_2 + \text{HO}_2 \rightarrow \text{MACRO} + \text{OH}$	$k_{\text{R02_H02}}(\text{temp},4)*r_{\text{COCH202_OH}}$	Sander et al. (2019)
G44036b	TrGC	$\text{MACRO}_2 + \text{HO}_2 \rightarrow \text{MACROOH}$	$k_{\text{R02_H02}}(\text{temp},4)*r_{\text{COCH202_00H}}$	Sander et al. (2019)
G44037a	TrGCN	$\text{MACRO}_2 + \text{NO} \rightarrow \text{MACRO} + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(6,3,1,0,0,\text{temp},\text{cair}))$	Sander et al. (2019)
G44037b	TrGCN	$\text{MACRO}_2 + \text{NO} \rightarrow \text{MACRNO}_3$	$\text{KR02N0}*\alpha_{\text{AN}}(6,3,1,0,0,\text{temp},\text{cair})$	Sander et al. (2019)
G44038	TrGCN	$\text{MACRO}_2 + \text{NO}_3 \rightarrow \text{MACRO} + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44039a	TrGC	$\text{MACROOH} + \text{OH} \rightarrow \text{MACRO}_2$	k_{ROOHRO}	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44039b	TrGC	MACROOH + OH \rightarrow CO + CH ₃ COCH ₂ OH + OH	k_t*f_0*f_tCH2OH*f_alk	Sander et al. (2019)
G44039c	TrGC	MACROOH + OH \rightarrow CO + MGLYOX + HO ₂	(k_s*f_sOH*f_pCH2OH + k_R0HRO)	Sander et al. (2019)
G44040	TrGC	MACROH + OH \rightarrow CH ₃ COCH ₂ OH + CO + HO ₂	k_t*f_0*f_tCH2OH*f_alk	Sander et al. (2019)
G44041	TrGC	MACRO \rightarrow .885 CH ₃ COCH ₂ OH + .885 CO + .115 MGLYOX + .115 HCHO + HO ₂	KDEC	Sander et al. (2019)
G44042	TrGC	MACO2H + OH \rightarrow CH ₃ COCH ₂ OH + HO ₂ + CO ₂	((k_adt+k_adp)*a_CO2H+k_CO2H)	Sander et al. (2019)
G44043a	TrGC	MACO3H + OH \rightarrow CH ₃ COCH ₂ OH + CO ₂ + OH	(k_adt+k_adp)*a_CO2H	Sander et al. (2019)
G44043b	TrGC	MACO3H + OH \rightarrow MACO3	k_R00HRO	Sander et al. (2019)
G44044	TrGC	LHMKABO2 \rightarrow .024 CO2H3CHO + .072 MGLYOX + .072 HO ₂ + .072 HCHO + .5280 CH ₃ C(O) + .5280 HOCH ₂ CHO + .176 BIACETOH + .2 HO12CO3C4	(.12*k1_R02pOR02+.88*k1_R02sOR02)	Sander et al. (2019)
G44045a	TrGC	LHMKABO2 + HO ₂ \rightarrow OH + HOCH ₂ CHO + CH ₃ C(O)	k_R02_HO2(temp,4)*.88*r_COCH2O2_OH	Sander et al. (2019)
G44045b	TrGC	LHMKABO2 + HO ₂ \rightarrow LHMKABOOH	k_R02_HO2(temp,4)*((.12+.88*r_COCH2O2_OO)H)	Sander et al. (2019)
G44046a	TrGCN	LHMKABO2 + NO \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + NO ₂	KR02NO*(1-(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair)))	Sander et al. (2019)
G44046b	TrGCN	LHMKABO2 + NO \rightarrow MVKNO3	KR02NO*(.12*alpha_AN(6,1,0,1,0,temp,cair)+.88*alpha_AN(6,2,1,0,0,temp,cair))	Sander et al. (2019)*
G44047	TrGCN	LHMKABO2 + NO ₃ \rightarrow .12 MGLYOX + .12 HO ₂ + .88 HOCH ₂ CHO + .88 CH ₃ C(O) + .12 HCHO + .12 HO ₂ + NO ₂	KR02NO3	Sander et al. (2019)
G44048a	TrGC	LHMKABOOH + OH \rightarrow LHMKABO2	k_R00HRO	Sander et al. (2019)
G44048b	TrGC	LHMKABOOH + OH \rightarrow .12 CO2H3CHO + .88 BIACETOH + OH	(.12*k_s*f_sOOH*f_pCH2OH+.88*k_t*f_tOOH*f_pCH2OH*f_CO)	Sander et al. (2019)
G44049a	TrGC	CO2H3CHO + OH \rightarrow CO2H3CO3	k_t*f_0*f_alk	Sander et al. (2019)
G44049b	TrGC	CO2H3CHO + OH \rightarrow CH ₃ COCOCHO + HO ₂ + H ₂ O	k_t*f_CO*f_tOH*f_CHO	Sander et al. (2019)
G44050	TrGCN	CO2H3CHO + NO ₃ \rightarrow CO2H3CO3 + HNO ₃	KN03AL*4.0	Rickard (2022)
G44051	TrGC	CO2H3CO3 \rightarrow MGLYOX + HO ₂ + CO ₂	k1_R02RCO3	Sander et al. (2019)
G44052a	TrGC	CO2H3CO3 + HO ₂ \rightarrow OH + MGLYOX + HO ₂ + CO ₂	KAPH02*r_CO3_OH	Sander et al. (2019)
G44052b	TrGC	CO2H3CO3 + HO ₂ \rightarrow CO2H3CO2H + O ₃	KAPH02*r_CO3_O3	Sander et al. (2019)
G44052c	TrGC	CO2H3CO3 + HO ₂ \rightarrow CO2H3CO3H	KAPH02*r_CO3_OOH	Sander et al. (2019)
G44053	TrGCN	CO2H3CO3 + NO \rightarrow MGLYOX + HO ₂ + NO ₂ + CO ₂	KAPNO	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44054	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$\text{KRO2NO3} \cdot 1.74$	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	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{OH}$	$(k_{\text{t}*\text{f}_{\text{CO2H}*}\text{f}_{\text{CO}*}\text{f}_{\text{tOH}})$	Sander et al. (2019)
G44056	TrGC	$\text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCOCOC}_2\text{H} + \text{HO}_2$	$k_{\text{t}*\text{f}_{\text{CO2H}*}\text{f}_{\text{CO}*}\text{f}_{\text{tOH}}+k_{\text{CO2H}}}$	Sander et al. (2019)
G44057a	TrGC	$\text{HO}_2\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{BIACETOH} + \text{HO}_2$	$k_{\text{t}*\text{f}_{\text{tOH}*}\text{f}_{\text{alk}*}\text{f}_{\text{CO}}}$	Sander et al. (2019)
G44057b	TrGC	$\text{HO}_2\text{CO}_3\text{C}_4 + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$	$k_{\text{s}*\text{f}_{\text{sOH}*}\text{f}_{\text{alk}}}$	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	$\text{LHMVKABO}_2 \rightarrow .88 \text{MGLYOX} + .88 \text{HCHO} + .12 \text{HOOCH}_2\text{CHO} + .12 \text{CH}_3\text{C}(\text{O}) + \text{OH}$	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	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}*\text{f}_{\text{sOOH}*}\text{f}_{\text{CH2ON02}}+k_{\text{ROHR0}}}$	Sander et al. (2019)*
G44061b	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{BIACETOH} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t}*\text{f}_{\text{ON02}*}\text{f}_{\text{CO}*}\text{f}_{\text{pCH2OH}}}$	Sander et al. (2019)*
G44062a	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t}*\text{f}_{\text{O}*}\text{f}_{\text{CH2ON02}}}$	Sander et al. (2019)*
G44062b	TrGCN	$\text{MACRNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{ROHR0}}+k_{\text{s}*\text{f}_{\text{sOOH}*}\text{f}_{\text{CH2ON02}}}$	Sander et al. (2019)*
G44063	TrGC	$\text{MACRO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH} + \text{CO}$	$k_{14\text{hsa1}}$	Sander et al. (2019)
G44064	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow .9 \text{CH}_3\text{COCHCO} + .1 \text{CH}_3\text{C}(\text{O}) + .01 \text{GLYOX} + .18 \text{CO} + .09 \text{HO}_2 + \text{OH}$	$k_{15\text{hs24vynal}}$	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	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	KRO2NO	Sander et al. (2019)*
G44067	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	KRO2NO3	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	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KRO2NO	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	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO}_3 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	KRO2NO3	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	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$	KRO2NO	Sander et al. (2019)*
G44077	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$	KRO2NO3	Sander et al. (2019)
G44078	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 4)$	Sander et al. (2019)*
G44079	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX}$	$k_{1_R02\text{sOR02}}$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44080	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$	$k1_R02t0R02$	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	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_R02_H02(\text{temp}, 4)$	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	$\text{HCOCCH}_3\text{CO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$1\text{E}-10*a_CH0$	Hatakeyama et al. (1985), Sander et al. (2019)
G44085	TrGC	$\text{CH}_3\text{COCHCO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	$7.6\text{E}-11*a_COCH3$	Hatakeyama et al. (1985), Sander et al. (2019)*
G44086	TrGCN	$\text{LMEKNO}_3 + \text{OH} \rightarrow .62 \text{ MGLYOX} + .62 \text{ HCHO} + .62 \text{ HO}_2 + .62 \text{ NO}_2 + .38 \text{ CH}_3\text{C(O)} + .38 \text{ NO}_3\text{CH}_2\text{CHO}$	$.62*(k_p*(f_CO+f_CH2ON02)) + .38*(k_s*f_CH2ON02*f_CO)$	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)
G44088a	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_2\text{OO}^*$	$2.7\text{E}-15*\text{EXP}(-1630./\text{temp})*0.33$	Atkinson et al. (2006), Sander et al. (2019)
G44088b	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{OH} + \text{HCHO}$	$2.7\text{E}-15*\text{EXP}(-1630./\text{temp})*0.67$	Atkinson et al. (2006), Sander et al. (2019)
G44089	TrGCN	$\text{MEPROPENE} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2$	$3.4\text{E}-13$	Atkinson et al. (2006), Sander et al. (2019)*
G44090	TrGC	$\text{IBUTOLBO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$	$k1_R02t0R02$	Sander et al. (2019)
G44091a	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{IBUTOLBOOH}$	$k_R02_H02(\text{temp}, 4)*r_COCH202_00H$	Sander et al. (2019)
G44091b	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	$k_R02_H02(\text{temp}, 4)*r_COCH202_0H$	Sander et al. (2019)
G44092a	TrGCN	$\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_AN(5,3,0,0,0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44092b	TrGCN	$\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{IBUTOLBNO}_3$	$\text{KR02N0}*\alpha_AN(5,3,0,0,0, \text{temp}, \text{cair})$	Sander et al. (2019)
G44093	TrGCN	$\text{IBUTOLBO}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Sander et al. (2019)
G44094a	TrGC	$\text{IBUTOLBOOH} + \text{OH} \rightarrow \text{IBUTOLBO}_2$	k_R00HRO	Sander et al. (2019)
G44094b	TrGC	$\text{IBUTOLBOOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$	$k_s*f_s00H*f_pCH20H$	Sander et al. (2019)
G44095	TrGCN	$\text{IBUTOLBNO}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$3.*k_p$	Sander et al. (2019)
G44096	TrGC	$\text{BUT1ENE} + \text{OH} \rightarrow \text{LBUT1ENO}_2$	$6.6\text{E}-12*\text{EXP}(465./\text{temp})$	Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
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_00H	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_0H	Sander et al. (2019)
G44101a	TrGCN	LBUT1ENO2 + NO → C ₂ H ₅ CHO + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(5,2,0,0,0, temp, cair))	Sander et al. (2019)
G44101b	TrGCN	LBUT1ENO2 + NO → LBUT1ENNO3	KR02N0*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2019)
G44102	TrGCN	LBUT1ENO2 + NO ₃ → C ₂ H ₅ CHO + HCHO + HO ₂ + NO ₂	KR02N03	Sander et al. (2019)
G44103a	TrGC	LBUT1ENOOH + OH → LBUT1ENO2	k_R00HRO	Sander et al. (2019)
G44103b	TrGC	LBUT1ENOOH + OH → C ₂ H ₅ CO ₃ + HCHO + HO ₂	k_t*f_t00H*f_pCH20H	Sander et al. (2019)*
G44104	TrGCN	LBUT1ENNO3 + OH → C ₂ H ₅ CHO + CO + HO ₂ + NO ₂	k_s*f_sOH*f_CH20N02	Sander et al. (2019)*
G44105	TrGC	CBUT2ENE + OH → BUT2OLO2	1.1E-11*EXP(485./temp)	Atkinson et al. (2006)
G44106	TrGC	CBUT2ENE + O ₃ → CH ₃ CHO + .16 CH ₃ CHOHOOH + .50 OH + .50 HCOCH ₂ O ₂ + .05 CH ₂ CO + .09 CH ₃ OH + .09 CO + .2 CH ₄ + .2 CO ₂	3.2E-15*EXP(-965./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44107	TrGCN	CBUT2ENE + NO ₃ → 2 CH ₃ CHO + NO ₂	3.5E-13	Atkinson et al. (2006), Sander et al. (2019)*
G44108	TrGC	TBUT2ENE + OH → BUT2OLO2	1.0E-11*EXP(553./temp)	Atkinson et al. (2006)
G44109	TrGC	TBUT2ENE + O ₃ → CH ₃ CHO + .16 CH ₃ CHOHOOH + .50 OH + .50 HCOCH ₂ O ₂ + .05 CH ₂ CO + .09 CH ₃ OH + .09 CO + .2 CH ₄ + .2 CO ₂	6.6E-15*EXP(-1060./temp)	Atkinson et al. (2006), Sander et al. (2019)
G44110	TrGCN	TBUT2ENE + NO ₃ → 2 CH ₃ CHO + NO ₂	1.78E-12*EXP(-530./temp) +1.28E-14*EXP(570./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44111	TrGC	BUT2OLO2 → C ₂ H ₅ CHO + HCHO + HO ₂	k1_R02sOR02	Sander et al. (2019)
G44112a	TrGC	BUT2OLO2 + HO ₂ → BUT2OLOOH	k_R02_H02(temp,4)*r_COCH202_00H	Sander et al. (2019)
G44112b	TrGC	BUT2OLO2 + HO ₂ → 2 CH ₃ CHO + HO ₂ + OH	k_R02_H02(temp,4)*r_COCH202_0H	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44113a	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{KRO2NO} \cdot (1 - \alpha_{\text{AN}}(5, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Sander et al. (2019)
G44113b	TrGCN	$\text{BUT2OLO2} + \text{NO} \rightarrow \text{BUT2OLNO3}$	$\text{KRO2NO} \cdot \alpha_{\text{AN}}(5, 2, 0, 0, 0, \text{temp}, \text{cair})$	Sander et al. (2019)
G44114	TrGCN	$\text{BUT2OLO2} + \text{NO}_3 \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	KRO2NO3	Sander et al. (2019)
G44115a	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO2}$	k_R00HRO	Sander et al. (2019)
G44115b	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{LMEKOOH} + \text{HO}_2$	k_t*f_tOH*f_pCH2OH	Sander et al. (2019)
G44115c	TrGC	$\text{BUT2OLOOH} + \text{OH} \rightarrow \text{BUT2OLO} + \text{OH}$	k_t*f_tOOH*f_pCH2OH	Sander et al. (2019)
G44116	TrGCN	$\text{BUT2OLNO3} + \text{OH} \rightarrow \text{LMEKNO3} + \text{HO}_2$	k_t*f_tOH*f_CH2ON02	Sander et al. (2019)
G44117	TrGC	$\text{BUT2OLO} + \text{OH} \rightarrow \text{BIACET} + \text{HO}_2$	k_t*f_tOH*f_CO	Sander et al. (2019)
G44118	TrGC	$\text{IPRCHO} + \text{OH} \rightarrow \text{IPRCO3} + \text{H}_2\text{O}$	$6.8\text{E}-12 \cdot \text{EXP}(410./\text{temp})$	Atkinson et al. (2006)
G44119	TrGCN	$\text{IPRCHO} + \text{NO}_3 \rightarrow \text{IPRCO3} + \text{HNO}_3$	$1.67\text{E}-12 \cdot \text{EXP}(-1460./\text{temp})$	Atkinson et al. (2006)
G44120	TrGC	$\text{IPRCO3} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2$	k1_R02RCO3	Rickard (2022)
G44121a	TrGC	$\text{IPRCO3} + \text{HO}_2 \rightarrow \text{PERIBUACID}$	KAPH02*r_C03_OOH	Rickard (2022), Sander et al. (2019)
G44121b	TrGC	$\text{IPRCO3} + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*(1.-r_C03_OOH)	Rickard (2022), Sander et al. (2019)
G44122	TrGCN	$\text{IPRCO3} + \text{NO}_2 \rightarrow \text{PIPn}$	k_CH3CO3_N02	Rickard (2022)
G44123	TrGCN	$\text{IPRCO3} + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G44124a	TrGC	$\text{PERIBUACID} + \text{OH} \rightarrow \text{IPRCO3} + \text{H}_2\text{O}$	k_R00HRO	Rickard (2022)
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	$\text{PIPn} \rightarrow \text{IPRCO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G44126	TrGCN	$\text{PIPn} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{NO}_2$	k_s*f_cpan	Sander et al. (2019)*
G44127	TrGC	$\text{MPROPENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{COCH}_3$	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	$\text{BUTENOL} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{C}_2\text{H}_5\text{CHO}$	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)*

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

#	labels	reaction	rate coefficient	reference
G44133	TrGC	HVMK + OH \rightarrow HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	HVMK + HCOOH \rightarrow CO ₂ C ₃ CHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44135	TrGC	CO ₂ C ₃ CHO + HCOOH \rightarrow HVMK + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44136	TrGC	HMAC + OH \rightarrow HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	HMAC + HCOOH \rightarrow IBUTDIAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44138	TrGC	IBUTDIAL + HCOOH \rightarrow HMAC + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44139	TrGC	CO ₂ C ₃ CHO + OH \rightarrow CH ₃ COCH ₂ O ₂ + CO ₂ + H ₂ O	k_t*f_0*f_alk+k_s*f_CHO*f_CO	Sander et al. (2019)*
G44140	TrGCN	CO ₂ C ₃ CHO + NO ₃ \rightarrow CH ₃ COCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*4.0	Sander et al. (2019)*
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 (2022)
G44201	TrGTerC	CH ₃ COCOCH ₂ O ₂ + HO ₂ \rightarrow CH ₃ COCOCH ₂ OOH	k_R02_H02(temp,4)	Rickard (2022)
G44202	TrGTerCN	CH ₃ COCOCH ₂ O ₂ + NO \rightarrow CH ₃ C(O) + HCHO + CO + NO ₂	KR02NO	Rickard (2022)*
G44203a	TrGTerC	CH ₃ COCOCH ₂ OOH + OH \rightarrow CH ₃ COCOCHO + OH	k_s*f_CO*f_s00H	Rickard (2022)*
G44203b	TrGTerC	CH ₃ COCOCH ₂ OOH + OH \rightarrow CH ₃ COCOCH ₂ O ₂	k_R00HR0	Rickard (2022)
G44204	TrGTerC	C44O ₂ + HO ₂ \rightarrow C44OOH	k_R02_H02(temp,4)	Rickard (2022)
G44205	TrGTerCN	C44O ₂ + NO \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂ + NO ₂	KR02NO	Rickard (2022)*
G44206	TrGTerC	C44O ₂ \rightarrow HCOCH ₂ CHO + CO ₂ + HO ₂	k1_R02sOR02	Rickard (2022)
G44207	TrGTerC	C44OOH + OH \rightarrow C44O ₂	7.46E-11	Rickard (2022)
G44208	TrGTerC	CHOC ₃ COO ₂ \rightarrow HCOCH ₂ CO ₃ + HCHO	k1_R02pOR02	Rickard (2022)
G44209	TrGTerC	CHOC ₃ COO ₂ + HO ₂ \rightarrow C413COOOH	k_R02_H02(temp,4)	Rickard (2022)
G44210	TrGTerCN	CHOC ₃ COO ₂ + NO \rightarrow HCOCH ₂ CO ₃ + HCHO + NO ₂	KR02NO	Rickard (2022)*
G44211	TrGTerC	C413COOOH + OH \rightarrow CHOC ₃ COO ₂	8.33E-11	Rickard (2022)
G44212	TrGTerC	C4CODIAL + OH \rightarrow C312COCO ₃	3.39E-11	Rickard (2022)
G44213	TrGTerCN	C4CODIAL + NO ₃ \rightarrow C312COCO ₃ + HNO ₃	2.*KN03AL*4.0	Rickard (2022)
G44214	TrGTerC	C312COCO ₃ \rightarrow HCOCOCH ₂ O ₂ + CO ₂	k1_R02RCO3	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G44215a	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{C312COCO3H}$	KAPH02*r_C03_00H	Rickard (2022)
G44215b	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02*(1.-r_C03_00H)}$	Rickard (2022)
G44216	TrGTerCN	$\text{C312COCO3} + \text{NO}_2 \rightarrow \text{C312COPAN}$	k_CH3C03_N02	Rickard (2022)
G44217	TrGTerCN	$\text{C312COCO3} + \text{NO} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G44218	TrGTerC	$\text{C312COCO3H} + \text{OH} \rightarrow \text{C312COCO3}$	$1.63\text{E-}11$	Rickard (2022)
G44219	TrGTerCN	$\text{C312COPAN} \rightarrow \text{C312COCO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G44220	TrGTerCN	$\text{C312COPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO} + \text{NO}_2$	$1.27\text{E-}11$	Rickard (2022)
G44221	TrGTerC	$\text{CH}_3\text{COCOCHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + 2 \text{CO}$	$8.4\text{E-}13*\text{EXP}(830./\text{temp})$	Sander et al. (2019)*
G44222	TrGTerCN	$\text{CH}_3\text{COCOCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + 2 \text{CO} + \text{HNO}_3$	KN03AL*4.0	Rickard (2022)
G44223	TrGTerC	$\text{IBUTALOH} + \text{OH} \rightarrow \text{IPRHOCO3}$	$1.4\text{E-}11$	Rickard (2022)
G44224a	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022), Sander et al. (2019)
G44224b	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO2H} + \text{O}_3$	KAPH02*r_C03_O3	Rickard (2022), Sander et al. (2019)
G44224c	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO3H}$	KAPH02*r_C03_00H	Rickard (2022), Sander et al. (2019)
G44225	TrGTerCN	$\text{IPRHOCO3} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G44226	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_2 \rightarrow \text{C4PAN5}$	k_CH3C03_N02	Rickard (2022)
G44227	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard (2022)
G44228a	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.7	Rickard (2022)
G44228b	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{IPRHOCO2H}$	k1_R02RC03*0.3	Rickard (2022)
G44229	TrGTerC	$\text{IPRHOCO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$1.72\text{E-}12$	Rickard (2022)
G44230	TrGTerC	$\text{OH} + \text{IPRHOCO3H} \rightarrow \text{IPRHOCO3}$	$4.80\text{E-}12$	Rickard (2022)
G44231	TrGTerCN	$\text{C4PAN5} \rightarrow \text{IPRHOCO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G44232	TrGTerCN	$\text{C4PAN5} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO} + \text{NO}_2$	$4.75\text{E-}13$	Rickard (2022)
G44233a	TrGTerC	$\text{MBOOO} \rightarrow \text{IPRHOCO2H}$	$1.60\text{E-}17*\text{C}(\text{ind_H20})*(0.08+0.15)$	Rickard (2022), Sander et al. (2019)
G44233b	TrGTerC	$\text{MBOOO} \rightarrow \text{IBUTALOH} + \text{H}_2\text{O}_2$	$1.60\text{E-}17*\text{C}(\text{ind_H20})*0.77$	Rickard (2022), Sander et al. (2019)
G44234	TrGTerC	$\text{MBOOO} + \text{CO} \rightarrow \text{IBUTALOH} + \text{CO}_2$	$1.20\text{E-}15$	Rickard (2022)
G44235	TrGTerCN	$\text{MBOOO} + \text{NO} \rightarrow \text{IBUTALOH} + \text{NO}_2$	$1.00\text{E-}14$	Rickard (2022)
G44236	TrGTerCN	$\text{MBOOO} + \text{NO}_2 \rightarrow \text{IBUTALOH} + \text{NO}_3$	$1.00\text{E-}15$	Rickard (2022)
G44400	TrGAroC	$\text{MALANHY} + \text{OH} \rightarrow \text{MALANHYO2}$	$1.4\text{E-}12$	Rickard (2022)
G44401a	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{HOCOC4DIAL} + \text{OH}$	$1.22\text{E-}10$	Rickard (2022)
G44401b	TrGAroC	$\text{MALDIALOOH} + \text{OH} \rightarrow \text{MALDIALO2}$	k_ROOHR0	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G44402	TrGAroCN	NC4DCO2H + OH \rightarrow MALANHY + NO ₂	k_R00HRO	Rickard (2022)*
G44403	TrGAroC	CO14O3CO2H + OH \rightarrow HCOCH ₂ O ₂ + 2 CO ₂	2.19E-11	Rickard (2022)
G44404	TrGAroC	BZFUOOH + OH \rightarrow BZFUO2	3.68E-11	Rickard (2022)
G44405	TrGAroC	HOCOC4DIAL + OH \rightarrow CO2C4DIAL + HO ₂	3.67E-11	Rickard (2022)
G44406a	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow MALDALCO2H + O ₃	KAPH02*r_C03_03	Rickard (2022)
G44406b	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow MALDALCO3H	KAPH02*r_C03_00H	Rickard (2022)
G44406c	TrGAroC	MALDIALCO3 + HO ₂ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + OH	KAPH02*r_C03_0H	Rickard (2022)*
G44407	TrGAroCN	MALDIALCO3 + NO \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KAPNO	Rickard (2022)*
G44408	TrGAroCN	MALDIALCO3 + NO ₂ \rightarrow MALDIALPAN	k_CH3C03_N02	Rickard (2022)
G44409	TrGAroCN	MALDIALCO3 + NO ₃ \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)*
G44410	TrGAroC	MALDIALCO3 \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	k1_R02RC03	Rickard (2022)*
G44411	TrGAroCN	BZFUONE + NO ₃ \rightarrow NBZFUO2	3.00E-13	Rickard (2022)
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 (2022)
G44414	TrGAroCN	NBZFUOOH + OH \rightarrow NBZFUO2	6.18E-12	Rickard (2022)
G44415	TrGAroC	MALDALCO3H + OH \rightarrow MALDIALCO3	4.00E-11	Rickard (2022)
G44416	TrGAroC	EPXDLCO2H + OH \rightarrow C3DIALO2 + CO ₂	2.31E-11	Rickard (2022)
G44417a	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow C3DIALO2 + CO ₂ + OH	KAPH02*r_C03_0H	Rickard (2022)
G44417b	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO2H + O ₃	KAPH02*r_C03_03	Rickard (2022)
G44417c	TrGAroC	EPXDLCO3 + HO ₂ \rightarrow EPXDLCO3H	KAPH02*r_C03_00H	Rickard (2022)
G44418	TrGAroCN	EPXDLCO3 + NO \rightarrow C3DIALO2 + CO ₂ + NO ₂	KAPNO	Rickard (2022)
G44419	TrGAroCN	EPXDLCO3 + NO ₂ \rightarrow EPXDLPAN	k_CH3C03_N02	Rickard (2022)
G44420	TrGAroCN	EPXDLCO3 + NO ₃ \rightarrow C3DIALO2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)
G44421	TrGAroC	EPXDLCO3 \rightarrow C3DIALO2 + CO ₂	k1_R02RC03	Rickard (2022)*
G44422	TrGAroC	MALNHYOHCO + OH \rightarrow CO + CO + CO + CO ₂ + HO ₂	5.68E-12	Rickard (2022)
G44423	TrGAroCN	MALDIAL + NO ₃ \rightarrow MALDIALCO3 + HNO ₃	2.*KN03AL*2.0	Rickard (2022)
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 (2022)*

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

#	labels	reaction	rate coefficient	reference
G44425	TrGAroC	MALDIAL + OH \rightarrow .83 MALDIALCO3 + .17 MALDIALO2	5.20E-11	Rickard (2022)*
G44426	TrGAroC	MALANHYOOH + OH \rightarrow MALNHYOHCO + OH	4.66E-11	Rickard (2022)
G44427	TrGAroCN	MALDIALPAN + OH \rightarrow GLYOX + CO + CO + NO ₂	3.70E-11	Rickard (2022)
G44428	TrGAroCN	MALDIALPAN \rightarrow MALDIALCO3 + NO ₂	k_PAN_M	Rickard (2022)
G44429a	TrGAroC	MALANHYO2 + HO ₂ \rightarrow MALANHYOOH	k_R02_H02(temp,4)*(1.-r_COCH202_OH-r_CHOCH202_OH)	Rickard (2022), Sander et al. (2019)
G44429b	TrGAroC	MALANHYO2 + HO ₂ \rightarrow HCOCOHC03 + CO ₂ + OH	k_R02_H02(temp,4)*(r_COCH202_OH+r_CHOCH202_OH)	Rickard (2022), Sander et al. (2019)
G44430	TrGAroCN	MALANHYO2 + NO \rightarrow HCOCOHC03 + CO ₂ + NO ₂	KR02N0	Rickard (2022)*
G44431	TrGAroCN	MALANHYO2 + NO ₃ \rightarrow HCOCOHC03 + CO ₂ + NO ₂	KR02N03	Rickard (2022)*
G44432	TrGAroC	MALANHYO2 \rightarrow HCOCOHC03 + CO ₂	k1_R02s0R02	Rickard (2022)*
G44433	TrGAroC	EPXDLC03H + OH \rightarrow EPXDLC03	2.62E-11	Rickard (2022)
G44434	TrGAroC	CO2C4DIAL + OH \rightarrow CO + CO + CO + CO + HO ₂	2.45E-11	Rickard (2022)
G44435a	TrGAroCN	NBZFUO2 + HO ₂ \rightarrow NBZFUOOH	k_R02_H02(temp,4)*(1.-r_COCH202_OH)	Rickard (2022), Sander et al. (2019)
G44435b	TrGAroCN	NBZFUO2 + HO ₂ \rightarrow .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + OH	k_R02_H02(temp,4)*r_COCH202_OH	Rickard (2022), Sander et al. (2019)
G44436	TrGAroCN	NBZFUO2 + NO \rightarrow .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂	KR02N0	Rickard (2022)*
G44437	TrGAroCN	NBZFUO2 + NO ₃ \rightarrow .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂ + NO ₂	KR02N03	Rickard (2022)*
G44438	TrGAroCN	NBZFUO2 \rightarrow .5 CO14O3CHO + .5 NO ₂ + .5 NBZFUONE + .5 HO ₂	k1_R02s0R02	Rickard (2022)*
G44439	TrGAroC	MALDALCO2H + OH \rightarrow .6 MALANHY + HO ₂ + .4 GLYOX + .4 CO + .4 CO ₂	3.70E-11	Rickard (2022)*
G44440	TrGAroCN	EPXC4DIAL + NO ₃ \rightarrow EPXDLC03 + HNO ₃	2.*KN03AL*4.0	Rickard (2022)
G44441	TrGAroC	EPXC4DIAL + OH \rightarrow EPXDLC03	4.32E-11	Rickard (2022)
G44442a	TrGAroC	MECOACETO2 + HO ₂ \rightarrow MECOACEOOH	k_R02_H02(temp,4)*(1.-r_COCH202_OH)	Rickard (2022), Sander et al. (2019)
G44442b	TrGAroC	MECOACETO2 + HO ₂ \rightarrow CH ₃ C(O)OO + HCHO + CO ₂ + OH	k_R02_H02(temp,4)*r_COCH202_OH	Rickard (2022), Sander et al. (2019)
G44443	TrGAroCN	MECOACETO2 + NO \rightarrow CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂	KR02N0	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G44444	TrGAroCN	MECOACETO2 + NO ₃ → CH ₃ C(O)OO + HCHO + CO ₂ + NO ₂	KR02NO3	Rickard (2022)*
G44445	TrGAroC	MECOACETO2 → CH ₃ C(O)OO + HCHO + CO ₂	k1_R02pOR02	Rickard (2022)*
G44446	TrGAroCN	CO14O3CHO + NO ₃ → CO + HCOCH ₂ O ₂ + CO ₂ + HNO ₃	KN03AL*8.0	Rickard (2022)
G44447	TrGAroC	CO14O3CHO + OH → CO + HCOCH ₂ O ₂ + CO ₂	3.44E-11	Rickard (2022)
G44448	TrGAroCN	NBZFUONE + OH → BZFUCO + NO ₂	1.16E-12	Rickard (2022)
G44449a	TrGAroC	BZFUO2 + HO ₂ → BZFUOOH	k_R02_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOCH2O2_OH)	Rickard (2022), Sander et al. (2019)
G44449b	TrGAroC	BZFUO2 + HO ₂ → CO14O3CHO + HO ₂ + OH	k_R02_HO2(temp,4)*(r_COCH2O2_OH+r_CHOCH2O2_OH)	Rickard (2022), Sander et al. (2019)
G44450	TrGAroCN	BZFUO2 + NO → CO14O3CHO + HO ₂ + NO ₂	KR02NO	Rickard (2022)*
G44451	TrGAroCN	BZFUO2 + NO ₃ → CO14O3CHO + HO ₂ + NO ₂	KR02NO3	Rickard (2022)*
G44452	TrGAroC	BZFUO2 → CO14O3CHO + HO ₂	k1_R02sOR02	Rickard (2022)*
G44453	TrGAroC	BZFUCO + OH → CO14O3CHO + HO ₂	1.78E-11	Rickard (2022)
G44456a	TrGAroC	MALDIALO2 + HO ₂ → MALDIALOOH	k_R02_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOCH2O2_OH)	Rickard (2022)
G44456b	TrGAroC	MALDIALO2 + HO ₂ → GLYOX + GLYOX + HO ₂ + OH	k_R02_HO2(temp,4)*(r_COCH2O2_OH+r_CHOCH2O2_OH)	Rickard (2022)
G44457	TrGAroCN	MALDIALO2 + NO → GLYOX + GLYOX + HO ₂ + NO ₂	KR02NO	Rickard (2022)*
G44458	TrGAroCN	MALDIALO2 + NO ₃ → GLYOX + GLYOX + HO ₂ + NO ₂	KR02NO3	Rickard (2022)*
G44459	TrGAroC	MALDIALO2 → GLYOX + GLYOX + HO ₂	k1_R02sOR02	Rickard (2022)*
G44460	TrGAroCN	EPXDL PAN + OH → HCOCOCHO + CO + NO ₂	2.29E-11	Rickard (2022)
G44461	TrGAroCN	EPXDL PAN → EPXDLCO3 + NO ₂	k_PAN_M	Rickard (2022)*
G44462	TrGAroC	MECOACEOOH + OH → MECOACETO2	3.59E-12	Rickard (2022)
G45000	TrGC	C ₅ H ₈ + O ₃ → .3508 MACR + .01518 MACO2H + .2440 MVK + .7085 HCHO + .11 CH ₂ OO + .1275 C ₃ H ₆ + .1575 CH ₃ C(O) + .0510 CH ₃ + .2625 HO ₂ + .27 OH + .09482 H ₂ O ₂ + .255 CO ₂ + .522 CO + .07182 HCHO + .03618 HCOCH ₂ O ₂ + .01782 CO + 0.05408 LCARBON	1.03E-14*EXP(-1995./temp)	Atkinson et al. (2006), Sander et al. (2019)
G45001	TrGC	C ₅ H ₈ + OH → .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 → NISOPO2	3.0E-12*EXP(-450./temp)	Atkinson et al. (2006)
G45003a	TrGC	LISOPAB + O ₂ → LISOPACO2	5.530E-13	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45003b	TrGC	LISOPAB + O ₂ → ISOPBO2	3.E-12	Sander et al. (2019)
G45004a	TrGC	LISOPCD + O ₂ → LDISOPACO2	6.780E-13	Sander et al. (2019)
G45004b	TrGC	LISOPCD + O ₂ → ISOPDO2	3.E-12	Sander et al. (2019)
G45005	TrGC	LISOPACO2 → LISOPAB + O ₂	3.1E12*exp(-7900./temp)*.6+ 7.8E13*exp(-8600./temp)*.4	Sander et al. (2019)
G45006	TrGC	ISOPBO2 → LISOPAB + O ₂	3.7E14*exp(-9570./temp) +4.2E14*exp(-9970./temp)	Sander et al. (2019)
G45007	TrGC	LDISOPACO2 → LISOPCD + O ₂	5.65E12*exp(-8410./temp) *.42+1.4E14*exp(-9110./temp)*.58	Sander et al. (2019)
G45008	TrGC	ISOPDO2 → LISOPCD + O ₂	5.0E14*exp(-10120./temp) +8.25E14*exp(-10220./temp)	Sander et al. (2019)
G45009a	TrGC	LISOPACO2 → C1ODC2O2C4OOH	k_16hsz14 * 2./3.*(1.-f_HPAl)	Sander et al. (2019)
G45009b	TrGC	LISOPACO2 → LZCODC23DBCOOH + HO ₂	k_16hsz14 * (2./3.*f_HPAl + 1./3.)	Sander et al. (2019)
G45010a	TrGC	LDISOPACO2 → C1OOHC3O2C4OD	k_16hsz41 * 2./3.*(1.-f_HPAl)	Sander et al. (2019)
G45010b	TrGC	LDISOPACO2 → LZCODC23DBCOOH + HO ₂	k_16hsz41 * (2./3.*f_HPAl + 1./3.)	Sander et al. (2019)
G45011	TrGC	LISOPACO2 → .9 LISOPACO + .1 ISOPAOh	k1_R02LISOPAC02	Rickard (2022), Sander et al. (2019)
G45012	TrGC	LISOPACO2 + HO ₂ → LISOPACOOH	k_R02_H02(temp,5)	Rickard (2022)
G45013a	TrGCN	LISOPACO2 + NO → LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45013b	TrGCN	LISOPACO2 + NO → LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45014	TrGCN	LISOPACO2 + NO ₃ → LISOPACO + NO ₂	KR02N03	Rickard (2022)
G45015	TrGC	LDISOPACO2 → .9 LISOPACO + .1 ISOPAOh	k1_R02LISOPAC02	Rickard (2022), Sander et al. (2019)
G45016	TrGC	LDISOPACO2 + HO ₂ → LISOPACOOH	k_R02_H02(temp,5)	Rickard (2022)
G45017a	TrGCN	LDISOPACO2 + NO → LISOPACO + NO ₂	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45017b	TrGCN	LDISOPACO2 + NO → LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Sander et al. (2019)
G45018	TrGCN	LDISOPACO2 + NO ₃ → LISOPACO + NO ₂	KR02N03	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45019a	TrGC	LISOPACOOH + OH \rightarrow LISOPACO2	k_R00HRO	Sander et al. (2019)
G45019b	TrGC	LISOPACOOH + OH \rightarrow LZCODC23DBCOOH + HO ₂	k_s*f_allyl*f_sOH	Sander et al. (2019)
G45019c	TrGC	LISOPACOOH + OH \rightarrow LHC4ACCHO + OH	(k_s*f_s00H*f_allyl+ k_R0HRO)	Sander et al. (2019)
G45019d	TrGC	LISOPACOOH + OH \rightarrow LIEPOX + OH	(k_adt+k_ads)*a_CH2OH*a_CH200H	Sander et al. (2019)*
G45020	TrGC	ISOPAOH + OH \rightarrow LHC4ACCHO + HO ₂	(k_adt+k_ads)*a_CH2OH*a_CH20H+k_s*f_sOH*f_allyl+k_R0HRO	Sander et al. (2019)
G45021	TrGCN	LISOPACNO3 + OH \rightarrow LISOPACNO3O2	(k_adt+k_ads)*a_CH2ON02*a_CH2OH	Sander et al. (2019)*
G45022	TrGC	ISOPBO2 \rightarrow .8 MVK + .8 HCHO + .8 HO ₂ + .2 ISOPBOH	k1_R02ISOPBO2	Rickard (2022)
G45023a	TrGC	ISOPBO2 + HO ₂ \rightarrow ISOPBOOH	k_R02_HO2(temp,5)*(1.-r_CHOCH202_OH)	Sander et al. (2019)
G45023b	TrGC	ISOPBO2 + HO ₂ \rightarrow MVK + HCHO + HO ₂ + OH	k_R02_HO2(temp,5)*r_CHOCH202_OH	Sander et al. (2019)
G45024a	TrGCN	ISOPBO2 + NO \rightarrow MVK + HCHO + HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(6,3,0,0,0,temp,cair))	Lockwood et al. (2010), Sander et al. (2019)
G45024b	TrGCN	ISOPBO2 + NO \rightarrow ISOPBNO3	KR02N0*alpha_AN(6,3,0,0,0,temp,cair)	Lockwood et al. (2010), Sander et al. (2019)
G45025	TrGCN	ISOPBO2 + NO ₃ \rightarrow MVK + .75 HCHO + .75 HO ₂ + .25 CH ₃ + NO ₂	KR02N03	Rickard (2022)
G45026a	TrGC	ISOPBOOH + OH \rightarrow LIEPOX + OH	(k_ads+k_adp)*a_CH200H	Paulot et al. (2009b), Sander et al. (2019)
G45026b	TrGC	ISOPBOOH + OH \rightarrow ISOPBO2	k_R00HRO	Sander et al. (2019)
G45026c	TrGC	ISOPBOOH + OH \rightarrow MGLYOX + HOCH ₂ CHO	k_R0HRO+k_s*f_alk*f_sOH	Sander et al. (2019)
G45027	TrGC	ISOPBOOH + O ₃ \rightarrow .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 \rightarrow 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 \rightarrow ISOPBDNO3O2	(k_adt+k_adp)*f_CH2ON02	Sander et al. (2019)
G45030	TrGC	ISOPDO2 \rightarrow .8 MACR + .8 HCHO + .8 HO ₂ + .1 HCOC5 + .1 ISOPDOH	k1_R02ISOPDO2	Rickard (2022)
G45031a	TrGC	ISOPDO2 + HO ₂ \rightarrow ISOPDOOH	k_R02_HO2(temp,5)*(1.-r_CHOCH202_OH)	Sander et al. (2019)
G45031b	TrGC	ISOPDO2 + HO ₂ \rightarrow MACR + HCHO + HO ₂ + OH	k_R02_HO2(temp,5)*r_CHOCH202_OH	Sander et al. (2019)
G45032a	TrGCN	ISOPDO2 + NO \rightarrow 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)

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

#	labels	reaction	rate coefficient	reference
G45032b	TrGCN	ISOPDO2 + NO \rightarrow ISOPDNO3	KR02N0*alpha_AN(6,2,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45033	TrGCN	ISOPDO2 + NO ₃ \rightarrow MACR + HCHO + HO ₂ + NO ₂	KR02N03	Rickard (2022)
G45034a	TrGC	ISOPDOOH + OH \rightarrow LIEPOX + OH	(k_adt+k_adp)*a_CH200H	Paulot et al. (2009b), Sander et al. (2019)
G45034b	TrGC	ISOPDOOH + OH \rightarrow ISOPDO2	k_R00HRO	Sander et al. (2019)
G45034c	TrGC	ISOPDOOH + OH \rightarrow HCOC5 + OH	k_t*f_t00H*f_allyl*f_pCH20H	Sander et al. (2019)
G45034d	TrGC	ISOPDOOH + OH \rightarrow CH ₃ COCH ₂ OH + GLYOX + OH	k_s*f_pCH20H*f_sOH	Sander et al. (2019)
G45035	TrGC	ISOPDOOH + O ₃ \rightarrow 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 \rightarrow HCOC5 + HO ₂	2.*k_R0HRO+(k_t*f_t0H*f_allyl+k_s*f_sOH)*f_pCH20H+(k_adt+k_adp)*a_CH20H	Sander et al. (2019)
G45037	TrGCN	ISOPDNO3 + OH \rightarrow ISOPBDNO3O2	(k_adp+k_ads)*a_CH20N02	Sander et al. (2019)*
G45038	TrGCN	NISOP02 \rightarrow .8 NC4CHO + .6 HO ₂ + .2 LISOPACNO3	k1_R02LISOPAC02	Rickard (2022)
G45039	TrGCN	NISOP02 + HO ₂ \rightarrow NISOP0OH	k_R02_H02(temp,5)	Rickard (2022)
G45040	TrGCN	NISOP02 + NO \rightarrow NC4CHO + HO ₂ + NO ₂	KR02N0	Rickard (2022)*
G45041	TrGCN	NISOP02 + NO ₃ \rightarrow NC4CHO + HO ₂ + NO ₂	KR02N03	Rickard (2022)
G45042	TrGCN	NISOP0OH + OH \rightarrow NC4CHO + OH	1.03E-10	Rickard (2022)
G45043	TrGCN	NC4CHO + OH \rightarrow LNISO3	(k_adt+k_ads)*a_CH0*a_CH20N02	Sander et al. (2019)*
G45044	TrGCN	NC4CHO + O ₃ \rightarrow .27 NOA + .027 HCOCO ₂ H + .0162 GLYOX + .0162 H ₂ O ₂ + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO ₂ + 0.7705 HCHO + .4055 CO ₂ + .73 GLYOX	2.40E-17	Sander et al. (2019)
G45045	TrGCN	NC4CHO + NO ₃ \rightarrow LNISO3 + HNO ₃	KN03AL*4.25	Rickard (2022)
G45046	TrGCN	LNISO3 + HO ₂ \rightarrow LNISOOH	0.5*k_R02_H02(temp,5)+0.5*KAPH02	Rickard (2022)
G45047	TrGCN	LNISO3 + NO \rightarrow NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	0.5*KAPN0+0.5*KR02N0	Rickard (2022)*
G45048	TrGCN	LNISO3 + NO ₃ \rightarrow NOA + .5 HOCHCHO + .5 CO + .5 HO ₂ + NO ₂ + .5 CO ₂	KR02N03*1.37	Rickard (2022)
G45049	TrGCN	LNISOOH + OH \rightarrow LNISO3	2.65E-11	Rickard (2022)
G45050a	TrGC	LHC4ACCHO + OH \rightarrow LC578O2	(k_adtertprim+k_ads)*a_CH0*a_CH20H	Sander et al. (2019)
G45050b	TrGC	LHC4ACCHO + OH \rightarrow LHC4ACCO3	k_t*f_0	Sander et al. (2019)
G45050c	TrGC	LHC4ACCHO + OH \rightarrow C4MDIAL + HO ₂	k_s*f_sOH*f_allyl	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45051	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow .2225 \text{ CH}_3\text{C(O)} + .89 \text{ CO} + .0171875 \text{ HOCH}_2\text{CO}_2\text{H} + .075625 \text{ H}_2\text{O}_2 + .0171875 \text{ HCOCO}_2\text{H} + .2775 \text{ CH}_3\text{COCH}_2\text{OH} + .6675 \text{ HO}_2 + .2603125 \text{ GLYOX} + .2225 \text{ HCHO} + .89 \text{ OH} + .2603125 \text{ HOCH}_2\text{CHO} + .5 \text{ MGLYOX}$	2.40E-17	Rickard (2022)
G45052	TrGCN	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO}_3 + \text{HNO}_3$	KN03AL*4.25	Rickard (2022)
G45053	TrGC	$\text{LC578O}_2 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2$	k1_R02t0R02	Rickard (2022)
G45054a	TrGC	$\text{LC578O}_2 + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO} + \text{OH}$	k_R02_H02(temp,5)*r_COCH202_OH	Rickard (2022)
G45054b	TrGC	$\text{LC578O}_2 + \text{HO}_2 \rightarrow \text{LC578OOH}$	k_R02_H02(temp,5)*r_COCH202_OOH	Rickard (2022)
G45055	TrGCN	$\text{LC578O}_2 + \text{NO} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45056	TrGCN	$\text{LC578O}_2 + \text{NO}_3 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCHCHO} + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)
G45057	TrGC	$\text{LC578O}_2 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCH}_2\text{CHO} + .75 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	k_hsb	Sander et al. (2019)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O}_2$	k_R00HRO	Sander et al. (2019)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C1ODC2OOHC4OD} + \text{HO}_2$	k_t*f_0*f_tCH20H*f_alk+k_t*f_tOH*f_pCH20H*f_pCH20H+k_s*f_sOH*f_pCH20H	Sander et al. (2019)
G45059a	TrGC	$\text{LHC4ACCO}_3 \rightarrow \text{OH} + .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{CO}_2$	k1_R02RC03*0.9	Sander et al. (2019)
G45059b	TrGC	$\text{LHC4ACCO}_3 \rightarrow \text{LHC4ACCO}_2\text{H}$	k1_R02RC03*0.1	Sander et al. (2019)
G45060a	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow 2 \text{ OH} + .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{CO}_2$	KAPH02*r_C03_OH	Sander et al. (2019)
G45060b	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow \text{LHC4ACCO}_3\text{H}$	KAPH02*r_C03_OOH	Sander et al. (2019)
G45060c	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow \text{LHC4ACCO}_2\text{H} + \text{O}_3$	KAPH02*r_C03_O3	Sander et al. (2019)
G45061	TrGCN	$\text{LHC4ACCO}_3 + \text{NO} \rightarrow .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{NO}_2 + \text{CO}_2$	KAPN0	Sander et al. (2019)
G45062	TrGCN	$\text{LHC4ACCO}_3 + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	k_CH3C03_N02	Rickard (2022)
G45063	TrGCN	$\text{LHC4ACCO}_3 + \text{NO}_3 \rightarrow .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{NO}_2 + \text{CO}_2$	KR02N03*1.74	Sander et al. (2019)
G45064a	TrGC	$\text{LHC4ACCO}_2\text{H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{CO}_2$	2.52E-11	Sander et al. (2019)
G45064b	TrGC	$\text{LHC4ACCO}_3\text{H} + \text{OH} \rightarrow \text{LHC4ACCO}_3$	2.88E-11	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45065	TrGCN	LC5PAN1719 \rightarrow LHC4ACCO3 + NO ₂	k_PAN_M	Rickard (2022)
G45066	TrGCN	LC5PAN1719 + OH \rightarrow .5 MACROH + .5 HO12CO3C4 + CO + NO ₂	2.52E-11	Rickard (2022)
G45067	TrGC	HCOC5 + OH \rightarrow C59O2	3.81E-11	Rickard (2022)
G45068	TrGC	HCOC5 + O ₃ \rightarrow BIACETOH + .335 H ₂ O ₂ + .67 HCHO + .2079 CO + .1221 CH ₂ OO + .05280 OH	7.51E-16*EXP(-1521./temp)	Sander et al. (2019)
G45069	TrGC	C59O2 \rightarrow CH ₃ COCH ₂ OH + HOCH ₂ CO	k1_R02t0R02	Sander et al. (2019)
G45070a	TrGC	C59O2 + HO ₂ \rightarrow OH + CH ₃ COCH ₂ OH + HOCH ₂ CO	k_R02_H02(temp,5)*r_COCH202_OH	Sander et al. (2019)
G45070b	TrGC	C59O2 + HO ₂ \rightarrow C59OOH	k_R02_H02(temp,5)*r_COCH202_OOH	Sander et al. (2019)
G45071	TrGCN	C59O2 + NO \rightarrow CH ₃ COCH ₂ OH + HOCH ₂ CO + NO ₂	KR02N0	Sander et al. (2019)*
G45072	TrGCN	C59O2 + NO ₃ \rightarrow CH ₃ COCH ₂ OH + HOCH ₂ CO + NO ₂	KR02N03	Sander et al. (2019)
G45073	TrGC	C59OOH + OH \rightarrow C59O2	9.7E-12	Rickard (2022)
G45074	TrGC	LIEPOX + OH \rightarrow DB1O2 + 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 CO2H3CHO + .22 HCHO + .22 OH	k1_R02t0R02	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45080	TrGCN	$\text{C10OHC2O2C4OD} + \text{NO} \rightarrow .78 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .78 \text{ HOCHCHO} + .22 \text{ CO}_2\text{H}_3\text{CHO} + .22 \text{ HCHO} + .22 \text{ OH} + \text{NO}_2$	KR02N0	Sander et al. (2019)*
G45081a	TrGC	$\text{C10OHC2O2C4OD} + \text{HO}_2 \rightarrow \text{C10OHC2OOHC4OD}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{COCH202_00H}}$	Sander et al. (2019)
G45081b	TrGC	$\text{C10OHC2O2C4OD} + \text{HO}_2 \rightarrow .78 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .78 \text{ HOCHCHO} + .22 \text{ CO}_2\text{H}_3\text{CHO} + .22 \text{ HCHO} + 1.22 \text{ OH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{COCH202_OH}}$	Sander et al. (2019)
G45082	TrGC	$\text{C10OHC2O2C4OD} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{GLYOX} + \text{OH}$	k_{hsb}	Sander et al. (2019)
G45083	TrGC	$\text{C1ODC2O2C4OOH} \rightarrow \text{OH} + \text{C1ODC2OOHC4OD}$	$k_{15\text{hsd}\text{hb}}$	Sander et al. (2019)
G45084a	TrGC	$\text{C10OHC2OOHC4OD} + \text{OH} \rightarrow \text{C1ODC2OOHC4OD} + \text{OH}$	$2 * k_{\text{s}} * f_{\text{s00H}} * f_{\text{tCH2OH}}$	Sander et al. (2019)
G45084b	TrGC	$\text{C10OHC2OOHC4OD} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + 2 \text{ CO} + 2 \text{ HO}_2 + \text{OH}$	$k_{\text{t}} * f_{\text{tOH}} * f_{\text{pCH2OH}} * f_{\text{pCH2OH}}$	Sander et al. (2019)
G45084c	TrGC	$\text{C10OHC2OOHC4OD} + \text{OH} \rightarrow \text{C10OHC2O2C4OD}$	k_{R00HRO}	Sander et al. (2019)
G45085	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{CO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t}} * f_{\text{O}} * f_{\text{tCH2OH}} + k_{\text{t}} * f_{\text{tOH}} * f_{\text{tOH}} * f_{\text{CHO}}$	Sander et al. (2019)
G45086	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{HOOCH}_2\text{CHO} + \text{HO}_2$	$k_{1\text{R02sOR02}}$	Sander et al. (2019)
G45087	TrGCN	$\text{C1ODC3O2C4OOH} + \text{NO} \rightarrow \text{MGLYOX} + \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Sander et al. (2019)
G45088	TrGC	$\text{C1ODC3O2C4OOH} + \text{HO}_2 \rightarrow .5 \text{ CH}_3\text{C(O)} + .5 \text{ CO} + .5 \text{ MGLYOX} + .5 \text{ HO}_2 + \text{HOOCH}_2\text{CO}_3$	$k_{\text{R02_H02}}(\text{temp}, 5)$	Sander et al. (2019)
G45089	TrGC	$\text{C1ODC3O2C4OOH} \rightarrow \text{MGLYOX} + \text{OH} + \text{HOOCH}_2\text{CHO}$	k_{hsd}	Sander et al. (2019)
G45090	TrGC	$\text{C10OHC3O2C4OD} \rightarrow .625 \text{ MGLYOX} + 2 \text{ CO} + 1.625 \text{ HO}_2 + .375 \text{ CH}_3\text{C(O)} + .375 \text{ CO}_2 + \text{OH}$	$k_{15\text{hsd}\text{hb}}$	Sander et al. (2019)
G45091	TrGC	$\text{LHC4ACCO}_3 \rightarrow \text{LZCO}_3\text{HC23DBCOD} + \text{HO}_2$	$k_{16\text{hs}}$	Sander et al. (2019)
G45092a	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{C1ODC2O2C4OD}$	$(k_{\text{adt}} + k_{\text{ads}}) * a_{\text{CHO}} * a_{\text{CHO}}$	Sander et al. (2019)*
G45092b	TrGC	$\text{C4MDIAL} + \text{OH} \rightarrow \text{LZCO}_3\text{C23DBCOD}$	$2 * k_{\text{t}} * f_{\text{O}} * f_{\text{alk}}$	Sander et al. (2019)*
G45093	TrGCN	$\text{C4MDIAL} + \text{NO}_3 \rightarrow \text{LZCO}_3\text{C23DBCOD} + \text{HNO}_3$	$\text{KN03AL} * 4.25 * 2.$	Sander et al. (2019)*
G45094a	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{COCH202_OH}}$	Sander et al. (2019)
G45094b	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1ODC2OOHC4OD}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{COCH202_00H}}$	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	$\text{C1ODC2O2C4OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$	$k_{1\text{R02tOR02}}$	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45097a	TrGC	$\text{C10DC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO}$	$(2.*k_tf_0*f_t\text{CH2OH}*f_alk+k_tf_t\text{OH}*f_CHO*f_p\text{CH2OH})*.5$	Sander et al. (2019)
G45097b	TrGC	$\text{C10DC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + \text{OH}$	$(2.*k_tf_0*f_t\text{CH2OH}*f_alk+k_tf_t\text{OH}*f_CHO*f_p\text{CH2OH})*.5$	Sander et al. (2019)
G45098	TrGCN	$\text{LISOPACNO3O2} + \text{NO} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2 + \text{NO}_2$	KR02NO	Sander et al. (2019)*
G45099	TrGCN	$\text{LISOPACNO3O2} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2$	$k1_R02t\text{OR02}+k_R02_H02(\text{temp},5)*c(\text{ind_H02})$	Sander et al. (2019)
G45100	TrGCN	$\text{ISOPBDNO3O2} + \text{NO} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRNO3} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + 1.6 \text{ NO}_2$	KR02NO	Sander et al. (2019)*
G45101	TrGCN	$\text{ISOPBDNO3O2} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRNO3} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + .6 \text{ NO}_2$	$k1_R02s\text{OR02}+k_R02_H02(\text{temp},5)*c(\text{ind_H02})$	Sander et al. (2019)
G45102	TrGCN	$\text{LISOPACNO3} + \text{O}_3 \rightarrow .8704 \text{ OH} + .365 \text{ HO}_2 + .73 \text{ MGLYOX} + .4325 \text{ NO}_3\text{CH}_2\text{CHO} + .135 \text{ CH}_3\text{COCH}_2\text{OH} + .0675 \text{ GLYOX} + .4325 \text{ NO}_2 + .0891 \text{ H}_2\text{O}_2 + .135 \text{ NOA} + .0675 \text{ HOCHCHO} + .3866 \text{ HOCH}_2\text{CHO} + .0405 \text{ CH}_3\text{OH} + .0405 \text{ CO} + .0054 \text{ HOCH}_2\text{CO}$	2.8E-17	Feierabend et al. (2008), Sander et al. (2019)
G45103	TrGC	$\text{DB1O2} \rightarrow \text{DB1O2}$	$k1_R02s\text{OR02}$	Sander et al. (2019)
G45104a	TrGC	$\text{DB1O2} + \text{HO}_2 \rightarrow \text{DB1OOH}$	$k_R02_H02(\text{temp},5)*(1-r_CHOHCH2O2_OH)$	Sander et al. (2019)*
G45104b	TrGC	$\text{DB1O2} + \text{HO}_2 \rightarrow \text{DB1O2} + \text{OH}$	$k_R02_H02(\text{temp},5)*r_CHOHCH2O2_OH$	Sander et al. (2019)
G45105a	TrGCN	$\text{DB1O2} + \text{NO} \rightarrow \text{DB1O2} + \text{NO}_2$	$\text{KR02NO}*(1.-\alpha_AN(7,2,0,0,0,\text{temp},\text{cair}))$	Sander et al. (2019)
G45105b	TrGCN	$\text{DB1O2} + \text{NO} \rightarrow \text{DB1NO3}$	$\text{KR02NO}*\alpha_AN(7,2,0,0,0,\text{temp},\text{cair})$	Sander et al. (2019)
G45106	TrGCN	$\text{DB1O2} + \text{NO}_3 \rightarrow \text{DB1O2} + \text{NO}_2$	KR02NO3	Sander et al. (2019)
G45107	TrGC	$\text{DB1O2} \rightarrow \text{DB1O2} + \text{OH}$	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	$\text{DB1O2} \rightarrow \text{DB1O2}$	KDEC*0.72	see note*
G45108b	TrGC	$\text{DB1O2} \rightarrow .5 \text{ HVMK} + .5 \text{ HMAc} + \text{HCHO} + \text{HO}_2$	KDEC*0.28	see note*

