The Chemical Mechanism of MECCA

KPP version: `2.2.3_rs3`

MECCA version: `4.4.2`

Date: 2020-11-09

MECCA config (*.ini) file: `latex.ini`

Integrator: `rosenbrock_posdef`

Gas equation file: `gas.eqn`

Replacement file:

Selected reactions:
“`True`”

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase:	708
Aqueous phase:	482
All species:	1190

Number of reactions in selected mechanism:

Gas phase (Gnnn):	1815
Aqueous phase (Annn):	402
Henry (Hnnn):	735
Photolysis (Jnnn):	385
Aqueous phase photolysis (PHnnn):	27
Heterogeneous (HETnnn):	21
Equilibria (EQnn):	138
Isotope exchange (IEXnnn):	0
Tagging equations (TAGnnn):	0
Dummy (Dnn):	1
All equations:	3524

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.3E-11*EXP(55./temp)	Burkholder et al. (2015)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	6.0E-34*((temp/300.)**(-2.4)) *cair	Burkholder et al. (2015)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2\ O_2$	1.2E-10	Burkholder et al. (2015)*
G1002b	UpG	$O_3 + O(^1D) \rightarrow O_2 + 2\ O(^3P)$	1.2E-10	Burkholder et al. (2015)
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2\ O_2$	8.0E-12*EXP(-2060./temp)	Burkholder et al. (2015)
G1004	UpG	$O_2 + O^+ \rightarrow O_2^+ + O(^3P)$	k_Op_O2(temp,temp_ion)	Fuller-Rowell (1993)
G1101	UpG	$O_2^+ + e^- \rightarrow 2\ O(^3P)$	2.7E-7*(300./temp_elec)**(.7)	Fuller-Rowell (1993)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	k_3rd(temp,cair,4.4E-32,1.3, 7.5E-11,-0.2,0.6)	Burkholder et al. (2015)
G2101	UpStG	$H + O_3 \rightarrow OH + O_2$	1.4E-10*EXP(-470./temp)	Burkholder et al. (2015)
G2102	UpStG	$H_2 + O(^1D) \rightarrow H + OH$	1.2E-10	Burkholder et al. (2015)
G2103	UpStG	$OH + O(^3P) \rightarrow H + O_2$	1.8E-11*EXP(180./temp)	Burkholder et al. (2015)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	1.7E-12*EXP(-940./temp)	Burkholder et al. (2015)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	2.8E-12*EXP(-1800./temp)	Burkholder et al. (2015)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow OH + O_2$	3.E-11*EXP(200./temp)	Burkholder et al. (2015)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	1.E-14*EXP(-490./temp)	Burkholder et al. (2015)
G2108a	UpStG	$HO_2 + H \rightarrow 2\ OH$	7.2E-11	Burkholder et al. (2015)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Burkholder et al. (2015)
G2108c	UpStG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	Burkholder et al. (2015)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	4.8E-11*EXP(250./temp)	Burkholder et al. (2015)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_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)
G2113	UpG	$H_2 + O(^3P) \rightarrow H + OH$	1.60E-11*EXP(-4570./temp)	Roble (1995)
G2114a	UpG	$OH + OH \rightarrow H_2O + O(^3P)$	4.20E-12*EXP(-240./temp)	Sander et al. (2003)
G2114b	UpG	$OH + OH \rightarrow H_2O_2$	k_3rd(temp,cair,6.9E-31,1.0, 2.6E-11,0.,0.6)	Burkholder et al. (2015)
G2115	UpG	$H + H \rightarrow H_2$	5.7E-32*(300./temp)**(1.6)*cair	Roble (1995)
G2116	UpG	$H_2O_2 + O(^3P) \rightarrow OH + HO_2$	1.40E-12*EXP(-2000./temp)	Sander et al. (2003)
G2117	UpStTrG	$H_2O + H_2O \rightarrow (H_2O)_2$	6.521E-26*temp*EXP(1851.09/temp) *EXP(-5.10485E-3*temp)	Scribano et al. (2006)*
G2118	UpStTrG	$(H_2O)_2 \rightarrow H_2O + H_2O$	1.E0	see note*
G3001	UpGN	$NO^+ + e^- \rightarrow .15\ N + .85\ N(^2D) + O(^3P)$	4.2E-7*(300./temp_elec)**(0.85)	Bailey et al. (2002)