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

#	labels	reaction	rate coefficient	reference
G45109	TrGC	DB1O2 \rightarrow .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 \rightarrow DB2OOH	k_R02_H02(temp,5)*(1.-r_CHOHCH2O2_OH)	Sander et al. (2019)
G45110b	TrGC	DB1O2 + HO ₂ \rightarrow .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 \rightarrow .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02NO	see note*
G45112	TrGCN	DB1O2 + NO ₃ \rightarrow .48 CH ₃ COCH ₂ OH + .52 HOCH ₂ CHO + .52 MGLYOX + .48 GLYOX + HO ₂ + NO ₂	KR02NO3	Sander et al. (2019)
G45113	TrGC	DB1O2 \rightarrow .48 MACROOH + .52 LHMVKABOOH + CO + OH	k_14hsa1	Sander et al. (2019)
G45114a	TrGC	DB1OOH + OH \rightarrow DB1O2	k_R00HRO	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_R00HRO	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	LISOPEFO ₂ \rightarrow LISOPEFO	k1_R02pOR02	Sander et al. (2019)
G45121a	TrGCN	LISOPEFO ₂ + NO \rightarrow LISOPEFO + NO ₂	KR02NO*(1.-alpha_AN(6,1,0,0,0,temp,cair))	Sander et al. (2019)
G45121b	TrGCN	LISOPEFO ₂ + NO \rightarrow ISOPDNO ₃	KR02NO*alpha_AN(6,1,0,0,0,temp,cair)	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G45122a	TrGC	LISOPEFO2 + HO ₂ → .7143 ISOPDOOH + .2857 ISOPBOOH	k_R02_H02(temp,5)*(1.-r_CHOHCH202_OH)	Sander et al. (2019)
G45122b	TrGC	LISOPEFO2 + HO ₂ → LISOPEFO + OH	k_R02_H02(temp,5)*r_CHOHCH202_OH	Sander et al. (2019)
G45123	TrGCN	LISOPEFO2 + NO ₃ → LISOPEFO + NO ₂	KR02N03	Sander et al. (2019)
G45124	TrGC	LISOPEFO2 → .7143 MACR + .2857 MVK + HCHO + OH	0.7143*k_hsd+.2857*k_hsb	Sander et al. (2019)
G45125	TrGC	LISOPEFO → .7143 MACR + .2857 MVK + HCHO + HO ₂	KDEC	Sander et al. (2019)
G45126a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO ₂ + .35 DB1O2	KDEC*(1.-0.37)	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO → 3METHYLFURAN + HO ₂	KDEC*0.37	Sander et al. (2019), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	LISOPACO → .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 → L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Sander et al. (2019)*
G45129	TrGCN	3METHYLFURAN + NO ₃ → L3METHYLFURANO2 + NO ₂	1.9E-11	Sander et al. (2019), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 → C4MDIAL + HO ₂	k1_R02s0R02	Sander et al. (2019)
G45131	TrGCN	L3METHYLFURANO2 + NO → C4MDIAL + HO ₂ + NO ₂	KR02N0	Sander et al. (2019)*
G45132	TrGC	L3METHYLFURANO2 + HO ₂ → C4MDIAL + HO ₂	k_R02_H02(temp,5)	Sander et al. (2019)*
G45133	TrGC	LZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂	k1_R02RC03	Sander et al. (2019)
G45134a	TrGC	LZCO3C23DBCOD + HO ₂ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + OH	KAPH02*r_C03_OH	Sander et al. (2019)
G45134b	TrGC	LZCO3C23DBCOD + HO ₂ → LZCO3HC23DBCOD	KAPH02*(r_C03_00H+r_C03_03)	Sander et al. (2019)*
G45135	TrGCN	LZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO ₂ + NO ₂	KAPN0	Sander et al. (2019)
G45136	TrGCN	LZCO3C23DBCOD + NO ₂ → LZCPANC23DBCOD	k_CH3C03_N02	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45137	TrGCN	$\text{LZCO}_3\text{C}_{23}\text{DBCOD} + \text{NO}_3 \rightarrow .62 \text{EZCH}_3\text{CO}_2\text{CHCHO} + .38 \text{EZCHOCCH}_3\text{CHO}_2 + \text{CO}_2 + \text{NO}_2$	$\text{KR02N03} \times 1.74$	Sander et al. (2019)
G45138	TrGCN	$\text{LZCPANC}_{23}\text{DBCOD} \rightarrow \text{LZCO}_3\text{C}_{23}\text{DBCOD} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G45139	TrGCN	$\text{LZCPANC}_{23}\text{DBCOD} + \text{OH} \rightarrow .62 \text{EZCH}_3\text{CO}_2\text{CHCHO} + .38 \text{EZCHOCCH}_3\text{CHO}_2 + \text{CO}_2 + \text{NO}_2$	$2.52\text{E}-11$	Sander et al. (2019)*
G45200	TrGTerC	$\text{C}_{511}\text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCH}_2\text{CHO}$	$k_{1_R02s0R02}$	Rickard (2022)
G45201	TrGTerCN	$\text{C}_{511}\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCH}_2\text{CHO} + \text{NO}_2$	KR02N0	Rickard (2022)*
G45202a	TrGTerC	$\text{C}_{511}\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_{511}\text{OOH}$	$k_{R02_H02}(\text{temp}, 5) \times r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G45202b	TrGTerC	$\text{C}_{511}\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCH}_2\text{CHO} + \text{OH}$	$k_{R02_H02}(\text{temp}, 5) \times r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G45203	TrGTerC	$\text{C}_{511}\text{OOH} + \text{OH} \rightarrow \text{C}_{511}\text{O}_2$	$7.49\text{E}-11$	Rickard (2022)
G45204	TrGTerC	$\text{CO}_{23}\text{C}_4\text{CHO} + \text{OH} \rightarrow \text{CO}_{23}\text{C}_4\text{CO}_3$	$6.65\text{E}-11$	Rickard (2022)
G45205	TrGTerCN	$\text{CO}_{23}\text{C}_4\text{CHO} + \text{NO}_3 \rightarrow \text{CO}_{23}\text{C}_4\text{CO}_3 + \text{HNO}_3$	$\text{KN03AL} \times 5.5$	Rickard (2022)
G45206	TrGTerC	$\text{CO}_{23}\text{C}_4\text{CO}_3 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2$	$k_{1_R02RC03}$	Rickard (2022)
G45207	TrGTerCN	$\text{CO}_{23}\text{C}_4\text{CO}_3 + \text{NO} \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard (2022)*
G45208	TrGTerCN	$\text{CO}_{23}\text{C}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_{5\text{PAN}9}$	$k_{\text{CH3CO3_N02}}$	Rickard (2022)
G45209a	TrGTerC	$\text{CO}_{23}\text{C}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_{23}\text{C}_4\text{CO}_3\text{H}$	$\text{KAPH02} \times (r_{\text{C03_00H}} + r_{\text{C03_03}})$	Rickard (2022)
G45209b	TrGTerC	$\text{CO}_{23}\text{C}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \times r_{\text{C03_OH}}$	Rickard (2022)
G45210	TrGTerCN	$\text{C}_{5\text{PAN}9} \rightarrow \text{CO}_{23}\text{C}_4\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G45211	TrGTerCN	$\text{C}_{5\text{PAN}9} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{CO} + \text{NO}_2$	$3.12\text{E}-13$	Rickard (2022)
G45212	TrGTerC	$\text{C}_{512}\text{O}_2 \rightarrow \text{C}_{513}\text{O}_2$	$k_{1_R02pR02}$	Rickard (2022)
G45213	TrGTerC	$\text{C}_{512}\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_{512}\text{OOH}$	$k_{R02_H02}(\text{temp}, 5)$	Rickard (2022)
G45214	TrGTerCN	$\text{C}_{512}\text{O}_2 + \text{NO} \rightarrow \text{C}_{513}\text{O}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45215	TrGTerC	$\text{C}_{512}\text{OOH} + \text{OH} \rightarrow \text{CO}_{13}\text{C}_4\text{CHO} + \text{OH}$	$1.01\text{E}-10$	Rickard (2022)
G45216	TrGTerC	$\text{C}_{513}\text{O}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3$	$k_{1_R02s0R02}$	Rickard (2022)
G45217	TrGTerCN	$\text{C}_{513}\text{O}_2 + \text{NO} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45218a	TrGTerC	$\text{C}_{513}\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_{513}\text{OOH}$	$k_{R02_H02}(\text{temp}, 5) \times r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G45218b	TrGTerC	$\text{C}_{513}\text{O}_2 + \text{HO}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$k_{R02_H02}(\text{temp}, 5) \times r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G45219	TrGTerC	$\text{CO}_{13}\text{C}_4\text{CHO} + \text{OH} \rightarrow \text{CHOC}_3\text{COCO}_3$	$1.33\text{E}-10$	Rickard (2022)
G45220	TrGTerCN	$\text{CO}_{13}\text{C}_4\text{CHO} + \text{NO}_3 \rightarrow \text{CHOC}_3\text{COCO}_3 + \text{HNO}_3$	$2 \times \text{KN03AL} \times 5.5$	Rickard (2022)
G45221	TrGTerC	$\text{C}_{513}\text{OOH} + \text{OH} \rightarrow \text{C}_{513}\text{CO} + \text{OH}$	$9.23\text{E}-11$	Rickard (2022)
G45222	TrGTerC	$\text{CHOC}_3\text{COCO}_3 \rightarrow \text{CHOC}_3\text{COO}_2 + \text{CO}_2$	$k_{1_R02RC03}$	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45223	TrGTerC	$\text{CHOC3COCO3} + \text{HO}_2 \rightarrow \text{CHOC3COOOH}$	KAPH02	Rickard (2022)
G45224	TrGTerCN	$\text{CHOC3COCO3} + \text{NO}_2 \rightarrow \text{CHOC3COPAN}$	k_CH3C03_N02	Rickard (2022)
G45225	TrGTerCN	$\text{CHOC3COCO3} + \text{NO} \rightarrow \text{CHOC3COO2} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard (2022)*
G45226	TrGTerC	$\text{C513CO} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{CO} + \text{CO}$	2.64E-11	Rickard (2022)
G45227	TrGTerC	$\text{C514O2} + \text{HO}_2 \rightarrow \text{C514OOH}$	k_R02_H02(temp,5)	Rickard (2022)
G45228a	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-alpha_AN(7,2,0,1,0, temp, cair))	Rickard (2022), Sander et al. (2019)
G45228b	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{C514NO3}$	KR02N0*alpha_AN(7,2,0,1,0,temp, cair)	Rickard (2022), Sander et al. (2019)
G45229	TrGTerCN	$\text{C514O2} + \text{NO}_3 \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)
G45230	TrGTerC	$\text{C514O2} \rightarrow \text{CO13C4CHO} + \text{HO}_2$	k1_R02sR02	Rickard (2022)
G45231	TrGTerC	$\text{C514OOH} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{OH}$	1.10E-10	Rickard (2022)
G45232	TrGTerCN	$\text{C514NO3} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{NO}_2$	4.33E-11	Rickard (2022)
G45233	TrGTerC	$\text{CHOC3COOOH} + \text{OH} \rightarrow \text{CHOC3COCO3}$	7.55E-11	Rickard (2022)
G45234	TrGTerCN	$\text{CHOC3COPAN} \rightarrow \text{CHOC3COCO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G45235	TrGTerCN	$\text{CHOC3COPAN} + \text{OH} \rightarrow \text{C4CODIAL} + \text{CO} + \text{NO}_2$	7.19E-11	Rickard (2022)
G45236	TrGTerC	$\text{MBO} + \text{OH} \rightarrow \text{LMBOABO2}$	8.1E-12*EXP(610./temp)	Rickard (2022), Sander et al. (2019)*
G45237a	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{COCH}_3 + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH} + .84 \text{MBOOO}$	1.0E-17*0.57	Rickard (2022), Sander et al. (2019)
G45237b	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{IBUTALOH} + .63 \text{CO} + .37 \text{HOCH}_2\text{OOH} + .16 \text{OH} + .16 \text{HO}_2$	1.0E-17*0.43	Rickard (2022), Sander et al. (2019)
G45238	TrGTerCN	$\text{MBO} + \text{NO}_3 \rightarrow \text{LNMBOABO2}$	4.6E-14*EXP(-400./temp)	Rickard (2022), Sander et al. (2019)
G45239	TrGTerC	$\text{LMBOABO2} + \text{HO}_2 \rightarrow \text{LMBOABOOH}$	k_R02_H02(temp,5)	Rickard (2022), Sander et al. (2019)
G45240a	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{LMBOABNO3}$	KR02N0*(.67*alpha_AN(7,2,0,0,0, temp, cair)+.33*alpha_AN(7,1,0,0,0,temp, cair))	Rickard (2022), Sander et al. (2019)
G45240b	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-(.67*alpha_AN(7,2,0,0,0,temp, cair)+.33*alpha_AN(7,1,0,0,0,temp, cair)))*.67	Rickard (2022), Sander et al. (2019)
G45240c	TrGTerCN	$\text{LMBOABO2} + \text{NO} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-(.67*alpha_AN(7,2,0,0,0,temp, cair)+.33*alpha_AN(7,1,0,0,0,temp, cair)))*.33	Rickard (2022), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45241a	TrGTerC	LMBOABO2 \rightarrow HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂	k1_R02s0R02*.67	Rickard (2022), Sander et al. (2019)
G45241b	TrGTerC	LMBOABO2 \rightarrow IBUTALOH + HCHO + HO ₂	k1_R02p0R02*.33	Rickard (2022), Sander et al. (2019)
G45242a	TrGTerC	LMBOABOOH + OH \rightarrow MBOACO	0.67*2.93E-11+.33*2.05E-12	Rickard (2022), Sander et al. (2019)
G45242b	TrGTerC	LMBOABOOH + OH \rightarrow LMBOABO2	k_R00HR0	Rickard (2022), Sander et al. (2019)
G45243	TrGTerCN	LMBOABNO3 + OH \rightarrow MBOACO + NO ₂	0.67*1.75E-12+.33*2.69E-12	Rickard (2022), Sander et al. (2019)
G45244	TrGTerC	MBOACO + OH \rightarrow MBOCOCO + HO ₂	3.79E-12	Rickard (2022)
G45245	TrGTerC	MBOCOCO + OH \rightarrow CO + IPRHOCO3	1.38E-11	Rickard (2022)
G45246	TrGTerCN	LNMBOABO2 + HO ₂ \rightarrow LNMBOABOOH	k_R02_H02(temp,5)	Rickard (2022), 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 (2022), 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 (2022), 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 (2022), Sander et al. (2019)
G45250a	TrGTerCN	LNMBOABOOH + OH \rightarrow .65 C4MCONO3OH + .35 NMBOBCO	0.65*4.89E-12+.35*2.52E-12	Rickard (2022), Sander et al. (2019)
G45250b	TrGTerCN	LNMBOABOOH + OH \rightarrow LNMBOABO2	k_R00HR0	Rickard (2022), Sander et al. (2019)
G45251	TrGTerCN	NMBOBCO + OH \rightarrow NC4OHCO3	4.26E-12	Rickard (2022)
G45252a	TrGTerCN	NC4OHCO3 + HO ₂ \rightarrow IBUTALOH + CO ₂ + NO ₂ + OH	KAPH02*r_C03_OH	Rickard (2022), Sander et al. (2019)
G45252b	TrGTerCN	NC4OHCO3 + HO ₂ \rightarrow NC4OHCO3H	KAPH02*(r_C03_03+r_C03_00H)	Rickard (2022), Sander et al. (2019)
G45253	TrGTerCN	NC4OHCO3 + NO \rightarrow IBUTALOH + CO ₂ + NO ₂ + NO ₂	KAPN0	Rickard (2022)
G45254	TrGTerCN	NC4OHCO3 + NO ₂ \rightarrow NC4OHCPAN	k_CH3C03_N02	Rickard (2022)
G45255	TrGTerCN	NC4OHCO3 + NO ₃ \rightarrow IBUTALOH + CO ₂ + NO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)
G45256	TrGTerCN	NC4OHCO3 \rightarrow IBUTALOH + CO ₂ + NO ₂	k1_R02RC03	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45257	TrGTerCN	$\text{NC4OHCO3H} + \text{OH} \rightarrow \text{NC4OHCO3}$	4.50E-12	Rickard (2022)
G45258	TrGTerCN	$\text{NC4OHCPAN} + \text{OH} \rightarrow \text{IBUTALOH} + \text{CO} + \text{NO}_2 + \text{NO}_2$	1.27E-12	Rickard (2022)
G45259	TrGTerCN	$\text{NC4OHCPAN} \rightarrow \text{NC4OHCO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G45260	TrGTerCN	$\text{C4MCONO3OH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{CO}_2 + \text{NO}_2$	1.23E-12	Rickard (2022), Sander et al. (2019)
G45400	TrGAroCN	$\text{NC4MDCO2HN} + \text{OH} \rightarrow \text{MMALANHY} + \text{NO}_2$	k_R00HRO	Rickard (2022)*
G45401	TrGAroCN	$\text{C54CO} + \text{NO}_3 \rightarrow 3 \text{CO} + \text{CH}_3\text{C(O)OO} + \text{HNO}_3$	KN03AL*5.5	Rickard (2022)
G45402	TrGAroC	$\text{C54CO} + \text{OH} \rightarrow 3 \text{CO} + \text{CH}_3\text{C(O)OO}$	1.72E-11	Rickard (2022)
G45403a	TrGAroCN	$\text{NTLFUO2} + \text{HO}_2 \rightarrow \text{NTLFUOOH}$	k_R02_H02(temp,5)*(1.-r_COCH202_OH)	Rickard (2022)
G45403b	TrGAroCN	$\text{NTLFUO2} + \text{HO}_2 \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{OH}$	k_R02_H02(temp,5)*r_COCH202_OH	Rickard (2022)
G45404	TrGAroCN	$\text{NTLFUO2} + \text{NO} \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02NO	Rickard (2022)*
G45405	TrGAroCN	$\text{NTLFUO2} + \text{NO}_3 \rightarrow \text{ACCOMMECHO} + \text{NO}_2 + \text{NO}_2$	KR02NO3	Rickard (2022)*
G45406	TrGAroCN	$\text{NTLFUO2} \rightarrow \text{ACCOMMECHO} + \text{NO}_2$	k1_R02tOR02	Rickard (2022)*
G45407	TrGAroC	$\text{C5134CO2OH} + \text{OH} \rightarrow \text{C54CO} + \text{HO}_2$	7.48E-11	Rickard (2022)
G45408	TrGAroCN	$\text{C5COO2NO2} + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{CO} + \text{NO}_2$	5.43E-11	Rickard (2022)
G45409	TrGAroCN	$\text{C5COO2NO2} \rightarrow \text{C5CO14O2} + \text{NO}_2$	k_PAN_M	Rickard (2022)*
G45410	TrGAroC	$\text{C5DIALOOH} + \text{OH} \rightarrow \text{C5DIALCO} + \text{OH}$	7.52E-11	Rickard (2022)
G45411a	TrGAroC	$\text{C4CO2DBC03} + \text{HO}_2 \rightarrow \text{C4CO2DCO3H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard (2022)
G45411b	TrGAroC	$\text{C4CO2DBC03} + \text{HO}_2 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022), Sander et al. (2019)
G45412	TrGAroCN	$\text{C4CO2DBC03} + \text{NO} \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G45413	TrGAroCN	$\text{C4CO2DBC03} + \text{NO}_2 \rightarrow \text{C4CO2DBPAN}$	k_CH3C03_N02	Rickard (2022)*
G45414	TrGAroCN	$\text{C4CO2DBC03} + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KR02NO3*1.74	Rickard (2022)
G45415	TrGAroC	$\text{C4CO2DBC03} \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2$	k1_R02RC03	Rickard (2022)
G45416	TrGAroC	$\text{MMALANHY} + \text{OH} \rightarrow \text{MMALANHYO2}$	1.50E-12	Rickard (2022)
G45421a	TrGAroC	$\text{MMALANHYO2} + \text{HO}_2 \rightarrow \text{MMALNHYOOH}$	k_R02_H02(temp,5)*(1.-r_COCH202_OH-r_CHOHCH202_OH)	Rickard (2022), Sander et al. (2019)
G45421b	TrGAroC	$\text{MMALANHYO2} + \text{HO}_2 \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{OH}$	k_R02_H02(temp,5)*(r_COCH202_OH+r_CHOHCH202_OH)	Rickard (2022), Sander et al. (2019)
G45422	TrGAroCN	$\text{MMALANHYO2} + \text{NO} \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{NO}_2$	KR02NO	Rickard (2022)*
G45423	TrGAroCN	$\text{MMALANHYO2} + \text{NO}_3 \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{NO}_2$	KR02NO3	Rickard (2022)*
G45424	TrGAroC	$\text{MMALANHYO2} \rightarrow \text{CO2H3CO3} + \text{CO}_2$	k1_R02tOR02	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G45428	TrGAroCN	$\text{C4CO2DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO}_2 + \text{CO} + \text{NO}_2$	2.74E-11	Rickard (2022)
G45429	TrGAroCN	$\text{C4CO2DBPAN} \rightarrow \text{C4CO2DBC03} + \text{NO}_2$	k_PAN_M	Rickard (2022)*
G45430a	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022)*
G45430b	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow \text{C5CO14OH} + \text{O}_3$	KAPH02*r_C03_03	Rickard (2022)
G45430c	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow \text{C5CO14OOH}$	KAPH02*r_C03_00H	Rickard (2022)
G45431	TrGAroCN	$\text{C5CO14O2} + \text{NO} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)*
G45432	TrGAroCN	$\text{C5CO14O2} + \text{NO}_2 \rightarrow \text{C5COO2NO2}$	k_CH3C03_N02	Rickard (2022)*
G45433	TrGAroCN	$\text{C5CO14O2} + \text{NO}_3 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard (2022)*
G45434	TrGAroC	$\text{C5CO14O2} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	k1_R02RC03	Rickard (2022)*
G45436	TrGAroC	$\text{C5CO14OH} + \text{OH} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	5.44E-11	Rickard (2022)*
G45441	TrGAroCN	$\text{C5DICARB} + \text{NO}_3 \rightarrow \text{C5CO14O2} + \text{HNO}_3$	KN03AL*2.75	Rickard (2022)
G45442	TrGAroC	$\text{C5DICARB} + \text{O}_3 \rightarrow .5338 \text{ GLYOX} + .063 \text{ CH}_3\text{CHO} + .348 \text{ CH}_3\text{C(O)OO} + .918 \text{ CO} + .57 \text{ OH} + .473 \text{ HO}_2 + .0563 \text{ CH}_3\text{COCO}_2\text{H} + .5338 \text{ MGLYOX} + .676 \text{ H}_2\text{O}_2 + .063 \text{ HCHO} + .0563 \text{ HCOCO}_2\text{H} + .2465 \text{ CO}_2$	2.00E-18	Rickard (2022)
G45443	TrGAroC	$\text{C5DICARB} + \text{OH} \rightarrow .48 \text{ C5CO14O2} + .52 \text{ C5DICARBO2}$	6.2E-11	Rickard (2022)
G45444	TrGAroC	$\text{MC3ODBCO2H} + \text{OH} \rightarrow .35 \text{ GLYOX} + .35 \text{ CH}_3 + .35 \text{ CO} + .35 \text{ CO}_2 + .65 \text{ MMALANHY} + .65 \text{ HO}_2$	4.38E-11	Rickard (2022)*
G45451	TrGAroCN	$\text{TLFUONE} + \text{NO}_3 \rightarrow \text{NTLFUO2}$	1.00E-12	Rickard (2022)
G45452	TrGAroC	$\text{TLFUONE} + \text{O}_3 \rightarrow .5 \text{ CO} + .5 \text{ OH} + .5 \text{ MECOACETO2} + .3125 \text{ C24O3CCO2H} + .1875 \text{ ACCOMECHO} + .1875 \text{ H}_2\text{O}_2$	8.00E-19	see note*
G45453	TrGAroC	$\text{TLFUONE} + \text{OH} \rightarrow \text{TLFUO2}$	6.90E-11	Rickard (2022)
G45454a	TrGAroC	$\text{ACCOMECO3} + \text{HO}_2 \rightarrow \text{ACCOMECO3H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard (2022)
G45454b	TrGAroC	$\text{ACCOMECO3} + \text{HO}_2 \rightarrow \text{MECOACETO2} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022)
G45455	TrGAroCN	$\text{ACCOMECO3} + \text{NO} \rightarrow \text{MECOACETO2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G45456	TrGAroCN	$\text{ACCOMECO3} + \text{NO}_2 \rightarrow \text{ACCOMEPAN}$	k_CH3C03_N02	Rickard (2022)*
G45457	TrGAroCN	$\text{ACCOMECO3} + \text{NO}_3 \rightarrow \text{MECOACETO2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard (2022)
G45458	TrGAroC	$\text{ACCOMECO3} \rightarrow \text{MECOACETO2} + \text{CO}_2$	k1_R02RC03	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G45459	TrGAroC	$\text{C4CO2DCO3H} + \text{OH} \rightarrow \text{C4CO2DBCO3}$	$3.06\text{E-}11$	Rickard (2022)
G45464	TrGAroCN	$\text{ACCOMMECHO} + \text{NO}_3 \rightarrow \text{ACCOMECO3} + \text{HNO}_3$	KN03AL*5.5	Rickard (2022)
G45465	TrGAroC	$\text{ACCOMMECHO} + \text{OH} \rightarrow \text{ACCOMECO3}$	$7.09\text{E-}11$	Rickard (2022)
G45466	TrGAroC	$\text{MMALNHYOOH} + \text{OH} \rightarrow \text{MMALANHYO2}$	$1.69\text{E-}11$	Rickard (2022)
G45467a	TrGAroC	$\text{C5DICAROOH} + \text{OH} \rightarrow \text{C5134CO2OH} + \text{OH}$	$1.21\text{E-}10$	Rickard (2022)
G45467b	TrGAroC	$\text{C5DICAROOH} + \text{OH} \rightarrow \text{C5DICARBO2}$	k_{R00HR0}	Rickard (2022)
G45468	TrGAroC	$\text{C24O3CCO2H} + \text{OH} \rightarrow \text{MECOACETO2} + \text{CO}_2$	$8.76\text{E-}13$	Rickard (2022)
G45469	TrGAroCN	$\text{NTLFUOOH} + \text{OH} \rightarrow \text{NTLFUO2}$	$4.44\text{E-}12$	Rickard (2022)
G45470	TrGAroCN	$\text{ACCOMEPAN} + \text{OH} \rightarrow \text{METACETHO} + \text{CO} + \text{CO} + \text{NO}_2$	$1.00\text{E-}14$	Rickard (2022)
G45471	TrGAroCN	$\text{ACCOMEPAN} \rightarrow \text{ACCOMECO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G45476a	TrGAroC	$\text{TLFUO2} + \text{HO}_2 \rightarrow \text{TLFUOOH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * (1 - r_{\text{COCH202_OH}} - r_{\text{CHOHCH202_OH}})$	Rickard (2022)
G45476b	TrGAroC	$\text{TLFUO2} + \text{HO}_2 \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * (r_{\text{COCH202_OH}} + r_{\text{CHOHCH202_OH}})$	Rickard (2022)*
G45477	TrGAroCN	$\text{TLFUO2} + \text{NO} \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45478	TrGAroCN	$\text{TLFUO2} + \text{NO}_3 \rightarrow \text{ACCOMMECHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*
G45479	TrGAroC	$\text{TLFUO2} \rightarrow \text{ACCOMMECHO} + \text{HO}_2$	$k1_{\text{R02t0R02}}$	Rickard (2022)*
G45480	TrGAroC	$\text{C5CO14OOH} + \text{OH} \rightarrow \text{C5CO14O2}$	$3.59\text{E-}12$	Rickard (2022)
G45483	TrGAroC	$\text{TLFUOOH} + \text{OH} \rightarrow \text{TLFUO2}$	$2.53\text{E-}11$	Rickard (2022)
G45485	TrGAroC	$\text{ACCOMECO3H} + \text{OH} \rightarrow \text{ACCOMECO3}$	$3.59\text{E-}12$	Rickard (2022)
G45486a	TrGAroC	$\text{C5DIALO2} + \text{HO}_2 \rightarrow \text{C5DIALOOH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * (1 - r_{\text{COCH202_OH}})$	Rickard (2022)
G45486b	TrGAroC	$\text{C5DIALO2} + \text{HO}_2 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{COCH202_OH}}$	Rickard (2022)*
G45487	TrGAroCN	$\text{C5DIALO2} + \text{NO} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45488	TrGAroCN	$\text{C5DIALO2} + \text{NO}_3 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*
G45489	TrGAroC	$\text{C5DIALO2} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2$	$k1_{\text{R02s0R02}}$	Rickard (2022)*
G45490a	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{C5DICAROOH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * (r_{\text{C03_00H}} + r_{\text{C03_03}})$	Rickard (2022)
G45491b	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 5) * r_{\text{C03_OH}}$	Rickard (2022)*
G45492	TrGAroCN	$\text{C5DICARBO2} + \text{NO} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G45493	TrGAroCN	$\text{C5DICARBO2} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G45494	TrGAroC	$\text{C5DICARBO2} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2$	$k_{1_R02sOR02}$	Rickard (2022)*
G46200a	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO235C6OOH}$	$k_{R02_H02}(\text{temp}, 6) * r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G46200b	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$	$k_{R02_H02}(\text{temp}, 6) * r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G46201	TrGTerCN	$\text{CO235C6O2} + \text{NO} \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{NO}_2$	K_{R02N0}	Rickard (2022)*
G46202	TrGTerC	$\text{CO235C6O2} \rightarrow \text{CO23C4CO3} + \text{HCHO}$	$k_{1_R02pOR02}$	Rickard (2022)
G46203	TrGTerC	$\text{CO235C6OOH} + \text{OH} \rightarrow \text{CO235C6O2}$	$1.01\text{E-}11$	Rickard (2022)
G46204	TrGTerC	$\text{C614O2} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2$	$k_{1_R02sOR02}$	Rickard (2022)
G46205a	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$K_{R02N0} * (1 - \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair}))$	Rickard (2022)
G46205b	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{C614NO3}$	$K_{R02N0} * \alpha_{\text{AN}}(9, 2, 0, 1, 0, \text{temp}, \text{cair})$	Rickard (2022)
G46206a	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{C614OOH}$	$k_{R02_H02}(\text{temp}, 6) * (1 - r_{\text{CHOHCH202_OH}})$	Rickard (2022), Sander et al. (2019)
G46206b	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$k_{R02_H02}(\text{temp}, 6) * r_{\text{CHOHCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G46207	TrGTerCN	$\text{C614NO3} + \text{OH} \rightarrow \text{C614CO} + \text{NO}_2$	$7.11\text{E-}12$	Rickard (2022)
G46208	TrGTerC	$\text{C614OOH} + \text{OH} \rightarrow \text{C614CO} + \text{OH}$	$8.69\text{E-}11$	Rickard (2022)
G46209	TrGTerC	$\text{C614CO} + \text{OH} \rightarrow \text{CO235C5CHO} + \text{HO}_2$	$3.22\text{E-}12$	Rickard (2022)
G46210	TrGTerC	$\text{CO235C5CHO} + \text{OH} \rightarrow \text{CO23C4CO3} + \text{CO}$	$1.33\text{E-}11$	Rickard (2022)
G46211	TrGTerCN	$\text{CO235C5CHO} + \text{NO}_3 \rightarrow \text{CO23C4CO3} + \text{CO} + \text{HNO}_3$	$K_{N03AL} * 5.5$	Rickard (2022)
G46400	TrGAroC	$\text{PHENOOH} + \text{OH} \rightarrow \text{PHENO2}$	$1.16\text{E-}10$	Rickard (2022)
G46401	TrGAroC	$\text{C6CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{CO} + \text{HCOCOCHO}$	$7.70\text{E-}11$	Rickard (2022)
G46402	TrGAroC	$\text{C5CO2DCO3H} + \text{OH} \rightarrow \text{C5CO2DBCO3}$	$3.60\text{E-}11$	Rickard (2022)
G46403	TrGAroCN	$\text{NDNPHENOOH} + \text{OH} \rightarrow \text{NDNPHENO2}$	k_{R00HR0}	Rickard (2022)
G46404a	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C615CO2OOH}$	$k_{R02_H02}(\text{temp}, 6) * (1 - r_{\text{COCH202_OH}})$	Rickard (2022)
G46404b	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{R02_H02}(\text{temp}, 6) * r_{\text{COCH202_OH}}$	Rickard (2022)*
G46405	TrGAroCN	$\text{C615CO2O2} + \text{NO} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	K_{R02N0}	Rickard (2022)*
G46406	TrGAroCN	$\text{C615CO2O2} + \text{NO}_3 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	K_{R02N03}	Rickard (2022)*
G46407	TrGAroC	$\text{C615CO2O2} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2$	$k_{1_R02sOR02}$	Rickard (2022)*
G46408	TrGAroCN	$\text{BZEMUCPAN} + \text{OH} \rightarrow \text{MALDIAL} + \text{CO} + \text{CO}_2 + \text{NO}_2$	$4.05\text{E-}11$	Rickard (2022)
G46409	TrGAroCN	$\text{BZEMUCPAN} \rightarrow \text{BZEMUCCO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G46410	TrGAroCN	BZBIPERNO3 + OH → BZOBIPEROH + NO ₂	7.30E-11	Rickard (2022)
G46411	TrGAroCN	HOC6H4NO2 + NO ₃ → NPHEN1O + HNO ₃	9.00E-14	Rickard (2022)
G46412	TrGAroCN	HOC6H4NO2 + OH → NPHEN1O	9.00E-13	Rickard (2022)
G46413a	TrGAroCN	NDNPHENO2 + HO ₂ → NDNPHENO2OH	k_R02_H02(temp,6)*(1.-r_ CHOHCH2O2_OH)	Rickard (2022)
G46413b	TrGAroCN	NDNPHENO2 + HO ₂ → NC4DCO2H + HNO ₃ + CO + CO + NO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH2O2_OH	Rickard (2022)*
G46414	TrGAroCN	NDNPHENO2 + NO → NC4DCO2H + HNO ₃ + CO + CO + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G46415	TrGAroCN	NDNPHENO2 + NO ₃ → NC4DCO2H + HNO ₃ + CO + CO + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G46416	TrGAroCN	NDNPHENO2 → NC4DCO2H + HNO ₃ + CO + CO + NO ₂	k1_R02ISOPD02	Rickard (2022)*
G46417	TrGAroC	PBZQCO + OH → C5CO2OHCO3	6.07E-11	Rickard (2022)
G46418	TrGAroCN	CATECHOL + NO ₃ → CATEC1O + HNO ₃	9.9E-11	Rickard (2022)*
G46419	TrGAroC	CATECHOL + O ₃ → MALDALCO2H + HCOCO ₂ H + HO ₂ + OH	9.2E-18	Rickard (2022)
G46420	TrGAroC	CATECHOL + OH → CATEC1O	1.0E-10	Rickard (2022)
G46421	TrGAroC	C5COOHCO3H + OH → C5CO2OHCO3	8.01E-11	Rickard (2022)
G46422	TrGAroCN	NCATECHOL + NO ₃ → NNCATECO2	2.60E-12	Rickard (2022)
G46423	TrGAroCN	NCATECHOL + OH → NCATECO2	3.47E-12	Rickard (2022)
G46424a	TrGAroC	C5CO2OHCO3 + HO ₂ → C5COOHCO3H	KAPH02*(r_C03_00H+r_C03_03)	Rickard (2022)
G46424b	TrGAroC	C5CO2OHCO3 + HO ₂ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + OH	KAPH02*r_C03_OH	Rickard (2022)
G46425	TrGAroCN	C5CO2OHCO3 + NO → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KAPN0	Rickard (2022)
G46426	TrGAroCN	C5CO2OHCO3 + NO ₂ → C5CO2OHPAN	k_CH3C03_N02	Rickard (2022)*
G46427	TrGAroCN	C5CO2OHCO3 + NO ₃ → HOCOC4DIAL + HO ₂ + CO + CO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)
G46428	TrGAroC	C5CO2OHCO3 → HOCOC4DIAL + HO ₂ + CO + CO ₂	k1_R02RC03	Rickard (2022)
G46429	TrGAroCN	BZEPOXMUC + NO ₃ → BZEMUCCO3 + HNO ₃	2.*KN03AL*2.75	Rickard (2022)
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 (2022)*

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

#	labels	reaction	rate coefficient	reference
G46431	TrGAroC	BZEPOXMUC + OH \rightarrow .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard (2022)
G46432a	TrGAroCN	NCATECO2 + HO ₂ \rightarrow NCATECOOH	k_R02_H02(temp,6)*(1.-r_CHOHCH202_OH)	Rickard (2022)
G46432b	TrGAroCN	NCATECO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard (2022)*
G46433	TrGAroCN	NCATECO2 + NO \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard (2022)*
G46434	TrGAroCN	NCATECO2 + NO ₃ \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard (2022)*
G46435	TrGAroCN	NCATECO2 \rightarrow NC4DCO2H + HCOCO ₂ H + HO ₂	k1_R02IS0PD02	Rickard (2022)*
G46436	TrGAroCN	NPHEN1OOH + OH \rightarrow NPHEN1O2	9.00E-13	Rickard (2022)
G46437a	TrGAroCN	NPHENO2 + HO ₂ \rightarrow NPHENOOH	k_R02_H02(temp,6)*(1.-r_CHOHCH202_OH)	Rickard (2022)
G46437b	TrGAroCN	NPHENO2 + HO ₂ \rightarrow MALDALCO2H + GLYOX + NO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard (2022)*
G46438	TrGAroCN	NPHENO2 + NO \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G46439	TrGAroCN	NPHENO2 + NO ₃ \rightarrow MALDALCO2H + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G46440	TrGAroCN	NPHENO2 \rightarrow MALDALCO2H + GLYOX + NO ₂	k1_R02IS0PD02	Rickard (2022)*
G46441	TrGAroC	BENZENE + OH \rightarrow .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO ₂ + .53 PHENOL + .53 HO ₂	2.3E-12*EXP(-190./temp)	Rickard (2022)*
G46442	TrGAroCN	C5CO2OHPAN + OH \rightarrow HOCOC4DIAL + CO + CO + NO ₂	7.66E-11	Rickard (2022)
G46443	TrGAroCN	C5CO2OHPAN \rightarrow C5CO2OHCO3 + NO ₂	k_PAN_M	Rickard (2022)
G46444	TrGAroCN	CATEC1O + NO ₂ \rightarrow NCATECHOL	k_C6H50_N02	Rickard (2022), Platz et al. (1998)
G46445	TrGAroC	CATEC1O + O ₃ \rightarrow CATEC1O2	k_C6H50_O3	Rickard (2022), Tao and Li (1999)
G46446	TrGAroC	BZEMUCCO + OH \rightarrow EPXDLCO3 + GLYOX	9.20E-11	Rickard (2022)
G46447a	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NNCATECOOH	k_R02_H02(temp,6)*(1.-r_CHOHCH202_OH)	Rickard (2022)
G46447b	TrGAroCN	NNCATECO2 + HO ₂ \rightarrow NC4DCO2H + HCOCO ₂ H + NO ₂ + OH	k_R02_H02(temp,6)*r_CHOHCH202_OH	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G46448	TrGAroCN	$\text{NNCATECO}_2 + \text{NO} \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	KR02N0	Rickard (2022)*
G46449	TrGAroCN	$\text{NNCATECO}_2 + \text{NO}_3 \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*
G46450	TrGAroCN	$\text{NNCATECO}_2 \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02IS0PD02	Rickard (2022)*
G46451	TrGAroC	$\text{BZEMUCCO}_2\text{H} + \text{OH} \rightarrow \text{C}_5\text{DIALO}_2 + \text{CO}_2$	4.06E-11	Rickard (2022)
G46452	TrGAroCN	$\text{NNCATECOOH} + \text{OH} \rightarrow \text{NNCATECO}_2$	k_R00HR0	Rickard (2022)
G46453	TrGAroCN	$\text{NPHEN1O} + \text{NO}_2 \rightarrow \text{DNPHEN}$	k_C6H50_N02	Rickard (2022), Platz et al. (1998)
G46454	TrGAroCN	$\text{NPHEN1O} + \text{O}_3 \rightarrow \text{NPHEN1O}_2$	k_C6H50_03	Rickard (2022), Tao and Li (1999)
G46455	TrGAroCN	$\text{DNPHEN} + \text{NO}_3 \rightarrow \text{NDNPHENO}_2$	2.25E-15	Rickard (2022)
G46456	TrGAroCN	$\text{DNPHEN} + \text{OH} \rightarrow \text{DNPHENO}_2$	3.00E-14	Rickard (2022)
G46457	TrGAroCN	$\text{PHENOL} + \text{NO}_3 \rightarrow .742 \text{ C}_6\text{H}_5\text{O} + .742 \text{ HNO}_3 + .258 \text{ NPHENO}_2$	3.8E-12	Rickard (2022)*
G46458	TrGAroC	$\text{PHENOL} + \text{OH} \rightarrow .06 \text{ C}_6\text{H}_5\text{O} + .8 \text{ CATECHOL} + .8 \text{ HO}_2 + .14 \text{ PHENO}_2$	4.7E-13*EXP(1220./temp)	Rickard (2022)*
G46459	TrGAroCN	$\text{PBZQONE} + \text{NO}_3 \rightarrow \text{NBZQO}_2$	3.00E-13	Rickard (2022)
G46460	TrGAroC	$\text{PBZQONE} + \text{OH} \rightarrow \text{PBZQO}_2$	4.6E-12	Rickard (2022)
G46461a	TrGAroC	$\text{PHENO}_2 + \text{HO}_2 \rightarrow \text{PHENOOH}$	k_R02_H02(temp,6)*(1.-r_CHOCH202_OH)	Rickard (2022)
G46461b	TrGAroC	$\text{PHENO}_2 + \text{HO}_2 \rightarrow .71 \text{ MALDALCO}_2\text{H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{OH}$	k_R02_H02(temp,6)*r_CHOCH202_OH	Rickard (2022)*
G46462	TrGAroCN	$\text{PHENO}_2 + \text{NO} \rightarrow .71 \text{ MALDALCO}_2\text{H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G46463	TrGAroCN	$\text{PHENO}_2 + \text{NO}_3 \rightarrow .71 \text{ MALDALCO}_2\text{H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard (2022)*
G46464	TrGAroC	$\text{PHENO}_2 \rightarrow .71 \text{ MALDALCO}_2\text{H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2$	k1_R02IS0PD02	Rickard (2022)*
G46465	TrGAroC	$\text{C}_6\text{H}_5\text{CO}_2\text{OOH} + \text{OH} \rightarrow \text{C}_6\text{H}_5\text{CO} + \text{OH}$	9.42E-11	Rickard (2022)
G46466a	TrGAroC	$\text{C}_5\text{CO}_2\text{DBCO}_3 + \text{HO}_2 \rightarrow \text{C}_5\text{CO}_2\text{DCO}_3\text{H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard (2022)
G46466b	TrGAroC	$\text{C}_5\text{CO}_2\text{DBCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022)
G46467	TrGAroCN	$\text{C}_5\text{CO}_2\text{DBCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G46468	TrGAroCN	$\text{C5CO2DBCO3} + \text{NO}_2 \rightarrow \text{C5CO2DBPAN}$	$k_{\text{CH3CO3_NO2}}$	Rickard (2022)*
G46469	TrGAroCN	$\text{C5CO2DBCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	$\text{KR02NO3} \times 1.74$	Rickard (2022)
G46470	TrGAroC	$\text{C5CO2DBCO3} \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2$	$k1_{\text{R02RCO3}}$	Rickard (2022)
G46471	TrGAroCN	$\text{NPHEN1O2} + \text{HO}_2 \rightarrow \text{NPHEN1OOH}$	$k_{\text{R02_HO2}}(\text{temp}, 6)$	Rickard (2022)
G46472a	TrGAroCN	$\text{NPHEN1O2} + \text{NO} \rightarrow \text{NPHEN1O} + \text{NO}_2$	KR02NO	Rickard (2022)
G46472b	TrGAroCN	$\text{NPHEN1O2} + \text{NO}_2 \rightarrow \text{NPHEN1O} + \text{NO}_3$	$k_{\text{C6H5O2_NO2}}$	Jagiella and Zabel (2007)*
G46473	TrGAroCN	$\text{NPHEN1O2} + \text{NO}_3 \rightarrow \text{NPHEN1O} + \text{NO}_2$	KR02NO3	Rickard (2022)
G46474	TrGAroCN	$\text{NPHEN1O2} \rightarrow \text{NPHEN1O}$	$k1_{\text{R02sR02}}$	Rickard (2022)
G46475	TrGAroCN	$\text{NPHENOOH} + \text{OH} \rightarrow \text{NPHENO2}$	$1.07\text{E-}10$	Rickard (2022)
G46476	TrGAroCN	$\text{C6H5O} + \text{NO}_2 \rightarrow \text{HOC6H4NO2}$	$k_{\text{C6H5O_NO2}}$	Rickard (2022), Platz et al. (1998)*
G46477	TrGAroC	$\text{C6H5O} + \text{O}_3 \rightarrow \text{C6H5O2}$	$k_{\text{C6H5O_O3}}$	Rickard (2022), Tao and Li (1999)
G46478	TrGAroCN	$\text{NCATECOOH} + \text{OH} \rightarrow \text{NCATECO2}$	k_{R00HRO}	Rickard (2022)
G46479	TrGAroC	$\text{PBZQOOH} + \text{OH} \rightarrow \text{PBZQCO} + \text{OH}$	$1.23\text{E-}10$	Rickard (2022)
G46480a	TrGAroC	$\text{PBZQO2} + \text{HO}_2 \rightarrow \text{PBZQOOH}$	$k_{\text{R02_HO2}}(\text{temp}, 6) \times (1 - r_{\text{CHOHCH2O2_OH}} - r_{\text{COCH2O2_OH}})$	Rickard (2022)
G46480b	TrGAroC	$\text{PBZQO2} + \text{HO}_2 \rightarrow \text{C5CO2OHCO3} + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp}, 6) \times (r_{\text{CHOHCH2O2_OH}} + r_{\text{COCH2O2_OH}})$	Rickard (2022)*
G46481	TrGAroCN	$\text{PBZQO2} + \text{NO} \rightarrow \text{C5CO2OHCO3} + \text{NO}_2$	KR02NO	Rickard (2022)*
G46482	TrGAroCN	$\text{PBZQO2} + \text{NO}_3 \rightarrow \text{C5CO2OHCO3} + \text{NO}_2$	KR02NO3	Rickard (2022)*
G46483	TrGAroC	$\text{PBZQO2} \rightarrow \text{C5CO2OHCO3}$	$k1_{\text{R02sOR02}}$	Rickard (2022)*
G46484	TrGAroC	$\text{BZOBIPEROH} + \text{OH} \rightarrow \text{MALDIALCO3} + \text{GLYOX}$	$8.16\text{E-}11$	Rickard (2022)
G46485a	TrGAroCN	$\text{DNPHENO2} + \text{HO}_2 \rightarrow \text{DNPHENOOH}$	$k_{\text{R02_HO2}}(\text{temp}, 6) \times (1 - r_{\text{CHOHCH2O2_OH}})$	Rickard (2022)
G46485b	TrGAroCN	$\text{DNPHENO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$k_{\text{R02_HO2}}(\text{temp}, 6) \times r_{\text{CHOHCH2O2_OH}}$	Rickard (2022)*
G46486	TrGAroCN	$\text{DNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02NO	Rickard (2022)*
G46487	TrGAroCN	$\text{DNPHENO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{NO}_2$	KR02NO3	Rickard (2022)*
G46488	TrGAroCN	$\text{DNPHENO2} \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2$	$k1_{\text{R02ISOPD02}}$	Rickard (2022)*
G46489	TrGAroC	$\text{BZBIPEROOH} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{OH}$	$9.77\text{E-}11$	Rickard (2022)
G46490a	TrGAroC	$\text{BZEMUCO2} + \text{HO}_2 \rightarrow \text{BZEMUCOOH}$	$k_{\text{R02_HO2}}(\text{temp}, 6)$	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G46490b	TrGAroC	BZEMUCO ₂ + HO ₂ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO ₂ + .5 C32OH13CO + OH	k_R02_H02(temp,6)	Rickard (2022)*
G46491a	TrGAroCN	BZEMUCO ₂ + NO → BZEMUCNO ₃	KR02N0*alpha_AN(10,2,0,1,0, temp, cair)	Rickard (2022)
G46491b	TrGAroCN	BZEMUCO ₂ + NO → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO ₂ + .5 C32OH13CO + NO ₂	KR02N0*(1.-alpha_AN(10,2,0,1,0, temp, cair))	Rickard (2022)*
G46492	TrGAroCN	BZEMUCO ₂ + NO ₃ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO ₂ + .5 C32OH13CO + NO ₂	KR02N03	Rickard (2022)*
G46493	TrGAroC	BZEMUCO ₂ → .5 EPXC4DIAL + .5 GLYOX + .5 HO ₂ + .5 C3DIALO ₂ + .5 C32OH13CO	k1_R02sOR02	Rickard (2022)*
G46494	TrGAroCN	C5CO2DBPAN + OH → HCOCOCHO + CH ₃ CHO + CO ₂ + NO ₂	3.28E-11	Rickard (2022)
G46495	TrGAroCN	C5CO2DBPAN → C5CO2DBCO ₃ + NO ₂	k_PAN_M	Rickard (2022)
G46496	TrGAroCN	NBZQOOH + OH → NBZQO ₂	6.68E-11	Rickard (2022)
G46497	TrGAroC	CATEC1OOH + OH → CATEC1O ₂	k_R00HRO	Rickard (2022)
G46498	TrGAroC	C6125CO + OH → C5CO14O ₂ + CO	6.45E-11	Rickard (2022)
G46499a	TrGAroCN	NBZQO ₂ + HO ₂ → NBZQOOH	k_R02_H02(temp,6)*(1.-r_COCH2O2_OH)	Rickard (2022)
G46499b	TrGAroCN	NBZQO ₂ + HO ₂ → C6CO4DB + NO ₂ + OH	k_R02_H02(temp,6)*r_COCH2O2_OH	Rickard (2022)*
G46500	TrGAroCN	NBZQO ₂ + NO → C6CO4DB + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G46501	TrGAroCN	NBZQO ₂ + NO ₃ → C6CO4DB + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G46502	TrGAroCN	NBZQO ₂ → C6CO4DB + NO ₂	k1_R02sOR02	Rickard (2022)*
G46503	TrGAroCN	DNPHEOOH + OH → DNPHEO ₂	k_R00HRO	Rickard (2022)
G46504	TrGAroC	CATEC1O ₂ + HO ₂ → CATEC1OOH	k_R02_H02(temp,6)	Rickard (2022)
G46505a	TrGAroCN	CATEC1O ₂ + NO → CATEC1O + NO ₂	KR02N0	Rickard (2022)
G46505b	TrGAroCN	CATEC1O ₂ + NO ₂ → CATEC1O + NO ₃	k_C6H5O2_N02	Jagiella and Zabel (2007)*
G46506	TrGAroCN	CATEC1O ₂ + NO ₃ → CATEC1O + NO ₂	KR02N03	Rickard (2022)
G46507	TrGAroC	CATEC1O ₂ → CATEC1O	k1_R02sOR02	Rickard (2022)
G46508	TrGAroC	BZEMUCCO ₃ H + OH → BZEMUCCO ₃	4.37E-11	Rickard (2022)
G46509	TrGAroC	C6H5OOH + OH → C6H5O ₂	3.60E-12	Rickard (2022)
G46510	TrGAroC	BZEMUCOOH + OH → BZEMUCCO + OH	1.31E-10	Rickard (2022)
G46511a	TrGAroC	BZEMUCCO ₃ + HO ₂ → BZEMUCCO ₂ H + O ₃	KAPH02*r_C03_03	Rickard (2022)
G46511b	TrGAroC	BZEMUCCO ₃ + HO ₂ → BZEMUCCO ₃ H	KAPH02*r_C03_00H	Rickard (2022)
G46511c	TrGAroC	BZEMUCCO ₃ + HO ₂ → C5DIALO ₂ + CO ₂ + OH	KAPH02*r_C03_0H	Rickard (2022)
G46512	TrGAroCN	BZEMUCCO ₃ + NO → C5DIALO ₂ + CO ₂ + NO ₂	KAPNO	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G46513	TrGAroCN	BZEMUCCO3 + NO ₂ → BZEMUCPAN	k_CH3CO3_NO2	Rickard (2022)
G46514	TrGAroCN	BZEMUCCO3 + NO ₃ → C5DIALO2 + CO ₂ + NO ₂	KR02NO3*1.74	Rickard (2022)
G46515	TrGAroC	BZEMUCCO3 → C5DIALO2 + CO ₂	k1_R02RCO3	Rickard (2022)*
G46516	TrGAroC	C6H5O2 + HO ₂ → C6H5OOH	k_R02_H02(temp,6)	Rickard (2022)
G46517	TrGAroCN	C6H5O2 + NO → C6H5O + NO ₂	KR02NO	Rickard (2022)
G46518	TrGAroCN	C6H5O2 + NO ₃ → C6H5O + NO ₂	KR02NO3	Rickard (2022)
G46519	TrGAroC	C6H5O2 → C6H5O	k1_R02sR02	Rickard (2022)
G46520	TrGAroCN	C6H5O2 + NO ₂ → C6H5O + NO ₃	k_C6H5O2_NO2	Jagiella and Zabel (2007)
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO ₂	4.38E-11	Rickard (2022)
G46522a	TrGAroC	BZBIPERO2 + HO ₂ → BZBIPEROOH	k_R02_H02(temp,6)*(1.-r_BIPERO2_OH)	Rickard (2022)
G46522b	TrGAroC	BZBIPERO2 + HO ₂ → OH + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	k_R02_H02(temp,6)*r_BIPERO2_OH	Rickard (2022), Birdsall et al. (2010)*
G46523a	TrGAroCN	BZBIPERO2 + NO → BZBIPERNO3	KR02NO*alpha_AN(9,2,0,0,1,temp,cair)	Rickard (2022)
G46523b	TrGAroCN	BZBIPERO2 + NO → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02NO*(1.-alpha_AN(9,2,0,0,1,temp,cair))	Rickard (2022)*
G46524	TrGAroCN	BZBIPERO2 + NO ₃ → NO ₂ + GLYOX + HO ₂ + .5 BZFUONE + .5 BZFUONE	KR02NO3	Rickard (2022)*
G46525	TrGAroC	BZBIPERO2 → GLYOX + HO ₂ + BZFUONE	k1_R02sOR02	Rickard (2022)*
G47200	TrGTerCN	CO235C6CHO + NO ₃ → CO235C6CO3 + HNO ₃	KN03AL*5.5	Rickard (2022)
G47201	TrGTerC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard (2022)
G47202a	TrGTerC	CO235C6CO3 + HO ₂ → C235C6CO3H	KAPH02*(r_C03_OOH+r_C03_O3)	Rickard (2022)
G47202b	TrGTerC	CO235C6CO3 + HO ₂ → CO235C6O2 + CO ₂ + OH	KAPH02*r_C03_OH	Rickard (2022)
G47203	TrGTerCN	CO235C6CO3 + NO → CO235C6O2 + CO ₂ + NO ₂	KAPNO	Rickard (2022)
G47204	TrGTerCN	CO235C6CO3 + NO ₂ → C7PAN3	k_CH3CO3_NO2	Rickard (2022)
G47205	TrGTerC	CO235C6CO3 → CO235C6O2 + CO ₂	k1_R02RCO3	Rickard (2022)
G47206	TrGTerC	C235C6CO3H + OH → CO235C6CO3	4.75E-12	Rickard (2022)
G47207	TrGTerCN	C7PAN3 + OH → CO235C5CHO + CO + NO ₂	8.83E-13	Rickard (2022)
G47208	TrGTerCN	C7PAN3 → CO235C6CO3 + NO ₂	k_PAN_M	Rickard (2022)
G47209a	TrGTerC	C716O2 + HO ₂ → C716OOH	k_R02_H02(temp,7)*r_COCH202_OOH	Rickard (2022), Sander et al. (2019)
G47209b	TrGTerC	C716O2 + HO ₂ → CO13C4CHO + CH ₃ C(O) + OH	k_R02_H02(temp,7)*r_COCH202_OH	Rickard (2022), Sander et al. (2019)
G47210	TrGTerCN	C716O2 + NO → CO13C4CHO + CH ₃ C(O) + NO ₂	KR02NO	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G47211	TrGTerC	$C716O2 \rightarrow CO13C4CHO + CH_3C(O)$	k1_R02s0R02	Rickard (2022)
G47212	TrGTerC	$C716OOH + OH \rightarrow CO235C6CHO + OH$	1.20E-10	Rickard (2022)
G47213	TrGTerC	$C721O2 + HO_2 \rightarrow C721OOH$	k_R02_H02(temp, 7)	Rickard (2022)
G47214	TrGTerCN	$C721O2 + NO \rightarrow C722O2 + NO_2$	KR02N0	Rickard (2022)*
G47215	TrGTerC	$C721O2 \rightarrow C722O2$	k1_R02pR02	Rickard (2022)
G47216	TrGTerC	$C721OOH + OH \rightarrow C721O2$	1.27E-11	Rickard (2022)
G47217	TrGTerC	$C722O2 + HO_2 \rightarrow C722OOH$	k_R02_H02(temp, 7)	Rickard (2022)
G47218	TrGTerCN	$C722O2 + NO \rightarrow CH_3COCH_3 + C44O2 + NO_2$	KR02N0	Rickard (2022)*
G47219	TrGTerC	$C722O2 \rightarrow CH_3COCH_3 + C44O2$	k1_R02tR02	Rickard (2022)
G47220	TrGTerC	$C722OOH + OH \rightarrow C722O2$	3.31E-11	Rickard (2022)
G47221	TrGTerC	$ROO6R3O2 \rightarrow ROO6R5O2$	5.68E10*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*EXP(-2949./temp)	Vereecken and Peeters (2012)*
G47226	TrGTerC	$ROO6R5O2 \rightarrow 7 \text{ L CARBON} + OH$	9.17E10*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*EXP(340./temp)	Rickard (2022)*
G47401	TrGAroC	$C6H5CH2O2 + HO_2 \rightarrow C6H5CH2OOH$	1.5E-13*EXP(1310./temp)	Rickard (2022)
G47402a	TrGAroCN	$C6H5CH2O2 + NO \rightarrow C6H5CH2NO3$	KR02N0*alpha_AN(7,1,0,0,0,temp, cair)	Rickard (2022)*
G47402b	TrGAroCN	$C6H5CH2O2 + NO \rightarrow BENZAL + HO_2 + NO_2$	KR02N0*(1.-alpha_AN(7,1,0,0,0,temp, cair))	Rickard (2022)*
G47403	TrGAroCN	$C6H5CH2O2 + NO_3 \rightarrow BENZAL + HO_2 + NO_2$	KR02N03	Rickard (2022)*
G47404	TrGAroC	$C6H5CH2O2 \rightarrow BENZAL + HO_2$	2.*(k_CH302*2.4E-14*EXP(1620./temp))**(0.5)*R02	Rickard (2022)*
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 (2022)*
G47406	TrGAroC	$CRESOL + OH \rightarrow .2 \text{ CRESO2} + .727 \text{ MCATECHOL} + .727 \text{ HO}_2 + .073 \text{ TOL1O}$	4.65E-11	Rickard (2022)*
G47407a	TrGAroC	$TLBIPERO2 + HO_2 \rightarrow TLBIPEROOH$	k_R02_H02(temp, 7)*(1.-r_BIPERO2_OH)	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G47407b	TrGAroC	TLBIPERO2 + HO ₂ → OH + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k_R02_H02(temp,7)*r_BIPERO2_OH	Rickard (2022), Birdsall et al. (2010)*
G47408a	TrGAroCN	TLBIPERO2 + NO → NO ₂ + .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KR02N0*(1.-alpha_AN(11,2,0,0,1, temp, cair))	Rickard (2022)*
G47408b	TrGAroCN	TLBIPERO2 + NO → TLBIPERNO3	KR02N0*alpha_AN(11,2,0,0,1, temp, cair)	Rickard (2022)*
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 (2022)*
G47410	TrGAroC	TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k1_R02sOR02	Rickard (2022)*
G47411	TrGAroCN	TLEPOXMUC + NO ₃ → TLEMUCCO3 + HNO ₃	KN03AL*2.75	Rickard (2022)
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 (2022)*
G47413	TrGAroC	TLEPOXMUC + OH → .31 TLEMUCCO3 + .69 TLEMUCO2	7.99E-11	Rickard (2022)*
G47414	TrGAroC	C6H5CH2OOH + OH → BENZAL + OH	2.05E-11	Rickard (2022)
G47415	TrGAroCN	C6H5CH2NO3 + OH → BENZAL + NO ₂	6.03E-12	Rickard (2022)
G47416	TrGAroCN	BENZAL + NO ₃ → C6H5CO3 + HNO ₃	2.40E-15	Rickard (2022)
G47417	TrGAroC	BENZAL + OH → C6H5CO3	5.9E-12*EXP(225./temp)	Rickard (2022)
G47418a	TrGAroC	CRESO2 + HO ₂ → CRESOOH	k_R02_H02(temp,7)*(1.-r_CHOCH202_OH)	Rickard (2022)
G47418b	TrGAroC	CRESO2 + HO ₂ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	k_R02_H02(temp,7)*r_CHOCH202_OH	Rickard (2022)*
G47419	TrGAroCN	CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N0	Rickard (2022)*
G47420	TrGAroCN	CRESO2 + NO ₃ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + NO ₂	KR02N03	Rickard (2022)*
G47421	TrGAroC	CRESO2 → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE	k1_R02ISOPD02	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G47422a	TrGAroCN	NCRESO2 + HO ₂ → NCRESOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH)	Rickard (2022)
G47422b	TrGAroCN	NCRESO2 + HO ₂ → C5CO14OH + GLYOX + NO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard (2022)*
G47423	TrGAroCN	NCRESO2 + NO → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G47424	TrGAroCN	NCRESO2 + NO ₃ → C5CO14OH + GLYOX + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47425	TrGAroCN	NCRESO2 → C5CO14OH + GLYOX + NO ₂	k1_R02IS0PD02	Rickard (2022)*
G47426	TrGAroCN	TOL1O + NO ₂ → TOL1OHNO2	k_C6H50_N02	Rickard (2022), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O ₃ → OXYL1O2	k_C6H50_03	Rickard (2022), Tao and Li (1999)
G47428	TrGAroCN	MCATECHOL + NO ₃ → MCATEC1O + HNO ₃	1.7E-10*1.0	Rickard (2022)
G47429	TrGAroC	MCATECHOL + O ₃ → MC3ODBCO2H + HCOCO ₂ H + HO ₂ + OH	2.8E-17	Rickard (2022)*
G47430	TrGAroC	MCATECHOL + OH → MCATEC1O	2.0E-10*1.0	Rickard (2022)
G47431	TrGAroC	TLBIPEROOH + OH → TLOBIPEROH + OH	9.64E-11	Rickard (2022)
G47432	TrGAroCN	TLBIPERNO3 + OH → TLOBIPEROH + NO ₂	7.16E-11	Rickard (2022)
G47433	TrGAroC	TLOBIPEROH + OH → C5CO14O2 + GLYOX	7.99E-11	Rickard (2022)
G47434a	TrGAroC	TLEMUCCO3 + HO ₂ → C615CO2O2 + CO ₂ + OH	KAPH02*r_C03_OH	Rickard (2022)
G47434b	TrGAroC	TLEMUCCO3 + HO ₂ → TLEMUCCO2H + O ₃	KAPH02*r_C03_03	Rickard (2022)
G47434c	TrGAroC	TLEMUCCO3 + HO ₂ → TLEMUCCO3H	KAPH02*r_C03_00H	Rickard (2022)
G47435	TrGAroCN	TLEMUCCO3 + NO → C615CO2O2 + CO ₂ + NO ₂	KAPN0	Rickard (2022)
G47436	TrGAroCN	TLEMUCCO3 + NO ₂ → TLEMUCPAN	k_CH3C03_N02	Rickard (2022)*
G47437	TrGAroCN	TLEMUCCO3 + NO ₃ → C615CO2O2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)
G47438	TrGAroC	TLEMUCCO3 → C615CO2O2 + CO ₂	k1_R02RC03	Rickard (2022)*
G47439a	TrGAroC	TLEMUCO2 + HO ₂ → TLEMUCOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH-r_COCH202_OH)	Rickard (2022)
G47439b	TrGAroC	TLEMUCO2 + HO ₂ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH	k_R02_H02(temp,7)*(r_CHOHCH202_OH+r_COCH202_OH)	Rickard (2022)*
G47440a	TrGAroCN	TLEMUCO2 + NO → TLEMUCNO3	KR02N0*alpha_AN(11,2,1,0,0, temp, cair)	Rickard (2022)
G47440b	TrGAroCN	TLEMUCO2 + NO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + NO ₂	KR02N0*(1.-alpha_AN(11,2,1,0,0, temp, cair))	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G47441	TrGAroCN	TLEMUCO2 + NO ₃ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47442	TrGAroC	TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂	k1_R02s0R02	Rickard (2022)*
G47443a	TrGAroC	C6H5CO3 + HO ₂ → C6H5CO3H	1.1E-11*EXP(364./temp)*0.65	Roth et al. (2010)
G47443b	TrGAroC	C6H5CO3 + HO ₂ → C6H5O2 + CO ₂ + OH	1.1E-11*EXP(364./temp)*0.20	Roth et al. (2010)
G47443c	TrGAroC	C6H5CO3 + HO ₂ → PHCOOH + O ₃	1.1E-11*EXP(364./temp)*0.15	Roth et al. (2010)
G47444	TrGAroCN	C6H5CO3 + NO → C6H5O2 + CO ₂ + NO ₂	KAPN0	Rickard (2022)
G47445	TrGAroCN	C6H5CO3 + NO ₂ → PBZN	k_CH3CO3_N02	Rickard (2022)*
G47446	TrGAroCN	C6H5CO3 + NO ₃ → C6H5O2 + CO ₂ + NO ₂	KR02N03*1.74	Rickard (2022)
G47447	TrGAroC	C6H5CO3 → C6H5O2 + CO ₂	k1_R02RC03	Rickard (2022)*
G47448	TrGAroC	CRESOOH + OH → CRESO2	1.15E-10	Rickard (2022)
G47449	TrGAroCN	NCRESOOH + OH → NCRESO2	1.07E-10	Rickard (2022)
G47450	TrGAroCN	TOL1OHNO2 + NO ₃ → NCRES1O + HNO ₃	3.13E-13*1.0	Rickard (2022)
G47451	TrGAroCN	TOL1OHNO2 + OH → NCRES1O	2.8E-12	Rickard (2022)
G47452	TrGAroC	OXYL1O2 + HO ₂ → OXYL1OOH	k_R02_H02(temp, 7)	Rickard (2022)
G47453	TrGAroCN	OXYL1O2 + NO → TOL1O + NO ₂	KR02N0	Rickard (2022)
G47454	TrGAroCN	OXYL1O2 + NO ₂ → TOL1O + NO ₃	k_C6H502_N02	Jagiella and Zabel (2007)*
G47455	TrGAroCN	OXYL1O2 + NO ₃ → TOL1O + NO ₂	KR02N03	Rickard (2022)
G47456	TrGAroC	OXYL1O2 → TOL1O	k1_R02sR02	Rickard (2022)
G47457	TrGAroCN	MCATEC1O + NO ₂ → MNCATECH	k_C6H50_N02	Rickard (2022), Platz et al. (1998)
G47458	TrGAroC	MCATEC1O + O ₃ → MCATEC1O2	k_C6H50_03	Rickard (2022), Tao and Li (1999)
G47459	TrGAroC	TLEMUCCO2H + OH → C615CO2O2 + CO ₂	5.98E-11	Rickard (2022)
G47460	TrGAroC	TLEMUCCO3H + OH → TLEMUCCO3	6.29E-11	Rickard (2022)
G47461	TrGAroCN	TLEMUCPAN + OH → C5DICARB + CO + CO ₂ + NO ₂	5.96E-11	Rickard (2022)
G47462	TrGAroCN	TLEMUCPAN → TLEMUCCO3 + NO ₂	k_PAN_M	Rickard (2022)
G47463	TrGAroC	TLEMUCOOH + OH → TLEMUCCO + OH	7.04E-11	Rickard (2022)
G47464	TrGAroCN	TLEMUCNO3 + OH → TLEMUCCO + NO ₂	3.06E-11	Rickard (2022)
G47465	TrGAroC	TLEMUCCO + OH → CH ₃ C(O) + EPXC4DIAL + CO	4.06E-11	Rickard (2022)
G47466	TrGAroC	C6H5CO3H + OH → C6H5CO3	4.66E-12	Rickard (2022)
G47467	TrGAroC	PHCOOH + OH → C6H5O2 + CO ₂	1.10E-12	Rickard (2022)
G47468	TrGAroCN	PBZN + OH → C6H5OOH + CO + NO ₂	1.06E-12	Rickard (2022)
G47469	TrGAroCN	PBZN → C6H5CO3 + NO ₂	k_PAN_M*0.67	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G47470	TrGAroCN	PTLQONE + NO ₃ → NPTLQO2	1.00E-12	Rickard (2022)
G47471	TrGAroC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard (2022)
G47472	TrGAroCN	NCRES1O + NO ₂ → DNCRES	k_C6H50_N02	Rickard (2022), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O ₃ → NCRES1O2	k_C6H50_O3	Rickard (2022), Tao and Li (1999)
G47474	TrGAroC	OXYL1OOH + OH → OXYL1O2	4.65E-11	Rickard (2022)
G47475	TrGAroCN	MNCATECH + NO ₃ → MNNCATECO2	5.03E-12	Rickard (2022)
G47476	TrGAroCN	MNCATECH + OH → MNCATECO2	6.83E-12	Rickard (2022)
G47477	TrGAroC	MCATEC1O2 + HO ₂ → MCATEC1OOH	k_R02_H02(temp, 7)	Rickard (2022)
G47478	TrGAroCN	MCATEC1O2 + NO → MCATEC1O + NO ₂	KR02N0	Rickard (2022)
G47479	TrGAroCN	MCATEC1O2 + NO ₂ → MCATEC1O + NO ₃	k_C6H502_N02	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO ₃ → MCATEC1O + NO ₂	KR02N03	Rickard (2022)
G47481	TrGAroC	MCATEC1O2 → MCATEC1O	k1_R02sOR02	Rickard (2022)
G47482a	TrGAroCN	NPTLQO2 + HO ₂ → NPTLQOOH	k_R02_H02(temp, 7) * (1 - r_COCH202_OH)	Rickard (2022)
G47482b	TrGAroCN	NPTLQO2 + HO ₂ → C7CO4DB + NO ₂ + OH	k_R02_H02(temp, 7) * r_COCH202_OH	Rickard (2022)*
G47483	TrGAroCN	NPTLQO2 + NO → C7CO4DB + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G47484	TrGAroCN	NPTLQO2 + NO ₃ → C7CO4DB + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47485	TrGAroCN	NPTLQO2 → C7CO4DB + NO ₂	k1_R02sOR02	Rickard (2022)*
G47486a	TrGAroC	PTLQO2 + HO ₂ → PTLQOOH	k_R02_H02(temp, 7) * (1 - r_CHOCH202_OH - r_COCH202_OH)	Rickard (2022)
G47486b	TrGAroC	PTLQO2 + HO ₂ → C6CO2OHCO3 + OH	k_R02_H02(temp, 7) * (r_CHOCH202_OH + r_COCH202_OH)	Rickard (2022)*
G47487	TrGAroCN	PTLQO2 + NO → C6CO2OHCO3 + NO ₂	KR02N0	Rickard (2022)*
G47488	TrGAroCN	PTLQO2 + NO ₃ → C6CO2OHCO3 + NO ₂	KR02N03	Rickard (2022)*
G47489	TrGAroC	PTLQO2 → C6CO2OHCO3	k1_R02sOR02	Rickard (2022)*
G47490	TrGAroCN	DNCRES + NO ₃ → NDNCRESO2	7.83E-15	Rickard (2022)
G47491	TrGAroCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard (2022)
G47492	TrGAroCN	NCRES1O2 + HO ₂ → NCRES1OOH	k_R02_H02(temp, 7)	Rickard (2022)
G47493	TrGAroCN	NCRES1O2 + NO → NCRES1O + NO ₂	KR02N0	Rickard (2022)
G47494	TrGAroCN	NCRES1O2 + NO ₂ → NCRES1O + NO ₃	k_C6H502_N02	Jagiella and Zabel (2007)*
G47495	TrGAroCN	NCRES1O2 + NO ₃ → NCRES1O + NO ₂	KR02N03	Rickard (2022)
G47496	TrGAroCN	NCRES1O2 → NCRES1O	k1_R02sR02	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G47497a	TrGAroCN	MNNCATECO ₂ + HO ₂ → MNNCATCOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH)	Rickard (2022)
G47497b	TrGAroCN	MNNCATECO ₂ + HO ₂ → NC4MDCO ₂ HN + HCOCO ₂ H + NO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard (2022)*
G47498	TrGAroCN	MNNCATECO ₂ + NO → NC4MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G47499	TrGAroCN	MNNCATECO ₂ + NO ₃ → NC4MDCO ₂ HN + HCOCO ₂ H + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47500	TrGAroCN	MNNCATECO ₂ → NC4MDCO ₂ HN + HCOCO ₂ H + NO ₂	k1_R02IS0PD02	Rickard (2022)
G47501a	TrGAroCN	MNCATECO ₂ + HO ₂ → MNCATECOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH)	Rickard (2022)
G47501b	TrGAroCN	MNCATECO ₂ + HO ₂ → NC4MDCO ₂ HN + HCOCO ₂ H + HO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard (2022)*
G47502	TrGAroCN	MNCATECO ₂ + NO → NC4MDCO ₂ HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N0	Rickard (2022)*
G47503	TrGAroCN	MNCATECO ₂ + NO ₃ → NC4MDCO ₂ HN + HCOCO ₂ H + HO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47504	TrGAroCN	MNCATECO ₂ → NC4MDCO ₂ HN + HCOCO ₂ H + HO ₂	k1_R02IS0PD02	Rickard (2022)*
G47505	TrGAroC	MCATEC10OH + OH → MCATEC1O2	2.05E-10	Rickard (2022)
G47506	TrGAroCN	NPTLQOOH + OH → NPTLQO2	8.56E-11	Rickard (2022)
G47507	TrGAroC	PTLQOOH + OH → PTLQCO + OH	1.42E-10	Rickard (2022)
G47508	TrGAroC	PTLQCO + OH → C6CO2OHCO3	7.95E-11	Rickard (2022)
G47509a	TrGAroCN	NDNCRESO ₂ + HO ₂ → NDNCRESOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH)	Rickard (2022)
G47509b	TrGAroCN	NDNCRESO ₂ + HO ₂ → NC4MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard (2022)*
G47510	TrGAroCN	NDNCRESO ₂ + NO → NC4MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N0	Rickard (2022)*
G47511	TrGAroCN	NDNCRESO ₂ + NO ₃ → NC4MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂ + NO ₂	KR02N03	Rickard (2022)*
G47512	TrGAroCN	NDNCRESO ₂ → NC4MDCO ₂ HN + HNO ₃ + 2 CO + NO ₂	k1_R02IS0PD02	Rickard (2022)*
G47513a	TrGAroCN	DNCRESO ₂ + HO ₂ → DNCRESOOH	k_R02_H02(temp,7)*(1.-r_ CHOHCH202_OH)	Rickard (2022)
G47513b	TrGAroCN	DNCRESO ₂ + HO ₂ → NC4MDCO ₂ HN + HCOCO ₂ H + NO ₂ + OH	k_R02_H02(temp,7)*r_CHOHCH202_OH	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
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 (2022)*
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 (2022)*
G47516	TrGAroCN	$\text{DNCRESO}_2 \rightarrow \text{NC4MDCO}_2\text{HN} + \text{HCOCO}_2\text{H} + \text{NO}_2$	k1_R02IS0PD02	Rickard (2022)*
G47517	TrGAroCN	$\text{NCRES1OOH} + \text{OH} \rightarrow \text{NCRES1O}_2$	1.53E-12	Rickard (2022)
G47518	TrGAroCN	$\text{MNNCATCOOH} + \text{OH} \rightarrow \text{MNNCATECO}_2$	k_R00HRO	Rickard (2022)
G47519	TrGAroCN	$\text{MNCATECOOH} + \text{OH} \rightarrow \text{MNCATECO}_2$	k_R00HRO	Rickard (2022)
G47520	TrGAroC	$\text{C7CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{CH}_3\text{C(O)} + \text{HCOCOCHO}$	9.58E-11	Rickard (2022)
G47521a	TrGAroC	$\text{C6CO2OHCO}_3 + \text{HO}_2 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022)
G47521b	TrGAroC	$\text{C6CO2OHCO}_3 + \text{HO}_2 \rightarrow \text{C6COOHCO}_3\text{H}$	KAPH02*(r_C03_00H+r_C03_03)	Rickard (2022)
G47522	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO} \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard (2022)
G47523	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO}_2 \rightarrow \text{C6CO}_2\text{OHPAN}$	k_CH3C03_N02	Rickard (2022)
G47524	TrGAroCN	$\text{C6CO2OHCO}_3 + \text{NO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard (2022)
G47525	TrGAroC	$\text{C6CO2OHCO}_3 \rightarrow \text{C5134CO}_2\text{OH} + \text{HO}_2 + \text{CO} + \text{CO}_2$	k1_R02RC03	Rickard (2022)
G47526	TrGAroCN	$\text{NDNCRESOOH} + \text{OH} \rightarrow \text{NDNCRESO}_2$	k_R00HRO	Rickard (2022)
G47527	TrGAroCN	$\text{DNCRESOOH} + \text{OH} \rightarrow \text{DNCRESO}_2$	k_R00HRO	Rickard (2022)
G47528	TrGAroC	$\text{C6COOHCO}_3\text{H} + \text{OH} \rightarrow \text{C6CO}_2\text{OHCO}_3$	9.29E-11	Rickard (2022)
G47529	TrGAroCN	$\text{C6CO}_2\text{OHPAN} + \text{OH} \rightarrow \text{C5134CO}_2\text{OH} + \text{CO} + \text{CO} + \text{NO}_2$	8.96E-11	Rickard (2022)
G47530	TrGAroCN	$\text{C6CO}_2\text{OHPAN} \rightarrow \text{C6CO}_2\text{OHCO}_3 + \text{NO}_2$	k_PAN_M	Rickard (2022)
G48200	TrGTerC	$\text{C85O}_2 \rightarrow \text{C86O}_2$	k1_R02tR02	Rickard (2022)
G48201	TrGTerC	$\text{C85O}_2 + \text{HO}_2 \rightarrow \text{C85OOH}$	k_R02_H02(temp,8)	Rickard (2022)
G48202	TrGTerCN	$\text{C85O}_2 + \text{NO} \rightarrow \text{C86O}_2 + \text{NO}_2$	KR02N0	Rickard (2022)*
G48203	TrGTerC	$\text{C85OOH} + \text{OH} \rightarrow \text{C85O}_2$	1.29E-11	Rickard (2022)
G48204	TrGTerC	$\text{C86O}_2 \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3$	k1_R02tR02	Rickard (2022)
G48205	TrGTerCN	$\text{C86O}_2 + \text{NO} \rightarrow \text{C511O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	KR02N0	Rickard (2022)*
G48206	TrGTerC	$\text{C86O}_2 + \text{HO}_2 \rightarrow \text{C86OOH}$	k_R02_H02(temp,8)	Rickard (2022)
G48207	TrGTerC	$\text{C86OOH} + \text{OH} \rightarrow \text{C86O}_2$	3.45E-11	Rickard (2022)
G48208	TrGTerC	$\text{C811O}_2 \rightarrow \text{C812O}_2$	k1_R02pR02	Rickard (2022)
G48209	TrGTerC	$\text{C811O}_2 + \text{HO}_2 \rightarrow 8 \text{ L CARBON}$	k_R02_H02(temp,8)	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G48210	TrGTerCN	$\text{C811O2} + \text{NO} \rightarrow \text{C812O2} + \text{NO}_2$	KR02NO	Rickard (2022)*
G48211	TrGTerC	$\text{C812O2} \rightarrow \text{C813O2}$	k1_R02t0R02	Rickard (2022)
G48212	TrGTerCN	$\text{C812O2} + \text{NO} \rightarrow \text{C813O2} + \text{NO}_2$	KR02NO	Rickard (2022)*
G48213	TrGTerC	$\text{C812O2} + \text{HO}_2 \rightarrow \text{C812OOH}$	k_R02_H02(temp,8)	Rickard (2022)
G48214	TrGTerC	$\text{C812OOH} + \text{OH} \rightarrow \text{C812O2}$	1.09E-11	Rickard (2022)
G48215	TrGTerC	$\text{C813O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2}$	k1_R02tR02	Rickard (2022)
G48216	TrGTerCN	$\text{C813O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{NO}_2$	KR02NO	Rickard (2022)*
G48217	TrGTerC	$\text{C813O2} + \text{HO}_2 \rightarrow \text{C813OOH}$	k_R02_H02(temp,8)	Rickard (2022)
G48218	TrGTerC	$\text{C813OOH} + \text{OH} \rightarrow \text{C813O2}$	1.86E-11	Rickard (2022)
G48219	TrGTerCN	$\text{C721CHO} + \text{NO}_3 \rightarrow \text{C721CO3} + \text{HNO}_3$	KN03AL*8.5	Rickard (2022)
G48220	TrGTerC	$\text{C721CHO} + \text{OH} \rightarrow \text{C721CO3}$	2.63E-11	Rickard (2022)
G48221a	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721CO3H}$	KAPH02*r_C03_OOH	Rickard (2022)
G48221b	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	KAPH02*r_C03_OH	Rickard (2022)
G48221c	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{NORPINIC} + \text{O}_3$	KAPH02*r_C03_O3	Rickard (2022)
G48222	TrGTerCN	$\text{C721CO3} + \text{NO} \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)*
G48223	TrGTerCN	$\text{C721CO3} + \text{NO}_2 \rightarrow \text{C721PAN}$	k_CH3C03_N02	Rickard (2022)
G48224	TrGTerCN	$\text{C721CO3} + \text{NO}_3 \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard (2022)
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 (2022)
G48228	TrGTerC	$\text{NORPINIC} + \text{OH} \rightarrow \text{C721O2} + \text{CO}_2$	6.57E-12	Rickard (2022)
G48229	TrGTerCN	$\text{C721PAN} + \text{OH} \rightarrow \text{C721OOH} + \text{CO} + \text{NO}_2$	2.96E-12	Rickard (2022)
G48230	TrGTerCN	$\text{C721PAN} \rightarrow \text{C721CO3} + \text{NO}_2$	k_PAN_M	Rickard (2022)
G48231	TrGTerC	$\text{C8BC} + \text{OH} \rightarrow \text{C8BCO2}$	3.04E-12	Rickard (2022)
G48232	TrGTerC	$\text{C8BCO2} + \text{HO}_2 \rightarrow \text{C8BCOOH}$	k_R02_H02(temp,8)	Rickard (2022)
G48233a	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C89O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard (2022)
G48233b	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C8BCNO3}$	KR02N0*alpha_AN(8,2,0,0,0,temp, cair)	Rickard (2022)
G48234	TrGTerC	$\text{C8BCO2} \rightarrow \text{C89O2}$	k1_R02sR02	Rickard (2022)
G48235	TrGTerC	$\text{C8BCOOH} + \text{OH} \rightarrow \text{C8BCCO} + \text{OH}$	1.62E-11	Rickard (2022)
G48236	TrGTerCN	$\text{C8BCNO3} + \text{OH} \rightarrow \text{C8BCCO} + \text{NO}_2$	1.84E-12	Rickard (2022)
G48237	TrGTerC	$\text{C8BCCO} + \text{OH} \rightarrow \text{C89O2}$	3.94E-12	Rickard (2022)
G48238	TrGTerC	$\text{C89O2} + \text{HO}_2 \rightarrow \text{C89OOH}$	k_R02_H02(temp,8)	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G48239a	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C810O2} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard (2022)
G48239b	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C89NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair})$	Rickard (2022)
G48240	TrGTerCN	$\text{C89O2} + \text{NO}_3 \rightarrow \text{C810O2} + \text{NO}_2$	KR02N03	Rickard (2022)
G48241	TrGTerC	$\text{C89O2} \rightarrow \text{C810O2}$	k1_R02tR02	Rickard (2022)
G48242	TrGTerC	$\text{C89OOH} + \text{OH} \rightarrow \text{C89O2}$	3.61E-11	Rickard (2022)
G48243	TrGTerCN	$\text{C89NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	2.56E-11	Rickard (2022)
G48244	TrGTerC	$\text{C810O2} + \text{HO}_2 \rightarrow \text{C810OOH}$	k_R02_H02(temp, 8)	Rickard (2022)
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 (2022)
G48245b	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{C810NO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(10, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard (2022)
G48246	TrGTerCN	$\text{C810O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KR02N03	Rickard (2022)
G48247	TrGTerC	$\text{C810O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2}$	k1_R02tR02	Rickard (2022)
G48248	TrGTerC	$\text{C810OOH} + \text{OH} \rightarrow \text{C810O2}$	8.35E-11	Rickard (2022)
G48249	TrGTerCN	$\text{C810NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	4.96E-11	Rickard (2022)
G48400a	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + \text{LCARBON}$	0.401E-11	Rickard (2022)*
G48400b	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{C6H5CH2O2} + \text{LCARBON}$	0.101E-11	Rickard (2022)*
G48400c	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{CRESOL} + \text{LCARBON}$	0.261E-11	Rickard (2022)*
G48400d	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLBIPERO2} + \text{HO}_2 + \text{LCARBON}$	0.932E-11	Rickard (2022)*
G48401	TrGAroCN	$\text{LXYL} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	3.9E-16	Rickard (2022)*
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 (2022)*
G48403	TrGAroCN	$\text{EBENZ} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	1.20E-16	Rickard (2022)*
G48404	TrGAroCN	$\text{STYRENE} + \text{NO}_3 \rightarrow \text{NSTYRENO2}$	1.50E-12	Rickard (2022)
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 (2022)*
G48406	TrGAroC	$\text{STYRENE} + \text{OH} \rightarrow \text{STYRENO2}$	5.80E-11	Rickard (2022)
G48407	TrGAroCN	$\text{NSTYRENO2} + \text{HO}_2 \rightarrow \text{NSTYRENOOH}$	k_R02_H02(temp, 8)	Rickard (2022)
G48408	TrGAroCN	$\text{NSTYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N0	Rickard (2022)*
G48409	TrGAroCN	$\text{NSTYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N03	Rickard (2022)*
G48410	TrGAroCN	$\text{NSTYRENO2} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	k1_R02sR02	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G48411	TrGAroCN	NSTYRENOOH + OH \rightarrow NSTYRENO2	6.16E-11	Rickard (2022)
G48412a	TrGAroC	STYRENO2 + HO ₂ \rightarrow STYRENOOH	k_R02_H02(temp,8)*(1.-r_ CHOHCH2O2_OH)	Rickard (2022)
G48412b	TrGAroC	STYRENO2 + HO ₂ \rightarrow HO ₂ + OH + HCHO + BENZAL	k_R02_H02(temp,8)*r_CHOHCH2O2_OH	Rickard (2022)*
G48413	TrGAroCN	STYRENO2 + NO \rightarrow NO ₂ + HO ₂ + HCHO + BENZAL	KR02NO	Rickard (2022)*
G48414	TrGAroCN	STYRENO2 + NO ₃ \rightarrow NO ₂ + HO ₂ + HCHO + BENZAL	KR02NO3	Rickard (2022)*
G48415	TrGAroC	STYRENO2 \rightarrow HO ₂ + HCHO + BENZAL	k1_R02sR02	Rickard (2022)*
G48416	TrGAroC	STYRENOOH + OH \rightarrow STYRENO2	6.16E-11	Rickard (2022)
G49200	TrGTerC	C96O2 \rightarrow C97O2	k1_R02pR02	Rickard (2022)
G49201	TrGTerC	C96O2 + HO ₂ \rightarrow C96OOH	k_R02_H02(temp,9)	Rickard (2022)
G49202a	TrGTerCN	C96O2 + NO \rightarrow C97O2 + NO ₂	KR02NO*(1.-alpha_AN(10,1,0,0,0, temp,cair))	Rickard (2022)
G49202b	TrGTerCN	C96O2 + NO \rightarrow C96NO3	KR02NO*alpha_AN(10,1,0,0,0, temp,cair)	Rickard (2022)
G49203	TrGTerCN	C96NO3 + OH \rightarrow NORPINAL + NO ₂	2.88E-12	Rickard (2022)
G49204a	TrGTerC	C96OOH + OH \rightarrow C96O2	k_R00HRO	Rickard (2022)
G49205b	TrGTerC	C96OOH + OH \rightarrow NORPINAL + OH	1.30E-11	Rickard (2022)
G49206	TrGTerC	C97O2 \rightarrow C98O2	k1_R02tR02	Rickard (2022)
G49207	TrGTerCN	C97O2 + NO \rightarrow C98O2 + NO ₂	KR02NO	Rickard (2022)*
G49208a	TrGTerC	C97O2 + HO ₂ \rightarrow C97OOH	k_R02_H02(temp,9)*r_COCH2O2_OOH	Rickard (2022), Sander et al. (2019)
G49208b	TrGTerC	C97O2 + HO ₂ \rightarrow C98O2 + OH	k_R02_H02(temp,9)*r_COCH2O2_OH	Rickard (2022), Sander et al. (2019)
G49209	TrGTerC	C97OOH + OH \rightarrow C97O2	1.05E-11	Rickard (2022)
G49210	TrGTerC	C98O2 \rightarrow C614O2 + CH ₃ COCH ₃	k1_R02tR02	Rickard (2022)
G49211a	TrGTerCN	C98O2 + NO \rightarrow C614O2 + CH ₃ COCH ₃ + NO ₂	KR02NO*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Rickard (2022)
G49211b	TrGTerCN	C98O2 + NO \rightarrow 9 LCARBON + LNITROGEN	KR02NO*alpha_AN(12,3,0,0,0, temp,cair)	Rickard (2022)
G49212	TrGTerC	C98O2 + HO ₂ \rightarrow C98OOH	k_R02_H02(temp,9)	Rickard (2022)
G49213	TrGTerC	C98OOH + OH \rightarrow C98O2	2.05E-11	Rickard (2022)
G49214	TrGTerC	NORPINAL + OH \rightarrow C85CO3	2.64E-11	Rickard (2022)
G49215	TrGTerCN	NORPINAL + NO ₃ \rightarrow C85CO3 + HNO ₃	KN03AL*8.5	Rickard (2022)
G49216	TrGTerC	C85CO3 \rightarrow C85O2 + CO ₂	k1_R02RCO3	Rickard (2022)
G49217	TrGTerCN	C85CO3 + NO \rightarrow C85O2 + CO ₂ + NO ₂	KAPNO	Rickard (2022)

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

#	labels	reaction	rate coefficient	reference
G49218	TrGTerCN	$\text{C85CO3} + \text{NO}_2 \rightarrow \text{C9PAN2}$	$k_{\text{CH3CO3_NO2}}$	Rickard (2022)
G49219a	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85CO3H}$	$\text{KAPH02}*(r_{\text{C03_00H}}+r_{\text{C03_03}})$	Rickard (2022)
G49219b	TrGTerC	$\text{C85CO3} + \text{HO}_2 \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{C03_OH}}$	Rickard (2022)
G49220	TrGTerCN	$\text{C9PAN2} \rightarrow \text{C85CO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G49221	TrGTerCN	$\text{C9PAN2} + \text{OH} \rightarrow \text{C85OOH} + \text{CO} + \text{NO}_2$	6.60E-12	Rickard (2022)
G49222	TrGTerC	$\text{C85CO3H} + \text{OH} \rightarrow \text{C85CO3}$	1.02E-11	Rickard (2022)
G49223a	TrGTerC	$\text{C89CO3} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	$k1_{\text{R02RC03}}*0.9$	Sander et al. (2019)
G49223b	TrGTerC	$\text{C89CO3} \rightarrow \text{C89CO2H}$	$k1_{\text{R02RC03}}*0.1$	Sander et al. (2019)
G49224a	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO3H}$	$\text{KAPH02}*r_{\text{C03_00H}}$	Rickard (2022)
G49224b	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO2H} + \text{O}_3$	$\text{KAPH02}*r_{\text{C03_03}}$	Rickard (2022)
G49224c	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow .80 \text{ C811CO3} + .20 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{C03_OH}}$	Rickard (2022)
G49225	TrGTerCN	$\text{C89CO3} + \text{NO}_2 \rightarrow \text{C89PAN}$	$k_{\text{CH3CO3_NO2}}$	Rickard (2022)
G49226	TrGTerCN	$\text{C89CO3} + \text{NO} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G49227	TrGTerC	$\text{C89CO2H} + \text{OH} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	2.69E-11	Rickard (2022)
G49228	TrGTerC	$\text{C89CO3H} + \text{OH} \rightarrow \text{C89CO3}$	3.00E-11	Rickard (2022)
G49229	TrGTerCN	$\text{C89PAN} \rightarrow \text{C89CO3} + \text{NO}_2$	$k_{\text{PAN_M}}$	Rickard (2022)
G49230	TrGTerCN	$\text{C89PAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{CO} + \text{NO}_2$	2.52E-11	Rickard (2022)
G49231a	TrGTerC	$\text{C811CO3} \rightarrow \text{C811O2} + \text{CO}_2$	$k1_{\text{R02RC03}}*0.9$	Sander et al. (2019)
G49231b	TrGTerC	$\text{C811CO3} \rightarrow \text{PINIC}$	$k1_{\text{R02RC03}}*0.1$	Sander et al. (2019)
G49232a	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811CO3H}$	$\text{KAPH02}*r_{\text{C03_00H}}$	Rickard (2022)
G49232b	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{PINIC} + \text{O}_3$	$\text{KAPH02}*r_{\text{C03_03}}$	Rickard (2022)
G49232c	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02}*r_{\text{C03_OH}}$	Rickard (2022)
G49233	TrGTerCN	$\text{C811CO3} + \text{NO} \rightarrow \text{C811O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard (2022)
G49234	TrGTerCN	$\text{C811CO3} + \text{NO}_2 \rightarrow \text{C811PAN}$	$k_{\text{CH3CO3_NO2}}$	Rickard (2022)
G49235	TrGTerC	$\text{PINIC} + \text{OH} \rightarrow \text{C811O2} + \text{CO}_2$	7.29E-12	Rickard (2022)
G49236	TrGTerC	$\text{NOPINONE} + \text{OH} \rightarrow \text{NOPINDO2}$	1.55E-11	Capouet et al. (2008), Rickard (2022)
G49237a	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{NOPINDOOH}$	$k_{\text{R02_H02}}(\text{temp}, 9)*r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 9)*r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	KR02NO	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G49239	TrGTerC	NOPINDO2 \rightarrow C89CO3	k1_R02p0R02	Rickard (2022)
G49240	TrGTerC	NOPINDOOH \rightarrow NOPINDCO	2.63E-11	Rickard (2022)
G49241	TrGTerC	NOPINDCO + OH \rightarrow C89CO3	3.07E-12	Rickard (2022)
G49242	TrGTerC	NOPINOO \rightarrow NOPINONE + H ₂ O ₂	6.00E-18*c(ind_H20)	Rickard (2022)
G49243	TrGTerC	NOPINOO + CO \rightarrow NOPINONE + CO ₂	1.2E-15	Rickard (2022)
G49244	TrGTerCN	NOPINOO + NO \rightarrow NOPINONE + NO ₂	1.E-14	Rickard (2022)
G49245	TrGTerCN	NOPINOO + NO ₂ \rightarrow NOPINONE + NO ₃	1.E-15	Rickard (2022)
G49246	TrGTerC	NORPINENOL + OH \rightarrow HCOOH + OH + C86O2	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
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 (2022)
G49250	TrGTerCN	C811PAN \rightarrow C811CO3 + NO ₂	k_PAN_M	Rickard (2022)
G49251	TrGTerCN	C811PAN + OH \rightarrow C721CHO + CO + NO ₂	6.77E-12	Rickard (2022)
G49400a	TrGAroC	LTMB + OH \rightarrow TLEPOXMUC + HO ₂ + 2 LCARBON	0.827E-11	Rickard (2022)*
G49400b	TrGAroC	LTMB + OH \rightarrow C6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard (2022)*
G49400c	TrGAroC	LTMB + OH \rightarrow CRESOL + 2 LCARBON	0.141E-11	Rickard (2022)*
G49400d	TrGAroC	LTMB + OH \rightarrow TLBIPERO2 + HO ₂ + 2 LCARBON	2.917E-11	Rickard (2022)*
G49401	TrGAroCN	LTMB + NO ₃ \rightarrow C6H5CH2O2 + HNO ₃ + 2 LCARBON	1.52E-15	Rickard (2022)*
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 (2022), 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 (2022), Sander et al. (2019)
G40202a	TrGTerC	LAPINABO2 + HO ₂ \rightarrow LAPINABOOH	k_R02_HO2(temp,10)*(1-r_CHOHCH2O2_OH)	Rickard (2022), Sander et al. (2019)
G40202b	TrGTerC	LAPINABO2 + HO ₂ \rightarrow PINAL + HO ₂ + OH	k_R02_HO2(temp,10)*r_CHOHCH2O2_OH	Rickard (2022), Sander et al. (2019)
G40203	TrGTerC	LAPINABO2 \rightarrow PINAL + HO ₂	R02*(0.65*k1_R02t0R02+.35*k1_R02s0R02)	Rickard (2022)*

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

#	labels	reaction	rate coefficient	reference
G40204	TrGTerC	LAPINABOOH + OH \rightarrow .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard (2022)*
G40205	TrGTerCN	LAPINABNO3 + OH \rightarrow .35 PINAL + .65 C96CO3 + NO ₂	4.29E-12	Rickard (2022)*
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_R02t0R02	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH \rightarrow 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH \rightarrow .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./temp)	Wallington et al. (2018)*
G40212	TrGTerCN	PINAL + NO ₃ \rightarrow C96CO3 + HNO ₃	2.0E-14	Wallington et al. (2018)*
G40213a	TrGTerC	C96CO3 \rightarrow C96O2 + CO ₂	k1_R02RC03*0.9	Rickard (2022)
G40213b	TrGTerC	C96CO3 \rightarrow PINONIC	k1_R02RC03*0.1	Rickard (2022)
G40214a	TrGTerC	C96CO3 + HO ₂ \rightarrow PERPINONIC	KAPH02*r_C03_00H	Rickard (2022)
G40214b	TrGTerC	C96CO3 + HO ₂ \rightarrow PINONIC + O ₃	KAPH02*r_C03_03	Rickard (2022)
G40214c	TrGTerC	C96CO3 + HO ₂ \rightarrow C96O2 + OH + CO ₂	KAPH02*r_C03_0H	Rickard (2022)
G40215	TrGTerCN	C96CO3 + NO ₂ \rightarrow C10PAN2	k_CH3C03_N02	Rickard (2022)
G40216	TrGTerCN	C96CO3 + NO \rightarrow C96O2 + NO ₂ + CO ₂	KAPNO	Rickard (2022)
G40217	TrGTerCN	C96CO3 + NO ₃ \rightarrow C96O2 + NO ₂ + CO ₂	KR02NO3*1.74	Rickard (2022)
G40218	TrGTerCN	C10PAN2 \rightarrow C96CO3 + NO ₂	k_PAN_M	Rickard (2022)
G40219	TrGTerCN	C10PAN2 + OH \rightarrow NORPINAL + CO + NO ₂	3.66E-12	Rickard (2022)
G40220	TrGTerC	PINONIC + OH \rightarrow C96O2 + CO ₂	6.65E-12	Rickard (2022)
G40221	TrGTerC	PERPINONIC + OH \rightarrow C96CO3	9.73E-12	Rickard (2022)
G40222	TrGTerC	PINALO2 + HO ₂ \rightarrow PINALOOH	k_R02_H02(temp,10)	Rickard (2022)
G40223a	TrGTerCN	PINALO2 + NO \rightarrow C106O2 + NO ₂	KR02NO*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard (2022), Sander et al. (2019)
G40223b	TrGTerCN	PINALO2 + NO \rightarrow PINALNO3	KR02NO*alpha_AN(12,3,0,1,0, temp, cair)	Rickard (2022), Sander et al. (2019)
G40224	TrGTerC	PINALO2 \rightarrow C106O2	k1_R02tR02	Rickard (2022)
G40225	TrGTerC	PINALOOH + OH \rightarrow PINALO2	2.75E-11	Rickard (2022)
G40226	TrGTerCN	PINALNO3 + OH \rightarrow CO235C6CHO + CH ₃ COCH ₃ + NO ₂	2.25E-11	Rickard (2022)
G40227	TrGTerC	C106O2 + HO ₂ \rightarrow C106OOH	k_R02_H02(temp,10)	Rickard (2022)
G40228a	TrGTerCN	C106O2 + NO \rightarrow C716O2 + CH ₃ COCH ₃ + NO ₂	KR02NO*0.875*(1.-alpha_AN(13,3,0,0,0,temp, cair))	Rickard (2022), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G40228b	TrGTerCN	$\text{C106O2} + \text{NO} \rightarrow \text{C106NO3}$	$\text{KRO2NO} * 0.875 * \alpha_{\text{AN}}(13, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard (2022), Sander et al. (2019)
G40229	TrGTerC	$\text{C106O2} \rightarrow \text{C716O2} + \text{CH}_3\text{COCH}_3$	$k1_{\text{R02tR02}}$	Rickard (2022)
G40230	TrGTerC	$\text{C106OOH} + \text{OH} \rightarrow \text{C106O2}$	$8.01\text{E-}11$	Rickard (2022)
G40231	TrGTerCN	$\text{C106NO3} + \text{OH} \rightarrow \text{CO235C6CHO} + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$7.03\text{E-}11$	Rickard (2022)
G40232	TrGTerC	$\text{APINENE} + \text{O}_3 \rightarrow .09 \text{ APINBOO} + .08 \text{ PINONIC} + .77 \text{ OH} + .33 \text{ NORPINAL} + .33 \text{ CO} + .33 \text{ HO}_2 + .06 \text{ APINAOO} + .44 \text{ C109O2}$	$8.05\text{E-}16 * \text{EXP}(-640./\text{temp})$	Wallington et al. (2018)*
G40233	TrGTerC	$\text{APINAOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * c(\text{ind_H2O})$	Rickard (2022)
G40234	TrGTerC	$\text{APINAOO} + \text{CO} \rightarrow \text{PINAL} + \text{CO}_2$	$1.20\text{E-}15$	Rickard (2022)
G40235	TrGTerCN	$\text{APINAOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2$	$1.00\text{E-}14$	Rickard (2022)
G40236	TrGTerCN	$\text{APINAOO} + \text{NO}_2 \rightarrow \text{PINAL} + \text{NO}_3$	$1.00\text{E-}15$	Rickard (2022)
G40237a	TrGTerC	$\text{APINBOO} \rightarrow \text{PINONIC}$	$1.00\text{E-}17 * c(\text{ind_H2O}) * (0.08 + 0.15)$	Rickard (2022)
G40237b	TrGTerC	$\text{APINBOO} \rightarrow \text{PINAL} + \text{H}_2\text{O}_2$	$1.00\text{E-}17 * c(\text{ind_H2O}) * 0.77$	Rickard (2022)
G40238	TrGTerC	$\text{APINBOO} + \text{CO} \rightarrow \text{PINAL} + \text{CO}_2$	$1.20\text{E-}15$	Rickard (2022)
G40239	TrGTerCN	$\text{APINBOO} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2$	$1.00\text{E-}14$	Rickard (2022)
G40240	TrGTerCN	$\text{APINBOO} + \text{NO}_2 \rightarrow \text{PINAL} + \text{NO}_3$	$1.00\text{E-}15$	Rickard (2022)
G40241	TrGTerC	$\text{C109O2} \rightarrow \text{C89CO3} + \text{HCHO}$	$k1_{\text{R02pOR02}}$	Rickard (2022)
G40242	TrGTerCN	$\text{C109O2} + \text{NO} \rightarrow \text{C89CO3} + \text{HCHO} + \text{NO}_2$	KRO2NO	Rickard (2022)*
G40243a	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C109OOH}$	$k_{\text{R02_H02}}(\text{temp}, 10) * r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G40243b	TrGTerC	$\text{C109O2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{HCHO} + \text{OH}$	$k_{\text{R02_H02}}(\text{temp}, 10) * r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G40244	TrGTerC	$\text{C109OOH} + \text{OH} \rightarrow \text{C109CO} + \text{OH}$	$5.47\text{E-}11$	Rickard (2022)
G40245	TrGTerC	$\text{C109CO} + \text{OH} \rightarrow \text{C89CO3} + \text{CO}$	$5.47\text{E-}11$	Rickard (2022)
G40246	TrGTerCN	$\text{APINENE} + \text{NO}_3 \rightarrow \text{LNAPINABO2}$	$1.2\text{E-}12 * \text{EXP}(490./\text{temp})$	Wallington et al. (2018)*
G40247	TrGTerCN	$\text{LNAPINABO2} \rightarrow \text{PINAL} + \text{NO}_2$	$(0.65 * k1_{\text{R02tR02}} + 0.35 * k1_{\text{R02sR02}})$	Rickard (2022)
G40248	TrGTerCN	$\text{LNAPINABO2} + \text{NO} \rightarrow \text{PINAL} + \text{NO}_2 + \text{NO}_2$	KRO2NO	Rickard (2022)*
G40249	TrGTerCN	$\text{LNAPINABO2} + \text{HO}_2 \rightarrow \text{LNAPINABOOH}$	$k_{\text{R02_H02}}(\text{temp}, 10)$	Rickard (2022)
G40250	TrGTerCN	$\text{LNAPINABO2} + \text{NO}_3 \rightarrow \text{PINAL} + \text{NO}_2 + \text{NO}_2$	KRO2NO3	Rickard (2022)
G40251	TrGTerCN	$\text{LNAPINABOOH} + \text{OH} \rightarrow \text{LNAPINABO2}$	$(.65 * 6.87\text{E-}12 + .35 * 1.23\text{E-}11)$	Rickard (2022)
G40252a	TrGTerC	$\text{BPINENE} + \text{OH} \rightarrow \text{BPINAO2}$	$1.47\text{E-}11 * \text{EXP}(467./\text{temp})$ $* (0.8326 * 0.3 + 0.068) / (0.8326 + 0.068)$	Gill and Hites (2002)*