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

#	labels	reaction	rate coefficient	reference
G3002	UpGN	$N_2^+ + e^- \rightarrow .88\ N + 1.12\ N(^2D)$	1.8E-7*(temp_elec/300.)**(-0.39)	Swaminathan et al. (1998)
G3003	UpGN	$N(^2D) + e^- \rightarrow N + e^-$	3.8E-12*(temp_elec)**(.81)	Swaminathan et al. (1998)
G3100	UpStGN	$N + O_2 \rightarrow NO + O(^3P)$	1.5E-11*EXP(-3600./temp)	Burkholder et al. (2015)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	2.15E-11*EXP(110./temp)	Burkholder et al. (2015)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow 2\ NO$	7.259E-11*EXP(20./temp)	Burkholder et al. (2015)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.641E-11*EXP(20./temp)	Burkholder et al. (2015)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.0E-12*EXP(-1500./temp)	Burkholder et al. (2015)
G3104	UpStGN	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Burkholder et al. (2015)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.1E-12*EXP(210./temp)	Burkholder et al. (2015)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Burkholder et al. (2015)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./temp)	Burkholder et al. (2015)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Burkholder et al. (2015)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Burkholder et al. (2015)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(5.8E-27*EXP(10840./temp))	Burkholder et al. (2015)*
G3111	UpGN	$N(^2D) + NO \rightarrow N_2 + O(^3P)$	6.70E-11	Fuller-Rowell (1993)
G3112	UpGN	$N(^2D) + O_2 \rightarrow NO + O(^3P)$	6.20E-12*(temp/300.)	Duff et al. (2003)
G3113	UpGN	$N(^2D) + O(^3P) \rightarrow N + O(^3P)$	6.90E-13	Fell et al. (1990)
G3114	UpGN	$N(^2D) + O_3 \rightarrow NO + O_2$	0.80E-16	Sander et al. (2003)
G3115	UpGN	$NO + O(^3P) \rightarrow NO_2$	k_3rd(temp,cair,9.0E-32,1.5,3.0E-11,0.0,0.6)	Burkholder et al. (2015)
G3116	UpGN	$NO_2 + O(^3P) \rightarrow NO_3$	k_3rd(temp,cair,2.5E-31,1.8,2.2E-11,0.7,0.6)	Burkholder et al. (2015)
G3117	UpGN	$N(^2D) \rightarrow N$	10.6	Fuller-Rowell (1993)
G3118	UpGN	$N^+ + O_2 \rightarrow NO + O^+$	3.66E-11	Barth (1992)
G3119	UpGN	$N_2^+ + O(^3P) \rightarrow NO^+ + N(^2D)$	k_N2_O(temp,temp_ion)	Fuller-Rowell (1993)
G3120a	UpGN	$N^+ + O_2 \rightarrow NO^+ + O(^3P)$	2.60E-10	Fuller-Rowell (1993)
G3120b	UpGN	$N^+ + O_2 \rightarrow O_2^+ + N$	3.10E-10	Swaminathan et al. (1998)
G3121	UpGN	$N^+ + O(^3P) \rightarrow O^+ + N$	1.00E-12	Fuller-Rowell (1993)
G3122	UpGN	$O_2^+ + N \rightarrow NO^+ + O(^3P)$	1.20E-10	Fuller-Rowell (1993)
G3123	UpGN	$O_2^+ + NO \rightarrow NO^+ + O_2$	4.40E-10	Fuller-Rowell (1993)
G3124	UpGN	$O^+ + N_2 \rightarrow NO^+ + N$	k_Op_N2(temp,temp_ion)	Fuller-Rowell (1993)
G3125	UpGN	$N_2^+ + O_2 \rightarrow N_2 + O_2^+$	5.10E-11*(temp/300.)**(-0.8)	Fuller-Rowell (1993)
G3200	TrGN	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.0E-31,2.6,3.6E-11,0.1,0.6)	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G3201	UpStTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.3E-12*EXP(270./temp)	Burkholder et al. (2015)
G3202a	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	(1.-alpha_HOONO) * k_NO2_OH	Amedro et al. (2020)
G3202b	UpStTrGN	$NO_2 + OH \rightarrow HOONO$	alpha_HOONO * k_NO2_OH	Amedro et al. (2020)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_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_HNO3_OH	Dulitz et al. (2018)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_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)
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	1.7E-12*EXP(-710./temp)	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow NH_2O + O_2$	4.3E-12*EXP(-930./temp)	Kohlmann and Poppe (1999)
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	4.8E-07*EXP(-628./temp)*(temp)**(-1.32)	Kohlmann and Poppe (1999)
G3212	TrGN	$NH_2 + HO_2 \rightarrow HNO + H_2O$	9.4E-09*EXP(-356./temp)*(temp)**(-1.12)	Kohlmann and Poppe (1999)