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

#	labels	reaction	rate coefficient	reference
G40252b	TrGTerC	BPINENE + OH \rightarrow ROO6R1O2	$1.47\text{E}-11 \cdot \text{EXP}(467./\text{temp})$ $\cdot 0.8326 \cdot 0.7 / (0.8326 + 0.068)$	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO ₂ \rightarrow BPINAOOH	$k_{\text{R02_H02}}(\text{temp}, 10) \cdot r_{\text{COCH202_00H}}$	Rickard (2022), Sander et al. (2019)
G40253b	TrGTerC	BPINAO2 + HO ₂ \rightarrow NOPINONE + HCHO + HO ₂ + OH	$k_{\text{R02_H02}}(\text{temp}, 10) \cdot r_{\text{COCH202_OH}}$	Rickard (2022), Sander et al. (2019)
G40254a	TrGTerCN	BPINAO2 + NO \rightarrow NOPINONE + HCHO + HO ₂ + NO ₂	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(11, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard (2022), Sander et al. (2019)
G40254b	TrGTerCN	BPINAO2 + NO \rightarrow BPINANO3	$\text{KR02N0} \cdot \alpha_{\text{AN}}(11, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard (2022), Sander et al. (2019)
G40255	TrGTerC	BPINAO2 \rightarrow NOPINONE + HCHO + HO ₂	$k1_{\text{R02t0R02}}$	Rickard (2022)
G40256	TrGTerC	BPINAOOH + OH \rightarrow BPINAO2	$1.33\text{E}-11$	Rickard (2022)
G40257	TrGTerCN	BPINANO3 + OH \rightarrow NOPINONE + HCHO + NO ₂	$4.70\text{E}-12$	Rickard (2022)
G40258a	TrGTerCN	ROO6R1O2 + NO \rightarrow ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(13, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO \rightarrow ROO6R1NO3	$\text{KR02N0} \cdot \alpha_{\text{AN}}(13, 3, 0, 0, 0, \text{temp}, \text{cair})$	Vereecken and Peeters (2012)
G40259	TrGTerC	ROO6R1O2 + HO ₂ \rightarrow 10 LCARBON	$k_{\text{R02_H02}}(\text{temp}, 10)$	Vereecken and Peeters (2012)*
G40260	TrGTerC	ROO6R1O2 \rightarrow ROO6R3O2 + CH ₃ COCH ₃	$k1_{\text{R02t0R02}}$	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO \rightarrow RO6R3O2 + NO ₂	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO \rightarrow RO6R1NO3	$\text{KR02N0} \cdot \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair})$	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO ₂ \rightarrow 10 LCARBON	$k_{\text{R02_H02}}(\text{temp}, 10)$	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 \rightarrow RO6R3O2	$k1_{\text{R02s0R02}}$	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO \rightarrow 9 LCARBON + HCHO + HO ₂ + NO ₂	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Vereecken and Peeters (2012)
G40264b	TrGTerCN	RO6R3O2 + NO \rightarrow 10 LCARBON + LNITROGEN	$\text{KR02N0} \cdot \alpha_{\text{AN}}(12, 3, 0, 0, 0, \text{temp}, \text{cair})$	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO ₂ \rightarrow 10 LCARBON	$k_{\text{R02_H02}}(\text{temp}, 10)$	Vereecken and Peeters (2012)
G40266	TrGTerC	RO6R3O2 \rightarrow 9 LCARBON + HCHO + HO ₂	$k1_{\text{R02sR02}}$	Vereecken and Peeters (2012)*
G40267a	TrGTerC	BPINENE + O ₃ \rightarrow NOPINONE + .63 CO + .37 CH ₂ OO + .16 OH + .16 HO ₂	$1.35\text{E}-15 \cdot \text{EXP}(-1270./\text{temp})$ $\cdot .051 / (1 - .027)$	Wallington et al. (2018)*
G40267b	TrGTerC	BPINENE + O ₃ \rightarrow NOPINOO + CO ₂	$1.35\text{E}-15 \cdot \text{EXP}(-1270./\text{temp})$ $\cdot .368 / (1 - .027)$	Nguyen et al. (2009), Wallington et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G40267c	TrGTerC	BPINENE + O ₃ → NOPINDO2 + CO ₂ + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267d	TrGTerC	BPINENE + O ₃ → C8BC + 2 CO ₂	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40268	TrGTerCN	BPINENE + NO ₃ → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40269	TrGTerCN	LNBPINABO2 + HO ₂ → LNBPINABOOH	k_R02_H02(temp,10)	Rickard (2022)
G40270	TrGTerCN	LNBPINABO2 + NO → NOPINONE + HCHO + NO ₂ + NO ₂	KR02NO	Rickard (2022)*
G40271	TrGTerCN	LNBPINABO2 + NO ₃ → NOPINONE + HCHO + NO ₂ + NO ₂	KR02NO3	Rickard (2022)
G40272a	TrGTerCN	LNBPINABO2 → NOPINONE + HCHO + NO ₂	k1_R02tR02*0.7	Rickard (2022)
G40272b	TrGTerCN	LNBPINABO2 → BPINAN03	k1_R02tR02*0.3	Rickard (2022)
G40273	TrGTerCN	LNBPINABOOH + OH → LNBPINABO2	9.58E-12	Rickard (2022)
G40274	TrGTerCN	ROO6R1NO3 + OH → ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40275	TrGTerCN	RO6R1NO3 + OH → 9 LCARBON + HCHO + HO ₂ + NO ₂	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)
G40276	TrGTerC	PINEOL + OH → HCOOH + OH + NORPINAL	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH → PINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G40278	TrGTerC	PINAL + HCOOH → PINEOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G40279a	TrGC	CARENE + OH → LAPINABO2	8.8E-11*(.50+.25)	Atkinson and Arey (2003)
G40279b	TrGC	CARENE + OH → MENTHEN6ONE + HO ₂	8.8E-11*.25*.60	Atkinson and Arey (2003)
G40279c	TrGC	CARENE + OH → ROO6R1O2	8.8E-11*.25*.40	Atkinson and Arey (2003)
G40280a	TrGC	CARENE + O ₃ → APINBOO	3.7E-17*.50*.18	Atkinson and Arey (2003)
G40280b	TrGC	CARENE + O ₃ → PINONIC	3.7E-17*.50*.16	Atkinson and Arey (2003)
G40280c	TrGC	CARENE + O ₃ → OH + NORPINAL + CO + HO ₂	3.7E-17*.50*.66	Atkinson and Arey (2003)
G40280d	TrGC	CARENE + O ₃ → APINA00	3.7E-17*.50*.12	Atkinson and Arey (2003)
G40280e	TrGC	CARENE + O ₃ → OH + C109O2	3.7E-17*.50*(.22+.66)	Atkinson and Arey (2003)
G40281	TrGCN	CARENE + NO ₃ → LNAPINABO2	9.1E-12	Atkinson and Arey (2003)
G40282a	TrGTerC	SABINENE + OH → BPINAO2	1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*

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

#	labels	reaction	rate coefficient	reference
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)*
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 (2022)*
G40401	TrGAroCN	LHAROM + NO ₃ \rightarrow C6H5CH2O2 + HNO ₃ + 4 LCARBON	2.60E-15	Rickard (2022)*
G6100	UpStTrGCl	Cl + O ₃ \rightarrow ClO + O ₂	2.8E-11*EXP(-250./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)

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

#	labels	reaction	rate coefficient	reference
G6103	StTrGCl	$\text{Cl}_2\text{O}_2 \rightarrow \text{ClO} + \text{ClO}$	$k_{\text{ClO-ClO}}/(2.16\text{E-}27*\text{EXP}(8537./\text{temp}))$	Burkholder et al. (2015)*
G69MS	StTrGCl	$\text{ClO} + \text{OCIO} \rightarrow \text{Cl}_2\text{O}_3$	1.2E-12	Atkinson et al. (2007)
G699MS	StTrGCl	$\text{Cl} + \text{Cl}_2\text{O} \rightarrow \text{Cl}_2 + \text{ClO}$	$6.2\text{E-}11*\text{EXP}(130./\text{temp})$	Atkinson et al. (2007)
G6202	StTrGCl	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	$1.1\text{E-}11*\text{EXP}(-980./\text{temp})$	Atkinson et al. (2007)
G6204	StTrGCl	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl} + \text{O}_2$	$2.2\text{E-}12*\text{EXP}(340./\text{temp})$	Atkinson et al. (2007)*
G6205	StTrGCl	$\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$	$1.7\text{E-}12*\text{EXP}(-230./\text{temp})$	Atkinson et al. (2007)
G67MS	StTrGCl	$\text{Cl}_2 + \text{OH} \rightarrow \text{HOCl} + \text{Cl}$	$3.6\text{E-}12*\text{EXP}(-1200./\text{temp})$	Atkinson et al. (2007)
G6300	UpStTrGCIN	$\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$	$6.2\text{E-}12*\text{EXP}(295./\text{temp})$	Atkinson et al. (2007)
G6301	StTrGCIN	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 1.6\text{E-}31, 3.4, 7\text{E-}11, 0., 0.4)$	Atkinson et al. (2007)
G6302	TrGCIN	$\text{ClNO}_3 \rightarrow \text{ClO} + \text{NO}_2$	$6.918\text{E-}7*\text{EXP}(-10909./\text{temp})*\text{cair}$	Anderson and Fahey (1990)
G6304	StTrGCIN	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	$6.2\text{E-}12*\text{EXP}(145./\text{temp})$	Atkinson et al. (2007)
G63MS	UpStTrGCIN	$\text{Cl} + \text{NO} \rightarrow \text{ClNO}$	$7.7\text{E-}32*(\text{temp}/298.)**(-1.80)*\text{cair}$	Burkholder et al. (2019)
G64MS	UpStTrGCIN	$\text{Cl} + \text{NO}_2 \rightarrow \text{ClONO}$	1.6E-11	Burkholder et al. (2015)
G65MS	UpStTrGCIN	$\text{Cl} + \text{NO}_2 \rightarrow \text{ClNO}_2$	3.6E-12	Burkholder et al. (2015)
G66MS	UpStTrGCIN	$\text{Cl} + \text{NO}_3 \rightarrow \text{ClO} + \text{NO}_2$	2.4E-11	Burkholder et al. (2019)
G68MS	StTrGCIN	$\text{ClNO}_2 + \text{OH} \rightarrow \text{HOCl} + \text{NO}_2$	$2.4\text{E-}12*\text{EXP}(-1250./\text{temp})$	Atkinson et al. (2007)
G688MS	UpStTrGCIN	$\text{OCIO} + \text{NO} \rightarrow \text{NO}_2 + \text{ClO}$	$1.1\text{E-}13*\text{EXP}(350./\text{temp})$	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)
G6400MS	TrGCCl	$\text{Cl} + \text{C}_3\text{H}_8 \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{HCl}$	$1.4\text{E-}10*0.43*\text{EXP}(75./\text{temp})$	Rickard (2022)
G6401MS	TrGCCl	$\text{Cl} + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{HCl}$	$1.4\text{E-}10*0.59*\text{EXP}(-90./\text{temp})$	Rickard (2022)
G6402MS	TrGCCl	$\text{Cl} + \text{iC}_4\text{H}_{10} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{HCl}$	1.43E-10*0.564	Rickard (2022)
G6403MS	TrGCCl	$\text{Cl} + \text{iC}_4\text{H}_{10} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{HCl}$	1.43E-10*0.436	Rickard (2022)
G6404MS	TrGCCl	$\text{Cl} + \text{C}_4\text{H}_{10} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{HCl}$	2.05E-10	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	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{HCHO} + \text{HCl} + \text{OH}$	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$1.8\text{E-}12*\text{EXP}(-600./\text{temp})$	Burkholder et al. (2015)
G6408	StTrGCCl	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow 2 \text{LCARBON} + \text{H}_2\text{O} + 3 \text{Cl}$	$1.64\text{E-}12*\text{EXP}(-1520./\text{temp})$	Burkholder et al. (2015)
G6409	TrGCCl	$\text{Cl} + \text{C}_2\text{H}_4 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 1.85\text{E-}29, 3.3, 6.0\text{E-}10, 0.0, 0.4)$	Atkinson et al. (2006)*
G6410	TrGCCl	$\text{Cl} + \text{CH}_3\text{CHO} \rightarrow \text{HCl} + \text{CH}_3\text{C}(\text{O})$	8.0e-11	Atkinson et al. (2006)
G6411	TrGCCl	$\text{C}_2\text{H}_2 + \text{Cl} \rightarrow \text{LCARBON} + \text{CH}_3 + \text{HCl}$	$k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 6.1\text{e-}30, 3.0, 2.0\text{e-}10, 0., 0.6)$	Atkinson et al. (2006)
G6412	TrGCCl	$\text{C}_2\text{H}_6 + \text{Cl} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$8.3\text{E-}11*\text{EXP}(-100./\text{temp})$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G6413	StTrGClN	$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{HCl} + \text{HCHO} + \text{NO}_2$	$1.3\text{E}-11 \cdot \text{EXP}(-1200./\text{temp})$	Burkholder et al. (2015)
G6414	StTrGClN	$\text{Cl} + \text{CH}_3\text{ONO} \rightarrow \text{HCl} + \text{HCHO} + \text{NO}$	$2.1\text{E}-12$	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	TrGCClN	$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{NCCH}_2\text{O}_2 + \text{HCl}$	$1.6\text{E}-11 \cdot \text{EXP}(-2104./\text{temp})$	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019)
G641MS	StTrGCCl	$\text{Cl} + \text{BENZENE} \rightarrow \text{C}_6\text{H}_5\text{O}_2 + \text{HCl}$	$1.3\text{E}-16$	Sokolov et al. (1998)
G642MS	StTrGCCl	$\text{Cl} + \text{TOLUENE} \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{HCl}$	$6.2\text{E}-11$	Wang et al. (2005)
G692MS	StTrGCCl	$\text{Cl} + \text{LXYL} \rightarrow \text{C}_6\text{H}_5\text{CH}_2\text{O}_2 + \text{LCARBON} + \text{HCl}$	$1.5\text{E}-10$	Shi and Bernhard (1997)
G643DT	TrGCCl	$\text{Cl} + \text{C}_5\text{H}_8 \rightarrow .63 \text{ LISOPAB} + .30 \text{ LISOPCD} + .07 \text{ LISOPEFO}_2 + \text{HCl}$	$7.6\text{E}-11 \cdot \text{EXP}(500./\text{temp}) * 1.1 \cdot \text{EXP}(-595./\text{temp})$	Wennberg et al. (2018)*
G644DT	TrGCCl	$\text{Cl} + \text{C}_5\text{H}_8 \rightarrow .63 \text{ LISOPAB} + .30 \text{ LISOPCD} + .07 \text{ LISOPEFO}_2 + \text{LCHLORINE}$	$7.6\text{E}-11 \cdot \text{EXP}(500./\text{temp}) * (1. - 1.1 \cdot \text{EXP}(-595./\text{temp}))$	Wennberg et al. (2018)*
G645DT	StTrGCl	$\text{Cl} + \text{CH}_3\text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{HCl}$	$7.1\text{E}-11 \cdot \text{EXP}(-75./\text{temp})$	Atkinson et al. (2006)
G646DT	StTrGCCl	$\text{Cl} + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HCl}$	$6.0\text{E}-11 \cdot \text{EXP}(155./\text{temp}) * 0.28 \cdot \text{EXP}(-350./\text{temp})$	Atkinson et al. (2006)
G647DT	StTrGCCl	$\text{Cl} + \text{C}_2\text{H}_5\text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HCl}$	$6.0\text{E}-11 \cdot \text{EXP}(155./\text{temp}) * (1. - 0.28 \cdot \text{EXP}(-350./\text{temp}))$	Atkinson et al. (2006)
G648DT	StTrGCCl	$\text{Cl} + \text{HOCH}_2\text{CHO} \rightarrow \text{HOCHCHO} + \text{HCl}$	$8.0\text{E}-12/0.9 * 0.35$	Niki et al. (1987), Atkinson et al. (2006)
G649DT	StTrGCCl	$\text{Cl} + \text{HOCH}_2\text{CHO} \rightarrow \text{HOCH}_2\text{CO} + \text{HCl}$	$8.0\text{E}-12/0.9 * (1. - 0.35)$	Niki et al. (1987), Atkinson et al. (2006)
G650DT	StTrGCCl	$\text{Cl} + \text{GLYOX} \rightarrow \text{HCOCO} + \text{HCl}$	$3.8\text{E}-11$	Niki et al. (1985)
G651DT	StTrGCCl	$\text{Cl} + \text{MGLYOX} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HCl}$	$4.8\text{E}-11$	Green et al. (1990)
G652DT	StTrGCCl	$\text{Cl} + \text{C}_2\text{H}_5\text{CHO} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HCl}$	$1.3\text{E}-10$	Atkinson et al. (2006)*
G653DT	StTrGCCl	$\text{Cl} + \text{CH}_3\text{COCH}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HCl}$	$1.5\text{E}-11 \cdot \text{EXP}(-590./\text{temp})$	Atkinson et al. (2006)
G654DT	StTrGCCl	$\text{Cl} + \text{MEK} \rightarrow \text{LMEKO}_2 + \text{HCl}$	$3.05\text{E}-11 \cdot \text{EXP}(80./\text{temp})$	Atkinson et al. (2006)*
G655MS	StTrGCCl	$\text{Cl} + \text{BENZAL} \rightarrow \text{C}_6\text{H}_5\text{CO}_3 + \text{HCl}$	$1.0\text{E}-10$	Thiault et al. (2002)
G7100	StTrGBr	$\text{Br} + \text{O}_3 \rightarrow \text{BrO} + \text{O}_2$	$1.7\text{E}-11 \cdot \text{EXP}(-800./\text{temp})$	Atkinson et al. (2007)
G7102a	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow 2 \text{Br} + \text{O}_2$	$2.7\text{E}-12$	Atkinson et al. (2007)
G7102b	StTrGBr	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$	$2.9\text{E}-14 \cdot \text{EXP}(840./\text{temp})$	Atkinson et al. (2007)
G7200	StTrGBr	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr} + \text{O}_2$	$7.7\text{E}-12 \cdot \text{EXP}(-450./\text{temp})$	Atkinson et al. (2007)
G7201	StTrGBr	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr} + \text{O}_2$	$4.5\text{E}-12 \cdot \text{EXP}(500./\text{temp})$	Atkinson et al. (2007)
G7202	StTrGBr	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$6.7\text{E}-12 \cdot \text{EXP}(155./\text{temp})$	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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	$\text{BrNO}_3 \rightarrow \text{BrO} + \text{NO}_2$	$k_{\text{BrO_NO2}} / (5.44\text{E}-9 \cdot \text{EXP}(14192./\text{temp}) \cdot 1.\text{E6} \cdot R_{\text{gas}} \cdot \text{temp} / (\text{atm2Pa} \cdot N_{\text{A}}))$	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)*
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0., 0.6)$	Burkholder et al. (2015)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E}-11 \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E}-13 \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGCS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{ SO}_2 + \text{HCHO} + .6 \text{ CH}_3 + .4 \text{ HO}_2 + .4 \text{ CH}_3\text{SO}_3\text{H}$	$1.\text{E}-10$	Hynes and Wine (1996)*

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	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	$k_{\text{CH200_SO2}}$	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 (2022)
G9410	TrGTerCS	$\text{APINAOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard (2022)
G9411	TrGTerCS	$\text{APINBOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard (2022)
G9412	TrGTerCS	$\text{MBOOO} + \text{SO}_2 \rightarrow \text{IBUTALOH} + \text{H}_2\text{SO}_4$	$7.00\text{E}-14$	Rickard (2022)
G9600	TrGCClS	$\text{DMS} + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCl} + \text{HCHO}$	$3.3\text{E}-10$	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)

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:

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

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

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

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

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:

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

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

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

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

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

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 $\text{cm}^{-3}\text{s}^{-1}$	
k_p	$4.49 \times 10^{-18} \times (T/\text{K})^2 \exp(-320 \text{ K}/T)$
k_s	$4.50 \times 10^{-18} \times (T/\text{K})^2 \exp(253 \text{ K}/T)$
k_t	$2.12 \times 10^{-18} \times (T/\text{K})^2 \exp(696 \text{ K}/T)$
k_ROHRO	$2.1 \times 10^{-18} \times (T/\text{K})^2 \exp(-85 \text{ K}/T)$
k_CO2H	$0.7 \times k_{\text{CH}_3\text{CO}_2\text{H}+\text{OH}}$
k_ROOHRO	$0.6 \times k_{\text{CH}_3\text{OOH}+\text{OH}}$
f_alk	1.23
f_sOH	3.44
f_tOH	2.68
f_sOOH	8.
f_tOOH	8.
f_ONO2	0.04
f_CH2ON02	0.20
f_cpan	0.25
f_allyl	3.6
f_CHO	0.55
f_CO2H	1.67
f_CO	0.73
f_O	8.15
f_pCH2OH	1.29
f_tCH2OH	0.53

k for OH-addition to double bonds in $\text{cm}^{-3}\text{s}^{-1}$	
k_adp	$4.5 \times 10^{-12} \times (T/300 \text{ K})^{-0.85}$
k_ads	$1/4 \times (1.1 \times 10^{-11} \times \exp(485 \text{ K}/T) + 1.0 \times 10^{-11} \times \exp(553 \text{ K}/T))$
k_adt	$1.922 \times 10^{-11} \times \exp(450 \text{ K}/T) - k_{\text{ads}}$
k_adsecprim	3.0×10^{-11}
k_adtertprim	5.7×10^{-11}
a_PAN	0.56
a_CHO	0.31
a_COCH3	0.76
a_CH2OH	1.7
a_CH2OOH	1.7
a_COH	2.2
a_COOH	2.2
a_CO2H	0.25
a_CH2ON02	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, 2022), 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 $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}} \times \mathbf{k_CH302}} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, $\mathbf{k_CH302}$ = second-order rate coefficient of the self reaction of CH_3O_2 , and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

G2110: The rate coefficient is: $k_{\text{H}_2\text{O}_2} = (3.0\text{E-}13 \cdot \text{EXP}(460./\text{temp}) + 2.1\text{E-}33 \cdot \text{EXP}(920./\text{temp}) \cdot \text{cair}) \cdot (1 + 1.4\text{E-}21 \cdot \text{EXP}(2200./\text{temp}) \cdot \text{C}(\text{ind_H}_2\text{O}))$.

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

G2118: Assuming fast equilibrium.

G3109: The rate coefficient is: $k_{\text{NO}_3\text{NO}_2} = k_{3\text{rd}}(\text{temp}, \text{cair}, 2.4\text{E-}30, 3.0, 1.6\text{E-}12, -0.1, 0.6)$.

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

G3203: The rate coefficient is: $k_{\text{NO}_2\text{H}_2\text{O}} = k_{3\text{rd}}(\text{temp}, \text{cair}, 1.9\text{E-}31, 3.4, 4.0\text{E-}12, 0.3, 0.6)$.

G3206: The rate coefficient is: $k_{\text{HNO}_3\text{OH}} = 1.32\text{E-}14 \cdot \text{EXP}(527/\text{temp}) + 1 / (1 / (7.39\text{E-}32 \cdot \text{EXP}(453/\text{temp}) \cdot \text{cair}) + 1 / (9.73\text{E-}17 \cdot \text{EXP}(1910/\text{temp})))$

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 (2022), 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: $k_{\text{CH}_3\text{CO}_3\text{NO}_2} = k_{3\text{rd}}(\text{temp}, \text{cair}, 9.7\text{E-}29, 5.6, 9.3\text{E-}12, 1.5, 0.6)$.

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

G42021: The rate coefficient is $k_{\text{PAN}_M} = k_{\text{CH}_3\text{CO}_3\text{NO}_2} / 9.0\text{E-}29 \cdot \text{EXP}(-14000./\text{temp})$, 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 $k = 1.1 \text{E-11 molec/cm}^3/\text{s}$ by Paulot et al. (2009a).

G42074b: Factor of 3 to match the estimate of $k = 1.1 \text{E-11 molec/cm}^3/\text{s}$ 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 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 $k=5.2\text{E-12}$ is combined with the major one producing HCOOH .

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

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

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 CHCH(OH)₂.

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

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

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

G43075a: Same value as for methanediol.

G43075b: Same value as for methanediol.

G43223: Products simplified

G43419: KDEC C3DIALO → GLYOX + CO + HO₂

G43420: KDEC C3DIALO → GLYOX + CO + HO₂

G43421: Permutation reaction (minor channels removed).

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

G44001b: sC₄H₉O₂ products are substituted with 0.636 MEK + HO₂ and 0.364 CH₃CHO + C₂H₅O₂ at 1 bar and 298 K.

G44003c: The alkyl nitrate yield is the weighted average yield for the two isomers forming from nC₄H₉O₂ and sC₄H₉O₂.

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

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

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

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

G44018: LHMVKABO₂ is 0.12 HMKVKAO₂ + 0.88 HMKVKB₂O₂.

G44019: LMEKO₂ represents 0.62 MEKBO₂ + 0.38 MEKAO₂.

G44021a: The products of MEKAO are substituted with HCHO + CO₂ + HOCH₂CH₂O₂.

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

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

G44025: Same value as for PAN.

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

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

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

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

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

G44062a: Simplified products.

G44062b: Simplified products.

G44066: Alkyl nitrate formation neglected.

G44070: Alkyl nitrate formation neglected.

G44076: Alkyl nitrate formation neglected.

G44078: Other channel neglected.

G44081: Alkyl nitrate formation neglected.

G44082: Other channel neglected.

G44085: k for CH₃CHCO from Hatakeyama et al. (1985) adjusted.

G44086: Simplified product distribution.

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

G44096: Both LBUT1ENO₂ isomers mostly C₂H₅CHO.

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

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

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

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH₃CHOOA products as from C₃H₆ + O₃ reaction.

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

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

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

G44127: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G44130: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G44133: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G44136: Only this channel considered as the intermediate radical is likely more stable than CHCH(OH)₂.

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

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

G44139: Simplified oxidation.

G44140: Simplified oxidation.

G44141: Simplified oxidation.

G44142: Simplified oxidation.

G44202: Alkyl nitrate formation neglected.

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

G44205: Alkyl nitrate formation neglected.

G44210: Alkyl nitrate formation neglected.

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

G44402: KDEC NC4DCO₂ → MALANHY + NO₂

G44406c: KDEC MALDIALCO₂ → 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 → HCOCO₂HCO₃

G44431: KDEC MALANHYO → HCOCO₂HCO₃

G44432: Only major channel. KDEC MALANHYO → HCOCO₂HCO₃

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), 4.2E-11.

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant 4.16E-11.

G45047: Alkyl nitrate formation neglected.

G45055: Alkyl nitrate formation neglected.

G45071: Alkyl nitrate formation neglected.

G45074: Formic acid production consistent with results of Bates et al. (2014). Here, the high yields of formic

acid and hydroxycarbonyls at low NO from oxidation of cis-beta-LIEPOX (the most abundant isomer) are approximated with the production of DB1O which undergo both the Dibble double H-transfer to DB2O2 and HOCH2 elimination yielding HVMK and HMAK (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting from the ring opening after H-abstraction). The rate constant is from Paulot et al. (2009b) and adjusted based on Bates et al. (2014) that determined the single rate constants for the cis- and trans- beta isomer.

G45080: Alkyl nitrate formation neglected.

G45092a: C4MDIAL = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

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

G45095: Alkyl nitrate formation neglected.

G45098: Alkyl nitrate formation neglected.

G45100: Alkyl nitrate formation neglected.

G45104a: DB1OOH is a hydroperoxide bearing a vinyl alcohol moiety that upon reaction with OH yields HCOOH (Davis et al., 1998).

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

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

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

G45111: Alkyl nitrate formation neglected.

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

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

G45116: As for DB1OOH + OH.

G45117: Additional sinks for DB2OOH are neglected.

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

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

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

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

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

G45139: LZCPANC₂3DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO₂ = 0.67 MBOAO₂ + 0.33 MBOBO₂

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO₂ → MMALANHY + NO₂

G45404: KDEC NTLFUO → ACCOMECHO + NO₂

G45405: KDEC NTLFUO → ACCOMECHO + NO₂

G45406: KDEC NTLFUO → ACCOMECHO

G45409: KBPAN → k_PAN_M(renaming)

G45413: KFPAN → k.CH₃CO₃_NO₂ (renaming)

G45422: KDEC MMALANHYO → CO₂H₃CO₃

G45423: KDEC MMALANHYO → CO₂H₃CO₃

G45424: KDEC MMALANHYO → CO₂H₃CO₃ and Only major channel.

G45429: KBPAN → k_PAN_M (renamed)

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

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

G45432: KFPAN → k.CH₃CO₃_NO₂ (renaming)

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

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

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

G45444: KDEC MC3CODBCO2 \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 ACCOMECHO + 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 NDNPHENO \rightarrow NC4DCO2H + HNO3 + CO + CO + NO2.

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

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

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

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

G46426: KFPAN \rightarrow k_CH3CO3_NO2

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

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

G46433: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46434: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

G46435: KDEC NCATECO \rightarrow NC4DCO2H + HCOCO2H + HO2

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

G46438: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46439: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46440: KDEC NPHENO \rightarrow MALDALCO2H + GLYOX + NO2

G46441: Merged equations.

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

G46448: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46449: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46450: KDEC NNCATECO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46457: Merged equations.

G46458: Merged equations.

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

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

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

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

G46468: KFPAN \rightarrow k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO \rightarrow C5CO2OHCO3

G46481: KDEC PBZQO \rightarrow C5CO2OHCO3

G46482: KDEC PBZQO \rightarrow C5CO2OHCO3

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

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

G46486: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHENO \rightarrow NC4DCO2H + HCOCO2H + NO2

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

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

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

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

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

G46500: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46501: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46502: KDEC NBZQO \rightarrow C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

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

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

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

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

G47210: Alkyl nitrate formation neglected.

G47214: Alkyl nitrate formation neglected.

G47218: Alkyl nitrate formation neglected.

G47222: Alkyl nitrate formation neglected.

G47223: ROO6R3OOH produced but no sink for it.

G47225: ROO6R4P produced but no sink for it.

G47226: ROO6R5P produced but no sink for it

G47400: Merged.

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

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

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

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

G47405: Merged.

G47406: Merged.

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

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

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

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

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

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

G47413: Merged.

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

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

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

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

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

G47423: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO \rightarrow C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

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

G47436: KFPAN \rightarrow k_CH3CO3_NO2

G47438: Only major channel.

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

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

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

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

G47445: KFPAN \rightarrow k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

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

G47483: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47484: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47485: KDEC NPTLQO \rightarrow C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO \rightarrow C6CO2OHCO3

G47487: KDEC PTLQO \rightarrow C6CO2OHCO3

G47488: KDEC PTLQO \rightarrow C6CO2OHCO3

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

G47494: New channel.

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

G47498: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2

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

G47502: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2

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

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

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

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

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

G47514: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2

G48202: Alkyl nitrate formation neglected.

G48205: Alkyl nitrate formation neglected.

G48210: Alkyl nitrate formation neglected.

G48212: Alkyl nitrate formation neglected.

G48216: Alkyl nitrate formation neglected.

G48222: Alkyl nitrate formation neglected.

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

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

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

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

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

G48402: merged under same rate constant

G48403: Same products as for toluene

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

G48408: KDEC NSTYRENEO \rightarrow NO2 + HCHO + BENZAL

G48409: KDEC NSTYRENEO \rightarrow NO₂ + HCHO + BENZAL

G48410: KDEC NSTYRENEO \rightarrow NO₂ + HCHO + BENZAL

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

G48413: KDEC STYRENO \rightarrow HO₂ + HCHO + BENZAL

G48414: KDEC STYRENO \rightarrow HO₂ + HCHO + BENZAL

G48415: KDEC STYRENO \rightarrow HO₂ + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

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

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

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

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to $(3.27\text{E-}11*0.21 + 3.25\text{E-}11*0.30 + 5.67\text{E-}11*0.14)/3$, 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 $(3.27\text{E-}11*0.06 + 3.25\text{E-}11*0.06 + 5.67\text{E-}11*0.03)/3$, 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 $(3.27\text{E-}11*0.03 + 3.25\text{E-}11*0.03 + 5.67\text{E-}11*0.04)/3$, 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 $(3.27\text{E-}11*0.70 + 3.25\text{E-}11*0.61 + 5.67\text{E-}11*0.79)/3$, 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, $k = 0.33*9.20\text{E-}14+0.67*8.80\text{E-}13$.

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

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

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

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard (2022).

G40212: Products from Rickard (2022).

G40232: Products from Capouet et al. (2008).

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard (2022).

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 (2022).

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 (2022).

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 (2022).

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 O₃+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

G6402: The initial products are probably HCl and CH₂OOH (Atkinson et al., 2006). It is assumed that CH₂OOH dissociates into HCHO and OH.

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

G643DT: H-abstraction channel producing HCl. Organic peroxy radicals (crudely) approximated with the ones from reaction with OH.

G644DT: Cl-addition channel. Chlorinated organic peroxy radicals (crudely) approximated with the ones from reaction with OH.

G652DT: Product distribution could be different.

G654DT: By using LMEKO2 (lumped RO2 from reaction with OH) the assumed yield of the isomer MEKBO2 is 0.62 instead of 0.79 as recommended by IUPAC.

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

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

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.

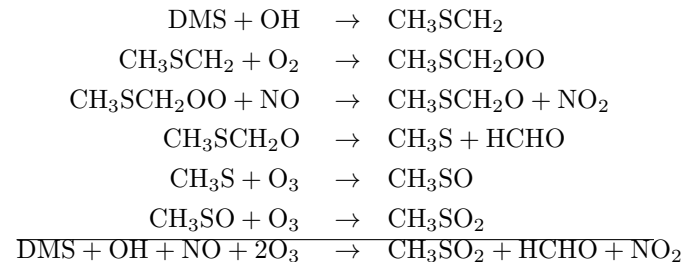
G7605: Same value as for G7408: CH₂Br₂+OH assumed. It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

G7606: Same value as for G7408: CH₂Br₂+OH assumed. It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

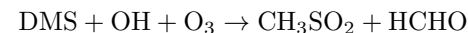
G7607: It is assumed that the reaction liberates all Br and Cl atoms. The fate of the carbon atom is currently not considered.

G9400a: For the abstraction path, the assumed reaction sequence (omitting H₂O and O₂ as products) according

to Yin et al. (1990) is:



Neglecting the effect on O₃ and NO_x, the remaining reaction is:



G9400b: For the addition path, the rate coefficient is: $k_{\text{DMS}_2\text{OH}} = 1.0\text{E-}39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{ind}_2) / (1. + 5.0\text{E-}30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{ind}_2))$.

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

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

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
J1000a	UpStTrGJ	$\text{O}_2 + h\nu \rightarrow \text{O}(^3\text{P}) + \text{O}(^3\text{P})$	jx(ip_02)	Sander et al. (2014)
J1001a	UpStTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^1\text{D}) + \text{O}_2$	jx(ip_01D)	Sander et al. (2014)
J1001b	UpStTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	jx(ip_03P)	Sander et al. (2014)
J2101	UpStTrGJ	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \text{OH}$	jx(ip_H202)	Sander et al. (2014)
J3101	UpStTrGJN	$\text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O}(^3\text{P})$	jx(ip_N02)	Sander et al. (2014)
J3103a	UpStTrGJN	$\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{O}(^3\text{P})$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGJN	$\text{NO}_3 + h\nu \rightarrow \text{NO} + \text{O}_2$	jx(ip_N002)	Sander et al. (2014)
J3104	StTrGJN	$\text{N}_2\text{O}_5 + h\nu \rightarrow \text{NO}_2 + \text{NO}_3$	jx(ip_N205)	Sander et al. (2014)
J3200	TrGJN	$\text{HONO} + h\nu \rightarrow \text{NO} + \text{OH}$	jx(ip_H0NO)	Sander et al. (2014)
J3201	StTrGJN	$\text{HNO}_3 + h\nu \rightarrow \text{NO}_2 + \text{OH}$	jx(ip_HN03)	Sander et al. (2014)
J3202	StTrGJN	$\text{HNO}_4 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{HO}_2 + .333 \text{NO}_3 + .333 \text{OH}$	jx(ip_HN04)	Sander et al. (2014)
J41000	StTrGJ	$\text{CH}_3\text{OOH} + h\nu \rightarrow \text{CH}_3\text{O} + \text{OH}$	jx(ip_CH300H)	Sander et al. (2014)
J41001a	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H}_2 + \text{CO}$	jx(ip_COH2)	Sander et al. (2014)
J41001b	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H} + \text{CO} + \text{HO}_2$	jx(ip_CH0H)	Sander et al. (2014)
J41004	StTrGJN	$\text{CH}_3\text{ONO} + h\nu \rightarrow \text{CH}_3\text{O} + \text{NO}$	jx(ip_CH30NO)	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_CH302N02)	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_CH302N02)	Sander et al. (2014)
J42000	TrGJC	$\text{C}_2\text{H}_5\text{OOH} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	von Kuhlmann (2001)
J42001a	TrGJC	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_3 + \text{HO}_2 + \text{CO}$	jx(ip_CH3CHO)	Sander et al. (2014)
J42001b	TrGJC	$\text{CH}_3\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHOH}$	jx(ip_CH3CHO2VINY)	Clubb et al. (2012)
J42002	TrGJC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + h\nu \rightarrow \text{CH}_3 + \text{OH} + \text{CO}_2$	jx(ip_CH3C03H)	Sander et al. (2014)
J42004	TrGJCN	$\text{PAN} + h\nu \rightarrow .7 \text{CH}_3\text{C}(\text{O}) + .7 \text{NO}_2 + .3 \text{CH}_3 + .3 \text{CO}_2 + .3 \text{NO}_3$	jx(ip_PAN)	Sander et al. (2014)*
J42005a	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{HCHO} + 2 \text{HO}_2 + \text{CO}$	jx(ip_HOCH2CHO)*0.83	Sander et al. (2014)*
J42005b	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{OH} + \text{HCOCH}_2\text{O}_2$	jx(ip_HOCH2CHO)*0.07	Sander et al. (2014)*
J42005c	TrGJC	$\text{HOCH}_2\text{CHO} + h\nu \rightarrow \text{CH}_3\text{OH} + \text{CO}$	jx(ip_HOCH2CHO)*0.10	Sander et al. (2014)*
J42006	TrGJC	$\text{HOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	jx(ip_CH300H)	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42007	TrGJCN	PHAN + $h\nu \rightarrow .7 \text{ HOCH}_2\text{CO} + .7 \text{ NO}_2 + .3 \text{ HCHO} + .3 \text{ HO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	see note*
J42008	TrGJC	GLYOX + $h\nu \rightarrow 2 \text{ CO} + 2 \text{ HO}_2$	jx(ip_GLYOX)	Sander et al. (2014)
J42009	TrGJC	HCOCO ₂ H + $h\nu \rightarrow 2 \text{ HO}_2 + \text{CO} + \text{CO}_2$	jx(ip_MGLYOX)	Rickard (2022)
J42010	TrGJC	HCOCO ₃ H + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard (2022)
J42011	TrGJC	HYETHO2H + $h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J42012	TrGJCN	ETHOHNO ₃ + $h\nu \rightarrow \text{HO}_2 + 2 \text{ HCHO} + \text{NO}_2$	j_IC3H7N03	Rickard (2022)
J42013	TrGJC	HOCH ₂ CO ₃ H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	2.*jx(ip_CH300H)	Sander et al. (2019)
J42014	TrGC	HOCH ₂ CO ₂ H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2$	jx(ip_CH300H)	Sander et al. (2019)
J42015	TrGC	CH ₂ 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)
J42016	TrGC	CH ₃ CHOHOOH + $h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	jx(ip_CH300H)	Sander et al. (2019)
J42017	TrGJCN	NO ₃ CH ₂ CHO + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	(jx(ip_C2H5N03)+jx(ip_CH3CHO)) *(jx(ip_NOA)+1E-10)/(0.59*j_IC3H7N03+jx(ip_CH3COCH3)+1E-10)	Sander et al. (2019)*
J42018	TrGJC	HOCH ₂ CHO + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Sander et al. (2019)
J42019	TrGJCN	C ₂ H ₅ ONO ₂ + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	jx(ip_C2H5N03)	Sander et al. (2019)
J42020	TrGJCN	NO ₃ CH ₂ CHO + $h\nu \rightarrow .7 \text{ NO}_3\text{CH}_2\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ HCHO} + .3 \text{ NO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	Sander et al. (2019)*
J42021	StTrGJCN	C ₂ H ₅ O ₂ NO ₂ + $h\nu \rightarrow .667 \text{ NO}_2 + .667 \text{ C}_2\text{H}_5\text{O}_2 + .333 \text{ NO}_3 + .333 \text{ CH}_3\text{CHO} + .333 \text{ HO}_2$	jx(ip_CH302N02)	Sander et al. (2019)*
J42022	TrGJC	HOCCOOH + $h\nu \rightarrow \text{CO}_2 + .72 \text{ HCOOH} + .28 \text{ CO} + .28 \text{ H}_2\text{O}$	jx(ip_H00CC00H)	Yamamoto and Back (1985)
J43000	TrGJC	iC ₃ H ₇ OOH + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	von Kuhlmann (2001)
J43001	TrGJC	CH ₃ COCH ₃ + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CH}_3$	jx(ip_CH3C0CH3)	Sander et al. (2014)
J43002	TrGJC	CH ₃ COCH ₂ 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	MGLYOX + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Sander et al. (2014)
J43004	TrGJC	CH ₃ COCH ₂ O ₂ H + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Rickard (2022)
J43005	TrGJC	HOCH ₂ COCH ₂ OOH + $h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+j_ACETOL	Sander et al. (2019)
J43006	TrGJCN	iC ₃ H ₇ ONO ₂ + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	j_IC3H7N03	von Kuhlmann et al. (2003)*
J43007	TrGJCN	NOA + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	jx(ip_NOA)	Barnes et al. (1993)
J43009	TrGJC	HYPROPO ₂ H + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J43010	TrGJCN	PR ₂ O ₂ HNO ₃ + $h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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 (2022)
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	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Sander et al. (2019)
J43014	TrGJTerC	$\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard (2022)
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 (2022)
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 (2022)
J43017	TrGJC	$\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$	$2 * \text{jx}(\text{ip_MGLYOX})$	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)
J43020	TrGC	$\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{j_ketene} * 0.36 * 2.$	Sander et al. (2019)
J43021	TrGCN	$\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	j_IC3H7N03	Sander et al. (2019)
J43022	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$	$\text{jx}(\text{ip_CH302N02}) + \text{jx}(\text{ip_CH3COCH}_3)$	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	$\text{C}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{NO}_2 + \text{HO}_2$	$0.59 * \text{j_IC3H7N03}$	see note*
J43025a	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{HCO})$	see note*
J43025b	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$	$\text{jx}(\text{ip_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$	Andrews et al. (2012), Sander et al. (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 (2022)
J43400	TrGJAroC	$\text{C}_3\text{DIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2. + \text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J43401	TrGJAroC	$\text{C}_3\text{OH}_2\text{CO} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO}) * 2.$	Rickard (2022)
J43402	TrGJAroC	$\text{HCOCOHCO}_3\text{H} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J44000a	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_p} / (\text{k_p} + \text{k_s}))$	Rickard (2022), Sander et al. (2019)
J44000b	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{MEK} + .636 \text{HO}_2 + .364 \text{CH}_3\text{CHO} + .364 \text{C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip_CH300H}) * (\text{k_s} / (\text{k_p} + \text{k_s}))$	Rickard (2022), 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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44002	TrGJC	$\text{MEK} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$	$0.42 \cdot j_x(\text{ip_CH0H})$	von Kuhlmann et al. (2003)
J44003	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$	$j_x(\text{ip_CH300H}) + 0.42 \cdot j_x(\text{ip_CH0H})$	Sander et al. (2019)
J44004	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C}(\text{O})$	$2.15 \cdot j_x(\text{ip_MGLYOX})$	see note*
J44005a	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$j_IC3H7N03 \cdot (k_p / (k_p + k_s))$	see note*
J44005b	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$	$j_IC3H7N03 \cdot (k_s / (k_p + k_s))$	see note*
J44006	TrGJCN	$\text{MPAN} + h\nu \rightarrow .7 \text{MACO}_3 + .7 \text{NO}_2 + .3 \text{MACO}_2 + .3 \text{NO}_3$	$j_x(\text{ip_PAN})$	see note*
J44007a	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$j_x(\text{ip_CH300H})$	Rickard (2022)
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 (2022)
J44008	TrGJC	$\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$	$j_x(\text{ip_MACR})$	Sander et al. (2014)
J44009	TrGJC	$\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$	$j_x(\text{ip_CH300H}) + 2.77 \cdot j_x(\text{ip_HOCH}_2\text{CHO})$	Sander et al. (2019)*
J44010	TrGJC	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$2.77 \cdot j_x(\text{ip_HOCH}_2\text{CHO})$	see note*
J44011	TrGJC	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$	$j_x(\text{ip_CH300H})$	Sander et al. (2019)
J44012	TrGJC	$\text{LHMKABOOH} + h\nu \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{CH}_3\text{C}(\text{O}) + .88 \text{HOCH}_2\text{CHO} + .12 \text{HCHO} + \text{OH}$	$j_x(\text{ip_CH300H}) + j_ACETOL$	Sander et al. (2019)
J44013	TrGJC	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$j_x(\text{ip_HOCH}_2\text{CHO}) + j_ACETOL$	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 (2022)
J44015	TrGJC	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	$2.15 \cdot j_x(\text{ip_MGLYOX})$	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	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{CH}_3\text{COCO}_2\text{H} + .1848 \text{H}_2\text{O}_2 + .2208 \text{MGLYOX} + .36 \text{OH} + .36 \text{CO} + .56 \text{CH}_3\text{C}(\text{O}) + .2 \text{CH}_3\text{CHO} + .2 \text{CO}_2 + .2 \text{HCHO} + .2 \text{HO}_2 + \text{CO}$	$j_ketene \cdot 0.5$	Sander et al. (2019), Rickard (2022)*
J44017b	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$	$j_ketene \cdot 0.5$	Sander et al. (2019)
J44018a	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$	$j_x(\text{ip_MGLYOX})$	Sander et al. (2019)
J44018b	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$	$2.15 \cdot j_x(\text{ip_MGLYOX})$	Sander et al. (2019)
J44019	TrGJC	$\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$	$3.15 \cdot j_x(\text{ip_MGLYOX})$	Sander et al. (2019)
J44020a	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$	$j_x(\text{ip_CH300H}) + j_ACETOL$	Rickard (2022)
J44020b	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$	$2.15 \cdot j_x(\text{ip_MGLYOX})$	Rickard (2022)
J44021	TrGJTerC	$\text{C44OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$j_x(\text{ip_CH300H})$	Rickard (2022)
J44022	TrGJTerC	$\text{C413COOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$	$j_x(\text{ip_CH300H}) + j_x(\text{ip_HOCH}_2\text{CHO}) + j_ACETOL$	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44023a	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_HOCH}_2\text{CHO})$	Rickard (2022)
J44023b	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
J44024	TrGJTerC	$\text{C312COCO}_3\text{H} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
J44025	TrGJCN	$\text{LMEKNO}_3 + h\nu \rightarrow .62 \text{ CH}_3\text{C}(\text{O}) + .62 \text{ CH}_3\text{CHO} + .38 \text{ HCHO}$ $+ .38 \text{ CO}_2 + .38 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{jx}(\text{ip_MEKNO}_3)$	Barnes et al. (1993), Sander et al. (2019)*
J44026	TrGJCN	$\text{MVKNO}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{NO}_2$	$\text{jx}(\text{ip_MEKNO}_3)$	Barnes et al. (1993), Sander et al. (2019)*
J44027	TrGJCN	$\text{MACRNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$(2.84 * \text{j_IC3H7NO}_3 + \text{jx}(\text{ip_CH3CHO}))$ $* (\text{jx}(\text{ip_MEKNO}_3) + 1\text{E-}10) / (\text{j_}$ $\text{IC3H7NO}_3 + 0.42 * \text{jx}(\text{ip_CHOH}) + 1\text{E-}10)$	Müller et al. (2014), Sander et al. (2019)*
J44028	TrGJCN	$\text{TC4H9NO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{NO}_2$	$2.84 * \text{j_IC3H7NO}_3$	Sander et al. (2019)
J44029	TrGJC	$\text{TC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44030	TrGJCN	$\text{IBUTOLBNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{j_IC3H7NO}_3$	Sander et al. (2019)
J44031	TrGJC	$\text{IBUTOLBOOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44032	TrGJC	$\text{LBUT1ENOOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	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_IC3H7NO_3	Sander et al. (2019)
J44034	TrGJC	$\text{BUT2OLOOH} + h\nu \rightarrow 2 \text{ CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	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_IC3H7NO_3	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	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_C3H7CHO2HCO})$	Sander et al. (2019)
J44037b	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{CHOH}$	$\text{jx}(\text{ip_C3H7CHO2VINY})$	Sander et al. (2019)*
J44038	TrGJC	$\text{IPRCHO} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_IPRCHO2HCO})$	Sander et al. (2019)
J44039	TrGJCN	$\text{IC4H9NO}_3 + h\nu \rightarrow \text{IPRCHO} + \text{NO}_2$	j_IC3H7NO_3	Sander et al. (2019)
J44040	TrGJC	$\text{IC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{IPRCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44041	TrGJC	$\text{PERIBUACID} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Sander et al. (2019)
J44042	TrGJCN	$\text{PIPN} + h\nu \rightarrow .7 \text{ IPRCO}_3 + .7 \text{ NO}_2 + .3 \text{ iC}_3\text{H}_7\text{O}_2 + .3 \text{ CO}_2 +$ $.3 \text{ NO}_3$	$\text{jx}(\text{ip_PAN})$	Sander et al. (2019), Sander et al. (2014)
J44043	TrGJC	$\text{HVMK} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + 2 \text{ OH}$	$\text{jx}(\text{ip_PeDIONE24})$	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	$\text{HMAC} + h\nu \rightarrow \text{HCOCCH}_3\text{CO} + 2 \text{ OH}$	$\text{jx}(\text{ip_PeDIONE24})$	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44045a	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_C2H5CHO2HCO})$	Rickard (2022)
J44045b	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$	$\text{jx}(\text{ip_C2H5CHO2ENOL})$	Andrews et al. (2012), Sander et al. (2019)
J44046a	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{jx}(\text{ip_C2H5CHO2HCO})*2.$	see note*
J44046b	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$	$\text{jx}(\text{ip_C2H5CHO2ENOL})*2.$	Andrews et al. (2012), Sander et al. (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 (2022)
J44201	TrGJTerC	$\text{IPRHOCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J44400a	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{C}_3\text{OH13CO} + \text{CO} + \text{OH} + \text{HO}_2$	$\text{jx}(\text{ip_HOCH2CHO})*2.$	Rickard (2022)
J44400b	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J44401	TrGJAroC	$\text{BZFUOOH} + h\nu \rightarrow \text{CO14O}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J44402	TrGJAroC	$\text{HOCOC4DIAL} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard (2022)
J44403	TrGJAroCN	$\text{NBZFUOOH} + h\nu \rightarrow .5 \text{ CO14O}_3\text{CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J44404a	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard (2022)
J44404b	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow .6 \text{ MALANHY} + \text{HO}_2 + .4 \text{ GLYOX} + .4 \text{ CO} + .4 \text{ CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J44405	TrGJAroC	$\text{EPXDLCO}_2\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO}_2 + \text{HO}_2$	$2.77*\text{jx}(\text{ip_HOCH2CHO})$	Rickard (2022)
J44406	TrGJAroC	$\text{MALDIAL} + h\nu \rightarrow .4 \text{ BZFUONE} + .6 \text{ MALDIALCO}_3 + .6 \text{ HO}_2$	$\text{jx}(\text{ip_NO}_2)*0.14$	Rickard (2022)
J44407	TrGJAroC	$\text{MALANHYOOH} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J44408	TrGJAroC	$\text{EPXDLCO}_3\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip_CH300H}) + 2.77*\text{jx}(\text{ip_HOCH2CHO})$	Rickard (2022)
J44409	TrGJAroC	$\text{CO}_2\text{C}_4\text{DIAL} + h\nu \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{HO}_2 + \text{CO} + \text{CO}$	$\text{jx}(\text{ip_MGLYOX})*2.$	Rickard (2022)
J44410	TrGJAroC	$\text{MALDALCO}_2\text{H} + h\nu \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip_MACR})$	Rickard (2022)
J44411	TrGJAroC	$\text{EPXC4DIAL} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO} + \text{HO}_2$	$2.77*\text{jx}(\text{ip_HOCH2CHO})*2.$	Rickard (2022)
J44412	TrGJAroC	$\text{CO14O}_3\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
J44414	TrGJAroC	$\text{MECOACEOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J45002	TrGJC	$\text{LISOPACOOH} + h\nu \rightarrow \text{LISOPACO} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J45003	TrGJCN	$\text{LISOPACNO}_3 + h\nu \rightarrow \text{LISOPACO} + \text{NO}_2$	$0.59*\text{j_IC3H7NO}_3$	see note*
J45004	TrGJC	$\text{ISOPBOOH} + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J45005	TrGJCN	$\text{ISOPBNO}_3 + h\nu \rightarrow \text{MVK} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84*\text{j_IC3H7NO}_3$	see note*
J45006	TrGJC	$\text{ISOPDOOH} + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J45007	TrGJCN	$\text{ISOPDNO}_3 + h\nu \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	j_IC3H7NO_3	see note*
J45008	TrGJCN	$\text{NISOPOOH} + h\nu \rightarrow \text{NC}_4\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45009	TrGJCN	$\text{NC4CHO} + h\nu \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	$(.59*j_IC3H7N03+jx(ip_MACR))$ $*(jx(ip_MEKN03)+1E-10)/(j_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)$	Müller et al. (2014), Sander et al. (2019)*
J45010	TrGJCN	$\text{LNISOOH} + h\nu \rightarrow \text{NOA} + \text{OH} + .5 \text{HOCHCHO} + .5 \text{CO} + .5 \text{HO}_2 + .5 \text{CO}_2$	$jx(ip_CH300H)$	Taraborrelli et al. (2009), Sander et al. (2019)
J45011	TrGJC	$\text{LHC4ACCHO} + h\nu \rightarrow .5 \text{LHC4ACCO3} + .5 \text{HO}_2 + .5 \text{CO} + .5 \text{OH} + .25 \text{MACRO2} + .25 \text{LHMKABO2}$	$jx(ip_MACR)$	Sander et al. (2019)
J45012	TrGJC	$\text{LC578OOH} + h\nu \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)+ 2.77*jx(ip_HOCH2CHO)$	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	$\text{LC5PAN1719} + h\nu \rightarrow .7 \text{LHC4ACCO3} + .7 \text{NO}_2 + .15 \text{MACRO2} + .15 \text{LHMKABO2} + .3 \text{CO}_2 + .3 \text{NO}_3$	$jx(ip_PAN)$	Sander et al. (2019)
J45015	TrGJC	$\text{HCOC5} + h\nu \rightarrow .65 \text{CH}_3 + .65 \text{CO} + .65 \text{HCHO} + .35 \text{OH} + .35 \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HOCH}_2\text{CO}$	$0.5*jx(ip_MVK)$	Sander et al. (2019)*
J45016	TrGJC	$\text{C59OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{OH}$	$j_ACETOL+jx(ip_CH300H)$	Sander et al. (2019)
J45017	TrGJTerC	$\text{C511OOH} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCH}_2\text{CHO} + \text{OH}$	$jx(ip_CH300H)+jx(ip_HOCH2CHO)$	Rickard (2022)
J45018a	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$jx(ip_HOCH2CHO)$	Rickard (2022)
J45018b	TrGJTerC	$\text{CO23C4CHO} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCH}_2\text{CO}_3$	$2.15*jx(ip_MGLYOX)$	Rickard (2022)
J45019	TrGJTerC	$\text{CO23C4CO3H} + h\nu \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$jx(ip_CH300H)+jx(ip_HOCH2CHO)$	Rickard (2022)
J45020	TrGJTerC	$\text{C512OOH} + h\nu \rightarrow \text{C513O}_2 + \text{OH}$	$jx(ip_CH300H)+jx(ip_HOCH2CHO)$	Rickard (2022)
J45021	TrGJTerC	$\text{CO13C4CHO} + h\nu \rightarrow \text{CHOC3COO}_2 + \text{CO} + \text{HO}_2$	$jx(ip_HOCH2CHO)*2.$	Rickard (2022)
J45022	TrGJTerC	$\text{C513OOH} + h\nu \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	$jx(ip_CH300H)+jx(ip_HOCH2CHO)$	Rickard (2022)
J45023	TrGJTerC	$\text{C513CO} + h\nu \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 + \text{CO} + \text{CO}$	$jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)$	Rickard (2022)
J45024	TrGJTerC	$\text{C514OOH} + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{OH}$	$jx(ip_CH300H)+jx(ip_HOCH2CHO)*2.$	Rickard (2022)
J45025	TrGJTerCN	$\text{C514NO}_3 + h\nu \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	$j_IC3H7N03+jx(ip_HOCH2CHO)*2.$	Rickard (2022)
J45026a	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HVMK} + \text{OH}$	$j_HPALD*0.6*0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CH}_3\text{C(O)} + \text{HOCH}_2\text{CHO}$	$j_HPALD*0.6*0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{HMAC} + \text{OH}$	$j_HPALD*0.4*0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45026d	TrGJC	$\text{LZCODC23DBCOOH} + h\nu \rightarrow \text{OH} + \text{CO} + \text{CO} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HO}_2$	$j_{\text{-HPALD}}*0.4*0.5$	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	$\text{LZCO3HC23DBCOD} + h\nu \rightarrow .62 \text{ EZCH3CO2CHCHO} + .38 \text{ EZCHOCCH3CHO2} + \text{OH} + \text{CO}_2$	$j_{\text{-HPALD}}$	Sander et al. (2019)
J45028a	TrGJC	$\text{C1OOHC2OOHC4OD} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} + 2 \text{ CO} + \text{HO}_2$	$2.77*jx(ip_{\text{HOCH2CHO}})$	Sander et al. (2019)
J45028b	TrGJC	$\text{C1OOHC2OOHC4OD} + h\nu \rightarrow .5 \text{ CH}_3\text{COCH}_2\text{O}_2\text{H} + .5 \text{ HOCHCHO} + .5 \text{ CO2H3CHO} + .5 \text{ HCHO} + 1.5 \text{ OH}$	$2.*jx(ip_{\text{CH300H}})$	Sander et al. (2019)
J45029	TrGC	$\text{DB1OOH} + h\nu \rightarrow \text{DB1O2} + \text{OH}$	$jx(ip_{\text{CH300H}})$	Sander et al. (2019)
J45030	TrGC	$\text{DB2OOH} + h\nu \rightarrow .48 \text{ CH}_3\text{COCH}_2\text{OH} + .52 \text{ HOCH}_2\text{CHO} + .52 \text{ MGLYOX} + .48 \text{ GLYOX} + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})$	Sander et al. (2019)
J45031a	TrGJC	$\text{C1ODC2OOHC4OD} + h\nu \rightarrow \text{MGLYOX} + \text{HOCHCHO} + \text{OH}$	$jx(ip_{\text{CH300H}})$	Sander et al. (2019)
J45031b	TrGJC	$\text{C1ODC2OOHC4OD} + h\nu \rightarrow \text{CO2H3CHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$2.*2.77*jx(ip_{\text{HOCH2CHO}})$	Sander et al. (2019)
J45032	TrGJC	$\text{C4MDIAL} + h\nu \rightarrow .5 \text{ CH}_3\text{COCHCO} + .5 \text{ HCOCCH}_3\text{CO} + \text{CO} + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{N02}})*0.1*0.5$	Sander et al. (2019)*
J45033	TrGCN	$\text{DB1NO3} + h\nu \rightarrow \text{DB1O2} + \text{NO}_2$	$j_{\text{-IC3H7N03}}$	Sander et al. (2019)
J45034	TrGJTerC	$\text{CHOC3COOOH} + h\nu \rightarrow \text{CHOC3COO2} + \text{CO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})+jx(ip_{\text{HOCH2CHO}})+j_{\text{-ACETOL}}$	Rickard (2022)
J45200a	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})*.67$	Rickard (2022), Sander et al. (2019)
J45200b	TrGJTerC	$\text{LMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})*.33$	Rickard (2022), Sander et al. (2019)
J45201	TrGJTerC	$\text{MBOACO} + h\nu \rightarrow \text{HCHO} + \text{HO}_2 + \text{IPRHOCO3}$	$j_{\text{-ACETOL}}$	Rickard (2022)
J45202	TrGJTerC	$\text{MBOCOCO} + h\nu \rightarrow \text{CO} + \text{HO}_2 + \text{IPRHOCO3}$	$jx(ip_{\text{MGLYOX}})$	Rickard (2022)
J45203a	TrGJTerCN	$\text{LNMBOABOOH} + h\nu \rightarrow \text{NO}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})*.65$	Rickard (2022), Sander et al. (2019)
J45203b	TrGJTerCN	$\text{LNMBOABOOH} + h\nu \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})*.35$	Rickard (2022), Sander et al. (2019)
J45204	TrGJTerCN	$\text{NC4OHCO3H} + h\nu \rightarrow \text{IBUTALOH} + \text{CO}_2 + \text{NO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})$	Rickard (2022)
J45400	TrGJAroC	$\text{C54CO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{CO} + \text{CO} + \text{CH}_3\text{C(O)}$	$jx(ip_{\text{MGLYOX}})+2.15*jx(ip_{\text{MGLYOX}})*2.$	Rickard (2022)
J45401	TrGJAroC	$\text{C5134CO2OH} + h\nu \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{CO} + \text{HO}_2$	$jx(ip_{\text{HOCH2CHO}})+2.15*jx(ip_{\text{MGLYOX}})$	Rickard (2022)
J45402	TrGJAroC	$\text{C5DIALOOH} + h\nu \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$jx(ip_{\text{CH300H}})+jx(ip_{\text{MACR}})$	Rickard (2022)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45406	TrGJAroC	$C_5CO_{14}OH + h\nu \rightarrow CH_3C(O) + HCOCO_2H + HO_2 + CO$	$jx(ip_MVK)$	Rickard (2022)
J45407	TrGJAroC	$C_5DICARB + h\nu \rightarrow .6 C_5CO_{14}O_2 + .6 HO_2 + .4 TLFUONE$	$jx(ip_N02)*0.2$	Rickard (2022)*
J45408	TrGJAroC	$MC_3ODBCO_2H + h\nu \rightarrow CH_3COCO_2H + HO_2 + CO + HO_2 + CO$	$jx(ip_MACR)$	Rickard (2022)
J45409	TrGJAroC	$ACCOMMECHO + h\nu \rightarrow MECOACETO_2 + HO_2 + CO$	$jx(ip_HOCH_2CHO)$	Rickard (2022)
J45410	TrGJAroC	$MMALNH_2OOH + h\nu \rightarrow CO_2H_3CO_3 + CO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J45411	TrGJAroC	$C_5DICAROOH + h\nu \rightarrow MGLYOX + GLYOX + HO_2 + OH$	$jx(ip_CH_3OOH)+jx(ip_HOCH_2CHO)+j_ACETOL$	Rickard (2022)*
J45412	TrGJAroCN	$NTLFUOOH + h\nu \rightarrow ACCOMECHO + NO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J45414	TrGJAroC	$C_5CO_{14}OOH + h\nu \rightarrow .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J45415	TrGJAroC	$TLFUOOH + h\nu \rightarrow ACCOMECHO + HO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J45417	TrGJAroC	$ACCOMMECO_3H + h\nu \rightarrow MECOACETO_2 + CO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)
J45418	TrGJAroC	$C_5DIALCO + h\nu \rightarrow MALDIALCO_3 + CO + HO_2$	$jx(ip_MGLYOX)+jx(ip_MACR)$	Rickard (2022)
J46200	TrGJTerCN	$C_6_{14}NO_3 + h\nu \rightarrow CO_2C_4CHO + HCHO + HO_2 + NO_2$	$2.15*jx(ip_MGLYOX)$	Rickard (2022)
J46201	TrGJTerC	$C_6_{14}OOH + h\nu \rightarrow CO_2C_4CHO + HCHO + HO_2 + OH$	$jx(ip_CH_3OOH)+2.15*jx(ip_MGLYOX)$	Rickard (2022)
J46202	TrGJTerC	$CO_2C_5CHO + h\nu \rightarrow CO_2C_4CO_3 + CO + HO_2$	$jx(ip_MGLYOX)$	Rickard (2022)
J46203	TrGJTerC	$CO_2C_5COOH + h\nu \rightarrow CO_2C_4CO_3 + HCHO + OH$	$jx(ip_CH_3OOH)+2.15*jx(ip_MGLYOX)$	Rickard (2022)
J46400	TrGJAroC	$PHENOOH + h\nu \rightarrow .71 MALDALCO_2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J46401	TrGJAroC	$C_6CO_4DB + h\nu \rightarrow C_4CO_2DBC_3 + HO_2 + CO$	$jx(ip_MGLYOX)*2.$	Rickard (2022)
J46402	TrGJAroC	$C_5CO_2DCO_3H + h\nu \rightarrow CH_3C(O) + HCOCOCHO + CO_2 + OH$	$jx(ip_CH_3OOH)+jx(ip_MGLYOX)$	Rickard (2022)
J46403	TrGJAroCN	$NDNPHENOOH + h\nu \rightarrow NC_4DCO_2H + HNO_3 + CO + CO + NO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)*
J46404	TrGJAroCN	$BZBIPERNO_3 + h\nu \rightarrow GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + NO_2$	$j_IC_3H_7NO_3$	Rickard (2022)*
J46405	TrGJAroCN	$HOC_6H_4NO_2 + h\nu \rightarrow HONO + CPDKETENE$	$jx(ip_HOC_6H_4NO_2)$	Chen et al. (2011)*
J46406	TrGJAroC	$CPDKETENE + h\nu \rightarrow CO_2 + CO + 2 HO_2 + MALDIAL$	j_ketene	see note*
J46407	TrGJAroC	$C_5COOHCO_3H + h\nu \rightarrow HOCOC_4DIAL + HO_2 + CO + CO_2 + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)
J46408	TrGJAroC	$BZEPOXMUC + h\nu \rightarrow .5 C_5DIALO_2 + 1.5 HO_2 + 1.5 CO + .5 MALDIAL$	$4.E3*jx(ip_MVK)*0.1$	Rickard (2022)
J46409	TrGJAroCN	$NPHEN_1OOH + h\nu \rightarrow NPHEN_1O + OH$	$jx(ip_CH_3OOH)$	Rickard (2022)
J46410	TrGJAroC	$BZEMUCCO + h\nu \rightarrow HCOCOHC_3 + C_3DIALO_2$	$jx(ip_HOCH_2CHO)*2.+j_ACETOL$	Rickard (2022)
J46411	TrGJAroC	$BZEMUCCO_2H + h\nu \rightarrow C_5DIALO_2 + CO_2 + HO_2$	$jx(ip_MACR)$	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46412	TrGJAroCN	$\text{NNCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46413	TrGJAroC	$\text{C615CO2OOH} + h\nu \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_MVK}) + \text{jx}(\text{ip_CH300H})$	Rickard (2022)
J46414	TrGJAroCN	$\text{NPHENO OH} + h\nu \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{OH} + \text{NO}_2$	$\text{j_IC3H7N03} + \text{jx}(\text{ip_CH300H})$	Rickard (2022)
J46415	TrGJAroCN	$\text{NCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46416	TrGJAroC	$\text{PBZQOOH} + h\nu \rightarrow \text{C5CO2OHCO3} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46417	TrGJAroC	$\text{BZOBIPEROH} + h\nu \rightarrow \text{MALDIALCO3} + \text{GLYOX} + \text{HO}_2$	j_ACETOL	Rickard (2022)
J46418	TrGJAroC	$\text{BZBIPEROOH} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46419	TrGJAroCN	$\text{NBZQOOH} + h\nu \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46420	TrGJAroC	$\text{CATEC1OOH} + h\nu \rightarrow \text{CATEC1O} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J46421	TrGJAroC	$\text{C6125CO} + h\nu \rightarrow \text{C5CO14O2} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip_MGLYOX}) + \text{jx}(\text{ip_MVK})$	Rickard (2022)
J46422	TrGJAroCN	$\text{DNPHENO OH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J46423	TrGJAroC	$\text{BZEMUCCO3H} + h\nu \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_MACR})$	Rickard (2022)
J46424	TrGJAroC	$\text{C6H5OOH} + h\nu \rightarrow \text{C6H5O} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J46425	TrGJAroC	$\text{BZEMUCOOH} + h\nu \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO}) * 2.$	Rickard (2022)*
J46427	TrGJAroCN	$\text{BZEMUCNO3} + h\nu \rightarrow \text{EPXC4DIAL} + \text{NO}_2 + \text{GLYOX} + \text{HO}_2$	$2.77 * \text{jx}(\text{ip_HOCH2CHO})$	Rickard (2022)
J46428	TrGJAroCN	$\text{DNPHEN} + h\nu \rightarrow \text{HONO} + \text{NCPDKETENE}$	$\text{jx}(\text{ip_HOC6H4N02})$	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	$\text{CO235C6CHO} + h\nu \rightarrow \text{CHOC3COCO3} + \text{CH}_3\text{C(O)}$	$2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
J47201	TrGJTerC	$\text{C235C6CO3H} + h\nu \rightarrow \text{CO235C6O2} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + 2.15 * \text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
J47202	TrGJTerC	$\text{C716OOH} + h\nu \rightarrow \text{CO13C4CHO} + \text{CH}_3\text{C(O)} + \text{OH}$	$\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO})$	Rickard (2022)
J47203	TrGJTerC	$\text{C721OOH} + h\nu \rightarrow \text{C722O2} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J47204	TrGJTerC	$\text{C722OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C44O2} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)
J47400	TrGJAroC	$\text{TLEPOXMUC} + h\nu \rightarrow .5 \text{ C615CO2O2} + \text{HO}_2 + \text{CO} + .5 \text{ EPXC4DIAL} + .5 \text{ CH}_3\text{C(O)}$	$4.E3 * \text{jx}(\text{ip_MVK}) * 0.1$	Rickard (2022)
J47401	TrGJAroC	$\text{C6H5CH2OOH} + h\nu \rightarrow \text{BENZAL} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
J47402	TrGJAroCN	$\text{C6H5CH2NO3} + h\nu \rightarrow \text{BENZAL} + \text{HO}_2 + \text{NO}_2$	$0.59 * \text{j_IC3H7N03}$	Rickard (2022)*
J47403	TrGJAroC	$\text{BENZAL} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{C6H5O2}$	$\text{jx}(\text{ip_BENZAL})$	Wallington et al. (2018)
J47404	TrGJAroC	$\text{TLBIPEROOH} + h\nu \rightarrow .6 \text{ GLYOX} + .4 \text{ MGLYOX} + \text{HO}_2 + .2 \text{ C4MDIAL} + .2 \text{ C5DICARB} + .2 \text{ TLFUONE} + .2 \text{ BZFUONE} + .2 \text{ MALDIAL} + \text{OH}$	$\text{jx}(\text{ip_CH300H})$	Rickard (2022)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47405	TrGJAroCN	TLBIPERNO3 + $h\nu$ → .6 GLYOX + .4 MGLYOX + HO ₂ + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO ₂	j_IC3H7N03	Rickard (2022)*
J47406	TrGJAroC	TLOBIPEROH + $h\nu$ → C5CO14O2 + GLYOX + HO ₂	j_ACETOL	Rickard (2022)
J47407	TrGJAroC	CRESOOH + $h\nu$ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH	jx(ip_CH300H)	Rickard (2022)*
J47408a	TrGJAroCN	NCRESOOH + $h\nu$ → .68 C5CO14OH + .68 GLYOX + HO ₂ + .32 PTLQONE + OH + NO ₂	j_IC3H7N03	Rickard (2022)*
J47408b	TrGJAroCN	NCRESOOH + $h\nu$ → C5CO14OH + GLYOX + NO ₂ + OH	jx(ip_CH300H)	Rickard (2022)*
J47409	TrGJAroCN	TOL1OHNO2 + $h\nu$ → HONO + MCPDKETENE	jx(ip_H0Ph3Me2N02)	see note*
J47410	TrGJAroC	TLEMUCCO2H + $h\nu$ → C615CO2O2 + CO ₂ + HO ₂	jx(ip_MACR)	Rickard (2022)
J47411	TrGJAroC	TLEMUCCO3H + $h\nu$ → C615CO2O2 + CO ₂ + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard (2022)
J47412	TrGJAroC	TLEMUCOOH + $h\nu$ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO ₂ + OH	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)+j_ACETOL	Rickard (2022)*
J47413	TrGJAroCN	TLEMUCNO3 + $h\nu$ → EPXC4DIAL + NO ₂ + CH ₃ C(O) + CO + HO ₂	2.77*jx(ip_HOCH2CHO)+j_ACETOL	Rickard (2022)
J47414	TrGJAroC	TLEMUCCO + $h\nu$ → CH ₃ C(O) + EPXC4DIAL + CO + HO ₂	2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard (2022)
J47415	TrGJAroC	C6H5CO3H + $h\nu$ → C6H5O2 + CO ₂ + OH	jx(ip_CH300H)	Rickard (2022)
J47416	TrGJAroC	OXYL1OOH + $h\nu$ → TOL1O + OH	jx(ip_CH300H)	Rickard (2022)
J47417	TrGJAroCN	MNCATECH + $h\nu$ → HONO + MCPDKETENE	jx(ip_H0Ph3Me2N02)	see note*
J47418	TrGJAroC	MCPDKETENE + $h\nu$ → CO ₂ + CO + 2 HO ₂ + C4MDIAL	j_ketene	see note*
J47419	TrGJAroCN	DNCRES + $h\nu$ → HONO + MNCPDKETENE	jx(ip_H0Ph3Me2N02)	see note*
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 (2022)
J47422	TrGJAroCN	NPTLQOOH + $h\nu$ → C7CO4DB + NO ₂ + OH	jx(ip_CH300H)	Rickard (2022)*
J47423	TrGJAroC	PTLQOOH + $h\nu$ → C6CO2OHCO3 + OH	jx(ip_CH300H)	Rickard (2022)*
J47424	TrGJAroCN	NCRES1OOH + $h\nu$ → NCRES1O + OH	jx(ip_CH300H)	Rickard (2022)
J47425	TrGJAroCN	MNNCATCOOH + $h\nu$ → NC4MDCO2HN + HCOCO ₂ H + NO ₂ + OH	jx(ip_CH300H)	Rickard (2022)*
J47426	TrGJAroCN	MNCATECOOH + $h\nu$ → NC4MDCO2HN + HCOCO ₂ H + HO ₂ + OH	jx(ip_CH300H)	Rickard (2022)*
J47427	TrGJAroC	C7CO4DB + $h\nu$ → C5CO2DBCO3 + HO ₂ + CO	jx(ip_MGLYOX)*2.	Rickard (2022)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47428	TrGJAroCN	$\text{NDNCRESOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)*
J47429	TrGJAroCN	$\text{DNCRESOOH} + h\nu \rightarrow \text{NC4MDCO2HN} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)*
J47430	TrGJAroC	$\text{C6COOHCO3H} + h\nu \rightarrow \text{C5134CO2OH} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J48200	TrGJTerC	$\text{C86OOH} + h\nu \rightarrow \text{C511O2} + \text{CH}_3\text{COCH}_3 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J48201	TrGJTerC	$\text{C812OOH} + h\nu \rightarrow \text{C813O2} + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J48202	TrGJTerC	$\text{C813OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_MGLYOX)}$	Rickard (2022)
J48203	TrGJTerC	$\text{C721CHO} + h\nu \rightarrow \text{C721O2} + \text{CO} + \text{HO}_2$	jx(ip_HOCH2CHO)	Rickard (2022)
J48204	TrGJTerC	$\text{C721CO3H} + h\nu \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J48205	TrGJTerC	$\text{C8BCOOH} + h\nu \rightarrow \text{C89O2} + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J48206	TrGJTerC	$\text{C89OOH} + h\nu \rightarrow \text{C810O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J48207	TrGJTerCN	$\text{C89NO3} + h\nu \rightarrow \text{C810O2} + \text{NO}_2$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J48208	TrGJTerC	$\text{C810OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J48209	TrGJTerCN	$\text{C810NO3} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	$2.84 * \text{j_IC3H7N03} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J48210	TrGJTerCN	$\text{C8BCNO3} + h\nu \rightarrow \text{C89O2} + \text{NO}_2$	j_IC3H7N03	Rickard (2022)
J48211	TrGJTerC	$\text{C85OOH} + h\nu \rightarrow \text{C86O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{j_ACETOL}$	Rickard (2022)
J48400	TrGJAroC	$\text{STYRENOOH} + h\nu \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL} + \text{OH}$	jx(ip_CH300H)	Rickard (2022)*
J49200	TrGJTerC	$\text{C96OOH} + h\nu \rightarrow \text{C97O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{j_ACETOL}$	Rickard (2022)
J49201	TrGJTerC	$\text{C97OOH} + h\nu \rightarrow \text{C98O2} + \text{OH}$	$\text{jx(ip_CH300H)} + \text{j_ACETOL}$	Rickard (2022)
J49202	TrGJTerC	$\text{C98OOH} + h\nu \rightarrow \text{C614O2} + \text{CH}_3\text{COCH}_3 + \text{OH}$	$(\text{jx(ip_CH300H)} + 2.15 * \text{jx(ip_MGLYOX)})$	Rickard (2022)
J49203a	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{C85O2} + \text{CO} + \text{HO}_2$	jx(ip_PINAL2HCO)	Rickard (2022), Sander et al. (2019)
J49203b	TrGJTerC	$\text{NORPINAL} + h\nu \rightarrow \text{NORPINENOL}$	jx(ip_PINAL2ENOL)	Sander et al. (2019), Andrews et al. (2012)
J49204	TrGJTerC	$\text{C85CO3H} + h\nu \rightarrow \text{C85O2} + \text{CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{j_ACETOL}$	Rickard (2022)
J49205	TrGJTerC	$\text{C89CO2H} + h\nu \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{HO}_2$	jx(ip_HOCH2CHO)	Rickard (2022)
J49206	TrGJTerC	$\text{C89CO3H} + h\nu \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	$\text{jx(ip_CH300H)} + \text{jx(ip_HOCH2CHO)}$	Rickard (2022)
J49207	TrGJTerC	$\text{C811CO3H} + h\nu \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J49208	TrGJTerC	$\text{NOPINDOOH} + h\nu \rightarrow \text{C89CO3} + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J40200	TrGJTerC	$\text{LAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard (2022)
J40201	TrGJTerC	$\text{MENTHEN6ONE} + h\nu \rightarrow \text{RO6R1O2} + \text{OH}$	jx(ip_CH300H)	Vereecken et al. (2007)
J40202	TrGJTerC	$\text{2OHMENTHEN6ONE} + h\nu \rightarrow 10 \text{ LCARBON} + \text{OH}$	jx(ip_CH300H)	Vereecken et al. (2007)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J40203a	TrGJTerC	PINAL + $h\nu \rightarrow$ C96O2 + CO + HO ₂	jx(ip_PINAL2HCO)	Rickard (2022)
J40203b	TrGJTerC	PINAL + $h\nu \rightarrow$ PINEOL	jx(ip_PINAL2ENOL)	Sander et al. (2019), Andrews et al. (2012)*
J40204	TrGJTerC	PERPINONIC + $h\nu \rightarrow$ C96O2 + CO ₂ + OH	jx(ip_CH300H)+j_ACETOL	Rickard (2022)
J40205	TrGJTerC	PINALOOH + $h\nu \rightarrow$ C106O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard (2022)
J40206	TrGJTerCN	PINALNO3 + $h\nu \rightarrow$ C106O2 + NO ₂	j_IC3H7N03+jx(ip_HOCH2CHO)	Rickard (2022)
J40207	TrGJTerC	C106OOH + $h\nu \rightarrow$ C716O2 + CH ₃ COCH ₃ + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard (2022)
J40208	TrGJTerCN	C106NO3 + $h\nu \rightarrow$ C716O2 + CH ₃ COCH ₃ + NO ₂	j_IC3H7N03+ jx(ip_HOCH2CHO)	Rickard (2022)
J40209	TrGJTerC	C109OOH + $h\nu \rightarrow$ C89CO3 + HCHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard (2022)
J40210	TrGJTerC	C109CO + $h\nu \rightarrow$ C89CO3 + CO + HO ₂	jx(ip_MGLY0X)+jx(ip_HOCH2CHO)	Rickard (2022)
J40211	TrGJTerCN	LNAPINABOOH + $h\nu \rightarrow$ PINAL + NO ₂ + OH	jx(ip_CH300H)	Rickard (2022)
J40212	TrGJTerC	BPINAOOH + $h\nu \rightarrow$ NOPINONE + HCHO + HO ₂ + OH	jx(ip_CH300H)	Rickard (2022)
J40213	TrGJTerCN	LNBPINABOOH + $h\nu \rightarrow$ NOPINONE + HCHO + NO ₂ + OH	jx(ip_CH300H)	Rickard (2022)
J40214	TrGJTerCN	ROO6R1NO3 + $h\nu \rightarrow$ ROO6R3O2 + CH ₃ COCH ₃ + NO ₂	2.84*j_IC3H7N03+jx(ip_CH300H)	Sander et al. (2019)
J40215	TrGJTerCN	RO6R1NO3 + $h\nu \rightarrow$ 9 LCARBON + HCHO + HO ₂ + NO ₂	2.84*j_IC3H7N03	Sander et al. (2019)
J6000	StTrGJCl	Cl ₂ + $h\nu \rightarrow$ Cl + Cl	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	Cl ₂ O ₂ + $h\nu \rightarrow$ 2 Cl	jx(ip_Cl202)	Sander et al. (2014)
J6101	StTrGJCl	OClo + $h\nu \rightarrow$ ClO + O(³ P)	jx(ip_0Cl0)	Sander et al. (2014)
J61MS	StTrGJCl	ClO + $h\nu \rightarrow$ Cl + O(³ P)	jx(ip_Cl0)	Atkinson et al. (2007)
J62MS	StTrGJCl	Cl ₂ O + $h\nu \rightarrow$ Cl + ClO	jx(ip_Cl20)	Atkinson et al. (2007)
J63MS	StTrGJCl	Cl ₂ O ₃ + $h\nu \rightarrow$ ClO + ClO ₂	jx(ip_Cl203)	Atkinson et al. (2007)
J6201	StTrGJCl	HOCl + $h\nu \rightarrow$ OH + Cl	jx(ip_HOCl)	Sander et al. (2014)
J6300	TrGJCIN	ClNO ₂ + $h\nu \rightarrow$ Cl + NO ₂	jx(ip_ClN02)	Sander et al. (2014)
J6301a	StTrGJCIN	ClNO ₃ + $h\nu \rightarrow$ Cl + NO ₃	jx(ip_ClN03)	Sander et al. (2014)
J6301b	StTrGJCIN	ClNO ₃ + $h\nu \rightarrow$ ClO + NO ₂	jx(ip_ClON02)	Sander et al. (2014)
J64MS	TrGJCIN	ClNO + $h\nu \rightarrow$ Cl + NO	jx(ip_ClN0)	Atkinson et al. (2007)
J65MS	TrGJCIN	ClONO + $h\nu \rightarrow$ Cl + NO ₂	jx(ip_ClON0)	Atkinson et al. (2007)
J7000	StTrGJBr	Br ₂ + $h\nu \rightarrow$ Br + Br	jx(ip_Br2)	Sander et al. (2014)
J7100	StTrGJBr	BrO + $h\nu \rightarrow$ Br + O(³ P)	jx(ip_Br0)	Sander et al. (2014)
J7200	StTrGJBr	HOBr + $h\nu \rightarrow$ Br + OH	jx(ip_HOBr)	Sander et al. (2014)
J7300	TrGJBrN	BrNO ₂ + $h\nu \rightarrow$ Br + NO ₂	jx(ip_BrN02)	Sander et al. (2014)
J7301	StTrGJBrN	BrNO ₃ + $h\nu \rightarrow$.85 Br + .85 NO ₃ + .15 BrO + .15 NO ₂	jx(ip_BrN03)	Sander et al. (2014)*
J7401	TrGJBr	CH ₂ Br ₂ + $h\nu \rightarrow$ LCARBON + 2 Br	jx(ip_CH2Br2)	Sander et al. (2014)
J7402	TrGJBr	CHBr ₃ + $h\nu \rightarrow$ LCARBON + 3 Br	jx(ip_CHBr3)	Sander et al. (2014)
J7600	StTrGJBrCl	BrCl + $h\nu \rightarrow$ Br + Cl	jx(ip_BrCl)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7602	TrGJBrCl	$\text{CH}_2\text{ClBr} + h\nu \rightarrow \text{LCARBON} + \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CH2ClBr})$	Sander et al. (2014)
J7603	TrGJBrCl	$\text{CHCl}_2\text{Br} + h\nu \rightarrow \text{LCARBON} + \text{Br} + 2 \text{Cl}$	$\text{jx}(\text{ip_CHCl2Br})$	Sander et al. (2014)
J7604	TrGJBrCl	$\text{CHClBr}_2 + h\nu \rightarrow \text{LCARBON} + 2 \text{Br} + \text{Cl}$	$\text{jx}(\text{ip_CHClBr2})$	Sander et al. (2014)
PH (aqueous)				
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	TrAa01ScJ	$\text{HOCH}_2\text{OOH}(\text{aq}) + h\nu \rightarrow \text{HCOOH}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	Sander et al. (2014)
PH4101_a01	TrAa01ScJ	$\text{CH}_3\text{OOH}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	Sander et al. (2014)
PH4200_a01	TrAa01ScJC	$\text{C}_2\text{H}_5\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{CHO}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	von Kuhlmann (2001)*
PH4201_a01	TrAa01ScJC	$\text{HOOCH}_2\text{CO}_2\text{H}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{CO}_2(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	Rickard (2022)*
PH4202_a01	TrAa01ScJC	$\text{CH}_2\text{OOHCO}_2^-(\text{aq}) + h\nu \rightarrow \text{CHOHOOC}_2^-(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	see note*
PH4203_a01	TrAa01ScJC	$\text{CH}_3\text{C}(\text{O})\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OO}(\text{aq}) + \text{CO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH3C03H})$	Sander et al. (2014)
PH4204_a01	TrAa01ScJC	$\text{HOCH}_2\text{CO}_3\text{H}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + \text{OH}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{CO}_2(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	Rickard (2022)
PH4205_a01	TrAa01ScJC	$\text{CH}_3\text{CHO}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OO}(\text{aq}) + \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH3CHO})$	Sander et al. (2014)
PH4206_a01	TrAa01ScJC	$\text{CH}_2\text{OOHCHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{CO}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33*\text{xaer}(01)*(\text{jx}(\text{ip_CH300H}) + \text{jx}(\text{ip_HOCH2CHO}))$	Sander et al. (2019)
PH4207a_a01	TrAa01ScJC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{HCHO}(\text{aq}) + 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_HOCH2CHO}) * 0.83$	Sander et al. (2014)*
PH4207b_a01	TrAa01ScJC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + .6 \text{HCHO}(\text{aq}) + .6 \text{CO}(\text{aq}) + .6 \text{HO}_2(\text{aq}) + .2 \text{GLYOX}(\text{aq}) + .2 \text{CH}_2\text{OHCHO}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_HOCH2CHO}) * 0.07$	Sander et al. (2014)*
PH4207c_a01	TrAa01ScJC	$\text{CH}_2\text{OHCHO}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{OH}(\text{aq}) + \text{CO}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_HOCH2CHO}) * 0.10$	Sander et al. (2014)*
PH4208_a01	TrAa01ScJC	$\text{CHOCOOH}(\text{aq}) + h\nu \rightarrow 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq}) + \text{CO}_2(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_MGLYOX})$	Rickard (2022)
PH4209_a01	TrAa01ScJC	$\text{GLYOX}(\text{aq}) + h\nu \rightarrow 2 \text{CO}(\text{aq}) + 2 \text{HO}_2(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_GLYOX})$	Sander et al. (2014)
PH4210a_a01	TrAa01ScJC	$\text{HOCCOOH}(\text{aq}) + h\nu \rightarrow \text{CO}_2(\text{aq}) + \text{HCOOH}(\text{aq})$	$2.33*\text{xaer}(01)*0.72*\text{jx}(\text{ip_HOCCOOH})$	Yamamoto and Back (1985)
PH4210b_a01	TrAa01ScJC	$\text{HOCCOOH}(\text{aq}) + h\nu \rightarrow \text{CO}_2(\text{aq}) + \text{CO}(\text{aq}) + \text{H}_2\text{O}(\text{aq})$	$2.33*\text{xaer}(01)*0.28*\text{jx}(\text{ip_HOCCOOH})$	Yamamoto and Back (1985)
PH4211_a01	TrAa01ScJC	$\text{CHOCHOHOH}(\text{aq}) + h\nu \rightarrow \text{HCOOH}(\text{aq}) + 2 \text{HO}_2(\text{aq}) + \text{CO}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_HOCH2CHO})$	Sander et al. (2014)*
PH4300_a01	TrAa01ScJC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{COOO}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*(\text{jx}(\text{ip_CH300H}) + 0.65*0.11*\text{jx}(\text{ip_CHOH}))$	see note*
PH4301_a01	TrAa01ScJC	$\text{iC}_3\text{H}_7\text{OOH}(\text{aq}) + h\nu \rightarrow \text{CH}_3\text{COCH}_3(\text{aq}) + \text{HO}_2(\text{aq}) + \text{OH}(\text{aq})$	$2.33*\text{xaer}(01)*\text{jx}(\text{ip_CH300H})$	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH4302_a01	TrAa01ScJC	$\text{CH}_3\text{COCH}_2\text{OH}(\text{aq}) + h\nu \rightarrow .5 \text{ OH}(\text{aq}) + .5 \text{ HCHO}(\text{aq}) + .5 \text{ CO}(\text{aq}) + .5 \text{ HCHO}(\text{aq}) + .5 \text{ HO}_2(\text{aq}) + .5 \text{ CH}_2\text{OHCO}_3(\text{aq}) + .5 \text{ CH}_3\text{OO}(\text{aq})$	$2.33 \times \text{xaer}(01) \times 0.65 \times 0.11 \times \text{jx}(\text{ip_CHOH})$	Sander et al. (2014)*
PH4303_a01	TrAa01ScJC	$\text{CH}_3\text{C}(\text{O})\text{CHO}(\text{aq}) + h\nu \rightarrow \text{OH}(\text{aq}) + \text{HCHO}(\text{aq}) + \text{CO}(\text{aq}) + \text{CO}(\text{aq}) + \text{HO}_2(\text{aq})$	$2.33 \times \text{xaer}(01) \times \text{jx}(\text{ip_MGLYOX})$	Sander et al. (2014)*
PH11200_a01	TrAa01JFe	$\text{FeOH}^{2+}(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{OH}(\text{aq})$	$\text{xaer}(01) \times 4.51\text{E-}3 \times 0.312$	Herrmann et al. (2000)
PH11201_a01	TrAa01JFe	$\text{Fe}(\text{OH})_2^+(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{OH}(\text{aq}) + \text{OH}^-(\text{aq})$	$\text{xaer}(01) \times 5.77\text{E-}3 \times 0.255$	Herrmann et al. (2000)
PH11800_a01	TrAa01JFeS	$\text{FeSO}_4^+(\text{aq}) + h\nu \rightarrow \text{Fe}^{2+}(\text{aq}) + \text{SO}_4^-(\text{aq})$	$\text{xaer}(01) \times 6.43\text{E-}3 \times 7.9\text{E-}3$	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 (2022) are translated accordingly in the following way:

$\text{j}(11) \rightarrow \text{jx}(\text{ip_COH}_2)$
 $\text{j}(12) \rightarrow \text{jx}(\text{ip_CHOH})$
 $\text{j}(15) \rightarrow \text{jx}(\text{ip_HOCH}_2\text{CHO})$
 $\text{j}(18) \rightarrow \text{jx}(\text{ip_MACR})$
 $\text{j}(22) \rightarrow \text{jx}(\text{ip_ACETOL})$
 $\text{j}(23)+\text{j}(24) \rightarrow \text{jx}(\text{ip_MVK})$
 $\text{j}(31)+\text{j}(32)+\text{j}(33) \rightarrow \text{jx}(\text{ip_GLYOX})$
 $\text{j}(34) \rightarrow \text{jx}(\text{ip_MGLYOX})$
 $\text{j}(41) \rightarrow \text{jx}(\text{ip_CH}_3\text{OOH})$
 $\text{j}(53) \rightarrow \text{j}(\text{isopropyl nitrate})$
 $\text{j}(54) \rightarrow \text{j}(\text{isopropyl nitrate})$
 $\text{j}(55) \rightarrow \text{j}(\text{isopropyl nitrate})$
 $\text{j}(56)+\text{j}(57) \rightarrow \text{jx}(\text{ip_NOA})$

Specific notes

J41006: product distribution as for HNO₄

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

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

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

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

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

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

J42020: It is assumed that *j*(NO₃CH₂CHO) is the same as *j*(PAN).

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

J43002: Following von Kuhlmann et al. (2003), we use *j*(CH₃COCH₂OH) = 0.11 × *jx*(ip_CHOH). As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a).

J43006: Following von Kuhlmann et al. (2003), we use J(iC₃H₇ONO₂) = 3.7 × *jx*(ip_PAN).

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

J43024: Assuming J(C₃H₇ONO₂) = 0.59 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

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

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

J43400: KDEC C3DIALO → GLYOX + CO + HO₂

J44004: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

J44005a: It is assumed that J(LC4H₉NO₃) is the same as J(iC₃H₇ONO₂).

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

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

J44009: It is assumed that J(MACROOH) is 2.77 times larger than J(HOCH₂CHO), consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

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, 2022).

J44015: It is assumed that $J(\text{BIACETOH})$ is 2.15 times larger than $J(\text{MGLYOX})$, consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

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

J44025: J values only for the secondary nitrate.

J44026: Like for LMEKNO3 photolysis

J44027: $2.84 \times J(\text{IC}_3\text{H}_7\text{NO}_3)$ like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to Müller et al. (2014).

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

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

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

J44046a: Simplified oxidation.

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

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

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

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

J44407: $\text{KDEC MALANHYO} \rightarrow \text{HCOCOHCO}_3$

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

J45003: It is assumed that $J(\text{LISOPACNO}_3) = 0.59 \times J(\text{IC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

J45005: It is assumed that $J(\text{ISOPBNO}_3) = 2.84 \times J(\text{IC}_3\text{H}_7\text{ONO}_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard, 2022).

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

J45009: $0.59 \times J(\text{IC}_3\text{H}_7\text{NO}_3)$ like for other primary alkyl nitrates (see J4503). Enhancement of J according to Müller et al. (2014).

J45015: Consistent with the MCM (Rickard, 2022), we assume that $J(\text{HCOC}_5)$ is half as large as $J(\text{MVK})$. With exception of HOCH_2CO the products of MACO_2 decomposition without CO_2 .

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

J45402: $\text{KDEC C}_5\text{DIALO} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2$

J45407: $\text{KDEC TLFUONE} \rightarrow 0.6 \text{ C}_5\text{CO}_2\text{HCHO} + 0.6 \text{ HO}_2 + 0.4 \text{ TLFUONE}$

J45410: $\text{KDEC MMALANHYO} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$

J45411: $\text{KDEC C}_5\text{DICARBO} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2$

J45412: $\text{KDEC NTLFUO} \rightarrow \text{ACCOMMECHO} + \text{NO}_2$

J45414: $\text{KDEC C}_5\text{CO}_2\text{HCHO} \rightarrow 0.83 \text{ MALANHY} + 0.83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$

J45415: $\text{KDEC TLFUO} \rightarrow \text{ACCOMMECHO} + \text{HO}_2$

J46400: $\text{KDEC PHENO} \rightarrow 0.71 \text{ MALDALCO}_2\text{H} + 0.71 \text{ GLYOX} + 0.29 \text{ PBZQONE} + \text{HO}_2$

J46403: $\text{KDEC NDNPHENO} \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2$

J46404: $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + 0.5 \text{ BZFUONE} + 0.5 \text{ BZFUONE}$

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: $\text{KDEC NNCATECO} \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$

J46415: $\text{KDEC NCATECO} \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{HO}_2$

J46416: $\text{KDEC PBZQO} \rightarrow \text{C}_5\text{CO}_2\text{OHCO}_3$

J46418: $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + 0.5 \text{ BZFUONE} + 0.5 \text{ BZFUONE}$

J46419: $\text{KDEC NBZQO} \rightarrow \text{C}_6\text{CO}_4\text{DB} + \text{NO}_2$

J46422: $\text{KDEC DNPHEO} \rightarrow \text{NC}_4\text{DCO}_2\text{H} + \text{HCOCO}_2\text{H} + \text{NO}_2$

J46425: $\text{KDEC BZEMUCO} \rightarrow 0.5 \text{ EPXC}_4\text{DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 + .5 \text{ C}_3\text{DIALO}_2 + .5 \text{ C}_3\text{OH}_2\text{CO}$

J46429: new channel

J47401: $\text{KROPRIM}^*\text{O}_2$ fast reaction $\text{C}_6\text{H}_5\text{CH}_2\text{O} = \text{BENZAL} + \text{HO}_2$

J47402: $\text{KROPRIM}^*\text{O}_2$ fast reaction $\text{C}_6\text{H}_5\text{CH}_2\text{O} = \text{BENZAL} + \text{HO}_2$

J47404: $\text{KDEC TLBIPERO} \rightarrow 0.6 \text{ GLYOX} + 0.4 \text{ MGLYOX} + \text{HO}_2 + 0.2 \text{ C}_4\text{MDIAL} + 0.2 \text{ C}_5\text{DICARB} + 0.2 \text{ TLFUONE} + 0.2 \text{ BZFUONE} + 0.2 \text{ MALDIAL}$

J47405: $\text{KDEC TLBIPERO} \rightarrow 0.6 \text{ GLYOX} + 0.4 \text{ MGLYOX} + \text{HO}_2 + 0.2 \text{ C}_4\text{MDIAL} + 0.2 \text{ C}_5\text{DICARB} + 0.2 \text{ TLFUONE} + 0.2 \text{ BZFUONE} + 0.2 \text{ MALDIAL}$

J47407: $\text{KDEC CRESO} \rightarrow 0.68 \text{ C}_5\text{CO}_2\text{HCHO} + 0.68 \text{ GLYOX} + \text{HO}_2 + 0.32 \text{ PTLQONE}$

J47408a: $\text{KDEC CRESO} \rightarrow 0.68 \text{ C}_5\text{CO}_2\text{HCHO} + 0.68 \text{ GLYOX} + \text{HO}_2 + 0.32 \text{ PTLQONE}$

J47408b: $\text{KDEC NCRESO} \rightarrow \text{C}_5\text{CO}_2\text{HCHO} + \text{GLYOX} + \text{NO}_2$

J47409: Using J for 3-methyl-2-nitrophenol.	J48400: KDEC STYRENO \rightarrow HO2 + HCHO + BEN-ZAL	PH4207b_a01: Quantum yields from Burkholder et al. (2015). HCOCH2O2 decomposes directly to .6 HCHO + .6 CO + .6 HO2 + .2 GLYOX + .2 HOCH2CHO
J47412: KDEC TLEMUCO \rightarrow 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2	J40203b: Substituted vinyl alcohol in analogy to CH3CHO photolysis.	PH4207c_a01: Quantum yields from Burkholder et al. (2015).
J47417: Using J for 3-methyl-2-nitrophenol.	J7301: The quantum yields are recommended by Burkholder et al. (2015) for $\lambda > 300\text{nm}$ and used here for the entire spectrum.	PH4211_a01: Assumed in analogy to the main channel for $j(\text{HOCH}_2\text{CHO})$.
J47418: new channel		
J47419: Using J for 3-methyl-2-nitrophenol.		
J47420: new channel	PH2100_a01: 2.33 times the gas-phase value	PH4300_a01: $2.33 * k$ from the gas-phase reaction, CH3CO directly reacts with O2 to form CH3CO3
J47422: KDEC NPTLQO \rightarrow C7CO4DB + NO2	PH3200_a01: Scaled to J(NO2) so that its lifetime is about 10.5 days, as suggested by Zellner et al. (1990).	PH4301_a01: $2.33 * k$ from the gas-phase reaction,
J47423: KDEC PTLQO \rightarrow C6CO2OHCO3	PH4200_a01: CH3CHOHO2 is assumed to directly decompose into CH3CHO + HO2	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
J47425: KDEC MNNCATECO \rightarrow NC4MDCO2H + HCOCO2H + NO2	PH4201_a01: COOHOO is not formed but directly dissociates into CO2 + HO2	
J47426: KDEC MNCATECO \rightarrow NC4MDCO2H + HCOCO2H + HO2	PH4202_a01: assumed to be the same as C2H5OOH + hv	
J47428: KDEC NDNCRESO \rightarrow NC4MDCO2H + HNO3 + CO + CO + NO2	PH4207a_a01: Quantum yields from Burkholder et al. (2015).	PH4303_a01: CH3CO reacts with O2 to form OH + HCHO + CO
J47429: KDEC DNCRESO \rightarrow NC4MDCO2H + HCOCO2H + NO2		

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*
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*
H320MSf_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow N_2O_5(aq)$	$k_{\text{exf}}(01, \text{ind}_{N2O5})$	see general notes*
H320MSb_a01	TrAa01MblScScmN	$N_2O_5(aq) \rightarrow N_2O_5$	$k_{\text{exb}}(01, \text{ind}_{N2O5})$	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	$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH300H})$	see general notes*
H41004b_a01	TrAa01ScScm	$\text{CH}_3\text{OOH}(\text{aq}) \rightarrow \text{CH}_3\text{OOH}$	$k_{\text{exb}}(01, \text{ind_CH300H})$	see general notes*
H41005f_a01	TrAa01Sc	$\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{OH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH30H})$	see general notes*
H41005b_a01	TrAa01Sc	$\text{CH}_3\text{OH}(\text{aq}) \rightarrow \text{CH}_3\text{OH}$	$k_{\text{exb}}(01, \text{ind_CH30H})$	see general notes*
H41006f_a01	TrAa01Sc	$\text{HOCH}_2\text{OH} \rightarrow \text{HOCH}_2\text{OH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH20H})$	see general notes*
H41006b_a01	TrAa01Sc	$\text{HOCH}_2\text{OH}(\text{aq}) \rightarrow \text{HOCH}_2\text{OH}$	$k_{\text{exb}}(01, \text{ind_HOCH20H})$	see general notes*
H41007f_a01	TrAa01Sc	$\text{HOCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH200H})$	see general notes*
H41007b_a01	TrAa01Sc	$\text{HOCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_HOCH200H})$	see general notes*
H41008f_a01	TrAa01Sc	$\text{CO} \rightarrow \text{CO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CO})$	see general notes*
H41008b_a01	TrAa01Sc	$\text{CO}(\text{aq}) \rightarrow \text{CO}$	$k_{\text{exb}}(01, \text{ind_CO})$	see general notes*
H41009MSf_a01	TrAa01ScN	$\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{ONO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3N03})$	see general notes*
H41010MSb_a01	TrAa01ScN	$\text{CH}_3\text{ONO}_2(\text{aq}) \rightarrow \text{CH}_3\text{ONO}_2$	$k_{\text{exb}}(01, \text{ind_CH3N03})$	see general notes*
H42000f_a01	TrAa01ScScmC	$\text{CH}_3\text{COOH} \rightarrow \text{CH}_3\text{COOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3C02H})$	see general notes*
H42000b_a01	TrAa01ScScmC	$\text{CH}_3\text{COOH}(\text{aq}) \rightarrow \text{CH}_3\text{COOH}$	$k_{\text{exb}}(01, \text{ind_CH3C02H})$	see general notes*
H42001f_a01	TrAa01ScC	$\text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{CHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3CHO})$	see general notes*
H42001b_a01	TrAa01ScC	$\text{CH}_3\text{CHO}(\text{aq}) \rightarrow \text{CH}_3\text{CHO}$	$k_{\text{exb}}(01, \text{ind_CH3CHO})$	see general notes*
H42002f_a01	TrAa01ScCN	$\text{PAN} \rightarrow \text{PAN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_PAN})$	see general notes*
H42002b_a01	TrAa01ScCN	$\text{PAN}(\text{aq}) \rightarrow \text{PAN}$	$k_{\text{exb}}(01, \text{ind_PAN})$	see general notes*
H42003f_a01	TrAa01ScC	$\text{C}_2\text{H}_5\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{OH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C2H50H})$	see general notes*
H42003b_a01	TrAa01ScC	$\text{CH}_3\text{CH}_2\text{OH}(\text{aq}) \rightarrow \text{C}_2\text{H}_5\text{OH}$	$k_{\text{exb}}(01, \text{ind_C2H50H})$	see general notes*
H42004f_a01	TrAa01ScC	$\text{ETHGLY} \rightarrow \text{ETHGLY}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ETHGLY})$	see general notes*
H42004b_a01	TrAa01ScC	$\text{ETHGLY}(\text{aq}) \rightarrow \text{ETHGLY}$	$k_{\text{exb}}(01, \text{ind_ETHGLY})$	see general notes*
H42006f_a01	TrAa01ScC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3C03})$	see general notes*
H42006b_a01	TrAa01ScC	$\text{CH}_3\text{COOO}(\text{aq}) \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$k_{\text{exb}}(01, \text{ind_CH3C03})$	see general notes*
H42007f_a01	TrAa01ScC	$\text{HOCH}_2\text{CHO} \rightarrow \text{CH}_2\text{OHCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH2CHO})$	see general notes*
H42007b_a01	TrAa01ScC	$\text{CH}_2\text{OHCHO}(\text{aq}) \rightarrow \text{HOCH}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HOCH2CHO})$	see general notes*
H42008f_a01	TrAa01ScC	$\text{GLYOX} \rightarrow \text{GLYOX}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_GLYOX})$	see general notes*
H42008b_a01	TrAa01ScC	$\text{GLYOX}(\text{aq}) \rightarrow \text{GLYOX}$	$k_{\text{exb}}(01, \text{ind_GLYOX})$	see general notes*
H42009f_a01	TrAa01ScC	$\text{CH}_3\text{C}(\text{O})\text{OOH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH3C03H})$	see general notes*
H42009b_a01	TrAa01ScC	$\text{CH}_3\text{C}(\text{O})\text{OOH}(\text{aq}) \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$k_{\text{exb}}(01, \text{ind_CH3C03H})$	see general notes*
H42010f_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_3\text{H} \rightarrow \text{HOCH}_2\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH2C03H})$	see general notes*
H42010b_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOCH2C03H})$	see general notes*
H42011f_a01	TrAa01ScC	$\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C2H500H})$	see general notes*
H42011b_a01	TrAa01ScC	$\text{C}_2\text{H}_5\text{OOH}(\text{aq}) \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$k_{\text{exb}}(01, \text{ind_C2H500H})$	see general notes*
H42012f_a01	TrAa01ScC	$\text{HOCCOOH} \rightarrow \text{HOCCOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_H00CC00H})$	see general notes*