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	1.92E-12*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3214	TrGN	$NH_2 + NO \rightarrow N_2 + H_2O$	1.41E-11*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3215	TrGN	$NH_2 + NO_2 \rightarrow N_2O + H_2O$	1.2E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3216	TrGN	$NH_2 + NO_2 \rightarrow NH_2O + NO$	0.8E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3217	TrGN	$NH_2O + O_3 \rightarrow NH_2 + O_2$	1.2E-14	Kohlmann and Poppe (1999)
G3218	TrGN	$NH_2O \rightarrow NHOH$	1.3E3	Kohlmann and Poppe (1999)
G3219	TrGN	$HNO + OH \rightarrow NO + H_2O$	8.0E-11*EXP(-500./temp)	Kohlmann and Poppe (1999)
G3220	TrGN	$HNO + NHOH \rightarrow NH_2OH + NO$	1.66E-12*EXP(-1500./temp)	Kohlmann and Poppe (1999)
G3221	TrGN	$HNO + NO_2 \rightarrow HONO + NO$	1.0E-12*EXP(-1000./temp)	Kohlmann and Poppe (1999)
G3222	TrGN	$NHOH + OH \rightarrow HNO + H_2O$	1.66E-12	Kohlmann and Poppe (1999)
G3223	TrGN	$NH_2OH + OH \rightarrow NHOH + H_2O$	4.13E-11*EXP(-2138./temp)	Kohlmann and Poppe (1999)
G3224	TrGN	$HNO + O_2 \rightarrow HO_2 + NO$	3.65E-14*EXP(-4600./temp)	Kohlmann and Poppe (1999)
G3225	UpGN	$N + OH \rightarrow NO + H$	5.00E-11	Roble (1995)
G3226	UpGN	$NO_2 + H \rightarrow NO + OH$	4.00E-10*EXP(-340./temp)	Sander et al. (2003)
G3227	UpStTrGN	$HOONO \rightarrow NO_2 + OH$	(alpha_HOONO*k_NO2_OH)/(3.5E-27*EXP(10135./temp))	see note*
G3228	UpStTrGN	$HOONO + OH \rightarrow H_2O + NO_3$	1.3E-12*EXP(380./temp)	Burkholder et al. (2015)*
G4100	UpStG	$CH_4 + O(^1D) \rightarrow .75\ CH_3 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	1.75E-10	Burkholder et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G4101	StTrG	$CH_4 + OH \rightarrow CH_3 + H_2O$	`1.85E-20*EXP(2.82*LOG(temp) -987./temp)`	Atkinson (2003)
G4102	TrG	$CH_3OH + OH \rightarrow .85\ HCHO + .85\ HO_2 + .15\ CH_3O + H_2O$	`6.38E-18*((temp)**2)*EXP(144./temp)`	Atkinson et al. (2006)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	`3.8E-13*EXP(780./temp)/(1.+1./498.*EXP(1160./temp))`	Atkinson et al. (2006)
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	`3.8E-13*EXP(780./temp)/(1.+498.*EXP(-1160./temp))`	Atkinson et al. (2006)
G4104a	StTrGN	$CH_3O_2 + NO \rightarrow CH_3O + NO_2$	`2.3E-12*EXP(360./temp)*(1.-beta_CH3NO3)`	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$CH_3O_2 + NO \rightarrow CH_3ONO_2$	`2.3E-12*EXP(360./temp)*beta_CH3NO3`	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow CH_3O + NO_2 + O_2$	`1.2E-12`	Atkinson et al. (2006)
G4106a	StTrG	$CH_3O_2 \rightarrow CH_3O + .5\ O_2$	`7.4E-13*EXP(-520./temp)*RO2*2.`	Atkinson et al. (2006)
G4106b	StTrG	$CH_3O_2 \rightarrow .5\ HCHO + .5\ CH_3OH + .5\ O_2$	`(k_CH3O2-7.4E-13*EXP(-520./temp))*RO2*2.`	Atkinson et al. (2006)
G4107	StTrG	$CH_3OOH + OH \rightarrow .6\ CH_3O_2 + .4\ HCHO + .4\ OH + H_2O$	`k_CH3OOH_OH`	Wallington et al. (2018)
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*LOG(temp) +636./temp)`	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Burkholder et al. (2015)*
G4110	UpStTrG	$CO + OH \rightarrow H + CO_2$	`(1.57E-13+cair*3.54E-33)`	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow CO_2 + HO_2 + H_2O$	`2.94E-14*exp(786./temp) +9.85E-13*EXP(-1036./temp)`	Paulot et al. (2011)
G4112	UpStG	$CO + O(^3P) \rightarrow CO_2$	`6.60E-33*EXP(-1103./temp)`	Roble (1995)
G4113	UpStG	$CH_4 + O(^3P) \rightarrow .51\ CH_3 + .51\ OH + .49\ CH_3O + .49\ H$	`6.03E-18*(temp)**(2.17) *EXP(-3619./temp)`	Roble (1995), Garton et al. (2003), Espinosa-Garcia and Garcia-Bernáldez (2000)
G4114	StTrGN	$CH_3O_2 + NO_2 \rightarrow CH_3O_2NO_2$	`k_NO2_CH3O2`	Burkholder et al. (2015)
G4115	StTrGN	$CH_3O_2NO_2 \rightarrow CH_3O_2 + NO_2$	`k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))`	Burkholder et al. (2015)*
G4116	StTrGN	$CH_3O_2NO_2 + OH \rightarrow HCHO + NO_3 + H_2O$	`3.00E-14`	see note*
G4117	StTrGN	$CH_3ONO_2 + OH \rightarrow H_2O + HCHO + NO_2$	`4.0E-13*EXP(-845./temp)`	Atkinson et al. (2006)
G4118	StTrG	$CH_3O \rightarrow HO_2 + HCHO$	`1.3E-14*exp(-663./temp)*c(ind_O2)`	Chai et al. (2014)