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H42012b_a01	TrAa01ScC	$\text{HOOC}\text{COOH}(\text{aq}) \rightarrow \text{HOOC}\text{COOH}$	$k_{\text{exb}}(01, \text{ind_HOOC}\text{COOH})$	see general notes*
H42013f_a01	TrAa01ScC	$\text{HOOC}\text{H}_2\text{CO}_2\text{H} \rightarrow \text{HOOC}\text{H}_2\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOC}\text{H}_2\text{CO}_2\text{H})$	see general notes*
H42013b_a01	TrAa01ScC	$\text{HOOC}\text{H}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOOC}\text{H}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOOC}\text{H}_2\text{CO}_2\text{H})$	see general notes*
H42014f_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightarrow \text{HOCH}_2\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	see general notes*
H42014b_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{CO}_2\text{H})$	see general notes*
H42015f_a01	TrAa01ScC	$\text{HCOC}\text{O}_2\text{H} \rightarrow \text{CHOC}\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOC}\text{O}_2\text{H})$	see general notes*
H42015b_a01	TrAa01ScC	$\text{CHOC}\text{OOH}(\text{aq}) \rightarrow \text{HCOC}\text{O}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOC}\text{O}_2\text{H})$	see general notes*
H42017f_a01	TrAa01ScCN	$\text{C}_2\text{H}_5\text{ONO}_2 \rightarrow \text{C}_2\text{H}_5\text{ONO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_C}_2\text{H}_5\text{NO}_3)$	see general notes*
H42017b_a01	TrAa01ScCN	$\text{C}_2\text{H}_5\text{ONO}_2(\text{aq}) \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$k_{\text{exb}}(01, \text{ind_C}_2\text{H}_5\text{NO}_3)$	see general notes*
H42018f_a01	TrAa01ScCN	$\text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{CN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CN})$	see general notes*
H42018b_a01	TrAa01ScCN	$\text{CH}_3\text{CN}(\text{aq}) \rightarrow \text{CH}_3\text{CN}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CN})$	see general notes*
H42019f_a01	TrAa01ScC	$\text{HOCH}_2\text{CHOHOH} \rightarrow \text{CH}_2\text{OHCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{CHOHOH})$	see general notes*
H42019b_a01	TrAa01ScC	$\text{CH}_2\text{OHCHOHOH}(\text{aq}) \rightarrow \text{HOCH}_2\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{CHOHOH})$	see general notes*
H42020f_a01	TrAa01ScC	$\text{CH}_3\text{CHOHOH} \rightarrow \text{CH}_3\text{CHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHOHOH})$	see general notes*
H42020b_a01	TrAa01ScC	$\text{CH}_3\text{CHOHOH}(\text{aq}) \rightarrow \text{CH}_3\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHOHOH})$	see general notes*
H42021f_a01	TrAa01ScC	$\text{CHOHOHCOOH} \rightarrow \text{CHOOHOHCOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOHOHCOOH})$	see general notes*
H42021b_a01	TrAa01ScC	$\text{CHOOHOHCOOH}(\text{aq}) \rightarrow \text{CHOHOHCOOH}$	$k_{\text{exb}}(01, \text{ind_CHOHOHCOOH})$	see general notes*
H42022f_a01	TrAa01ScC	$\text{CHOHOHCHOHOH} \rightarrow \text{CHOHOHCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOHOHCHOHOH})$	see general notes*
H42022b_a01	TrAa01ScC	$\text{CHOHOHCHOHOH}(\text{aq}) \rightarrow \text{CHOHOHCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CHOHOHCHOHOH})$	see general notes*
H42023f_a01	TrAa01ScC	$\text{HOOC}\text{H}_2\text{CHO} \rightarrow \text{CH}_2\text{OOHCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOC}\text{H}_2\text{CHO})$	see general notes*
H42023b_a01	TrAa01ScC	$\text{CH}_2\text{OOHCHO}(\text{aq}) \rightarrow \text{HOOC}\text{H}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HOOC}\text{H}_2\text{CHO})$	see general notes*
H42024f_a01	TrAa01ScC	$\text{CHOCHOHOH} \rightarrow \text{CHOCHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CHOCHOHOH})$	see general notes*
H42024b_a01	TrAa01ScC	$\text{CHOCHOHOH}(\text{aq}) \rightarrow \text{CHOCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CHOCHOHOH})$	see general notes*
H42025f_a01	TrAa01ScC	$\text{HOOC}\text{H}_2\text{CHOHOH} \rightarrow \text{HOOC}\text{H}_2\text{CHOHOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOOC}\text{H}_2\text{CHOHOH})$	see general notes*
H42025b_a01	TrAa01ScC	$\text{HOOC}\text{H}_2\text{CHOHOH}(\text{aq}) \rightarrow \text{HOOC}\text{H}_2\text{CHOHOH}$	$k_{\text{exb}}(01, \text{ind_HOOC}\text{H}_2\text{CHOHOH})$	see general notes*
H42026f_a01	TrAa01ScC	$\text{CH}_2\text{CO} \rightarrow \text{CH}_2\text{CO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_2\text{CO})$	see general notes*
H42026b_a01	TrAa01ScC	$\text{CH}_2\text{CO}(\text{aq}) \rightarrow \text{CH}_2\text{CO}$	$k_{\text{exb}}(01, \text{ind_CH}_2\text{CO})$	see general notes*
H42027f_a01	TrAa01ScC	$\text{CH}_3\text{CHOHOOH} \rightarrow \text{CH}_3\text{CHOHOOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHOHOOH})$	see general notes*
H42027b_a01	TrAa01ScC	$\text{CH}_3\text{CHOHOOH}(\text{aq}) \rightarrow \text{CH}_3\text{CHOHOOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHOHOOH})$	see general notes*
H42028f_a01	TrAa01ScCN	$\text{ETHOHNO}_3 \rightarrow \text{ETHOHNO}_3(\text{aq})$	$k_{\text{exf}}(01, \text{ind_ETHOHNO}_3)$	see general notes*
H42028b_a01	TrAa01ScCN	$\text{ETHOHNO}_3(\text{aq}) \rightarrow \text{ETHOHNO}_3$	$k_{\text{exb}}(01, \text{ind_ETHOHNO}_3)$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H42029f_a01	TrAa01ScC	$\text{HCOCO}_3\text{H} \rightarrow \text{HCOCO}_3\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HCOCO}_3\text{H})$	see general notes*
H42029b_a01	TrAa01ScC	$\text{HCOCO}_3\text{H(aq)} \rightarrow \text{HCOCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCO}_3\text{H})$	see general notes*
H42030f_a01	TrAa01ScC	$\text{HOOCH}_2\text{CO}_3\text{H} \rightarrow \text{HOOCH}_2\text{CO}_3\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HOOCH}_2\text{CO}_3\text{H})$	see general notes*
H42030b_a01	TrAa01ScC	$\text{HOOCH}_2\text{CO}_3\text{H(aq)} \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOOCH}_2\text{CO}_3\text{H})$	see general notes*
H42031f_a01	TrAa01ScC	$\text{HYETHO}_2\text{H} \rightarrow \text{HYETHO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HYETHO}_2\text{H})$	see general notes*
H42031b_a01	TrAa01ScC	$\text{HYETHO}_2\text{H(aq)} \rightarrow \text{HYETHO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYETHO}_2\text{H})$	see general notes*
H42032f_a01	TrAa01ScCN	$\text{PHAN} \rightarrow \text{PHAN(aq)}$	$k_{\text{exf}}(01, \text{ind_PHAN})$	see general notes*
H42032b_a01	TrAa01ScCN	$\text{PHAN(aq)} \rightarrow \text{PHAN}$	$k_{\text{exb}}(01, \text{ind_PHAN})$	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	TrAa01ScC	$\text{MGLYOX} \rightarrow \text{CH}_3\text{C(O)CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_MGLYOX})$	see general notes*
H43001b_a01	TrAa01ScC	$\text{CH}_3\text{C(O)CHO(aq)} \rightarrow \text{MGLYOX}$	$k_{\text{exb}}(01, \text{ind_MGLYOX})$	see general notes*
H43002f_a01	TrAa01ScC	$\text{CH}_3\text{COCO}_2\text{H} \rightarrow \text{CH}_3\text{COCO}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCO}_2\text{H})$	see general notes*
H43002b_a01	TrAa01ScC	$\text{CH}_3\text{COCO}_2\text{H(aq)} \rightarrow \text{CH}_3\text{COCO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCO}_2\text{H})$	see general notes*
H43003f_a01	TrAa01ScC	$\text{CH}_3\text{COCHOHOH} \rightarrow \text{CH}_3\text{COCHOHOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCHOHOH})$	see general notes*
H43003b_a01	TrAa01ScC	$\text{CH}_3\text{COCHOHOH(aq)} \rightarrow \text{CH}_3\text{COCHOHOH}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCHOHOH})$	see general notes*
H43005f_a01	TrAa01ScC	$\text{IPROPOL} \rightarrow \text{IPROPOL(aq)}$	$k_{\text{exf}}(01, \text{ind_IPROPOL})$	see general notes*
H43005b_a01	TrAa01ScC	$\text{IPROPOL(aq)} \rightarrow \text{IPROPOL}$	$k_{\text{exb}}(01, \text{ind_IPROPOL})$	see general notes*
H43006f_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H(aq)}$	$k_{\text{exf}}(01, \text{ind_HYPERACET})$	see general notes*
H43006b_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H(aq)} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYPERACET})$	see general notes*
H43007f_a01	TrAa01ScC	$\text{iC}_3\text{H}_7\text{OOH} \rightarrow \text{iC}_3\text{H}_7\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_IC}_3\text{H}_7\text{OOH})$	see general notes*
H43007b_a01	TrAa01ScC	$\text{iC}_3\text{H}_7\text{OOH(aq)} \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$k_{\text{exb}}(01, \text{ind_IC}_3\text{H}_7\text{OOH})$	see general notes*
H43008f_a01	TrAa01ScC	$\text{HCOCOCH}_2\text{OOH} \rightarrow \text{HCOCOCH}_2\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_ALCOCH}_2\text{OOH})$	see general notes*
H43008b_a01	TrAa01ScC	$\text{HCOCOCH}_2\text{OOH(aq)} \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_ALCOCH}_2\text{OOH})$	see general notes*
H43009f_a01	TrAa01ScC	$\text{C}_3\text{OH13CO} \rightarrow \text{C}_3\text{OH13CO(aq)}$	$k_{\text{exf}}(01, \text{ind_C}_3\text{OH13CO})$	see general notes*
H43009b_a01	TrAa01ScC	$\text{C}_3\text{OH13CO(aq)} \rightarrow \text{C}_3\text{OH13CO}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{OH13CO})$	see general notes*
H43010f_a01	TrAa01ScC	$\text{HCOCOCHO} \rightarrow \text{HCOCOCHO(aq)}$	$k_{\text{exf}}(01, \text{ind_C}_3\text{CO})$	see general notes*
H43010b_a01	TrAa01ScC	$\text{HCOCOCHO(aq)} \rightarrow \text{HCOCOCHO}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{CO})$	see general notes*
H43011f_a01	TrAa01ScC	$\text{C}_3\text{DIALOOH} \rightarrow \text{C}_3\text{DIALOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C}_3\text{DIALOOH})$	see general notes*
H43011b_a01	TrAa01ScC	$\text{C}_3\text{DIALOOH(aq)} \rightarrow \text{C}_3\text{DIALOOH}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{DIALOOH})$	see general notes*
H43012f_a01	TrAa01ScCN	$\text{C}_3\text{PAN1} \rightarrow \text{C}_3\text{PAN1(aq)}$	$k_{\text{exf}}(01, \text{ind_C}_3\text{PAN1})$	see general notes*
H43012b_a01	TrAa01ScCN	$\text{C}_3\text{PAN1(aq)} \rightarrow \text{C}_3\text{PAN1}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{PAN1})$	see general notes*
H43013f_a01	TrAa01ScCN	$\text{C}_3\text{PAN2} \rightarrow \text{C}_3\text{PAN2(aq)}$	$k_{\text{exf}}(01, \text{ind_C}_3\text{PAN2})$	see general notes*
H43013b_a01	TrAa01ScCN	$\text{C}_3\text{PAN2(aq)} \rightarrow \text{C}_3\text{PAN2}$	$k_{\text{exb}}(01, \text{ind_C}_3\text{PAN2})$	see general notes*
H43014f_a01	TrAa01ScC	$\text{CH}_3\text{CHCO} \rightarrow \text{CH}_3\text{CHCO(aq)}$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{CHCO})$	see general notes*

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H43014b_a01	TrAa01ScC	$\text{CH}_3\text{CHCO}(\text{aq}) \rightarrow \text{CH}_3\text{CHCO}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{CHCO})$	see general notes*
H43015f_a01	TrAa01ScCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCH}_2\text{O}_2\text{N}_2)$	see general notes*
H43015b_a01	TrAa01ScCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2(\text{aq}) \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCH}_2\text{O}_2\text{N}_2)$	see general notes*
H43016f_a01	TrAa01ScC	$\text{CH}_3\text{COCO}_3\text{H} \rightarrow \text{CH}_3\text{COCO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_CH}_3\text{COCO}_3\text{H})$	see general notes*
H43016b_a01	TrAa01ScC	$\text{CH}_3\text{COCO}_3\text{H}(\text{aq}) \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_CH}_3\text{COCO}_3\text{H})$	see general notes*
H43017f_a01	TrAa01ScC	$\text{HCOCH}_2\text{CHO} \rightarrow \text{HCOCH}_2\text{CHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH}_2\text{CHO})$	see general notes*
H43017b_a01	TrAa01ScC	$\text{HCOCH}_2\text{CHO}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CHO}$	$k_{\text{exb}}(01, \text{ind_HCOCH}_2\text{CHO})$	see general notes*
H43018f_a01	TrAa01ScC	$\text{HCOCH}_2\text{CO}_2\text{H} \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH}_2\text{CO}_2\text{H})$	see general notes*
H43018b_a01	TrAa01ScC	$\text{HCOCH}_2\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCH}_2\text{CO}_2\text{H})$	see general notes*
H43019f_a01	TrAa01ScC	$\text{HCOCH}_2\text{CO}_3\text{H} \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCH}_2\text{CO}_3\text{H})$	see general notes*
H43019b_a01	TrAa01ScC	$\text{HCOCH}_2\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCH}_2\text{CO}_3\text{H})$	see general notes*
H43020f_a01	TrAa01ScC	$\text{HCOCOCH}_2\text{OOH} \rightarrow \text{HCOCOCH}_2\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOCH}_2\text{OOH})$	see general notes*
H43020b_a01	TrAa01ScC	$\text{HCOCOCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HCOCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_HCOCOCH}_2\text{OOH})$	see general notes*
H43021f_a01	TrAa01ScC	$\text{HCOCOHC}_3\text{O}_3\text{H} \rightarrow \text{HCOCOHC}_3\text{O}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOHC}_3\text{O}_3\text{H})$	see general notes*
H43021b_a01	TrAa01ScC	$\text{HCOCOHC}_3\text{O}_3\text{H}(\text{aq}) \rightarrow \text{HCOCOHC}_3\text{O}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HCOCOHC}_3\text{O}_3\text{H})$	see general notes*
H43022f_a01	TrAa01ScCN	$\text{HCOCOHPAN} \rightarrow \text{HCOCOHPAN}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HCOCOHPAN})$	see general notes*
H43022b_a01	TrAa01ScCN	$\text{HCOCOHPAN}(\text{aq}) \rightarrow \text{HCOCOHPAN}$	$k_{\text{exb}}(01, \text{ind_HCOCOHPAN})$	see general notes*
H43023f_a01	TrAa01ScC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOC}_2\text{H}_4\text{CO}_2\text{H})$	see general notes*
H43023b_a01	TrAa01ScC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H}(\text{aq}) \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HOC}_2\text{H}_4\text{CO}_2\text{H})$	see general notes*
H43024f_a01	TrAa01ScC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOC}_2\text{H}_4\text{CO}_3\text{H})$	see general notes*
H43024b_a01	TrAa01ScC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H}(\text{aq}) \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$k_{\text{exb}}(01, \text{ind_HOC}_2\text{H}_4\text{CO}_3\text{H})$	see general notes*
H43025f_a01	TrAa01ScC	$\text{HOCH}_2\text{COCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{COCH}_2\text{OOH})$	see general notes*
H43025b_a01	TrAa01ScC	$\text{HOCH}_2\text{COCH}_2\text{OOH}(\text{aq}) \rightarrow \text{HOCH}_2\text{COCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{COCH}_2\text{OOH})$	see general notes*
H43026f_a01	TrAa01ScC	$\text{HOCH}_2\text{COCHO} \rightarrow \text{HOCH}_2\text{COCHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HOCH}_2\text{COCHO})$	see general notes*
H43026b_a01	TrAa01ScC	$\text{HOCH}_2\text{COCHO}(\text{aq}) \rightarrow \text{HOCH}_2\text{COCHO}$	$k_{\text{exb}}(01, \text{ind_HOCH}_2\text{COCHO})$	see general notes*
H43027f_a01	TrAa01ScC	$\text{HYPROPO}_2\text{H} \rightarrow \text{HYPROPO}_2\text{H}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_HYPROPO}_2\text{H})$	see general notes*
H43027b_a01	TrAa01ScC	$\text{HYPROPO}_2\text{H}(\text{aq}) \rightarrow \text{HYPROPO}_2\text{H}$	$k_{\text{exb}}(01, \text{ind_HYPROPO}_2\text{H})$	see general notes*
H43028f_a01	TrAa01ScC	$\text{METACETHO} \rightarrow \text{METACETHO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_METACETHO})$	see general notes*
H43028b_a01	TrAa01ScC	$\text{METACETHO}(\text{aq}) \rightarrow \text{METACETHO}$	$k_{\text{exb}}(01, \text{ind_METACETHO})$	see general notes*
H43029f_a01	TrAa01ScCN	$\text{NOA} \rightarrow \text{NOA}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_NOA})$	see general notes*
H43029b_a01	TrAa01ScCN	$\text{NOA}(\text{aq}) \rightarrow \text{NOA}$	$k_{\text{exb}}(01, \text{ind_NOA})$	see general notes*

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H43030f_a01	TrAa01ScCN	$\text{PR2O2HNO3} \rightarrow \text{PR2O2HNO3(aq)}$	$k_{\text{exf}}(01, \text{ind_PR2O2HNO3})$	see general notes*
H43030b_a01	TrAa01ScCN	$\text{PR2O2HNO3(aq)} \rightarrow \text{PR2O2HNO3}$	$k_{\text{exb}}(01, \text{ind_PR2O2HNO3})$	see general notes*
H43031f_a01	TrAa01ScCN	$\text{PROPOLNO3} \rightarrow \text{PROPOLNO3(aq)}$	$k_{\text{exf}}(01, \text{ind_PROPOLNO3})$	see general notes*
H43031b_a01	TrAa01ScCN	$\text{PROPOLNO3(aq)} \rightarrow \text{PROPOLNO3}$	$k_{\text{exb}}(01, \text{ind_PROPOLNO3})$	see general notes*
H43032f_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_2\text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH(aq)}$	$k_{\text{exf}}(01, \text{ind_ACETOL})$	see general notes*
H43032b_a01	TrAa01ScC	$\text{CH}_3\text{COCH}_2\text{OH(aq)} \rightarrow \text{CH}_3\text{COCH}_2\text{OH}$	$k_{\text{exb}}(01, \text{ind_ACETOL})$	see general notes*
H44000f_a01	TrAa01ScC	$\text{MACR} \rightarrow \text{MACR(aq)}$	$k_{\text{exf}}(01, \text{ind_MACR})$	see general notes*
H44000b_a01	TrAa01ScC	$\text{MACR(aq)} \rightarrow \text{MACR}$	$k_{\text{exb}}(01, \text{ind_MACR})$	see general notes*
H44001f_a01	TrAa01ScC	$\text{MVK} \rightarrow \text{MVK(aq)}$	$k_{\text{exf}}(01, \text{ind_MVK})$	see general notes*
H44001b_a01	TrAa01ScC	$\text{MVK(aq)} \rightarrow \text{MVK}$	$k_{\text{exb}}(01, \text{ind_MVK})$	see general notes*
H44002f_a01	TrAa01ScC	$\text{CH}_3\text{COCOCH}_2\text{O}_2 \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2(\text{aq})$	$k_{\text{exf}}(01, \text{ind_BIACETO2})$	see general notes*
H44002b_a01	TrAa01ScC	$\text{CH}_3\text{COCOCH}_2\text{O}_2(\text{aq}) \rightarrow \text{CH}_3\text{COCOCH}_2\text{O}_2$	$k_{\text{exb}}(01, \text{ind_BIACETO2})$	see general notes*
H44003f_a01	TrAa01ScC	$\text{BIACETOH} \rightarrow \text{BIACETOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BIACETOH})$	see general notes*
H44003b_a01	TrAa01ScC	$\text{BIACETOH(aq)} \rightarrow \text{BIACETOH}$	$k_{\text{exb}}(01, \text{ind_BIACETOH})$	see general notes*
H44004f_a01	TrAa01ScC	$\text{CH}_3\text{COCOCH}_2\text{OOH} \rightarrow \text{CH}_3\text{COCOCH}_2\text{OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BIACETO0H})$	see general notes*
H44004b_a01	TrAa01ScC	$\text{CH}_3\text{COCOCH}_2\text{OOH(aq)} \rightarrow \text{CH}_3\text{COCOCH}_2\text{OOH}$	$k_{\text{exb}}(01, \text{ind_BIACETO0H})$	see general notes*
H44005f_a01	TrAa01ScC	$\text{BUT2OLO} \rightarrow \text{BUT2OLO(aq)}$	$k_{\text{exf}}(01, \text{ind_BUT2OLO})$	see general notes*
H44005b_a01	TrAa01ScC	$\text{BUT2OLO(aq)} \rightarrow \text{BUT2OLO}$	$k_{\text{exb}}(01, \text{ind_BUT2OLO})$	see general notes*
H44006f_a01	TrAa01ScC	$\text{BUT2OLOOH} \rightarrow \text{BUT2OLOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BUT2OLOOH})$	see general notes*
H44006b_a01	TrAa01ScC	$\text{BUT2OLOOH(aq)} \rightarrow \text{BUT2OLOOH}$	$k_{\text{exb}}(01, \text{ind_BUT2OLOOH})$	see general notes*
H44007f_a01	TrAa01ScC	$\text{BZFUCO} \rightarrow \text{BZFUCO(aq)}$	$k_{\text{exf}}(01, \text{ind_BZFUCO})$	see general notes*
H44007b_a01	TrAa01ScC	$\text{BZFUCO(aq)} \rightarrow \text{BZFUCO}$	$k_{\text{exb}}(01, \text{ind_BZFUCO})$	see general notes*
H44008f_a01	TrAa01ScC	$\text{BZFUOOH} \rightarrow \text{BZFUOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_BZFUOOH})$	see general notes*
H44008b_a01	TrAa01ScC	$\text{BZFUOOH(aq)} \rightarrow \text{BZFUOOH}$	$k_{\text{exb}}(01, \text{ind_BZFUOOH})$	see general notes*
H44009f_a01	TrAa01ScC	$\text{C312COCO3H} \rightarrow \text{C312COCO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_C312COCO3H})$	see general notes*
H44009b_a01	TrAa01ScC	$\text{C312COCO3H(aq)} \rightarrow \text{C312COCO3H}$	$k_{\text{exb}}(01, \text{ind_C312COCO3H})$	see general notes*
H44010f_a01	TrAa01ScCN	$\text{C312COPAN} \rightarrow \text{C312COPAN(aq)}$	$k_{\text{exf}}(01, \text{ind_C312COPAN})$	see general notes*
H44010b_a01	TrAa01ScCN	$\text{C312COPAN(aq)} \rightarrow \text{C312COPAN}$	$k_{\text{exb}}(01, \text{ind_C312COPAN})$	see general notes*
H44011f_a01	TrAa01ScC	$\text{C413COOOH} \rightarrow \text{C413COOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C413COOOH})$	see general notes*
H44011b_a01	TrAa01ScC	$\text{C413COOOH(aq)} \rightarrow \text{C413COOOH}$	$k_{\text{exb}}(01, \text{ind_C413COOOH})$	see general notes*
H44012f_a01	TrAa01ScC	$\text{C44OOH} \rightarrow \text{C44OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C44OOH})$	see general notes*
H44012b_a01	TrAa01ScC	$\text{C44OOH(aq)} \rightarrow \text{C44OOH}$	$k_{\text{exb}}(01, \text{ind_C44OOH})$	see general notes*
H44013f_a01	TrAa01ScC	$\text{C4CODIAL} \rightarrow \text{C4CODIAL(aq)}$	$k_{\text{exf}}(01, \text{ind_C4CODIAL})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H44013b_a01	TrAa01ScC	C4CODIAL(aq) \rightarrow C4CODIAL	k_exb(01,ind_C4CODIAL)	see general notes*
H44014f_a01	TrAa01ScCN	C4PAN5 \rightarrow C4PAN5(aq)	k_exf(01,ind_C4PAN5)	see general notes*
H44014b_a01	TrAa01ScCN	C4PAN5(aq) \rightarrow C4PAN5	k_exb(01,ind_C4PAN5)	see general notes*
H44015f_a01	TrAa01ScC	CH ₃ COCHCO \rightarrow CH ₃ COCHCO(aq)	k_exf(01,ind_CH3COCHCO)	see general notes*
H44015b_a01	TrAa01ScC	CH ₃ COCHCO(aq) \rightarrow CH ₃ COCHCO	k_exb(01,ind_CH3COCHCO)	see general notes*
H44016f_a01	TrAa01ScC	CH ₃ COCOCO ₂ H \rightarrow CH ₃ COCOCO ₂ H(aq)	k_exf(01,ind_CH3COCOCO2H)	see general notes*
H44016b_a01	TrAa01ScC	CH ₃ COCOCO ₂ H(aq) \rightarrow CH ₃ COCOCO ₂ H	k_exb(01,ind_CH3COCOCO2H)	see general notes*
H44017f_a01	TrAa01ScC	CH ₃ COOHCHCHO \rightarrow CH ₃ COOHCHCHO(aq)	k_exf(01,ind_CH3COOHCHCHO)	see general notes*
H44017b_a01	TrAa01ScC	CH ₃ COOHCHCHO(aq) \rightarrow CH ₃ COOHCHCHO	k_exb(01,ind_CH3COOHCHCHO)	see general notes*
H44018f_a01	TrAa01ScC	CHOC3COO ₂ \rightarrow CHOC3COO ₂ (aq)	k_exf(01,ind_CHOC3COO2)	see general notes*
H44018b_a01	TrAa01ScC	CHOC3COO ₂ (aq) \rightarrow CHOC3COO ₂	k_exb(01,ind_CHOC3COO2)	see general notes*
H44019f_a01	TrAa01ScC	CO14O3CHO \rightarrow CO14O3CHO(aq)	k_exf(01,ind_CO14O3CHO)	see general notes*
H44019b_a01	TrAa01ScC	CO14O3CHO(aq) \rightarrow CO14O3CHO	k_exb(01,ind_CO14O3CHO)	see general notes*
H44020f_a01	TrAa01ScC	CO14O3CO ₂ H \rightarrow CO14O3CO ₂ H(aq)	k_exf(01,ind_CO14O3CO2H)	see general notes*
H44020b_a01	TrAa01ScC	CO14O3CO ₂ H(aq) \rightarrow CO14O3CO ₂ H	k_exb(01,ind_CO14O3CO2H)	see general notes*
H44021f_a01	TrAa01ScC	CH ₃ COCOCHO \rightarrow CH ₃ COCOCHO(aq)	k_exf(01,ind_CO23C3CHO)	see general notes*
H44021b_a01	TrAa01ScC	CH ₃ COCOCHO(aq) \rightarrow CH ₃ COCOCHO	k_exb(01,ind_CO23C3CHO)	see general notes*
H44022f_a01	TrAa01ScC	CO ₂ C ₃ CHO \rightarrow CO ₂ C ₃ CHO(aq)	k_exf(01,ind_CO2C3CHO)	see general notes*
H44022b_a01	TrAa01ScC	CO ₂ C ₃ CHO(aq) \rightarrow CO ₂ C ₃ CHO	k_exb(01,ind_CO2C3CHO)	see general notes*
H44023f_a01	TrAa01ScC	CO ₂ C ₄ DIAL \rightarrow CO ₂ C ₄ DIAL(aq)	k_exf(01,ind_CO2C4DIAL)	see general notes*
H44023b_a01	TrAa01ScC	CO ₂ C ₄ DIAL(aq) \rightarrow CO ₂ C ₄ DIAL	k_exb(01,ind_CO2C4DIAL)	see general notes*
H44024f_a01	TrAa01ScC	CO ₂ H ₃ CHO \rightarrow CO ₂ H ₃ CHO(aq)	k_exf(01,ind_CO2H3CHO)	see general notes*
H44024b_a01	TrAa01ScC	CO ₂ H ₃ CHO(aq) \rightarrow CO ₂ H ₃ CHO	k_exb(01,ind_CO2H3CHO)	see general notes*
H44025f_a01	TrAa01ScC	CO ₂ H ₃ CO ₂ H \rightarrow CO ₂ H ₃ CO ₂ H(aq)	k_exf(01,ind_CO2H3CO2H)	see general notes*
H44025b_a01	TrAa01ScC	CO ₂ H ₃ CO ₂ H(aq) \rightarrow CO ₂ H ₃ CO ₂ H	k_exb(01,ind_CO2H3CO2H)	see general notes*
H44026f_a01	TrAa01ScC	CO ₂ H ₃ CO ₃ H \rightarrow CO ₂ H ₃ CO ₃ H(aq)	k_exf(01,ind_CO2H3CO3H)	see general notes*
H44026b_a01	TrAa01ScC	CO ₂ H ₃ CO ₃ H(aq) \rightarrow CO ₂ H ₃ CO ₃ H	k_exb(01,ind_CO2H3CO3H)	see general notes*
H44027f_a01	TrAa01ScC	EPXC ₄ DIAL \rightarrow EPXC ₄ DIAL(aq)	k_exf(01,ind_EPXC4DIAL)	see general notes*
H44027b_a01	TrAa01ScC	EPXC ₄ DIAL(aq) \rightarrow EPXC ₄ DIAL	k_exb(01,ind_EPXC4DIAL)	see general notes*
H44028f_a01	TrAa01ScC	EPXDLCO ₂ H \rightarrow EPXDLCO ₂ H(aq)	k_exf(01,ind_EPXDLCO2H)	see general notes*
H44028b_a01	TrAa01ScC	EPXDLCO ₂ H(aq) \rightarrow EPXDLCO ₂ H	k_exb(01,ind_EPXDLCO2H)	see general notes*
H44029f_a01	TrAa01ScC	EPXDLCO ₃ H \rightarrow EPXDLCO ₃ H(aq)	k_exf(01,ind_EPXDLCO3H)	see general notes*
H44029b_a01	TrAa01ScC	EPXDLCO ₃ H(aq) \rightarrow EPXDLCO ₃ H	k_exb(01,ind_EPXDLCO3H)	see general notes*

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H44030f_a01	TrAa01ScC	$\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCCH}_3\text{CHOOH(aq)}$	$\rightarrow \text{k_exf}(01, \text{ind_HCOCCH}_3\text{CHOOH})$	see general notes*
H44030b_a01	TrAa01ScC	$\text{HCOCCH}_3\text{CHOOH(aq)} \rightarrow \text{HCOCCH}_3\text{CHOOH}$	$\rightarrow \text{k_exb}(01, \text{ind_HCOCCH}_3\text{CHOOH})$	see general notes*
H44031f_a01	TrAa01ScC	$\text{HCOCCH}_3\text{CO} \rightarrow \text{HCOCCH}_3\text{CO(aq)}$	$\text{k_exf}(01, \text{ind_HCOCCH}_3\text{CO})$	see general notes*
H44031b_a01	TrAa01ScC	$\text{HCOCCH}_3\text{CO(aq)} \rightarrow \text{HCOCCH}_3\text{CO}$	$\text{k_exb}(01, \text{ind_HCOCCH}_3\text{CO})$	see general notes*
H44032f_a01	TrAa01ScC	$\text{HMAC} \rightarrow \text{HMAC(aq)}$	$\text{k_exf}(01, \text{ind_HMAC})$	see general notes*
H44032b_a01	TrAa01ScC	$\text{HMAC(aq)} \rightarrow \text{HMAC}$	$\text{k_exb}(01, \text{ind_HMAC})$	see general notes*
H44033f_a01	TrAa01ScC	$\text{HO12CO3C4} \rightarrow \text{HO12CO3C4(aq)}$	$\text{k_exf}(01, \text{ind_HO12CO3C4})$	see general notes*
H44033b_a01	TrAa01ScC	$\text{HO12CO3C4(aq)} \rightarrow \text{HO12CO3C4}$	$\text{k_exb}(01, \text{ind_HO12CO3C4})$	see general notes*
H44034f_a01	TrAa01ScC	$\text{HOCOC4DIAL} \rightarrow \text{HOCOC4DIAL(aq)}$	$\text{k_exf}(01, \text{ind_HOCOC4DIAL})$	see general notes*
H44034b_a01	TrAa01ScC	$\text{HOCOC4DIAL(aq)} \rightarrow \text{HOCOC4DIAL}$	$\text{k_exb}(01, \text{ind_HOCOC4DIAL})$	see general notes*
H44035f_a01	TrAa01ScC	$\text{HVMK} \rightarrow \text{HVMK(aq)}$	$\text{k_exf}(01, \text{ind_HVMK})$	see general notes*
H44035b_a01	TrAa01ScC	$\text{HVMK(aq)} \rightarrow \text{HVMK}$	$\text{k_exb}(01, \text{ind_HVMK})$	see general notes*
H44036f_a01	TrAa01ScC	$\text{IBUTALOH} \rightarrow \text{IBUTALOH(aq)}$	$\text{k_exf}(01, \text{ind_IBUTALOH})$	see general notes*
H44036b_a01	TrAa01ScC	$\text{IBUTALOH(aq)} \rightarrow \text{IBUTALOH}$	$\text{k_exb}(01, \text{ind_IBUTALOH})$	see general notes*
H44037f_a01	TrAa01ScC	$\text{IBUTDIAL} \rightarrow \text{IBUTDIAL(aq)}$	$\text{k_exf}(01, \text{ind_IBUTDIAL})$	see general notes*
H44037b_a01	TrAa01ScC	$\text{IBUTDIAL(aq)} \rightarrow \text{IBUTDIAL}$	$\text{k_exb}(01, \text{ind_IBUTDIAL})$	see general notes*
H44038f_a01	TrAa01ScC	$\text{IBUTOLBOOH} \rightarrow \text{IBUTOLBOOH(aq)}$	$\text{k_exf}(01, \text{ind_IBUTOLBOOH})$	see general notes*
H44038b_a01	TrAa01ScC	$\text{IBUTOLBOOH(aq)} \rightarrow \text{IBUTOLBOOH}$	$\text{k_exb}(01, \text{ind_IBUTOLBOOH})$	see general notes*
H44039f_a01	TrAa01ScC	$\text{IPRHOCO2H} \rightarrow \text{IPRHOCO2H(aq)}$	$\text{k_exf}(01, \text{ind_IPRHOCO2H})$	see general notes*
H44039b_a01	TrAa01ScC	$\text{IPRHOCO2H(aq)} \rightarrow \text{IPRHOCO2H}$	$\text{k_exb}(01, \text{ind_IPRHOCO2H})$	see general notes*
H44040f_a01	TrAa01ScC	$\text{IPRHOCO3H} \rightarrow \text{IPRHOCO3H(aq)}$	$\text{k_exf}(01, \text{ind_IPRHOCO3H})$	see general notes*
H44040b_a01	TrAa01ScC	$\text{IPRHOCO3H(aq)} \rightarrow \text{IPRHOCO3H}$	$\text{k_exb}(01, \text{ind_IPRHOCO3H})$	see general notes*
H44041f_a01	TrAa01ScC	$\text{LBUT1ENOOH} \rightarrow \text{LBUT1ENOOH(aq)}$	$\text{k_exf}(01, \text{ind_LBUT1ENOOH})$	see general notes*
H44041b_a01	TrAa01ScC	$\text{LBUT1ENOOH(aq)} \rightarrow \text{LBUT1ENOOH}$	$\text{k_exb}(01, \text{ind_LBUT1ENOOH})$	see general notes*
H44042f_a01	TrAa01ScC	$\text{LHMKABOOH} \rightarrow \text{LHMKABOOH(aq)}$	$\text{k_exf}(01, \text{ind_LHMKABOOH})$	see general notes*
H44042b_a01	TrAa01ScC	$\text{LHMKABOOH(aq)} \rightarrow \text{LHMKABOOH}$	$\text{k_exb}(01, \text{ind_LHMKABOOH})$	see general notes*
H44043f_a01	TrAa01ScC	$\text{LMEKOOH} \rightarrow \text{LMEKOOH(aq)}$	$\text{k_exf}(01, \text{ind_LMEKOOH})$	see general notes*
H44043b_a01	TrAa01ScC	$\text{LMEKOOH(aq)} \rightarrow \text{LMEKOOH}$	$\text{k_exb}(01, \text{ind_LMEKOOH})$	see general notes*
H44044f_a01	TrAa01ScC	$\text{MACO2H} \rightarrow \text{MACO2H(aq)}$	$\text{k_exf}(01, \text{ind_MACO2H})$	see general notes*
H44044b_a01	TrAa01ScC	$\text{MACO2H(aq)} \rightarrow \text{MACO2H}$	$\text{k_exb}(01, \text{ind_MACO2H})$	see general notes*
H44045f_a01	TrAa01ScC	$\text{MACO3H} \rightarrow \text{MACO3H(aq)}$	$\text{k_exf}(01, \text{ind_MACO3H})$	see general notes*
H44045b_a01	TrAa01ScC	$\text{MACO3H(aq)} \rightarrow \text{MACO3H}$	$\text{k_exb}(01, \text{ind_MACO3H})$	see general notes*
H44046f_a01	TrAa01ScC	$\text{MACROH} \rightarrow \text{MACROH(aq)}$	$\text{k_exf}(01, \text{ind_MACROH})$	see general notes*

Table 3: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H44046b_a01	TrAa01ScC	MACROH(aq) \rightarrow MACROH	k_exb(01,ind_MACROH)	see general notes*
H44047f_a01	TrAa01ScC	MACROOH \rightarrow MACROOH(aq)	k_exf(01,ind_MACROOH)	see general notes*
H44047b_a01	TrAa01ScC	MACROOH(aq) \rightarrow MACROOH	k_exb(01,ind_MACROOH)	see general notes*
H44048f_a01	TrAa01ScC	MALANHYOOH \rightarrow MALANHYOOH(aq)	k_exf(01,ind_MALANHYOOH)	see general notes*
H44048b_a01	TrAa01ScC	MALANHYOOH(aq) \rightarrow MALANHYOOH	k_exb(01,ind_MALANHYOOH)	see general notes*
H44049f_a01	TrAa01ScC	MALDALCO2H \rightarrow MALDALCO2H(aq)	k_exf(01,ind_MALDALCO2H)	see general notes*
H44049b_a01	TrAa01ScC	MALDALCO2H(aq) \rightarrow MALDALCO2H	k_exb(01,ind_MALDALCO2H)	see general notes*
H44050f_a01	TrAa01ScC	MALDALCO3H \rightarrow MALDALCO3H(aq)	k_exf(01,ind_MALDALCO3H)	see general notes*
H44050b_a01	TrAa01ScC	MALDALCO3H(aq) \rightarrow MALDALCO3H	k_exb(01,ind_MALDALCO3H)	see general notes*
H44051f_a01	TrAa01ScC	MALDIAL \rightarrow MALDIAL(aq)	k_exf(01,ind_MALDIAL)	see general notes*
H44051b_a01	TrAa01ScC	MALDIAL(aq) \rightarrow MALDIAL	k_exb(01,ind_MALDIAL)	see general notes*
H44052f_a01	TrAa01ScC	MALDIALOOH \rightarrow MALDIALOOH(aq)	k_exf(01,ind_MALDIALOOH)	see general notes*
H44052b_a01	TrAa01ScC	MALDIALOOH(aq) \rightarrow MALDIALOOH	k_exb(01,ind_MALDIALOOH)	see general notes*
H44053f_a01	TrAa01ScC	MALNHYOHCO \rightarrow MALNHYOHCO(aq)	k_exf(01,ind_MALNHYOHCO)	see general notes*
H44053b_a01	TrAa01ScC	MALNHYOHCO(aq) \rightarrow MALNHYOHCO	k_exb(01,ind_MALNHYOHCO)	see general notes*
H44054f_a01	TrAa01ScC	MECOACEOOH \rightarrow MECOACEOOH(aq)	k_exf(01,ind_MECOACEOOH)	see general notes*
H44054b_a01	TrAa01ScC	MECOACEOOH(aq) \rightarrow MECOACEOOH	k_exb(01,ind_MECOACEOOH)	see general notes*
H44055f_a01	TrAa01ScCN	MVKNO3 \rightarrow MVKNO3(aq)	k_exf(01,ind_MVKNO3)	see general notes*
H44055b_a01	TrAa01ScCN	MVKNO3(aq) \rightarrow MVKNO3	k_exb(01,ind_MVKNO3)	see general notes*
H44056f_a01	TrAa01ScCN	NBZFUOOH \rightarrow NBZFUOOH(aq)	k_exf(01,ind_NBZFUOOH)	see general notes*
H44056b_a01	TrAa01ScCN	NBZFUOOH(aq) \rightarrow NBZFUOOH	k_exb(01,ind_NBZFUOOH)	see general notes*
H44057f_a01	TrAa01ScCN	NC4DCO2H \rightarrow NC4DCO2H(aq)	k_exf(01,ind_NC4DCO2H)	see general notes*
H44057b_a01	TrAa01ScCN	NC4DCO2H(aq) \rightarrow NC4DCO2H	k_exb(01,ind_NC4DCO2H)	see general notes*
H45000f_a01	TrAa01ScC	ACCOMMECHO \rightarrow ACCOMMECHO(aq)	k_exf(01,ind_ACCOMMECHO)	see general notes*
H45000b_a01	TrAa01ScC	ACCOMMECHO(aq) \rightarrow ACCOMMECHO	k_exb(01,ind_ACCOMMECHO)	see general notes*
H45001f_a01	TrAa01ScC	ACCOMMECO3H \rightarrow ACCOMMECO3H(aq)	k_exf(01,ind_ACCOMMECO3H)	see general notes*
H45001b_a01	TrAa01ScC	ACCOMMECO3H(aq) \rightarrow ACCOMMECO3H	k_exb(01,ind_ACCOMMECO3H)	see general notes*
H45002f_a01	TrAa01ScC	C1ODC2O2C4OOH \rightarrow C1ODC2O2C4OOH(aq)	k_exf(01,ind_C1ODC2O2C4OOH)	see general notes*
H45002b_a01	TrAa01ScC	C1ODC2O2C4OOH(aq) \rightarrow C1ODC2O2C4OOH	k_exb(01,ind_C1ODC2O2C4OOH)	see general notes*
H45003f_a01	TrAa01ScC	C1ODC2OOHC4OD \rightarrow C1ODC2OOHC4OD(aq)	k_exf(01,ind_C1ODC2OOHC4OD)	see general notes*
H45003b_a01	TrAa01ScC	C1ODC2OOHC4OD(aq) \rightarrow C1ODC2OOHC4OD	k_exb(01,ind_C1ODC2OOHC4OD)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45004f_a01	TrAa01ScC	C10DC3O2C4OOH C10DC3O2C4OOH(aq)	→ k_exf(01, ind_C10DC3O2C4OOH)	see general notes*
H45004b_a01	TrAa01ScC	C10DC3O2C4OOH(aq) C10DC3O2C4OOH	→ k_exb(01, ind_C10DC3O2C4OOH)	see general notes*
H45005f_a01	TrAa01ScC	C10OHC2OOHC4OD C10OHC2OOHC4OD(aq)	→ k_exf(01, ind_C10OHC2OOHC4OD)	see general notes*
H45005b_a01	TrAa01ScC	C10OHC2OOHC4OD(aq) C10OHC2OOHC4OD	→ k_exb(01, ind_C10OHC2OOHC4OD)	see general notes*
H45006f_a01	TrAa01ScC	C24O3CCO2H → C24O3CCO2H(aq)	k_exf(01, ind_C24O3CCO2H)	see general notes*
H45006b_a01	TrAa01ScC	C24O3CCO2H(aq) → C24O3CCO2H	k_exb(01, ind_C24O3CCO2H)	see general notes*
H45007f_a01	TrAa01ScC	C4CO2DBCO3 → C4CO2DBCO3(aq)	k_exf(01, ind_C4CO2DBCO3)	see general notes*
H45007b_a01	TrAa01ScC	C4CO2DBCO3(aq) → C4CO2DBCO3	k_exb(01, ind_C4CO2DBCO3)	see general notes*
H45008f_a01	TrAa01ScCN	C4CO2DBPAN → C4CO2DBPAN(aq)	k_exf(01, ind_C4CO2DBPAN)	see general notes*
H45008b_a01	TrAa01ScCN	C4CO2DBPAN(aq) → C4CO2DBPAN	k_exb(01, ind_C4CO2DBPAN)	see general notes*
H45009f_a01	TrAa01ScC	C4CO2DCO3H → C4CO2DCO3H(aq)	k_exf(01, ind_C4CO2DCO3H)	see general notes*
H45009b_a01	TrAa01ScC	C4CO2DCO3H(aq) → C4CO2DCO3H	k_exb(01, ind_C4CO2DCO3H)	see general notes*
H45010f_a01	TrAa01ScCN	C4MCONO3OH → C4MCONO3OH(aq)	k_exf(01, ind_C4MCONO3OH)	see general notes*
H45010b_a01	TrAa01ScCN	C4MCONO3OH(aq) → C4MCONO3OH	k_exb(01, ind_C4MCONO3OH)	see general notes*
H45011f_a01	TrAa01ScC	C511OOH → C511OOH(aq)	k_exf(01, ind_C511OOH)	see general notes*
H45011b_a01	TrAa01ScC	C511OOH(aq) → C511OOH	k_exb(01, ind_C511OOH)	see general notes*
H45012f_a01	TrAa01ScC	C512OOH → C512OOH(aq)	k_exf(01, ind_C512OOH)	see general notes*
H45012b_a01	TrAa01ScC	C512OOH(aq) → C512OOH	k_exb(01, ind_C512OOH)	see general notes*
H45013f_a01	TrAa01ScC	C5134CO2OH → C5134CO2OH(aq)	k_exf(01, ind_C5134CO2OH)	see general notes*
H45013b_a01	TrAa01ScC	C5134CO2OH(aq) → C5134CO2OH	k_exb(01, ind_C5134CO2OH)	see general notes*
H45014f_a01	TrAa01ScC	C513CO → C513CO(aq)	k_exf(01, ind_C513CO)	see general notes*
H45014b_a01	TrAa01ScC	C513CO(aq) → C513CO	k_exb(01, ind_C513CO)	see general notes*
H45015f_a01	TrAa01ScC	C513OOH → C513OOH(aq)	k_exf(01, ind_C513OOH)	see general notes*
H45015b_a01	TrAa01ScC	C513OOH(aq) → C513OOH	k_exb(01, ind_C513OOH)	see general notes*
H45016f_a01	TrAa01ScCN	C514NO3 → C514NO3(aq)	k_exf(01, ind_C514NO3)	see general notes*
H45016b_a01	TrAa01ScCN	C514NO3(aq) → C514NO3	k_exb(01, ind_C514NO3)	see general notes*
H45017f_a01	TrAa01ScC	C514OOH → C514OOH(aq)	k_exf(01, ind_C514OOH)	see general notes*
H45017b_a01	TrAa01ScC	C514OOH(aq) → C514OOH	k_exb(01, ind_C514OOH)	see general notes*
H45018f_a01	TrAa01ScC	C54CO → C54CO(aq)	k_exf(01, ind_C54CO)	see general notes*
H45018b_a01	TrAa01ScC	C54CO(aq) → C54CO	k_exb(01, ind_C54CO)	see general notes*
H45019f_a01	TrAa01ScC	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	TrAa01ScC	C59OOH(aq) \rightarrow C59OOH	k_exb(01,ind_C59OOH)	see general notes*
H45020f_a01	TrAa01ScC	C5CO14OH \rightarrow C5CO14OH(aq)	k_exf(01,ind_C5CO14OH)	see general notes*
H45020b_a01	TrAa01ScC	C5CO14OH(aq) \rightarrow C5CO14OH	k_exb(01,ind_C5CO14OH)	see general notes*
H45021f_a01	TrAa01ScC	C5CO14OOH \rightarrow C5CO14OOH(aq)	k_exf(01,ind_C5CO14OOH)	see general notes*
H45021b_a01	TrAa01ScC	C5CO14OOH(aq) \rightarrow C5CO14OOH	k_exb(01,ind_C5CO14OOH)	see general notes*
H45022f_a01	TrAa01ScC	C5DIALCO \rightarrow C5DIALCO(aq)	k_exf(01,ind_C5DIALCO)	see general notes*
H45022b_a01	TrAa01ScC	C5DIALCO(aq) \rightarrow C5DIALCO	k_exb(01,ind_C5DIALCO)	see general notes*
H45023f_a01	TrAa01ScC	C5DIALOOH \rightarrow C5DIALOOH(aq)	k_exf(01,ind_C5DIALOOH)	see general notes*
H45023b_a01	TrAa01ScC	C5DIALOOH(aq) \rightarrow C5DIALOOH	k_exb(01,ind_C5DIALOOH)	see general notes*
H45024f_a01	TrAa01ScC	C5DICARB \rightarrow C5DICARB(aq)	k_exf(01,ind_C5DICARB)	see general notes*
H45024b_a01	TrAa01ScC	C5DICARB(aq) \rightarrow C5DICARB	k_exb(01,ind_C5DICARB)	see general notes*
H45025f_a01	TrAa01ScC	C5DICAROOH \rightarrow C5DICAROOH(aq)	k_exf(01,ind_C5DICAROOH)	see general notes*
H45025b_a01	TrAa01ScC	C5DICAROOH(aq) \rightarrow C5DICAROOH	k_exb(01,ind_C5DICAROOH)	see general notes*
H45026f_a01	TrAa01ScCN	C5PAN9 \rightarrow C5PAN9(aq)	k_exf(01,ind_C5PAN9)	see general notes*
H45026b_a01	TrAa01ScCN	C5PAN9(aq) \rightarrow C5PAN9	k_exb(01,ind_C5PAN9)	see general notes*
H45027f_a01	TrAa01ScC	CHOC3COOOH \rightarrow CHOC3COOOH(aq)	k_exf(01,ind_CHOC3COOOH)	see general notes*
H45027b_a01	TrAa01ScC	CHOC3COOOH(aq) \rightarrow CHOC3COOOH	k_exb(01,ind_CHOC3COOOH)	see general notes*
H45028f_a01	TrAa01ScCN	CHOC3COPAN \rightarrow CHOC3COPAN(aq)	k_exf(01,ind_CHOC3COPAN)	see general notes*
H45028b_a01	TrAa01ScCN	CHOC3COPAN(aq) \rightarrow CHOC3COPAN	k_exb(01,ind_CHOC3COPAN)	see general notes*
H45029f_a01	TrAa01ScC	CO13C4CHO \rightarrow CO13C4CHO(aq)	k_exf(01,ind_CO13C4CHO)	see general notes*
H45029b_a01	TrAa01ScC	CO13C4CHO(aq) \rightarrow CO13C4CHO	k_exb(01,ind_CO13C4CHO)	see general notes*
H45030f_a01	TrAa01ScC	CO23C4CHO \rightarrow CO23C4CHO(aq)	k_exf(01,ind_CO23C4CHO)	see general notes*
H45030b_a01	TrAa01ScC	CO23C4CHO(aq) \rightarrow CO23C4CHO	k_exb(01,ind_CO23C4CHO)	see general notes*
H45031f_a01	TrAa01ScC	CO23C4CO3H \rightarrow CO23C4CO3H(aq)	k_exf(01,ind_CO23C4CO3H)	see general notes*
H45031b_a01	TrAa01ScC	CO23C4CO3H(aq) \rightarrow CO23C4CO3H	k_exb(01,ind_CO23C4CO3H)	see general notes*
H45032f_a01	TrAa01ScCN	DB1NO3 \rightarrow DB1NO3(aq)	k_exf(01,ind_DB1NO3)	see general notes*
H45032b_a01	TrAa01ScCN	DB1NO3(aq) \rightarrow DB1NO3	k_exb(01,ind_DB1NO3)	see general notes*
H45033f_a01	TrAa01ScC	DB1OOH \rightarrow DB1OOH(aq)	k_exf(01,ind_DB1OOH)	see general notes*
H45033b_a01	TrAa01ScC	DB1OOH(aq) \rightarrow DB1OOH	k_exb(01,ind_DB1OOH)	see general notes*
H45034f_a01	TrAa01ScC	DB2OOH \rightarrow DB2OOH(aq)	k_exf(01,ind_DB2OOH)	see general notes*
H45034b_a01	TrAa01ScC	DB2OOH(aq) \rightarrow DB2OOH	k_exb(01,ind_DB2OOH)	see general notes*
H45035f_a01	TrAa01ScC	ISOPA OH \rightarrow ISOPA OH(aq)	k_exf(01,ind_ISOPA OH)	see general notes*
H45035b_a01	TrAa01ScC	ISOPA OH(aq) \rightarrow ISOPA OH	k_exb(01,ind_ISOPA OH)	see general notes*
H45036f_a01	TrAa01ScCN	ISOPBNO3 \rightarrow ISOPBNO3(aq)	k_exf(01,ind_ISOPBNO3)	see general notes*
H45036b_a01	TrAa01ScCN	ISOPBNO3(aq) \rightarrow ISOPBNO3	k_exb(01,ind_ISOPBNO3)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H45037f_a01	TrAa01ScC	ISOPBOH \rightarrow ISOPBOH(aq)	k_exf(01,ind_ISOPBOH)	see general notes*
H45037b_a01	TrAa01ScC	ISOPBOH(aq) \rightarrow ISOPBOH	k_exb(01,ind_ISOPBOH)	see general notes*
H45038f_a01	TrAa01ScC	ISOPBOOH \rightarrow ISOPBOOH(aq)	k_exf(01,ind_ISOPBOOH)	see general notes*
H45038b_a01	TrAa01ScC	ISOPBOOH(aq) \rightarrow ISOPBOOH	k_exb(01,ind_ISOPBOOH)	see general notes*
H45039f_a01	TrAa01ScCN	ISOPDNO3 \rightarrow ISOPDNO3(aq)	k_exf(01,ind_ISOPDNO3)	see general notes*
H45039b_a01	TrAa01ScCN	ISOPDNO3(aq) \rightarrow ISOPDNO3	k_exb(01,ind_ISOPDNO3)	see general notes*
H45040f_a01	TrAa01ScC	ISOPDOH \rightarrow ISOPDOH(aq)	k_exf(01,ind_ISOPDOH)	see general notes*
H45040b_a01	TrAa01ScC	ISOPDOH(aq) \rightarrow ISOPDOH	k_exb(01,ind_ISOPDOH)	see general notes*
H45041f_a01	TrAa01ScC	ISOPDOOH \rightarrow ISOPDOOH(aq)	k_exf(01,ind_ISOPDOOH)	see general notes*
H45041b_a01	TrAa01ScC	ISOPDOOH(aq) \rightarrow ISOPDOOH	k_exb(01,ind_ISOPDOOH)	see general notes*
H45042f_a01	TrAa01ScC	LC578OOH \rightarrow LC578OOH(aq)	k_exf(01,ind_LC578OOH)	see general notes*
H45042b_a01	TrAa01ScC	LC578OOH(aq) \rightarrow LC578OOH	k_exb(01,ind_LC578OOH)	see general notes*
H45043f_a01	TrAa01ScCN	LC5PAN1719 \rightarrow LC5PAN1719(aq)	k_exf(01,ind_LC5PAN1719)	see general notes*
H45043b_a01	TrAa01ScCN	LC5PAN1719(aq) \rightarrow LC5PAN1719	k_exb(01,ind_LC5PAN1719)	see general notes*
H45044f_a01	TrAa01ScC	LHC4ACCHO \rightarrow LHC4ACCHO(aq)	k_exf(01,ind_LHC4ACCHO)	see general notes*
H45044b_a01	TrAa01ScC	LHC4ACCHO(aq) \rightarrow LHC4ACCHO	k_exb(01,ind_LHC4ACCHO)	see general notes*
H45045f_a01	TrAa01ScC	LHC4ACCO2H \rightarrow LHC4ACCO2H(aq)	k_exf(01,ind_LHC4ACCO2H)	see general notes*
H45045b_a01	TrAa01ScC	LHC4ACCO2H(aq) \rightarrow LHC4ACCO2H	k_exb(01,ind_LHC4ACCO2H)	see general notes*
H45046f_a01	TrAa01ScC	LHC4ACCO3H \rightarrow LHC4ACCO3H(aq)	k_exf(01,ind_LHC4ACCO3H)	see general notes*
H45046b_a01	TrAa01ScC	LHC4ACCO3H(aq) \rightarrow LHC4ACCO3H	k_exb(01,ind_LHC4ACCO3H)	see general notes*
H45047f_a01	TrAa01ScC	LIEPOX \rightarrow LIEPOX(aq)	k_exf(01,ind_LIEPOX)	see general notes*
H45047b_a01	TrAa01ScC	LIEPOX(aq) \rightarrow LIEPOX	k_exb(01,ind_LIEPOX)	see general notes*
H45048f_a01	TrAa01ScCN	LISOPACNO3 \rightarrow LISOPACNO3(aq)	k_exf(01,ind_LISOPACNO3)	see general notes*
H45048b_a01	TrAa01ScCN	LISOPACNO3(aq) \rightarrow LISOPACNO3	k_exb(01,ind_LISOPACNO3)	see general notes*
H45049f_a01	TrAa01ScC	LISOPACOOH \rightarrow LISOPACOOH(aq)	k_exf(01,ind_LISOPACOOH)	see general notes*
H45049b_a01	TrAa01ScC	LISOPACOOH(aq) \rightarrow LISOPACOOH	k_exb(01,ind_LISOPACOOH)	see general notes*
H45050f_a01	TrAa01ScCN	LMBOABNO3 \rightarrow LMBOABNO3(aq)	k_exf(01,ind_LMBOABNO3)	see general notes*
H45050b_a01	TrAa01ScCN	LMBOABNO3(aq) \rightarrow LMBOABNO3	k_exb(01,ind_LMBOABNO3)	see general notes*
H45051f_a01	TrAa01ScC	LMBOABOOH \rightarrow LMBOABOOH(aq)	k_exf(01,ind_LMBOABOOH)	see general notes*
H45051b_a01	TrAa01ScC	LMBOABOOH(aq) \rightarrow LMBOABOOH	k_exb(01,ind_LMBOABOOH)	see general notes*
H45052f_a01	TrAa01ScCN	LNMBOABOOH \rightarrow LNMBOABOOH(aq)	k_exf(01,ind_LNMBOABOOH)	see general notes*
H45052b_a01	TrAa01ScCN	LNMBOABOOH(aq) \rightarrow LNMBOABOOH	k_exb(01,ind_LNMBOABOOH)	see general notes*
H45053f_a01	TrAa01ScC	MBO \rightarrow MBO(aq)	k_exf(01,ind_MBO)	see general notes*
H45053b_a01	TrAa01ScC	MBO(aq) \rightarrow MBO	k_exb(01,ind_MBO)	see general notes*
H45054f_a01	TrAa01ScC	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	TrAa01ScC	MBOACO(aq) \rightarrow MBOACO	k_exb(01,ind_MBOACO)	see general notes*
H45055f_a01	TrAa01ScC	MBOCOCO \rightarrow MBOCOCO(aq)	k_exf(01,ind_MBOCOCO)	see general notes*
H45055b_a01	TrAa01ScC	MBOCOCO(aq) \rightarrow MBOCOCO	k_exb(01,ind_MBOCOCO)	see general notes*
H45056f_a01	TrAa01ScC	MC3ODBCO2H \rightarrow MC3ODBCO2H(aq)	k_exf(01,ind_MC3ODBCO2H)	see general notes*
H45056b_a01	TrAa01ScC	MC3ODBCO2H(aq) \rightarrow MC3ODBCO2H	k_exb(01,ind_MC3ODBCO2H)	see general notes*
H45057f_a01	TrAa01ScC	3METHYLFURAN \rightarrow 3METHYLFURAN(aq)	k_exf(01,ind_ME3FURAN)	see general notes*
H45057b_a01	TrAa01ScC	3METHYLFURAN(aq) \rightarrow 3METHYLFURAN	k_exb(01,ind_ME3FURAN)	see general notes*
H45058f_a01	TrAa01ScC	MMALNHYOOH \rightarrow MMALNHYOOH(aq)	k_exf(01,ind_MMALNHYOOH)	see general notes*
H45058b_a01	TrAa01ScC	MMALNHYOOH(aq) \rightarrow MMALNHYOOH	k_exb(01,ind_MMALNHYOOH)	see general notes*
H45059f_a01	TrAa01ScCN	NC4MDCO2HN \rightarrow NC4MDCO2HN(aq)	k_exf(01,ind_NC4MDCO2H)	see general notes*
H45059b_a01	TrAa01ScCN	NC4MDCO2HN(aq) \rightarrow NC4MDCO2HN	k_exb(01,ind_NC4MDCO2H)	see general notes*
H45060f_a01	TrAa01ScCN	NC4OHCO3H \rightarrow NC4OHCO3H(aq)	k_exf(01,ind_NC4OHCO3H)	see general notes*
H45060b_a01	TrAa01ScCN	NC4OHCO3H(aq) \rightarrow NC4OHCO3H	k_exb(01,ind_NC4OHCO3H)	see general notes*
H45061f_a01	TrAa01ScCN	NC4OHCPAN \rightarrow NC4OHCPAN(aq)	k_exf(01,ind_NC4OHCPAN)	see general notes*
H45061b_a01	TrAa01ScCN	NC4OHCPAN(aq) \rightarrow NC4OHCPAN	k_exb(01,ind_NC4OHCPAN)	see general notes*
H45062f_a01	TrAa01ScCN	NISOPOOH \rightarrow NISOPOOH(aq)	k_exf(01,ind_NISOPOOH)	see general notes*
H45062b_a01	TrAa01ScCN	NISOPOOH(aq) \rightarrow NISOPOOH	k_exb(01,ind_NISOPOOH)	see general notes*
H45063f_a01	TrAa01ScCN	NMBOBCO \rightarrow NMBOBCO(aq)	k_exf(01,ind_NMBOBCO)	see general notes*
H45063b_a01	TrAa01ScCN	NMBOBCO(aq) \rightarrow NMBOBCO	k_exb(01,ind_NMBOBCO)	see general notes*
H45064f_a01	TrAa01ScCN	NTLFUOOH \rightarrow NTLFUOOH(aq)	k_exf(01,ind_NTLFUOOH)	see general notes*
H45064b_a01	TrAa01ScCN	NTLFUOOH(aq) \rightarrow NTLFUOOH	k_exb(01,ind_NTLFUOOH)	see general notes*
H45065f_a01	TrAa01ScC	TLFUOOH \rightarrow TLFUOOH(aq)	k_exf(01,ind_TLFUOOH)	see general notes*
H45065b_a01	TrAa01ScC	TLFUOOH(aq) \rightarrow TLFUOOH	k_exb(01,ind_TLFUOOH)	see general notes*
H45066f_a01	TrAa01ScC	LZCO3HC23DBCOD \rightarrow LZCO3HC23DBCOD(aq)	k_exf(01,ind_LZCO3HC23DBCOD)	see general notes*
H45066b_a01	TrAa01ScC	LZCO3HC23DBCOD(aq) \rightarrow LZCO3HC23DBCOD	k_exb(01,ind_LZCO3HC23DBCOD)	see general notes*
H45067f_a01	TrAa01ScC	C4MDIAL \rightarrow C4MDIAL(aq)	k_exf(01,ind_C4MDIAL)	see general notes*
H45067b_a01	TrAa01ScC	C4MDIAL(aq) \rightarrow C4MDIAL	k_exb(01,ind_C4MDIAL)	see general notes*
H46000f_a01	TrAa01ScCN	BZBIPERNO3 \rightarrow BZBIPERNO3(aq)	k_exf(01,ind_BZBIPERNO3)	see general notes*
H46000b_a01	TrAa01ScCN	BZBIPERNO3(aq) \rightarrow BZBIPERNO3	k_exb(01,ind_BZBIPERNO3)	see general notes*
H46001f_a01	TrAa01ScC	BZBIPEROOH \rightarrow BZBIPEROOH(aq)	k_exf(01,ind_BZBIPEROOH)	see general notes*
H46001b_a01	TrAa01ScC	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	TrAa01ScC	BZEMUCCO \rightarrow BZEMUCCO(aq)	k_exf(01,ind_BZEMUCCO)	see general notes*
H46002b_a01	TrAa01ScC	BZEMUCCO(aq) \rightarrow BZEMUCCO	k_exb(01,ind_BZEMUCCO)	see general notes*
H46003f_a01	TrAa01ScC	BZEMUCCO2H \rightarrow BZEMUCCO2H(aq)	k_exf(01,ind_BZEMUCCO2H)	see general notes*
H46003b_a01	TrAa01ScC	BZEMUCCO2H(aq) \rightarrow BZEMUCCO2H	k_exb(01,ind_BZEMUCCO2H)	see general notes*
H46004f_a01	TrAa01ScC	BZEMUCCO3H \rightarrow BZEMUCCO3H(aq)	k_exf(01,ind_BZEMUCCO3H)	see general notes*
H46004b_a01	TrAa01ScC	BZEMUCCO3H(aq) \rightarrow BZEMUCCO3H	k_exb(01,ind_BZEMUCCO3H)	see general notes*
H46005f_a01	TrAa01ScCN	BZEMUCNO3 \rightarrow BZEMUCNO3(aq)	k_exf(01,ind_BZEMUCNO3)	see general notes*
H46005b_a01	TrAa01ScCN	BZEMUCNO3(aq) \rightarrow BZEMUCNO3	k_exb(01,ind_BZEMUCNO3)	see general notes*
H46006f_a01	TrAa01ScC	BZEMUCOOH \rightarrow BZEMUCOOH(aq)	k_exf(01,ind_BZEMUCOOH)	see general notes*
H46006b_a01	TrAa01ScC	BZEMUCOOH(aq) \rightarrow BZEMUCOOH	k_exb(01,ind_BZEMUCOOH)	see general notes*
H46007f_a01	TrAa01ScC	BZEPOXMUC \rightarrow BZEPOXMUC(aq)	k_exf(01,ind_BZEPOXMUC)	see general notes*
H46007b_a01	TrAa01ScC	BZEPOXMUC(aq) \rightarrow BZEPOXMUC	k_exb(01,ind_BZEPOXMUC)	see general notes*
H46008f_a01	TrAa01ScC	BZOBIPEROH \rightarrow BZOBIPEROH(aq)	k_exf(01,ind_BZOBIPEROH)	see general notes*
H46008b_a01	TrAa01ScC	BZOBIPEROH(aq) \rightarrow BZOBIPEROH	k_exb(01,ind_BZOBIPEROH)	see general notes*
H46009f_a01	TrAa01ScCN	C5CO2DBPAN \rightarrow C5CO2DBPAN(aq)	k_exf(01,ind_C5CO2DBPAN)	see general notes*
H46009b_a01	TrAa01ScCN	C5CO2DBPAN(aq) \rightarrow C5CO2DBPAN	k_exb(01,ind_C5CO2DBPAN)	see general notes*
H46010f_a01	TrAa01ScC	C5CO2DCO3H \rightarrow C5CO2DCO3H(aq)	k_exf(01,ind_C5CO2DCO3H)	see general notes*
H46010b_a01	TrAa01ScC	C5CO2DCO3H(aq) \rightarrow C5CO2DCO3H	k_exb(01,ind_C5CO2DCO3H)	see general notes*
H46011f_a01	TrAa01ScCN	C5CO2OHPAN \rightarrow C5CO2OHPAN(aq)	k_exf(01,ind_C5CO2OHPAN)	see general notes*
H46011b_a01	TrAa01ScCN	C5CO2OHPAN(aq) \rightarrow C5CO2OHPAN	k_exb(01,ind_C5CO2OHPAN)	see general notes*
H46012f_a01	TrAa01ScC	C5COOHCO3H \rightarrow C5COOHCO3H(aq)	k_exf(01,ind_C5COOHCO3H)	see general notes*
H46012b_a01	TrAa01ScC	C5COOHCO3H(aq) \rightarrow C5COOHCO3H	k_exb(01,ind_C5COOHCO3H)	see general notes*
H46013f_a01	TrAa01ScC	C6125CO \rightarrow C6125CO(aq)	k_exf(01,ind_C6125CO)	see general notes*
H46013b_a01	TrAa01ScC	C6125CO(aq) \rightarrow C6125CO	k_exb(01,ind_C6125CO)	see general notes*
H46014f_a01	TrAa01ScC	C614CO \rightarrow C614CO(aq)	k_exf(01,ind_C614CO)	see general notes*
H46014b_a01	TrAa01ScC	C614CO(aq) \rightarrow C614CO	k_exb(01,ind_C614CO)	see general notes*
H46015f_a01	TrAa01ScCN	C614NO3 \rightarrow C614NO3(aq)	k_exf(01,ind_C614NO3)	see general notes*
H46015b_a01	TrAa01ScCN	C614NO3(aq) \rightarrow C614NO3	k_exb(01,ind_C614NO3)	see general notes*
H46016f_a01	TrAa01ScC	C614OOH \rightarrow C614OOH(aq)	k_exf(01,ind_C614OOH)	see general notes*
H46016b_a01	TrAa01ScC	C614OOH(aq) \rightarrow C614OOH	k_exb(01,ind_C614OOH)	see general notes*
H46017f_a01	TrAa01ScC	C615CO2OOH \rightarrow C615CO2OOH(aq)	k_exf(01,ind_C615CO2OOH)	see general notes*
H46017b_a01	TrAa01ScC	C615CO2OOH(aq) \rightarrow C615CO2OOH	k_exb(01,ind_C615CO2OOH)	see general notes*
H46018f_a01	TrAa01ScC	C6CO4DB \rightarrow C6CO4DB(aq)	k_exf(01,ind_C6CO4DB)	see general notes*
H46018b_a01	TrAa01ScC	C6CO4DB(aq) \rightarrow C6CO4DB	k_exb(01,ind_C6CO4DB)	see general notes*
H46019f_a01	TrAa01ScC	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	TrAa01ScC	$\text{C6H5O(aq)} \rightarrow \text{C6H5O}$	$k_{\text{exb}}(01, \text{ind_C6H5O})$	see general notes*
H46020f_a01	TrAa01ScC	$\text{C6H5OOH} \rightarrow \text{C6H5OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C6H5OOH})$	see general notes*
H46020b_a01	TrAa01ScC	$\text{C6H5OOH(aq)} \rightarrow \text{C6H5OOH}$	$k_{\text{exb}}(01, \text{ind_C6H5OOH})$	see general notes*
H46021f_a01	TrAa01ScC	$\text{CATEC1O} \rightarrow \text{CATEC1O(aq)}$	$k_{\text{exf}}(01, \text{ind_CATEC1O})$	see general notes*
H46021b_a01	TrAa01ScC	$\text{CATEC1O(aq)} \rightarrow \text{CATEC1O}$	$k_{\text{exb}}(01, \text{ind_CATEC1O})$	see general notes*
H46022f_a01	TrAa01ScC	$\text{CATEC1OOH} \rightarrow \text{CATEC1OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CATEC1OOH})$	see general notes*
H46022b_a01	TrAa01ScC	$\text{CATEC1OOH(aq)} \rightarrow \text{CATEC1OOH}$	$k_{\text{exb}}(01, \text{ind_CATEC1OOH})$	see general notes*
H46023f_a01	TrAa01ScC	$\text{CATECHOL} \rightarrow \text{CATECHOL(aq)}$	$k_{\text{exf}}(01, \text{ind_CATECHOL})$	see general notes*
H46023b_a01	TrAa01ScC	$\text{CATECHOL(aq)} \rightarrow \text{CATECHOL}$	$k_{\text{exb}}(01, \text{ind_CATECHOL})$	see general notes*
H46024f_a01	TrAa01ScC	$\text{CO235C5CHO} \rightarrow \text{CO235C5CHO(aq)}$	$k_{\text{exf}}(01, \text{ind_CO235C5CHO})$	see general notes*
H46024b_a01	TrAa01ScC	$\text{CO235C5CHO(aq)} \rightarrow \text{CO235C5CHO}$	$k_{\text{exb}}(01, \text{ind_CO235C5CHO})$	see general notes*
H46025f_a01	TrAa01ScC	$\text{CO235C6OOH} \rightarrow \text{CO235C6OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_CO235C6OOH})$	see general notes*
H46025b_a01	TrAa01ScC	$\text{CO235C6OOH(aq)} \rightarrow \text{CO235C6OOH}$	$k_{\text{exb}}(01, \text{ind_CO235C6OOH})$	see general notes*
H46026f_a01	TrAa01ScCN	$\text{DNPHEN} \rightarrow \text{DNPHEN(aq)}$	$k_{\text{exf}}(01, \text{ind_DNPHEN})$	see general notes*
H46026b_a01	TrAa01ScCN	$\text{DNPHEN(aq)} \rightarrow \text{DNPHEN}$	$k_{\text{exb}}(01, \text{ind_DNPHEN})$	see general notes*
H46027f_a01	TrAa01ScCN	$\text{DNPHENOOH} \rightarrow \text{DNPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_DNPHENOOH})$	see general notes*
H46027b_a01	TrAa01ScCN	$\text{DNPHENOOH(aq)} \rightarrow \text{DNPHENOOH}$	$k_{\text{exb}}(01, \text{ind_DNPHENOOH})$	see general notes*
H46028f_a01	TrAa01ScCN	$\text{NBZQOOH} \rightarrow \text{NBZQOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NBZQOOH})$	see general notes*
H46028b_a01	TrAa01ScCN	$\text{NBZQOOH(aq)} \rightarrow \text{NBZQOOH}$	$k_{\text{exb}}(01, \text{ind_NBZQOOH})$	see general notes*
H46029f_a01	TrAa01ScCN	$\text{NCATECHOL} \rightarrow \text{NCATECHOL(aq)}$	$k_{\text{exf}}(01, \text{ind_NCATECHOL})$	see general notes*
H46029b_a01	TrAa01ScCN	$\text{NCATECHOL(aq)} \rightarrow \text{NCATECHOL}$	$k_{\text{exb}}(01, \text{ind_NCATECHOL})$	see general notes*
H46030f_a01	TrAa01ScCN	$\text{NCATECOOH} \rightarrow \text{NCATECOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NCATECOOH})$	see general notes*
H46030b_a01	TrAa01ScCN	$\text{NCATECOOH(aq)} \rightarrow \text{NCATECOOH}$	$k_{\text{exb}}(01, \text{ind_NCATECOOH})$	see general notes*
H46031f_a01	TrAa01ScCN	$\text{NDNPHENOOH} \rightarrow \text{NDNPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NDNPHENOOH})$	see general notes*
H46031b_a01	TrAa01ScCN	$\text{NDNPHENOOH(aq)} \rightarrow \text{NDNPHENOOH}$	$k_{\text{exb}}(01, \text{ind_NDNPHENOOH})$	see general notes*
H46032f_a01	TrAa01ScCN	$\text{NNCATECOOH} \rightarrow \text{NNCATECOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NNCATECOOH})$	see general notes*
H46032b_a01	TrAa01ScCN	$\text{NNCATECOOH(aq)} \rightarrow \text{NNCATECOOH}$	$k_{\text{exb}}(01, \text{ind_NNCATECOOH})$	see general notes*
H46033f_a01	TrAa01ScCN	$\text{NPHENOOH} \rightarrow \text{NPHENOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NPHENOOH})$	see general notes*
H46033b_a01	TrAa01ScCN	$\text{NPHENOOH(aq)} \rightarrow \text{NPHENOOH}$	$k_{\text{exb}}(01, \text{ind_NPHENOOH})$	see general notes*
H46034f_a01	TrAa01ScC	$\text{PBZQCO} \rightarrow \text{PBZQCO(aq)}$	$k_{\text{exf}}(01, \text{ind_PBZQCO})$	see general notes*
H46034b_a01	TrAa01ScC	$\text{PBZQCO(aq)} \rightarrow \text{PBZQCO}$	$k_{\text{exb}}(01, \text{ind_PBZQCO})$	see general notes*
H46035f_a01	TrAa01ScC	$\text{PBZQOOH} \rightarrow \text{PBZQOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_PBZQOOH})$	see general notes*
H46035b_a01	TrAa01ScC	$\text{PBZQOOH(aq)} \rightarrow \text{PBZQOOH}$	$k_{\text{exb}}(01, \text{ind_PBZQOOH})$	see general notes*
H46036f_a01	TrAa01ScC	$\text{PHENOL} \rightarrow \text{PHENOL(aq)}$	$k_{\text{exf}}(01, \text{ind_PHENOL})$	see general notes*
H46036b_a01	TrAa01ScC	$\text{PHENOL(aq)} \rightarrow \text{PHENOL}$	$k_{\text{exb}}(01, \text{ind_PHENOL})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H46037f_a01	TrAa01ScC	PHENOOH \rightarrow PHENOOH(aq)	k_exf(01,ind_PHENOOH)	see general notes*
H46037b_a01	TrAa01ScC	PHENOOH(aq) \rightarrow PHENOOH	k_exb(01,ind_PHENOOH)	see general notes*
H460MSf_a01	TrAa01ScCN	HOC6H4NO2 \rightarrow HOC6H4NO2(aq)	k_exf(01,ind_HOC6H4NO2)	see general notes*
H461MSb_a01	TrAa01ScCN	HOC6H4NO2(aq) \rightarrow HOC6H4NO2	k_exb(01,ind_HOC6H4NO2)	see general notes*
H47000f_a01	TrAa01ScC	C235C6CO3H \rightarrow C235C6CO3H(aq)	k_exf(01,ind_C235C6CO3H)	see general notes*
H47000b_a01	TrAa01ScC	C235C6CO3H(aq) \rightarrow C235C6CO3H	k_exb(01,ind_C235C6CO3H)	see general notes*
H47001f_a01	TrAa01ScCN	C6CO2OHPAN \rightarrow C6CO2OHPAN(aq)	k_exf(01,ind_C6CO2OHPAN)	see general notes*
H47001b_a01	TrAa01ScCN	C6CO2OHPAN(aq) \rightarrow C6CO2OHPAN	k_exb(01,ind_C6CO2OHPAN)	see general notes*
H47002f_a01	TrAa01ScC	C6COOHCO3H \rightarrow C6COOHCO3H(aq)	k_exf(01,ind_C6COOHCO3H)	see general notes*
H47002b_a01	TrAa01ScC	C6COOHCO3H(aq) \rightarrow C6COOHCO3H	k_exb(01,ind_C6COOHCO3H)	see general notes*
H47003f_a01	TrAa01ScC	C6H5CH2OOH \rightarrow C6H5CH2OOH(aq)	k_exf(01,ind_C6H5CH2OOH)	see general notes*
H47003b_a01	TrAa01ScC	C6H5CH2OOH(aq) \rightarrow C6H5CH2OOH	k_exb(01,ind_C6H5CH2OOH)	see general notes*
H47004f_a01	TrAa01ScC	C6H5CO3H \rightarrow C6H5CO3H(aq)	k_exf(01,ind_C6H5CO3H)	see general notes*
H47004b_a01	TrAa01ScC	C6H5CO3H(aq) \rightarrow C6H5CO3H	k_exb(01,ind_C6H5CO3H)	see general notes*
H47005f_a01	TrAa01ScC	C716OOH \rightarrow C716OOH(aq)	k_exf(01,ind_C716OOH)	see general notes*
H47005b_a01	TrAa01ScC	C716OOH(aq) \rightarrow C716OOH	k_exb(01,ind_C716OOH)	see general notes*
H47006f_a01	TrAa01ScC	C721OOH \rightarrow C721OOH(aq)	k_exf(01,ind_C721OOH)	see general notes*
H47006b_a01	TrAa01ScC	C721OOH(aq) \rightarrow C721OOH	k_exb(01,ind_C721OOH)	see general notes*
H47007f_a01	TrAa01ScC	C722OOH \rightarrow C722OOH(aq)	k_exf(01,ind_C722OOH)	see general notes*
H47007b_a01	TrAa01ScC	C722OOH(aq) \rightarrow C722OOH	k_exb(01,ind_C722OOH)	see general notes*
H47008f_a01	TrAa01ScC	C7CO4DB \rightarrow C7CO4DB(aq)	k_exf(01,ind_C7CO4DB)	see general notes*
H47008b_a01	TrAa01ScC	C7CO4DB(aq) \rightarrow C7CO4DB	k_exb(01,ind_C7CO4DB)	see general notes*
H47009f_a01	TrAa01ScCN	C7PAN3 \rightarrow C7PAN3(aq)	k_exf(01,ind_C7PAN3)	see general notes*
H47009b_a01	TrAa01ScCN	C7PAN3(aq) \rightarrow C7PAN3	k_exb(01,ind_C7PAN3)	see general notes*
H47010f_a01	TrAa01ScC	CO235C6CHO \rightarrow CO235C6CHO(aq)	k_exf(01,ind_CO235C6CHO)	see general notes*
H47010b_a01	TrAa01ScC	CO235C6CHO(aq) \rightarrow CO235C6CHO	k_exb(01,ind_CO235C6CHO)	see general notes*
H47011f_a01	TrAa01ScC	CRESOL \rightarrow CRESOL(aq)	k_exf(01,ind_CRESOL)	see general notes*
H47011b_a01	TrAa01ScC	CRESOL(aq) \rightarrow CRESOL	k_exb(01,ind_CRESOL)	see general notes*
H47012f_a01	TrAa01ScC	CRESOOH \rightarrow CRESOOH(aq)	k_exf(01,ind_CRESOOH)	see general notes*
H47012b_a01	TrAa01ScC	CRESOOH(aq) \rightarrow CRESOOH	k_exb(01,ind_CRESOOH)	see general notes*
H47013f_a01	TrAa01ScCN	DNCRES \rightarrow DNCRES(aq)	k_exf(01,ind_DNCRES)	see general notes*
H47013b_a01	TrAa01ScCN	DNCRES(aq) \rightarrow DNCRES	k_exb(01,ind_DNCRES)	see general notes*
H47014f_a01	TrAa01ScCN	DNCRESOOH \rightarrow DNCRESOOH(aq)	k_exf(01,ind_DNCRESOOH)	see general notes*
H47014b_a01	TrAa01ScCN	DNCRESOOH(aq) \rightarrow DNCRESOOH	k_exb(01,ind_DNCRESOOH)	see general notes*
H47015f_a01	TrAa01ScC	MCATEC1O \rightarrow MCATEC1O(aq)	k_exf(01,ind_MCATEC1O)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H47015b_a01	TrAa01ScC	MCATEC1O(aq) \rightarrow MCATEC1O	k_exb(01,ind_MCATEC1O)	see general notes*
H47016f_a01	TrAa01ScC	MCATEC1OOH \rightarrow MCATEC1OOH(aq)	k_exf(01,ind_MCATEC1OOH)	see general notes*
H47016b_a01	TrAa01ScC	MCATEC1OOH(aq) \rightarrow MCATEC1OOH	k_exb(01,ind_MCATEC1OOH)	see general notes*
H47017f_a01	TrAa01ScC	MCATECHOL \rightarrow MCATECHOL(aq)	k_exf(01,ind_MCATECHOL)	see general notes*
H47017b_a01	TrAa01ScC	MCATECHOL(aq) \rightarrow MCATECHOL	k_exb(01,ind_MCATECHOL)	see general notes*
H47018f_a01	TrAa01ScCN	MNCATECH \rightarrow MNCATECH(aq)	k_exf(01,ind_MNCATECH)	see general notes*
H47018b_a01	TrAa01ScCN	MNCATECH(aq) \rightarrow MNCATECH	k_exb(01,ind_MNCATECH)	see general notes*
H47019f_a01	TrAa01ScCN	MNCATECOOH \rightarrow MNCATECOOH(aq)	k_exf(01,ind_MNCATECOOH)	see general notes*
H47019b_a01	TrAa01ScCN	MNCATECOOH(aq) \rightarrow MNCATECOOH	k_exb(01,ind_MNCATECOOH)	see general notes*
H47020f_a01	TrAa01ScCN	MNNCATCOOH \rightarrow MNNCATCOOH(aq)	k_exf(01,ind_MNNCATCOOH)	see general notes*
H47020b_a01	TrAa01ScCN	MNNCATCOOH(aq) \rightarrow MNNCATCOOH	k_exb(01,ind_MNNCATCOOH)	see general notes*
H47021f_a01	TrAa01ScCN	NCRESOOH \rightarrow NCRESOOH(aq)	k_exf(01,ind_NCRESOOH)	see general notes*
H47021b_a01	TrAa01ScCN	NCRESOOH(aq) \rightarrow NCRESOOH	k_exb(01,ind_NCRESOOH)	see general notes*
H47022f_a01	TrAa01ScCN	NDNCRESOOH \rightarrow NDNCRESOOH(aq)	k_exf(01,ind_NDNCRESOOH)	see general notes*
H47022b_a01	TrAa01ScCN	NDNCRESOOH(aq) \rightarrow NDNCRESOOH	k_exb(01,ind_NDNCRESOOH)	see general notes*
H47023f_a01	TrAa01ScC	OXYL1OOH \rightarrow OXYL1OOH(aq)	k_exf(01,ind_OXYL1OOH)	see general notes*
H47023b_a01	TrAa01ScC	OXYL1OOH(aq) \rightarrow OXYL1OOH	k_exb(01,ind_OXYL1OOH)	see general notes*
H47024f_a01	TrAa01ScC	PHCOOH \rightarrow PHCOOH(aq)	k_exf(01,ind_PHCOOH)	see general notes*
H47024b_a01	TrAa01ScC	PHCOOH(aq) \rightarrow PHCOOH	k_exb(01,ind_PHCOOH)	see general notes*
H47025f_a01	TrAa01ScC	TLBIPEROOH \rightarrow TLBIPEROOH(aq)	k_exf(01,ind_TLBIPEROOH)	see general notes*
H47025b_a01	TrAa01ScC	TLBIPEROOH(aq) \rightarrow TLBIPEROOH	k_exb(01,ind_TLBIPEROOH)	see general notes*
H47026f_a01	TrAa01ScC	TLEMUCCO \rightarrow TLEMUCCO(aq)	k_exf(01,ind_TLEMUCCO)	see general notes*
H47026b_a01	TrAa01ScC	TLEMUCCO(aq) \rightarrow TLEMUCCO	k_exb(01,ind_TLEMUCCO)	see general notes*
H47027f_a01	TrAa01ScC	TLEMUCCO2H \rightarrow TLEMUCCO2H(aq)	k_exf(01,ind_TLEMUCCO2H)	see general notes*
H47027b_a01	TrAa01ScC	TLEMUCCO2H(aq) \rightarrow TLEMUCCO2H	k_exb(01,ind_TLEMUCCO2H)	see general notes*
H47028f_a01	TrAa01ScC	TLEMUCCO3H \rightarrow TLEMUCCO3H(aq)	k_exf(01,ind_TLEMUCCO3H)	see general notes*
H47028b_a01	TrAa01ScC	TLEMUCCO3H(aq) \rightarrow TLEMUCCO3H	k_exb(01,ind_TLEMUCCO3H)	see general notes*
H47029f_a01	TrAa01ScCN	TLEMUCNO3 \rightarrow TLEMUCNO3(aq)	k_exf(01,ind_TLEMUCNO3)	see general notes*
H47029b_a01	TrAa01ScCN	TLEMUCNO3(aq) \rightarrow TLEMUCNO3	k_exb(01,ind_TLEMUCNO3)	see general notes*
H47030f_a01	TrAa01ScC	TLEMUCOOH \rightarrow TLEMUCOOH(aq)	k_exf(01,ind_TLEMUCOOH)	see general notes*
H47030b_a01	TrAa01ScC	TLEMUCOOH(aq) \rightarrow TLEMUCOOH	k_exb(01,ind_TLEMUCOOH)	see general notes*
H47031f_a01	TrAa01ScC	TLOBIPEROH \rightarrow TLOBIPEROH(aq)	k_exf(01,ind_TLOBIPEROH)	see general notes*
H47031b_a01	TrAa01ScC	TLOBIPEROH(aq) \rightarrow TLOBIPEROH	k_exb(01,ind_TLOBIPEROH)	see general notes*
H47032f_a01	TrAa01ScC	TOL1O \rightarrow TOL1O(aq)	k_exf(01,ind_TOL1O)	see general notes*
H47032b_a01	TrAa01ScC	TOL1O(aq) \rightarrow TOL1O	k_exb(01,ind_TOL1O)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H48000f_a01	TrAa01ScC	C721CHO → C721CHO(aq)	k_exf(01,ind_C721CHO)	see general notes*
H48000b_a01	TrAa01ScC	C721CHO(aq) → C721CHO	k_exb(01,ind_C721CHO)	see general notes*
H48001f_a01	TrAa01ScC	C721CO3H → C721CO3H(aq)	k_exf(01,ind_C721CO3H)	see general notes*
H48001b_a01	TrAa01ScC	C721CO3H(aq) → C721CO3H	k_exb(01,ind_C721CO3H)	see general notes*
H48002f_a01	TrAa01ScCN	C721PAN → C721PAN(aq)	k_exf(01,ind_C721PAN)	see general notes*
H48002b_a01	TrAa01ScCN	C721PAN(aq) → C721PAN	k_exb(01,ind_C721PAN)	see general notes*
H48003f_a01	TrAa01ScCN	C810NO3 → C810NO3(aq)	k_exf(01,ind_C810NO3)	see general notes*
H48003b_a01	TrAa01ScCN	C810NO3(aq) → C810NO3	k_exb(01,ind_C810NO3)	see general notes*
H48004f_a01	TrAa01ScC	C810OOH → C810OOH(aq)	k_exf(01,ind_C810OOH)	see general notes*
H48004b_a01	TrAa01ScC	C810OOH(aq) → C810OOH	k_exb(01,ind_C810OOH)	see general notes*
H48005f_a01	TrAa01ScC	C812OOH → C812OOH(aq)	k_exf(01,ind_C812OOH)	see general notes*
H48005b_a01	TrAa01ScC	C812OOH(aq) → C812OOH	k_exb(01,ind_C812OOH)	see general notes*
H48006f_a01	TrAa01ScC	C813OOH → C813OOH(aq)	k_exf(01,ind_C813OOH)	see general notes*
H48006b_a01	TrAa01ScC	C813OOH(aq) → C813OOH	k_exb(01,ind_C813OOH)	see general notes*
H48007f_a01	TrAa01ScC	C85OOH → C85OOH(aq)	k_exf(01,ind_C85OOH)	see general notes*
H48007b_a01	TrAa01ScC	C85OOH(aq) → C85OOH	k_exb(01,ind_C85OOH)	see general notes*
H48008f_a01	TrAa01ScC	C86OOH → C86OOH(aq)	k_exf(01,ind_C86OOH)	see general notes*
H48008b_a01	TrAa01ScC	C86OOH(aq) → C86OOH	k_exb(01,ind_C86OOH)	see general notes*
H48009f_a01	TrAa01ScCN	C89NO3 → C89NO3(aq)	k_exf(01,ind_C89NO3)	see general notes*
H48009b_a01	TrAa01ScCN	C89NO3(aq) → C89NO3	k_exb(01,ind_C89NO3)	see general notes*
H48010f_a01	TrAa01ScC	C89OOH → C89OOH(aq)	k_exf(01,ind_C89OOH)	see general notes*
H48010b_a01	TrAa01ScC	C89OOH(aq) → C89OOH	k_exb(01,ind_C89OOH)	see general notes*
H48011f_a01	TrAa01ScC	C8BC → C8BC(aq)	k_exf(01,ind_C8BC)	see general notes*
H48011b_a01	TrAa01ScC	C8BC(aq) → C8BC	k_exb(01,ind_C8BC)	see general notes*
H48012f_a01	TrAa01ScC	C8BCCO → C8BCCO(aq)	k_exf(01,ind_C8BCCO)	see general notes*
H48012b_a01	TrAa01ScC	C8BCCO(aq) → C8BCCO	k_exb(01,ind_C8BCCO)	see general notes*
H48013f_a01	TrAa01ScCN	C8BCNO3 → C8BCNO3(aq)	k_exf(01,ind_C8BCNO3)	see general notes*
H48013b_a01	TrAa01ScCN	C8BCNO3(aq) → C8BCNO3	k_exb(01,ind_C8BCNO3)	see general notes*
H48014f_a01	TrAa01ScC	C8BCOOH → C8BCOOH(aq)	k_exf(01,ind_C8BCOOH)	see general notes*
H48014b_a01	TrAa01ScC	C8BCOOH(aq) → C8BCOOH	k_exb(01,ind_C8BCOOH)	see general notes*
H48015f_a01	TrAa01ScC	NORPINIC → NORPINIC(aq)	k_exf(01,ind_NORPINIC)	see general notes*
H48015b_a01	TrAa01ScC	NORPINIC(aq) → NORPINIC	k_exb(01,ind_NORPINIC)	see general notes*
H48016f_a01	TrAa01ScC	STYRENOOH → STYRENOOH(aq)	k_exf(01,ind_STYRENOOH)	see general notes*
H48016b_a01	TrAa01ScC	STYRENOOH(aq) → STYRENOOH	k_exb(01,ind_STYRENOOH)	see general notes*
H49000f_a01	TrAa01ScC	C811CO3H → C811CO3H(aq)	k_exf(01,ind_C811CO3H)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H49000b_a01	TrAa01ScC	$\text{C811CO3H(aq)} \rightarrow \text{C811CO3H}$	$k_{\text{exb}}(01, \text{ind_C811CO3H})$	see general notes*
H49001f_a01	TrAa01ScCN	$\text{C811PAN} \rightarrow \text{C811PAN(aq)}$	$k_{\text{exf}}(01, \text{ind_C811PAN})$	see general notes*
H49001b_a01	TrAa01ScCN	$\text{C811PAN(aq)} \rightarrow \text{C811PAN}$	$k_{\text{exb}}(01, \text{ind_C811PAN})$	see general notes*
H49002f_a01	TrAa01ScC	$\text{C85CO3H} \rightarrow \text{C85CO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_C85CO3H})$	see general notes*
H49002b_a01	TrAa01ScC	$\text{C85CO3H(aq)} \rightarrow \text{C85CO3H}$	$k_{\text{exb}}(01, \text{ind_C85CO3H})$	see general notes*
H49003f_a01	TrAa01ScC	$\text{C89CO2H} \rightarrow \text{C89CO2H(aq)}$	$k_{\text{exf}}(01, \text{ind_C89CO2H})$	see general notes*
H49003b_a01	TrAa01ScC	$\text{C89CO2H(aq)} \rightarrow \text{C89CO2H}$	$k_{\text{exb}}(01, \text{ind_C89CO2H})$	see general notes*
H49004f_a01	TrAa01ScC	$\text{C89CO3H} \rightarrow \text{C89CO3H(aq)}$	$k_{\text{exf}}(01, \text{ind_C89CO3H})$	see general notes*
H49004b_a01	TrAa01ScC	$\text{C89CO3H(aq)} \rightarrow \text{C89CO3H}$	$k_{\text{exb}}(01, \text{ind_C89CO3H})$	see general notes*
H49005f_a01	TrAa01ScCN	$\text{C89PAN} \rightarrow \text{C89PAN(aq)}$	$k_{\text{exf}}(01, \text{ind_C89PAN})$	see general notes*
H49005b_a01	TrAa01ScCN	$\text{C89PAN(aq)} \rightarrow \text{C89PAN}$	$k_{\text{exb}}(01, \text{ind_C89PAN})$	see general notes*
H49006f_a01	TrAa01ScCN	$\text{C96NO3} \rightarrow \text{C96NO3(aq)}$	$k_{\text{exf}}(01, \text{ind_C96NO3})$	see general notes*
H49006b_a01	TrAa01ScCN	$\text{C96NO3(aq)} \rightarrow \text{C96NO3}$	$k_{\text{exb}}(01, \text{ind_C96NO3})$	see general notes*
H49007f_a01	TrAa01ScC	$\text{C96OOH} \rightarrow \text{C96OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C96OOH})$	see general notes*
H49007b_a01	TrAa01ScC	$\text{C96OOH(aq)} \rightarrow \text{C96OOH}$	$k_{\text{exb}}(01, \text{ind_C96OOH})$	see general notes*
H49008f_a01	TrAa01ScC	$\text{C97OOH} \rightarrow \text{C97OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C97OOH})$	see general notes*
H49008b_a01	TrAa01ScC	$\text{C97OOH(aq)} \rightarrow \text{C97OOH}$	$k_{\text{exb}}(01, \text{ind_C97OOH})$	see general notes*
H49009f_a01	TrAa01ScC	$\text{C98OOH} \rightarrow \text{C98OOH(aq)}$	$k_{\text{exf}}(01, \text{ind_C98OOH})$	see general notes*
H49009b_a01	TrAa01ScC	$\text{C98OOH(aq)} \rightarrow \text{C98OOH}$	$k_{\text{exb}}(01, \text{ind_C98OOH})$	see general notes*
H49010f_a01	TrAa01ScCN	$\text{C9PAN2} \rightarrow \text{C9PAN2(aq)}$	$k_{\text{exf}}(01, \text{ind_C9PAN2})$	see general notes*
H49010b_a01	TrAa01ScCN	$\text{C9PAN2(aq)} \rightarrow \text{C9PAN2}$	$k_{\text{exb}}(01, \text{ind_C9PAN2})$	see general notes*
H49011f_a01	TrAa01ScC	$\text{NOPINDCO} \rightarrow \text{NOPINDCO(aq)}$	$k_{\text{exf}}(01, \text{ind_NOPINDCO})$	see general notes*
H49011b_a01	TrAa01ScC	$\text{NOPINDCO(aq)} \rightarrow \text{NOPINDCO}$	$k_{\text{exb}}(01, \text{ind_NOPINDCO})$	see general notes*
H49012f_a01	TrAa01ScC	$\text{NOPINDOOH} \rightarrow \text{NOPINDOOH(aq)}$	$k_{\text{exf}}(01, \text{ind_NOPINDOOH})$	see general notes*
H49012b_a01	TrAa01ScC	$\text{NOPINDOOH(aq)} \rightarrow \text{NOPINDOOH}$	$k_{\text{exb}}(01, \text{ind_NOPINDOOH})$	see general notes*
H49013f_a01	TrAa01ScC	$\text{NOPINONE} \rightarrow \text{NOPINONE(aq)}$	$k_{\text{exf}}(01, \text{ind_NOPINONE})$	see general notes*
H49013b_a01	TrAa01ScC	$\text{NOPINONE(aq)} \rightarrow \text{NOPINONE}$	$k_{\text{exb}}(01, \text{ind_NOPINONE})$	see general notes*
H49014f_a01	TrAa01ScC	$\text{NOPINOO} \rightarrow \text{NOPINOO(aq)}$	$k_{\text{exf}}(01, \text{ind_NOPINOO})$	see general notes*
H49014b_a01	TrAa01ScC	$\text{NOPINOO(aq)} \rightarrow \text{NOPINOO}$	$k_{\text{exb}}(01, \text{ind_NOPINOO})$	see general notes*
H49015f_a01	TrAa01ScC	$\text{NORPINAL} \rightarrow \text{NORPINAL(aq)}$	$k_{\text{exf}}(01, \text{ind_NORPINAL})$	see general notes*
H49015b_a01	TrAa01ScC	$\text{NORPINAL(aq)} \rightarrow \text{NORPINAL}$	$k_{\text{exb}}(01, \text{ind_NORPINAL})$	see general notes*
H49016f_a01	TrAa01ScC	$\text{NORPINENOL} \rightarrow \text{NORPINENOL(aq)}$	$k_{\text{exf}}(01, \text{ind_NORPINENOL})$	see general notes*
H49016b_a01	TrAa01ScC	$\text{NORPINENOL(aq)} \rightarrow \text{NORPINENOL}$	$k_{\text{exb}}(01, \text{ind_NORPINENOL})$	see general notes*
H49017f_a01	TrAa01ScC	$\text{PINIC} \rightarrow \text{PINIC(aq)}$	$k_{\text{exf}}(01, \text{ind_PINIC})$	see general notes*
H49017b_a01	TrAa01ScC	$\text{PINIC(aq)} \rightarrow \text{PINIC}$	$k_{\text{exb}}(01, \text{ind_PINIC})$	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410000f_a01	TrAa01ScCN	BPINANO3 \rightarrow BPINANO3(aq)	k_exf(01,ind_BPINANO3)	see general notes*
H410000b_a01	TrAa01ScCN	BPINANO3(aq) \rightarrow BPINANO3	k_exb(01,ind_BPINANO3)	see general notes*
H410001f_a01	TrAa01ScC	BPINAOOH \rightarrow BPINAOOH(aq)	k_exf(01,ind_BPINAOOH)	see general notes*
H410001b_a01	TrAa01ScC	BPINAOOH(aq) \rightarrow BPINAOOH	k_exb(01,ind_BPINAOOH)	see general notes*
H410002f_a01	TrAa01ScCN	C106NO3 \rightarrow C106NO3(aq)	k_exf(01,ind_C106NO3)	see general notes*
H410002b_a01	TrAa01ScCN	C106NO3(aq) \rightarrow C106NO3	k_exb(01,ind_C106NO3)	see general notes*
H410003f_a01	TrAa01ScC	C106OOH \rightarrow C106OOH(aq)	k_exf(01,ind_C106OOH)	see general notes*
H410003b_a01	TrAa01ScC	C106OOH(aq) \rightarrow C106OOH	k_exb(01,ind_C106OOH)	see general notes*
H410004f_a01	TrAa01ScC	C109CO \rightarrow C109CO(aq)	k_exf(01,ind_C109CO)	see general notes*
H410004b_a01	TrAa01ScC	C109CO(aq) \rightarrow C109CO	k_exb(01,ind_C109CO)	see general notes*
H410005f_a01	TrAa01ScC	C109OOH \rightarrow C109OOH(aq)	k_exf(01,ind_C109OOH)	see general notes*
H410005b_a01	TrAa01ScC	C109OOH(aq) \rightarrow C109OOH	k_exb(01,ind_C109OOH)	see general notes*
H410006f_a01	TrAa01ScCN	C10PAN2 \rightarrow C10PAN2(aq)	k_exf(01,ind_C10PAN2)	see general notes*
H410006b_a01	TrAa01ScCN	C10PAN2(aq) \rightarrow C10PAN2	k_exb(01,ind_C10PAN2)	see general notes*
H410007f_a01	TrAa01ScCN	LAPINABNO3 \rightarrow LAPINABNO3(aq)	k_exf(01,ind_LAPINABNO3)	see general notes*
H410007b_a01	TrAa01ScCN	LAPINABNO3(aq) \rightarrow LAPINABNO3	k_exb(01,ind_LAPINABNO3)	see general notes*
H410008f_a01	TrAa01ScC	LAPINABOOH \rightarrow LAPINABOOH(aq)	k_exf(01,ind_LAPINABOOH)	see general notes*
H410008b_a01	TrAa01ScC	LAPINABOOH(aq) \rightarrow LAPINABOOH	k_exb(01,ind_LAPINABOOH)	see general notes*
H410009f_a01	TrAa01ScCN	LNAPINABOOH \rightarrow LNAPINABOOH(aq)	k_exf(01,ind_LNAPINABOOH)	see general notes*
H410009b_a01	TrAa01ScCN	LNAPINABOOH(aq) \rightarrow LNAPINABOOH	k_exb(01,ind_LNAPINABOOH)	see general notes*
H410010f_a01	TrAa01ScCN	LNBPINABOOH \rightarrow LNBPINABOOH(aq)	k_exf(01,ind_LNBPINABOOH)	see general notes*
H410010b_a01	TrAa01ScCN	LNBPINABOOH(aq) \rightarrow LNBPINABOOH	k_exb(01,ind_LNBPINABOOH)	see general notes*
H410011f_a01	TrAa01ScC	MENTHEN6ONE \rightarrow MENTHEN6ONE(aq)	k_exf(01,ind_MENTHEN6ONE)	see general notes*
H410011b_a01	TrAa01ScC	MENTHEN6ONE(aq) \rightarrow MENTHEN6ONE	k_exb(01,ind_MENTHEN6ONE)	see general notes*
H410012f_a01	TrAa01ScC	2OHMENTHEN6ONE \rightarrow 2OHMENTHEN6ONE(aq)	k_exf(01,ind_OH2MENTHEN6ONE)	see general notes*
H410012b_a01	TrAa01ScC	2OHMENTHEN6ONE(aq) \rightarrow 2OHMENTHEN6ONE	k_exb(01,ind_OH2MENTHEN6ONE)	see general notes*
H410013f_a01	TrAa01ScC	PERPINONIC \rightarrow PERPINONIC(aq)	k_exf(01,ind_PERPINONIC)	see general notes*
H410013b_a01	TrAa01ScC	PERPINONIC(aq) \rightarrow PERPINONIC	k_exb(01,ind_PERPINONIC)	see general notes*
H410014f_a01	TrAa01ScC	PINAL \rightarrow PINAL(aq)	k_exf(01,ind_PINAL)	see general notes*
H410014b_a01	TrAa01ScC	PINAL(aq) \rightarrow PINAL	k_exb(01,ind_PINAL)	see general notes*
H410015f_a01	TrAa01ScCN	PINALNO3 \rightarrow PINALNO3(aq)	k_exf(01,ind_PINALNO3)	see general notes*
H410015b_a01	TrAa01ScCN	PINALNO3(aq) \rightarrow PINALNO3	k_exb(01,ind_PINALNO3)	see general notes*
H410016f_a01	TrAa01ScC	PINALOOH \rightarrow PINALOOH(aq)	k_exf(01,ind_PINALOOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410016b_a01	TrAa01ScC	PINALOOH(aq) \rightarrow PINALOOH	k_exb(01,ind_PINALOOH)	see general notes*
H410017f_a01	TrAa01ScC	PINEOL \rightarrow PINEOL(aq)	k_exf(01,ind_PINENOL)	see general notes*
H410017b_a01	TrAa01ScC	PINEOL(aq) \rightarrow PINEOL	k_exb(01,ind_PINENOL)	see general notes*
H410018f_a01	TrAa01ScC	PINONIC \rightarrow PINONIC(aq)	k_exf(01,ind_PINONIC)	see general notes*
H410018b_a01	TrAa01ScC	PINONIC(aq) \rightarrow PINONIC	k_exb(01,ind_PINONIC)	see general notes*
H410019f_a01	TrAa01ScCN	RO6R1NO3 \rightarrow RO6R1NO3(aq)	k_exf(01,ind_RO6R1NO3)	see general notes*
H410019b_a01	TrAa01ScCN	RO6R1NO3(aq) \rightarrow RO6R1NO3	k_exb(01,ind_RO6R1NO3)	see general notes*
H410020f_a01	TrAa01ScCN	ROO6R1NO3 \rightarrow ROO6R1NO3(aq)	k_exf(01,ind_ROO6R1NO3)	see general notes*
H410020b_a01	TrAa01ScCN	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*
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*
H631MS_a01	TrAa01MblClN	ClNO ₂ \rightarrow ClNO ₂ (aq)	k_exf(01,ind_ClN02)	see general notes*
H632MS_a01	TrAa01MblClN	ClNO ₂ (aq) \rightarrow ClNO ₂	k_exb(01,ind_ClN02)	see general notes*
H633MS_a01	TrAa01MblClN	ClNO \rightarrow ClNO(aq)	k_exf(01,ind_ClN0)	see general notes*
H634MS_a01	TrAa01MblClN	ClNO(aq) \rightarrow ClNO	k_exb(01,ind_ClN0)	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*

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

#	labels	reaction	rate coefficient	reference
H76002_a01	TrAa01MblBrClN	$\text{BrNO}_3 + \text{Cl}^-(\text{aq}) \rightarrow \text{BrCl}(\text{aq}) + \text{NO}_3^-(\text{aq})$	$k_{\text{exf_BrNO3}}(01) * 5.E2$	see general notes*
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	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$x_{\text{nom7sulf}} * k_{\text{exf}}(01, \text{ind_H2SO4})$	see general notes*
H94000f_a01	TrAa01CS	$\text{DMSO} \rightarrow \text{DMSO}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_DMSO})$	see general notes*
H94000b_a01	TrAa01CS	$\text{DMSO}(\text{aq}) \rightarrow \text{DMSO}$	$k_{\text{exb}}(01, \text{ind_DMSO})$	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	$\text{DMS} \rightarrow \text{DMS}(\text{aq})$	$k_{\text{exf}}(01, \text{ind_DMS})$	see general notes*
H94002b_a01	TrAa01CS	$\text{DMS}(\text{aq}) \rightarrow \text{DMS}$	$k_{\text{exb}}(01, \text{ind_DMS})$	see general notes*

General notes

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

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

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

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

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

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

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
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General notes

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

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
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*
EQ4201_a01	TrAa01ScC	$\text{CH}_3\text{C}(\text{O})\text{OOH} \rightleftharpoons \text{CH}_3\text{COOO}^- + \text{H}^+$	6.3E-9		Schuchmann and von Sonntag (1988)
EQ4202_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_3\text{H} \rightleftharpoons \text{CH}_2\text{OHCO}_2\text{O}^- + \text{H}^+$	6.3E-9		Schuchmann and von Sonntag (1988)*
EQ4203_a01	TrAa01ScC	$\text{HOCCOOH} \rightleftharpoons \text{H}^+ + \text{HOCCOO}^-$	5.6E-2		Martell (1977)
EQ4204_a01	TrAa01ScC	$\text{HOCCOO}^- \rightleftharpoons \text{H}^+ + \text{C}_2\text{O}_4^{2-}$	5.4E-5		Martell (1977)
EQ4205_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OOHCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4206_a01	TrAa01ScC	$\text{CH}_2\text{OOCOOH} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OOCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4207_a01	TrAa01ScC	$\text{CHOOHOOCOOH} \rightleftharpoons \text{H}^+ + \text{CHOOHOOCO}_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4208_a01	TrAa01ScC	$\text{HOCH}_2\text{CO}_2\text{H} \rightleftharpoons \text{H}^+ + \text{CH}_2\text{OHCO}_2^-$	1.5E-4		Rumble (2020)
EQ4209_a01	TrAa01ScC	$\text{CHOHOOCOOH} \rightleftharpoons \text{H}^+ + \text{CHOHOOCOO}_2^-$	1.5E-4		Rumble (2020)*
EQ4210_a01	TrAa01ScC	$\text{CHOCOOH} \rightleftharpoons \text{H}^+ + \text{CHOCOO}^-$	1.754E-5		Fisher and Barnes (1972)
EQ4211_a01	TrAa01ScC	$\text{COOHCO}_3 \rightleftharpoons \text{H}^+ + \text{CO}_2^- \text{CO}_3$	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	TrAa01ScC	$\text{CHOHOOCOHO} \rightleftharpoons \text{CHOHOOCOHOHOH}$	1.57E1		see note*
EQ4252_a01	TrAa01ScC	$\text{CH}_2\text{OHCHO} \rightleftharpoons \text{CH}_2\text{OHCHOHOH}$	1.56E1		Doussin and Monod (2013)
EQ4253_a01	TrAa01ScC	$\text{GLYOX} \rightleftharpoons \text{CHOCHOHOH}$	3.5E2		Ervens and Volkamer (2010)
EQ4254_a01	TrAa01ScC	$\text{CHOCHOHOH} \rightleftharpoons \text{CHOHOHCHOHOH}$	2.0E2		Ervens and Volkamer (2010)
EQ4255_a01	TrAa01ScC	$\text{CHOCOOH} \rightleftharpoons \text{CHOOHOHCOOH}$	1.1E3		Doussin and Monod (2013)
EQ4256_a01	TrAa01ScC	$\text{CHOCOO}^- \rightleftharpoons \text{CHOHOHCO}_2^-$	6.6E1		Doussin and Monod (2013)
EQ4257_a01	TrAa01ScC	$\text{CO}_2^- \text{CO}_3 \rightleftharpoons \text{CO}_2^- \text{COHOHO}_2$	6.6E1		see note*
EQ4258_a01	TrAa01ScC	$\text{CH}_2\text{OOHCHO} \rightleftharpoons \text{HOCH}_2\text{CHOHOH}$	1.56E1		see note*
EQ4300_a01	TrAa01ScScmC	$\text{CH}_3\text{COCOHOH} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COCO}_2^-$	4.1E-3		Rumble (2020)
EQ4350_a01	TrAa01ScC	$\text{CH}_3\text{C}(\text{O})\text{CHO} \rightleftharpoons \text{CH}_3\text{COCHOHOH}$	1.98E3		Doussin and Monod (2013)

Table 5: Acid-base and other equilibria

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

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)
A310MS_a01	TrAa01ScN	$N_2O_5 \rightarrow NO_2^+ + NO_3^-$	1.5E5		Staudt et al. (2019)
A311MS_a01	TrAa01ScN	$NO_2^+ + NO_3^- \rightarrow N_2O_5$	2.7E8		Staudt et al. (2019), Bertram and Thornton (2009)*
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)
A320MS_a01	TrAa01ScN	$NO_2^+ + H_2O \rightarrow HNO_3 + H^+$	1.6E7		Staudt et al. (2019)
A321MS_a01	TrAa01ScN	$HNO_3 + H^+ \rightarrow NO_2^+ + H_2O$	1.6E-9		Sampoli et al. (1985)*
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	$HCOO^- + NO_3 \rightarrow NO_3^- + H^+ + O_2^- + CO_2$	5.119E+07	-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)

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
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	$CH_3OO + CH_3OO \rightarrow 2 HCHO + H_2O_2$	$0.20 \times 2.145E+08$	-2139	Herrmann et al. (1999b)
A41012b_a01	TrAa01Sc	$CH_3OO + CH_3OO \rightarrow 2 HOCH_2O_2$	$0.80 \times 2.145E+08$	-2139	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	Herrmann and Zellner (1998)
A41015_a01	TrAa01Sc	$CH_3OH + CO_3^- \rightarrow HOCH_2O_2 + HCO_3^-$	5.431E+03	-3100	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	TrAa01Sc	$HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$	$0.25 \times 6.30E8$		see note*
A41019b_a01	TrAa01Sc	$HOCH_2OOH + OH \rightarrow CHOOOH + HO_2 + H_2O$	$0.75 \times 6.30E8$		see note*
A41020a_a01	TrAa01ScN	$HOCH_2OOH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$	$0.25 \times 4.90E6$	-2000	see note*
A41020b_a01	TrAa01ScN	$HOCH_2OOH + NO_3 \rightarrow CHOOOH + HO_2 + NO_3^- + H^+$	$0.75 \times 4.90E6$	-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	$HOCH_2O_2 + HOCH_2O_2 \rightarrow 2 HCOOH + H_2O_2$	7.367E+08	-1395	Huie and Clifton (1993)
A41025_a01	TrAa01Sc	$HCOOH + H_2O_2 + H^+ \rightarrow CHOOOH + H_2O + H^+$	3.080E-04	-5235	De Filippis et al. (2009)
A41026a_a01	TrAa01Sc	$CHOOOH + H^+ \rightarrow HCOOH + H_2O_2 + H^+$	3.790E-04	-5235	De Filippis et al. (2009)
A41026b_a01	TrAa01Sc	$CHOOOH + H^+ \rightarrow CO_2 + H_2O + H^+$	1.219E-03	-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	$HOCH_2OH + NO_3 \rightarrow NO_3^- + H^+ + HCOHOHO_2$	1.003E+06	-4500	Exner et al. (1993)
A41030_a01	TrAa01Sc	$HCOHOHO_2 \rightarrow HCOOH + HO_2$	1.00E6		see note*
A41030DT_a01	TrAa01ScN	$HCOO^- + NO_2^+ \rightarrow HCOO^- + NO_3^- + 2 H^+$	7.50E+09		Staudt et al. (2019)
A41030MS_a01	TrAa01ScN	$CH_3OH + NO_2^+ \rightarrow CH_3ONO_2 + H^+$	4.50E+08		Iraci et al. (2007)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42000a_a01	TrAa01ScC	$CH_3CH_2OH + OH \rightarrow CH_3CHO + HO_2 + H_2O$	$0.90 \times 2.002E+09$	-830	Monod et al. (2005)*
A42000b_a01	TrAa01ScC	$CH_3CH_2OH + OH \rightarrow CH_2OHCH_2OO + H_2O$	$0.10 \times 2.002E+09$	-830	Monod et al. (2005)
A42001a_a01	TrAa01ScCN	$CH_3CH_2OH + NO_3 \rightarrow CH_3CHO + HO_2 + NO_3^- + H^+$	$0.90 \times 2.184E+06$	-3300	Herrmann and Zellner (1998)*
A42001b_a01	TrAa01ScCN	$CH_3CH_2OH + NO_3 \rightarrow CH_2OHCH_2OO + NO_3^- + H^+$	$0.10 \times 2.184E+06$	-3300	Herrmann and Zellner (1998)
A42002a_a01	TrAa01ScC	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow CH_2OHCHO + CH_2OHCHO + H_2O_2$	$0.50 \times 1.00E8$		Piesiak et al. (1984)
A42002b_a01	TrAa01ScC	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow CH_2OHCHO + ETHGLY$	$0.33 \times 1.00E8$		Piesiak et al. (1984)
A42002c_a01	TrAa01ScC	$CH_2OHCH_2OO + CH_2OHCH_2OO \rightarrow 2 HOCH_2O_2 + 2 HCHO$	$0.17 \times 1.00E8$		Piesiak et al. (1984)
A42003_a01	TrAa01ScC	$CH_2OHCH_2OO + O_2^- \rightarrow HYETHO_2H + OH^-$	1.0E8	-900	see note*
A42004_a01	TrAa01ScC	$CH_2OHCH_2OO + HO_2 \rightarrow HYETHO_2H$	9.7E5	-2500	see note*
A42005_a01	TrAa01ScC	$HYETHO_2H + OH \rightarrow CH_2OHCHO$	1.10E9		see note*
A42006_a01	TrAa01ScC	$ETHGLY + OH \rightarrow CH_2OHCHO + HO_2 + H_2O$	1.657E+09	-1191	Hoffmann et al. (2009)*
A42007_a01	TrAa01ScCN	$ETHGLY + NO_3 \rightarrow CH_2OHCHO + HO_2 + NO_3^- + H^+$	5.856E+06	-2117	Hoffmann et al. (2009)*
A42008_a01	TrAa01ScC	$CH_3CHO + OH \rightarrow CH_3COOO + H_2O$	3.60E9		Schuchmann and von Sonntag (1988)
A42009_a01	TrAa01ScCN	$CH_3CHO + NO_3 \rightarrow CH_3COOO + NO_3^- + H^+$	3.10E6		Rousse and George (2004)
A42010_a01	TrAa01ScC	$CH_3COOO + CH_3COOO \rightarrow CH_3OO + CH_3OO + CO_2 + CO_2$	1.891E+08	1563	see note*
A42011_a01	TrAa01ScC	$CH_3COOO + O_2^- \rightarrow CH_3COOO^- + O_2$	1.00E9		Schuchmann and von Sonntag (1988)
A42012_a01	TrAa01ScC	$CH_3CHOHOH + OH \rightarrow CH_3COHOHOH + H_2O$	1.20E9		Schuchmann and von Sonntag (1988)
A42013_a01	TrAa01ScCN	$CH_3CHOHOH + NO_3 \rightarrow CH_3COHOHOH + NO_3^- + H^+$	1.10E6		Rousse and George (2004)
A42014_a01	TrAa01ScC	$CH_3COHOHOH \rightarrow CH_3COOH + HO_2$	1.00E6		see note*
A42015a_a01	TrAa01ScC	$CH_2OHCHO + OH \rightarrow CH_2OHCO_3 + H_2O$	$0.77 \times 1.40E9$		Doussin and Monod (2013)
A42015b_a01	TrAa01ScC	$CH_2OHCHO + OH \rightarrow CHOHOOCO_3 + H_2O$	$0.23 \times 1.40E9$		Doussin and Monod (2013)
A42016a_a01	TrAa01ScCN	$CH_2OHCHO + NO_3 \rightarrow CH_2OHCO_3 + NO_3^- + H^+$	$0.77 \times 3.10E6$		see note*
A42016b_a01	TrAa01ScCN	$CH_2OHCHO + NO_3 \rightarrow CHOHOOCO_3 + NO_3^- + H^+$	$0.23 \times 3.10E6$		see note*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A42017_a01	TrAa01ScC	$CH_2OHCO_3 + O_2^- \rightarrow CH_2OHCO_2O^-$	1.00E9		see note*
A42018_a01	TrAa01ScC	$CH_2OHCOHOHO_2 \rightarrow HOCH_2CO_2H + HO_2$	1.00E6		see note*
A42019_a01	TrAa01ScC	$CHOHOOCHO \rightarrow GLYOX + HO_2$	1.90E2		see note*
A42020_a01	TrAa01ScC	$CHOHOOCHOHOH \rightarrow CHOCHOHOH + HO_2$	1.90E2		see note*
A42021a_a01	TrAa01ScC	$CH_2OHCHOHOH + OH \rightarrow CH_2OHCOHOHO_2 + H_2O$	$0.33 \times 1.10E9$		Doussin and Monod (2013)
A42021b_a01	TrAa01ScC	$CH_2OHCHOHOH + OH \rightarrow CHOHOCHOHOH + H_2O$	$0.28 \times 1.10E9$		Doussin and Monod (2013)
A42021c_a01	TrAa01ScC	$CH_2OHCHOHOH + OH \rightarrow HCOOH + HOCH_2O_2 + H_2O$	$0.39 \times 1.10E9$		Doussin and Monod (2013)
A42022a_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow CH_2OHCOHOHO_2 + NO_3^- + H^+$	$0.33 \times 1.10E6$		see note*
A42022b_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow CHOHOCHOHOH + NO_3^- + H^+$	$0.28 \times 1.10E6$		see note*
A42022c_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow HCOOH + HOCH_2O_2 + NO_3^- + H^+$	$0.39 \times 1.10E6$		see note*
A42023a_a01	TrAa01ScC	$CHOHOHCHOHOH + OH \rightarrow CHOHOHCOHOHO_2 + H_2O$	$0.27 \times 1.114E+09$	-1516	Buxton et al. (1997)
A42023b_a01	TrAa01ScC	$CHOHOHCHOHOH + OH \rightarrow HCOOH + HCOHOHO_2 + HO_2 + H_2O$	$0.73 \times 1.114E+09$	-1516	Buxton et al. (1997)*
A42024a_a01	TrAa01ScCN	$CHOHOHCHOHOH + NO_3 \rightarrow CHOHOHCOHOHO_2 + NO_3^- + H^+$	$0.27 \times 1.00E6$		see note*
A42024b_a01	TrAa01ScCN	$CHOHOHCHOHOH + NO_3 \rightarrow HCOOH + HCOHOHO_2 + HO_2 + NO_3^- + H^+$	$0.73 \times 1.00E6$		see note*
A42025_a01	TrAa01ScC	$CHOHOHCOHOHO_2 \rightarrow CHOOHOHCOOH + HO_2$	$0.77 \times 1.00E6$		see note*
A42026_a01	TrAa01ScC	$CH_3COOH + OH \rightarrow CH_2OOCO_2H + H_2O$	1.50E7	-1330	Chin and Wine (1994)
A42027_a01	TrAa01ScCN	$CH_3COOH + NO_3 \rightarrow CH_2OOCO_2H + NO_3^- + H^+$	1.429E+04	-3800	Exner et al. (1994)
A42028_a01	TrAa01ScC	$CH_3COO^- + OH \rightarrow CH_2OOCO_2^- + H_2O$	1.00E8	-1800	Fisher and Hamill (1973)
A42029_a01	TrAa01ScCN	$CH_3COO^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$	2.916E+06	-3800	Exner et al. (1994)
A42030DT_a01	TrAa01ScCN	$CH_3COO^- + NO_2^+ \rightarrow CH_3COO^- + NO_3^- + 2 H^+$	7.50E+09		Staudt et al. (2019)
A42030a_a01	TrAa01ScC	$C_2H_5OOH + OH \rightarrow C_2H_5OO + H_2O$	$0.80 \times 5.80E8$		Monod et al. (2007)
A42030b_a01	TrAa01ScC	$C_2H_5OOH + OH \rightarrow CH_3COOH + HO_2 + H_2O$	$0.20 \times 5.80E8$		Monod et al. (2007)*
A42031a_a01	TrAa01ScC	$C_2H_5OO + C_2H_5OO \rightarrow CH_3CHO + CH_3CHO + H_2O_2$	$0.20 \times 1.891E+08$	1563	Herrmann et al. (1999b)
A42031b_a01	TrAa01ScC	$C_2H_5OO + C_2H_5OO \rightarrow 2 CH_3CHO + 2 HO_2$	$0.80 \times 1.891E+08$	1563	Herrmann et al. (1999b)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A42032_a01	TrAa01ScC	$C_2H_5OO + O_2^- \rightarrow C_2H_5OOH + OH^-$	1.0E8	-900	see note*
A42033_a01	TrAa01ScC	$C_2H_5OO + HO_2 \rightarrow C_2H_5OOH$	9.7E5	-2500	see note*
A42034_a01	TrAa01ScC	$CH_2OOCO_2H + HO_2 \rightarrow HOOCH_2CO_2H$	9.7E5	-2500	see note*
A42035_a01	TrAa01ScC	$CH_2OOCO_2H + O_2^- + H^+ \rightarrow HOOCH_2CO_2H$	1.0E8	-900	see note*
A42036a_a01	TrAa01ScC	$CH_2OOCO_2H + CH_2OOCO_2H \rightarrow CHOCO_2H + CHOCO_2H + H_2O_2$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42036b_a01	TrAa01ScC	$CH_2OOCO_2H + CH_2OOCO_2H \rightarrow 2 HCHO + 2 CO_2 + H_2O_2$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42036c_a01	TrAa01ScC	$CH_2OOCO_2H + CH_2OOCO_2H \rightarrow CHOCO_2H + HOCH_2CO_2H$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42036d_a01	TrAa01ScC	$CH_2OOCO_2H + CH_2OOCO_2H \rightarrow CHOHOOOCO_2H + CHOHOOOCO_2H$	$0.10 \times 7.50E7$		Schuchmann et al. (1985)
A42037_a01	TrAa01ScC	$CH_2OOCO_2^- + HO_2 \rightarrow CH_2OOHCO_2^- + O_2$	9.7E5	-2500	see note*
A42038_a01	TrAa01ScC	$CH_2OOCO_2^- + O_2^- + H^+ \rightarrow CH_2OOHCO_2^-$	1.0E8	-900	see note*
A42039a_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCO_2^- + CHOCO_2^- + H_2O_2$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039b_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2 HCHO + 2 CO_2 + H_2O_2 + 2 OH^-$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039c_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCO_2^- + CH_2OHCO_2^-$	$0.30 \times 7.50E7$		Schuchmann et al. (1985)
A42039d_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2 CHOHOOOCO_2^-$	$0.10 \times 7.50E7$		Schuchmann et al. (1985)
A42040_a01	TrAa01ScC	$CH_2OOCO_2^- + O_3 \rightarrow O_3^- + HOCH_2OOH + CO_2$	2.00E9		Sehested et al. (1984)
A42141_a01	TrAa01ScC	$HOCCOO^- + OH \rightarrow C_2O_4^- + H_2O$	2.086E+08	-2800	Ervens et al. (2003)
A42142_a01	TrAa01ScC	$C_2O_4^{2-} + OH \rightarrow C_2O_4^- + OH^-$	2.508E+08	-4300	Ervens et al. (2003)
A42143_a01	TrAa01ScC	$C_2O_4^- + O_2 \rightarrow 2 CO_2 + O_2^-$	2.40E9		Hislop and Bolton (1999)
A42144a_a01	TrAa01ScC	$HOOCH_2CO_2H + OH \rightarrow CH_2OOCO_2H + H_2O$	$0.80 \times 5.80E8$		see note*
A42144b_a01	TrAa01ScC	$HOOCH_2CO_2H + OH \rightarrow CHOOHOOCO_2H + H_2O$	$0.20 \times 5.80E8$		see note*
A42145a_a01	TrAa01ScCN	$HOOCH_2CO_2H + NO_3 \rightarrow CH_2OOCO_2H + NO_3^- + H^+$	$0.80 \times 1.70E6$		Herrmann and Zellner (1998)
A42145b_a01	TrAa01ScCN	$HOOCH_2CO_2H + NO_3 \rightarrow CHOOHOOCO_2H + NO_3^- + H^+$	$0.20 \times 1.70E6$		Herrmann and Zellner (1998)
A42146a_a01	TrAa01ScC	$CH_2OOHCO_2^- + OH \rightarrow CH_2OOCO_2^- + H_2O$	$0.80 \times 5.80E8$		see note*
A42146b_a01	TrAa01ScC	$CH_2OOHCO_2^- + OH \rightarrow CHOOHOOCO_2^- + H_2O$	$0.20 \times 5.80E8$		see note*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42147a_a01	TrAa01ScCN	$CH_2OOHCO_2^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$	$0.80 \times 7.10E6$		Herrmann and Zellner (1998)
A42147b_a01	TrAa01ScCN	$CH_2OOHCO_2^- + NO_3 \rightarrow CHOOHOOCO_2^- + NO_3^- + H^+$	$0.20 \times 7.10E6$		Herrmann and Zellner (1998)
A42148_a01	TrAa01ScC	$CHOOHOOCO_2^- \rightarrow HOCCOOH + HO_2$	1.90E2		see note*
A42149_a01	TrAa01ScC	$CHOOHOOCO_2^- \rightarrow HOCCOO^- + HO_2$	1.90E2		see note*
A42150a_a01	TrAa01ScC	$HOCH_2CO_2H + OH \rightarrow CHOHOOCO_2H + H_2O$	$0.62 \times 6.00E8$		see note*
A42150b_a01	TrAa01ScC	$HOCH_2CO_2H + OH \rightarrow HCHO + CO_2 + HO_2 + H_2O$	$0.38 \times 6.00E8$		see note*
A42151a_a01	TrAa01ScCN	$HOCH_2CO_2H + NO_3 \rightarrow CHOHOOCO_2H + NO_3^- + H^+$	$0.62 \times 7.445E+05$	-3969	see note*
A42151b_a01	TrAa01ScCN	$HOCH_2CO_2H + NO_3 \rightarrow HCHO + CO_2 + HO_2 + NO_3^- + H^+$	$0.38 \times 7.445E+05$	-3969	see note*
A42152_a01	TrAa01ScC	$CHOHOOCO_2H \rightarrow CHOCO_2H + HO_2$	1.90E2		von Sonntag (1987)
A42153a_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow CHOHOOCO_2^- + H_2O$	$0.60 \times 8.60E8$		Buxton et al. (1988)
A42153b_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow HCHO + CO_2 + O_2^- + H_2O$	$0.19 \times 8.60E8$		Buxton et al. (1988)
A42153c_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow HOCH_2O_2 + CO_2 + OH^-$	$0.21 \times 8.60E8$		Buxton et al. (1988)
A42154a_a01	TrAa01ScCN	$CH_2OHCO_2^- + NO_3 \rightarrow CHOHOOCO_2^- + NO_3^- + H^+$	$0.76 \times 7.502E+06$	-3007	Gaillard de Sémainville et al. (2007)
A42154b_a01	TrAa01ScCN	$CH_2OHCO_2^- + NO_3 \rightarrow HCHO + CO_2 + O_2^- + NO_3^- + H^+$	$0.24 \times 7.502E+06$	-3007	Gaillard de Sémainville et al. (2007)
A42155_a01	TrAa01ScC	$CHOHOOCO_2^- \rightarrow CHOCOO^- + HO_2$	1.90E2		von Sonntag (1987)
A42156a_a01	TrAa01ScC	$CHOOHOHCOOH + OH \rightarrow COOHCOHOHO_2 + H_2O$	$0.15 \times 2.830E+08$	-1000	Ervens et al. (2003)
A42156b_a01	TrAa01ScC	$CHOOHOHCOOH + OH \rightarrow HCOOH + CO_2 + HO_2 + H_2O$	$0.85 \times 2.830E+08$	-1000	Ervens et al. (2003)*
A42157a_a01	TrAa01ScCN	$CHOOHOHCOOH + NO_3 \rightarrow COOHCOHOHO_2 + NO_3^- + H^+$	$0.15 \times 1.00E6$		see note*
A42157b_a01	TrAa01ScCN	$CHOOHOHCOOH + NO_3 \rightarrow HCOOH + CO_2 + HO_2 + NO_3^- + H^+$	$0.85 \times 1.00E6$		see note*
A42158a_a01	TrAa01ScC	$CHOHOHCO_2^- + OH \rightarrow CO_2^-COHOHO_2 + H_2O$	$0.26 \times 3.271E+09$	-4300	Ervens et al. (2003)
A42158b_a01	TrAa01ScC	$CHOHOHCO_2^- + OH \rightarrow HCOOH + CO_2 + O_2^- + H_2O$	$0.74 \times 3.271E+09$	-4300	Ervens et al. (2003)
A42159a_a01	TrAa01ScCN	$CHOHOHCO_2^- + NO_3 \rightarrow CO_2^-COHOHO_2 + NO_3^- + H^+$	$0.26 \times 1.80E5$		Herrmann and Zellner (1998)

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42159b_a01	TrAa01ScCN	$\text{CHOHOHCO}_2^- + \text{NO}_3 \rightarrow \text{HCOOH} + \text{CO}_2 + \text{O}_2^- + \text{NO}_3^- + \text{H}^+$	$0.74 \times 1.80\text{E}5$		Herrmann and Zellner (1998)
A42160_a01	TrAa01ScC	$\text{CHOHOHCO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{HCOO}^- + \text{CO}_2 + \text{H}_2\text{O} + \text{H}_2\text{O}$	1.10E-1		Schöne and Herrmann (2014)
A42161_a01	TrAa01ScC	$\text{COOHCOHOHO}_2 \rightarrow \text{HOCCOOH} + \text{HO}_2$	1.00E6		see note*
A42162_a01	TrAa01ScC	$\text{CO}_2^- \text{COHOHO}_2 \rightarrow \text{HOCCOO}^- + \text{HO}_2$	1.00E6		see note*
A42163a_a01	TrAa01ScC	$\text{CH}_2\text{OOHCHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH} + \text{H}_2\text{O}$	$0.77 \times 1.40\text{E}9$		see note*
A42163b_a01	TrAa01ScC	$\text{CH}_2\text{OOHCHO} + \text{OH} \rightarrow \text{GLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$0.23 \times 1.40\text{E}9$		see note*
A42164a_a01	TrAa01ScCN	$\text{CH}_2\text{OOHCHO} + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{NO}_3 + \text{H}_2\text{O}$	$0.77 \times 3.10\text{E}6$		see note*
A42164b_a01	TrAa01ScCN	$\text{CH}_2\text{OOHCHO} + \text{NO}_3 \rightarrow \text{GLYOX} + \text{NO}_3^- + \text{H}_2\text{O} + \text{H}^+$	$0.23 \times 3.10\text{E}6$		see note*
A42165a_a01	TrAa01ScC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	$0.33 \times 1.10\text{E}9$		see note*
A42165b_a01	TrAa01ScC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{CHOCHOHOH} + \text{OH} + \text{H}_2\text{O}$	$0.28 \times 1.10\text{E}9$		see note*
A42165c_a01	TrAa01ScC	$\text{HOOCH}_2\text{CHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$0.39 \times 1.10\text{E}9$		see note*
A42166a_a01	TrAa01ScCN	$\text{HOOCH}_2\text{CHOHOH} + \text{NO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{NO}_3^- + \text{H}_2\text{O} + \text{H}^+$	$0.33 \times 1.10\text{E}6$		see note*
A42166b_a01	TrAa01ScCN	$\text{HOOCH}_2\text{CHOHOH} + \text{NO}_3 \rightarrow \text{CHOCHOHOH} + \text{NO}_3 + \text{H}_2\text{O}$	$0.28 \times 1.10\text{E}6$		see note*
A42166c_a01	TrAa01ScCN	$\text{HOOCH}_2\text{CHOHOH} + \text{NO}_3 \rightarrow \text{HCOOH} + \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$	$0.39 \times 1.10\text{E}6$		see note*
A42167_a01	TrAa01ScC	$\text{HOCH}_2\text{OH} + \text{HOCH}_2\text{OH} \rightarrow \text{MG2} + \text{H}_2\text{O}$	see note	see note	Hahnenstein et al. (1995)*
A42168_a01	TrAa01ScC	$\text{MG2} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OH} + \text{HOCH}_2\text{OH}$	see note	see note	Hahnenstein et al. (1995)
A42169_a01	TrAa01ScC	$\text{MG2} + \text{OH} \rightarrow \text{HMF} + \text{HO}_2$	1.54E9	-1020	see note*
A42470_a01	TrAa01ScC	$\text{CH}_3\text{COOO} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{HO}_2$	7.0E5		Villalta et al. (1996)
A42471_a01	TrAa01ScC	$\text{CH}_2\text{OHCO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{CO}_2\text{H} + \text{HO}_2$	7.0E5		see note*
A42472_a01	TrAa01ScC	$\text{CHOCO}_3 + \text{H}_2\text{O} \rightarrow \text{CHOCOOH} + \text{HO}_2$	7.0E5		see note*
A42473_a01	TrAa01ScC	$\text{COOHCO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCCOOH} + \text{HO}_2$	7.0E5		see note*
A43000a_a01	TrAa01ScC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{CH}_3\text{COCOOH} + \text{HO}_2$	$0.29 \times 9.215\text{E}+08$	-1235	Schaefer et al. (2015)*
A43000b_a01	TrAa01ScC	$\text{CH}_3\text{COCHOHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{CH}_3\text{COOO}$	$0.71 \times 9.215\text{E}+08$	-1235	Schaefer et al. (2015)
A43001_a01	TrAa01ScCN	$\text{CH}_3\text{COCHOHOH} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCOOH} + \text{NO}_3^- + \text{H}^+$	4.539E+06	-4213	Schaefer et al. (2015)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A43002_a01	TrAa01ScC	$CH_3COCOOH + OH \rightarrow CH_3COOH + HO_2 + CO_2$	2.592E+08	-1804	Schaefer et al. (2012)*
A43003_a01	TrAa01ScCN	$CH_3COCOOH + NO_3 \rightarrow CH_3COOH + NO_3^- + CO_2 + H^+$	2.828E+06	-1804	Gaillard de Sémainville et al. (2007)
A43004_a01	TrAa01ScC	$CH_3COCO2^- + OH \rightarrow CH_3COO^- + HO_2 + CO_2$	6.252E+08	-3007	Schaefer et al. (2012)*
A43005_a01	TrAa01ScCN	$CH_3COCO2^- + NO_3 \rightarrow CH_3COO^- + NO_3^- + CO_2 + H^+$	2.306E+07	-2887	Gaillard de Sémainville et al. (2007)
A43006_a01	TrAa01ScC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2$	1.80E8		Gligorovski et al. (2009)
A43007_a01	TrAa01ScCN	$CH_3COCH_3 + NO_3 \rightarrow CH_3COCH_2O_2 + NO_3^- + H^+$	3.721E+03	-4332	Herrmann and Zellner (1998)
A43008a_a01	TrAa01ScC	$CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow CH_3COCH_2OH + CH_3C(O)CHO$	$0.20 \times 4.00E8$		Zegota et al. (1986)
A43008b_a01	TrAa01ScC	$CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0 CH_3C(O)CHO + H_2O_2$	$0.45 \times 4.00E8$		Zegota et al. (1986)
A43009c_a01	TrAa01ScC	$CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0 HCHO + 2.0 CH_3COOO$	$0.15 \times 4.00E8$		Zegota et al. (1986)
A43009d_a01	TrAa01ScC	$CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow 2.0 CH_3C(O)CHO + 2.0 HO_2$	$0.20 \times 4.00E8$		Zegota et al. (1986)
A43010a_a01	TrAa01ScC	$CH_3COCH_2OH + OH \rightarrow CH_3COCHOHO_2$	$0.85 \times 5.10E8$		Doussin and Monod (2013)*
A43010b_a01	TrAa01ScC	$CH_3COCH_2OH + OH \rightarrow HCHO + CH_3COOO$	$0.15 \times 5.10E8$		Doussin and Monod (2013)
A43011_a01	TrAa01ScCN	$CH_3COCH_2OH + NO_3 \rightarrow CH_3COCHOHO_2 + NO_3^- + H^+$	2.108E+07	-1564	Gaillard de Sémainville et al. (2007)
A43012_a01	TrAa01ScC	$CH_3COCHOHO_2 \rightarrow CH_3C(O)CHO + HO_2$	1.90E2		von Sonntag (1987)
A43013_a01	TrAa01ScC	$IPROPOL + OH \rightarrow CH_3COCH_3 + HO_2$	1.90E9		see note*
A43014_a01	TrAa01ScCN	$IPROPOL + NO_3 \rightarrow CH_3COCH_3 + NO_3^- + H^+ + HO_2$	3.70E6		see note*
A43015a_a01	TrAa01ScC	$CH_3COCH_2O_2H + OH \rightarrow CH_3C(O)CHO + OH$	1.80E8		see note*
A43015b_a01	TrAa01ScC	$CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2$	4.70E8		see note*
A43016_a01	TrAa01ScCN	$CH_3COCH_2O_2H + NO_3 \rightarrow CH_3COCH_2O_2 + NO_3^- + H^+$	4.50E6		see note*
A43017_a01	TrAa01ScC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	4.30E5		see note*
A43018_a01	TrAa01ScC	$CH_3COCH_2O_2 + O_2^- \rightarrow CH_3COCH_2O_2H + O_2 + OH^-$	5.00E7		see note*
A43019a_a01	TrAa01ScC	$iC_3H_7OOH + OH \rightarrow CH_3COCH_3 + OH$	9.90E8		see note*
A43019b_a01	TrAa01ScC	$iC_3H_7OOH + OH \rightarrow iC_3H_7O_2$	1.80E8		see note*
A43020_a01	TrAa01ScCN	$iC_3H_7OOH + NO_3 \rightarrow iC_3H_7O_2 + NO_3^- + H^+$	4.50E6		see note*
A43021_a01	TrAa01ScC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	4.30E5		see note*

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

#	labels	reaction	$k_0 [M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A43022_a01	TrAa01ScC	$iC_3H_7O_2 + O_2^- \rightarrow iC_3H_7OOH + O_2 + OH^-$	5.00E7		see note*
A43023_a01	TrAa01ScC	$HOCH_2OH + MG2 \rightarrow MG3 + H_2O$	see note	see note	Hahnenstein et al. (1995)*
A43024_a01	TrAa01ScC	$MG3 + H_2O \rightarrow HOCH_2OH + MG2$	see note	see note	Hahnenstein et al. (1995)
A43025_a01	TrAa01ScC	$MG3 + OH \rightarrow HM2F + HO_2$	1.54E9	-1020	see note*
A44000_a01	TrAa01ScC	$MACR + OH \rightarrow CH_2OHCO_2CH_3CHO$	9.905E+09	-1203	Schöne and Herrmann (2014)
A44001_a01	TrAa01ScC	$CH_2OHCO_2CH_3CHO + CH_2OHCO_2CH_3CHO \rightarrow$ $CH_3C(O)CHO + CH_3COCH_2OH + HOCH_2O_2 +$ $HCOHOHO_2$	4.00E8		Schöne and Herrmann (2014)
A44002_a01	TrAa01ScC	$MVK + OH \rightarrow CH_3COCHO_2CH_2OH$	7.117E+09	-1443	Schöne and Herrmann (2014)
A44003_a01	TrAa01ScC	$CH_3COCHO_2CH_2OH + CH_3COCHO_2CH_2OH \rightarrow$ $1.1 CH_2COCOCH_2OH + .2 CH_2OHCHOOHCOCH_3$ $+ .35 CH_2OHCHO + .35 CH_3C(O)CHO + .35$ $HOCH_2O_2 + .35 CH_3COOO + .45 H_2O_2$	4.00E8		Schöne and Herrmann (2014)
A44004_a01	TrAa01ScC	$GLYOX + CHOCHOHOH \rightarrow GOLIG1 + H_2O$	1.00E2		Ervens and Volkamer (2010)
A44005_a01	TrAa01ScC	$GOLIG1 + H_2O \rightarrow GLYOX + CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44006_a01	TrAa01ScC	$CHOCHOHOH + CHOCHOHOH \rightarrow GOLIG2 +$ H_2O	1.00E2		Ervens and Volkamer (2010)
A44007_a01	TrAa01ScC	$GOLIG2 + H_2O \rightarrow CHOCHOHOH +$ $CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44008_a01	TrAa01ScC	$CHOHOHCHOHOH + CHOCHOHOH \rightarrow GOLIG3$ $+ H_2O$	1.00E2		Ervens and Volkamer (2010)
A44009_a01	TrAa01ScC	$GOLIG3 + H_2O \rightarrow CHOHOHCHOHOH +$ $CHOCHOHOH$	1.00E-1		Ervens and Volkamer (2010)
A44010_a01	TrAa01ScC	$GOLIG1 + OH \rightarrow GOLIGO1 + HO_2$	1.610E+09	-1516	see note*
A44011_a01	TrAa01ScC	$GOLIG2 + OH \rightarrow GOLIGO2 + HO_2$	1.610E+09	-1516	see note*
A44012_a01	TrAa01ScC	$GOLIG3 + OH \rightarrow GOLIGO3 + HO_2$	1.610E+09	-1516	see note*
A46000_a01	TrAa01ScC	$CH_3C(O)CHO + CH_3COCHOHOH \rightarrow$ $CH_3COCHOHOCHOHCOCH_3 + H_2O$	1.00E2		Ervens and Volkamer (2010)*
A46001_a01	TrAa01ScC	$CH_3COCHOHOCHOHCOCH_3 + H_2O \rightarrow$ $CH_3COCHOHOH + CH_3C(O)CHO$	1.00E-1		Ervens and Volkamer (2010)*
A46002_a01	TrAa01ScC	$CH_3COCHOHOCHOHCOCH_3 + OH \rightarrow$ $CH_3COCOHOCHOHCOCH_3 + HO_2$	1.303E+09	-1235	see note*
A46003_a01	TrAa01ScC	$CH_3COCHOHOH + CH_3COCHOHOH \rightarrow$ $CH_3COCHOHOCOHC_3CHOHOH + H_2O$	1.00E2		Ervens and Volkamer (2010)*

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
A46004_a01	TrAa01ScC	$CH_3COCHOHOCOHC_3CHOHOH + H_2O \rightarrow 2 CH_3COCHOHOH$	1.00E-1		Ervens and Volkamer (2010)*
A46005_a01	TrAa01ScC	$CH_3COCHOHOCOHC_3CHOHOH + OH \rightarrow CH_3COCOHOHOCOHC_3COHOH + HO_2$	1.303E+09	-1235	see note*
A460MS_a01	TrAa01CN	$PHENOL + NO_2^+ \rightarrow HOC_6H_4NO_2 + H^+$	7.5E9		Ryder et al. (2015), Heal et al. (2007)*
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)*
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	TrAa01MbICl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	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	TrAa01MbICl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	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)
A620MS_a01	TrAa01Cl	$ClOH^- + ClOH^- \rightarrow Cl_2 + 2 OH^-$	1.8E9		Knipping et al. (2000)
A621MS_a01	TrAa01Cl	$ClOH^- + Cl^- \rightarrow Cl_2^- + OH^-$	1.0E4		Grigorev et al. (1987)
A622MS_a01	TrAa01Cl	$OH^- + Cl_2^- \rightarrow ClOH^- + Cl^-$	4.5E7		Grigorev et al. (1987)
A63000_a01	TrAa01ClIN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A63001_a01	TrAa01ClIN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A63002_a01	TrAa01ClIN	$Cl_2^- + NO_2^- \rightarrow 2 Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A630MS_a01	TrAa01MbIClIN	$ClNO_2 \rightarrow Cl^- + NO_2^+$	2.70E2		Behnke et al. (1997)
A631MS_a01	TrAa01MbIClIN	$Cl^- + NO_2^+ \rightarrow ClNO_2$	7.5E9		Staudt et al. (2019)
A632MS_a01	TrAa01MbIClIN	$ClNO_2 + Cl^- \rightarrow Cl_2 + NO_2^-$	1.0E7		Roberts et al. (2008)
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)

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
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)*
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)
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)
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)

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

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
A92005_a01	TrAa01ScS	$\text{HSO}_3^- + \text{O}_2^- \rightarrow \text{SO}_4^{2-} + \text{OH}^-$	3.0E3		see note*
A92006_a01	TrAa01MblScScmS	$\text{HSO}_3^- + \text{O}_3 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	3.7E5	-5500	Hoffmann (1986)
A92007_a01	TrAa01ScS	$\text{HSO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^{2-}$	4.5E9		Buxton et al. (1988)
A92008_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HO}_2 \rightarrow \text{SO}_4^{2-} + \text{OH}^- + \text{H}^+$	3.0E3		see note*
A92009_a01	TrAa01MblScScmS	$\text{HSO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{SO}_4^{2-} + \text{H}^+$	5.2E6	-3650	Martin and Damschen (1981)
A92010_a01	TrAa01ScS	$\text{HSO}_3^- + \text{SO}_4^- \rightarrow \text{SO}_3^- + \text{SO}_4^{2-} + \text{H}^+$	8.0E8		Huie and Neta (1987)
A92011_a01	TrAa01S	$\text{HSO}_3^- + \text{SO}_5^- \rightarrow .75 \text{SO}_4^- + .75 \text{SO}_4^{2-} + .75 \text{H}^+ + .25 \text{SO}_3^- + .25 \text{HSO}_5^-$	1.0E5		Huie and Neta (1987)
A92012_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HSO}_5^- + \text{H}^+ \rightarrow 2 \text{HSO}_4^- + \text{H}^+$	7.1E6		Betterton and Hoffmann (1988)
A93001_a01	TrAa01ScNS	$\text{SO}_4^- + \text{NO}_3^- \rightarrow \text{SO}_4^{2-} + \text{NO}_3$	5.0E4		Exner et al. (1992)
A93002_a01	TrAa01ScNS	$\text{SO}_4^{2-} + \text{NO}_3 \rightarrow \text{NO}_3^- + \text{SO}_4^-$	1.0E5		Løgager et al. (1993)
A93004_a01	TrAa01ScNS	$\text{HSO}_3^- + \text{NO}_3 \rightarrow \text{SO}_3^- + \text{NO}_3^- + \text{H}^+$	1.4E9	-2000	Exner et al. (1992)
A93005_a01	TrAa01ScNS	$\text{HSO}_3^- + \text{HNO}_4 \rightarrow \text{HSO}_4^- + \text{NO}_3^- + \text{H}^+$	3.1E5		Warneck (1999)
A930MS_a01	TrAa01ScNS	$\text{SO}_4^{2-} + \text{NO}_2^+ \rightarrow \text{SO}_4^- + \text{NO}_3^- + 2 \text{H}^+$	7.5E9		Staudt et al. (2019)*
A94100_a01	TrAa01ScS	$\text{SO}_3^{2-} + \text{HCHO} \rightarrow \text{CH}_2\text{OH}\text{SO}_3^- + \text{OH}^-$	1.4E4		Boyce and Hoffmann (1984)*
A94101_a01	TrAa01ScS	$\text{SO}_3^{2-} + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A94102_a01	TrAa01ScS	$\text{HSO}_3^- + \text{HCHO} \rightarrow \text{CH}_2\text{OH}\text{SO}_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A94103_a01	TrAa01ScS	$\text{HSO}_3^- + \text{CH}_3\text{OOH} + \text{H}^+ \rightarrow \text{HSO}_4^- + \text{H}^+ + \text{CH}_3\text{OH}$	1.6E7	-3800	Lind et al. (1987)
A94104_a01	TrAa01ScS	$\text{HSO}_3^- + \text{CH}_3\text{OO} \rightarrow \text{SO}_3^- + \text{CH}_3\text{OOH}$	5.00E5		Herrmann et al. (1999b)
A94105_a01	TrAa01ScS	$\text{SO}_4^- + \text{HCOO}^- \rightarrow \text{SO}_4^{2-} + \text{CO}_2 + \text{HO}_2$	1.7E8	-1500	Jacob (1986)
A94106_a01	TrAa01ScS	$\text{SO}_4^- + \text{HCOOH} \rightarrow \text{SO}_4^{2-} + \text{CO}_2 + \text{H}^+ + \text{HO}_2$	1.7E8	-1500	Jacob (1986)
A94107_a01	TrAa01ScS	$\text{SO}_4^- + \text{CH}_3\text{OH} \rightarrow \text{SO}_4^{2-} + \text{HOCH}_2\text{O}_2 + \text{H}^+$	9.039E+06	-2190	Clifton and Huie (1989)
A94108a_a01	TrAa01ScS	$\text{SO}_4^- + \text{CH}_3\text{OOH} \rightarrow \text{SO}_4^{2-} + \text{CH}_3\text{OO} + \text{H}^+$	$0.25 \times 1.20\text{E}7$		see note*
A94108b_a01	TrAa01ScS	$\text{SO}_4^- + \text{CH}_3\text{OOH} \rightarrow \text{SO}_4^{2-} + \text{HCHO} + \text{HO}_2 + \text{H}^+$	$0.75 \times 1.20\text{E}7$		see note*
A94109_a01	TrAa01ScS	$\text{SO}_4^- + \text{HOCH}_2\text{OH} \rightarrow \text{SO}_4^{2-} + \text{HCOHOHO}_2 + \text{H}^+$	1.40E7	-1300	Buxton et al. (1990)
A94110_a01	TrAa01ScS	$\text{SO}_5^- + \text{HCOO}^- \rightarrow \text{HSO}_5^- + \text{CO}_2 + \text{O}_2^-$	1.4E4	-4000	Jacob (1986)
A94111_a01	TrAa01ScS	$\text{CH}_2\text{OH}\text{SO}_3^- + \text{OH}^- \rightarrow \text{SO}_3^{2-} + \text{HCHO}$	3.6E3		Seinfeld and Pandis (1998)
A94200_a01	TrAa01ScCS	$\text{HSO}_3^- + \text{CH}_2\text{OOC}\text{COOH} \rightarrow \text{SO}_3^- + \text{HOOCH}_2\text{CO}_2\text{H}$	5.00E5		see note*
A94201_a01	TrAa01ScCS	$\text{HSO}_3^- + \text{CH}_2\text{OOC}\text{CO}_2^- \rightarrow \text{SO}_3^- + \text{CH}_2\text{OOH}\text{CO}_2^-$	5.00E5		see note*
A94202a_a01	TrAa01ScCS	$\text{SO}_4^- + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{SO}_4^{2-} + \text{CH}_3\text{CHO} + \text{HO}_2 + \text{H}^+$	$0.90 \times 4.236\text{E}+07$	-1750	Clifton and Huie (1989)*
A94202b_a01	TrAa01ScCS	$\text{SO}_4^- + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{SO}_4^{2-} + \text{CH}_2\text{OHCH}_2\text{OO} + \text{H}^+$	$0.10 \times 4.236\text{E}+07$	-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	$SO_4^- + \text{CHOHOHCHOHOH} \rightarrow SO_4^{2-} + \text{HCOHOH}_2 + \text{HCOOH} + \text{HO}_2 + H^+$	$0.73 \times 2.40E7$		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)
A111001_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{O}_2^- \rightarrow \text{Fe}^{3+} + \text{HO}_2^- + \text{OH}^-$	1E7		de Laat and Le (2006)
A111002_a01	TrAa01Fe	$\text{Fe}^{3+} + \text{O}_2^- \rightarrow \text{O}_2 + \text{Fe}^{2+}$	5E7		de Laat and Le (2006)
A111003_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{O}_3 \rightarrow \text{FeO}^{2+} + \text{O}_2$	8.2E5		Løgager et al. (1992)
A112001a_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{OH} \rightarrow \text{Fe}^{3+} + \text{OH}^-$	2.7E8		de Laat and Le (2006)
A112001b_a01	TrAa01Fe	$\text{FeOH}^+ + \text{OH} \rightarrow \text{Fe}^{3+} + 2 \text{OH}^-$	2.7E8		de Laat and Le (2006)
A112002a_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \text{OH} + \text{OH}^-$	5.5E1		de Laat and Le (2006)
A112002b_a01	TrAa01Fe	$\text{FeOH}^+ + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \text{OH} + 2 \text{OH}^-$	5.9E6		de Laat and Le (2006)
A112003_a01	TrAa01Fe	$\text{FeHO}_2^+ \rightarrow \text{Fe}^{2+} + \text{HO}_2$	2.3E-3		de Laat and Le (2006)
A112004_a01	TrAa01Fe	$\text{Fe}(\text{OH})(\text{HO}_2)^+ \rightarrow \text{Fe}^{2+} + \text{HO}_2 + \text{OH}^-$	2.3E-3		de Laat and Le (2006)
A112006_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{HO}_2 \rightarrow \text{Fe}^{3+} + \text{HO}_2^-$	1.2E6		de Laat and Le (2006)
A112008a_a01	TrAa01Fe	$\text{FeOH}^{2+} + \text{O}_2^- \rightarrow \text{Fe}^{2+} + \text{O}_2 + \text{OH}^-$	1.5E8		Rush and Bielski (1985)
A112008b_a01	TrAa01Fe	$\text{Fe}(\text{OH})_2^+ + \text{O}_2^- \rightarrow \text{Fe}^{2+} + \text{O}_2 + 2 \text{OH}^-$	1.5E8		Rush and Bielski (1985)
A112009_a01	TrAa01Fe	$\text{Fe}^{2+} + \text{O}_2^- \rightarrow \text{Fe}^{3+} + \text{H}_2\text{O}_2 + 2 \text{OH}^-$	1.0E7		Rush and Bielski (1985)

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

#	labels	reaction	$k_0 [M^{1-n} s^{-1}]$	$-E_a/R[K]$	reference
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)*
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

Staudt et al. (2019).

(1985).

A311MS_a01: Rate constant derived from $k_3/k_2b = 6.E-2$ in Bertram and Thornton (2009) and $k_3 = 1.7E5$ in

A321MS_a01: Rate constant is derived from $k(NO_2p + H_2O)/K(NO_2p)$, where $K(NO_2p)$ is $1E16$ Sampoli et al.

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 CH₃O₂ would only produce 2 CH₃O radicals and thus HCHO + HO₂. Instead, the latter reaction has a 0.8 yield of HOCH₂O₂, which is a precursor of hydroxymethyl hydroperoxide and thus HCOOH.

A41016b_a01: The CH₂OOH radical has a lifetime of 10⁻⁹ s in the gas phase decomposing to HCHO and OH. O₂-addition in the aqueous-phase seems unlikely. It is hard to imagine how the HOOHCH₂O₂ radical would decompose into HCOOH and HO₂.

A41017a_a01: $k(\text{H}_2\text{O}_2 + \text{NO}_3)$, branching ratio as for CH₃OOH + OH

A41017b_a01: See branch a.

A41018a_a01: $k(\text{H}_2\text{O}_2 + \text{CO}_3^-)$, branching ratio as for CH₃OOH + OH

A41018b_a01: See branch a.

A41019a_a01: Branching ratio as for CH₃OOH + OH

A41019b_a01: HOCHOOHO₂ is assumed to directly decompose into CHOOOH and HO₂

A41020a_a01: $k(\text{H}_2\text{O}_2 + \text{NO}_3)$, branching ratio as for CH₃OOH + OH

A41020b_a01: HOCHOOHO₂ is assumed to directly decompose into CHOOOH and HO₂

A41021_a01: HO₂ elimination

A41022_a01: $k(\text{HO}_2 + \text{HO}_2)$

A41023_a01: $k(\text{HO}_2 + \text{O}_2^-)$

A41030_a01: HO₂ elimination

A42000a_a01: CH₃CHOHO₂ is assumed to directly decompose into CH₃CHO + HO₂

A42001a_a01: CH₃CHOHO₂ is assumed to directly decompose into CH₃CHO + HO₂

A42003_a01: $k(\text{HO}_2 + \text{O}_2^-)$

A42004_a01: $k(\text{HO}_2 + \text{HO}_2)$

A42005_a01: k approximated from $(k(\text{CH}_3\text{OOH} + \text{OH}) / k(\text{CH}_3\text{OH} + \text{OH}))$

A42006_a01: CH₂OHCHOHO₂ is assumed to directly decompose into HOCH₂CHO + HO₂

A42007_a01: CH₂OHCHOHO₂ is assumed to directly decompose into HOCH₂CHO + HO₂

A42010_a01: k based on Monod et al. (2005): $k = k(2 \text{CH}_3\text{CH}_2(\text{OO}))$

A42014_a01: HO₂ elimination

A42016a_a01: k assumed to be the same as for CH₃CHO + NO₃

A42016b_a01: See branch a.

A42017_a01: $k(\text{CH}_3\text{CHOHOH} + \text{O}_2^-)$

A42018_a01: HO₂ elimination

A42019_a01: k based on von Sonntag (1987)

A42020_a01: k based on von Sonntag (1987)

A42022a_a01: $k(\text{CH}_3\text{CHOHOH} + \text{NO}_3)$

A42022b_a01: See branch a.

A42022c_a01: See branch a.

A42023b_a01: CHOHOHO₂ directly decomposes into HCOOH + HO₂

A42024a_a01: k based on Neta and Huie (1986)

A42024b_a01: CHOHOHO₂ directly decomposes into HCOOH + HO₂

A42025_a01: HO₂ elimination

A42030b_a01: CH₃CHOOHO₂ is assumed to directly decompose into CH₃CO₂H and HO₂

A42031b_a01: CH₃CHOHO₂ is assumed to directly decompose into CH₃CHO + HO₂

A42032_a01: $k(\text{HO}_2 + \text{O}_2^-)$

A42033_a01: $k(\text{HO}_2 + \text{HO}_2)$

A42034_a01: $k(\text{HO}_2 + \text{HO}_2)$

A42035_a01: $k(\text{HO}_2 + \text{O}_2^-)$

A42037_a01: $k(\text{HO}_2 + \text{HO}_2)$

A42038_a01: $k(\text{HO}_2 + \text{O}_2^-)$

A42144a_a01: k assumed to be the same as C₂H₅OOH + OH based on Monod et al. (2007)

A42144b_a01: See branch a.

A42146a_a01: k assumed to be the same as C₂H₅OOH + OH based on Monod et al. (2007)

A42146b_a01: See branch a.

A42148_a01: HO₂ elimination

A42149_a01: HO₂ elimination

A42150a_a01: COOHOO is not formed but directly dissociates into CO₂ + HO₂. Rate coefficient based on Buxton et al. (1988)

A42150b_a01: See branch a.

A42151a_a01: COOHOO is not formed but directly dissociates into CO₂ + HO₂. Rate coefficient based on Gaillard de Sémainville et al. (2007)

A42151b_a01: See branch a.

A42156b_a01: COOHOO is not formed but directly dissociates into CO₂ + HO₂.

A42157a_a01: $k(\text{CHOHOHCHOHOH} + \text{NO}_3)$

A42157b_a01: COOHOO is not formed but directly dissociates into CO₂ + HO₂

A42161_a01: HO₂ elimination

A42162_a01: HO₂ elimination

A42163a_a01: $k(\text{HOCH}_2\text{CHO} + \text{OH})$

A42163b_a01: See branch a.

A42164a_a01: $k(\text{HOCH}_2\text{CHO}+\text{NO}_3)$	A43015a_a01: k calculated comparing the rates ($\text{CH}_3\text{OH} + \text{OH}/\text{CH}_3\text{OOH} + \text{OH}$) and ($\text{ACETOL} + \text{OH}/\text{HYPERACET} + \text{OH}$)	assume that only 2-nitrophenol is formed like in the gas phase.
A42164b_a01: See branch a.		
A42165a_a01: $k(\text{HOCH}_2\text{CHOHOH}+\text{OH})$	A43015b_a01: k from $\text{CH}_3\text{OOH} + \text{OH} \rightarrow \text{HCHO}$.	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.
A42165b_a01: See branch a.		
A42165c_a01: See branch a.	A43016_a01: k taken from the reaction of the hydrated form of MGLYOX and NO_3	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.
A42166a_a01: $k(\text{HOCH}_2\text{CHOHOH}+\text{NO}_3)$	A43017_a01: k from $\text{CH}_3\text{O}_2 + \text{HO}_2$	A64000_a01: k taken from $\text{H}_2\text{O}_2+\text{Cl}_2^-$ (Yu, 2004).
A42166b_a01: See branch a.	A43018_a01: k from $\text{CH}_3\text{O}_2 + \text{O}_2^-$	A74000_a01: Assumed to be the same as for $\text{Br}_2^- + \text{H}_2\text{O}_2$.
A42166c_a01: See branch a.	A43019a_a01: k calculated comparing $\text{CH}_3\text{OH} + \text{OH} / \text{CH}_3\text{OOH} + \text{OH}$ with $\text{IPROPL} + \text{OH}$	A76003_a01: The rate coefficient is defined as backward reaction divided by equilibrium constant.
A42167_a01: pH-dependent	A43019b_a01: k calculated comparing $\text{CH}_3\text{OH} + \text{OH} / \text{CH}_3\text{OOH} + \text{OH}$ with $\text{ACETOL} + \text{OH} / \text{HYPERCET} + \text{OH}$	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).
A42169_a01: $k = 2 \times k(\text{HOCH}_2\text{OH}+\text{OH})$	A43020_a01: k taken from the reaction of the hydrated form of MGLYOX and NO_3	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 $\text{S}_2\text{O}_8^{2-}$ as product. Since $\text{S}_2\text{O}_8^{2-}$ is not treated explicitly in the mechanism, SO_4^{2-} is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.
A42471_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)	A43021_a01: k from $\text{CH}_3\text{O}_2 + \text{HO}_2$	A92005_a01: D. Sedlak, pers. comm. (1993).
A42472_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)	A43022_a01: k from $\text{CH}_3\text{O}_2 + \text{O}_2^-$	A92008_a01: D. Sedlak, pers. comm. (1993).
A42473_a01: Assumed to be the same as $\text{CH}_3\text{CO}_3 + \text{H}_2\text{O}$, following Villalta et al. (1996)	A43023_a01: pH-dependent	A930MS_a01: As suggested in Staudt et al., 2019 intermediate product is NO_2SO_4^- , which readily reacts with H_2O and produce final products
A43000a_a01: Intermdiate reaction with O_2^- and $\text{CH}(\text{OH})_2\text{COCH}_2\text{O}_2$ neglected	A43025_a01: $k = 2 \times k(\text{HOCH}_2\text{OH}+\text{OH})$	A94100_a01: $2.48 \times 10^7 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.
A43001_a01: $\text{CH}(\text{OH})_2\text{COCH}_2\text{O}_2$ neglected	A44010_a01: $k = 2 \times k(\text{CHOHOHCHOHOH}+\text{OH})$	A94102_a01: $790 \times 5.5 \times 10^{-4}$, considering the hydrated form of HCHO.
A43002_a01: CO_2 added for mass balance intermediate reactions neglected	A44011_a01: $k = 2 \times k(\text{CHOHOHCHOHOH}+\text{OH})$	A94108a_a01: $k(\text{H}_2\text{O}_2+\text{SO}_4^-)$, branching ratio as for $\text{CH}_3\text{OOH} + \text{OH}$
A43004_a01: CO_2 added for mass balance intermediate reactions neglected	A44012_a01: $k = 2 \times k(\text{CHOHOHCHOHOH}+\text{OH})$	
A43010a_a01: $\text{CH}_2(\text{OH})\text{COCH}_2\text{O}_2$ was negected with a branching ratio 0.16 added to $\text{CH}_3\text{COCHOHO}_2$	A46000_a01: Assumed to be the same as for glyoxal	
A43013_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Monod et al., 2005)	A46001_a01: Assumed to be the same as for glyoxal	
A43014_a01: There is an intermediate reaction with branching ratio 0.87 and 0.13, the minor compound is neglected (Herrmann et al., 1994)	A46002_a01: $k = 2 \times k(\text{CH}_3\text{COCHOHOH}+\text{OH})$	
	A46003_a01: Assumed to be the same as for glyoxal	
	A46004_a01: Assumed to be the same as for glyoxal	
	A46005_a01: $k = 2 \times k(\text{CH}_3\text{COCHOHOH}+\text{OH})$	
	A460MS_a01: Ryder et al. say that k is the same as for $\text{NO}_2^+ + \text{chloride}$; In reality 6% 4-nitrophenol, 80% 4-nitrosophenol and 14% 2-nitrophenol is formed but we	

A94108b_a01: See branch a.	A96005_a01: Assumed to be the same as for SO_3^{2-} + 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 SO_3^{2-} + 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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