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

#	labels	reaction	rate coefficient	reference
G4119a	StTrGN	$CH_3O + NO_2 \rightarrow CH_3ONO_2$	k_3rd_iupac(temp,cair,8.1E-29, 4.5,2.1E-11,0.,0.44)	Atkinson et al. (2006)
G4119b	StTrGN	$CH_3O + NO_2 \rightarrow HCHO + HONO$	9.6E-12*EXP(-1150./temp)	Atkinson et al. (2006)
G4120a	StTrGN	$CH_3O + NO \rightarrow CH_3ONO$	k_3rd_iupac(temp,cair,2.6E-29, 2.8,3.3E-11,0.6,REAL(EXP(-temp/ 900.),SP))	Atkinson et al. (2006)
G4120b	StTrGN	$CH_3O + NO \rightarrow HCHO + HNO$	2.3E-12*(temp/300.)**(0.7)	Atkinson et al. (2006)
G4121	StTrG	$CH_3O_2 + O_3 \rightarrow CH_3O + 2\ O_2$	2.9E-16*exp(-1000./temp)	Burkholder et al. (2015)
G4122	StTrGN	$CH_3ONO + OH \rightarrow H_2O + HCHO + NO$	1.E-10*exp(-1764./temp)	Nielsen et al. (1991)
G4123	StTrG	$HCHO + HO_2 \rightarrow HOCH_2O_2$	9.7E-15*EXP(625./temp)	Atkinson et al. (2006)
G4124	StTrG	$HOCH_2O_2 \rightarrow HCHO + HO_2$	2.4E12*EXP(-7000./temp)	Atkinson et al. (2006)
G4125	StTrG	$HOCH_2O_2 + HO_2 \rightarrow .5\ HOCH_2OOH + .5\ HCOOH + .2\ OH + .2\ HO_2 + .3\ H_2O + .8\ O_2$	5.6E-15*EXP(2300./temp)	Atkinson et al. (2006)
G4126	StTrGN	$HOCH_2O_2 + NO \rightarrow NO_2 + HO_2 + HCOOH$	0.7275*2.3E-12*EXP(360./temp)	Atkinson et al. (2006)*
G4127	StTrGN	$HOCH_2O_2 + NO_3 \rightarrow NO_2 + HO_2 + HCOOH$	1.2E-12	see note*
G4129a	StTrG	$HOCH_2O_2 \rightarrow HCOOH + HO_2$	(k_CH3O2*5.5E-12)**(0.5)*RO2*2.	Atkinson et al. (2006)
G4129b	StTrG	$HOCH_2O_2 \rightarrow .5\ HCOOH + .5\ HOCH_2OH + .5\ O_2$	(k_CH3O2*5.7E-14*EXP(750./temp)) **(0.5)*RO2*2.	Atkinson et al. (2006)
G4130a	StTrG	$HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$	k_ROOHRO	Taraborrelli (2010)*
G4130b	StTrG	$HOCH_2OOH + OH \rightarrow HCOOH + H_2O + OH$	k_ROHRO + k_s*f_sOOH*f_sOH	Taraborrelli (2010)*
G4132	StTrG	$HOCH_2OH + OH \rightarrow HO_2 + HCOOH + H_2O$	2.*k_ROHRO + k_s*f_sOH*f_sOH	Taraborrelli (2010)*
G4133	StTrG	$CH_3O_2 + OH \rightarrow CH_3O + HO_2$	1.4E-10	Bossolasco et al. (2014)*
G4134	StTrG	$CH_2OO \rightarrow CO + HO_2 + OH$	1.124E+14*EXP(-10000./temp)	see note*
G4135	StTrG	$CH_2OO + H_2O \rightarrow HOCH_2OOH$	k_CH2OO_NO2*3.6E-6	Ouyang et al. (2013)*
G4136	StTrG	$CH_2OO + (H_2O)_2 \rightarrow HOCH_2OOH + H_2O$	5.2E-12	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$CH_2OO + NO \rightarrow HCHO + NO_2$	6.E-14	Welz et al. (2012)*
G4138	StTrGN	$CH_2OO + NO_2 \rightarrow HCHO + NO_3$	k_CH2OO_NO2	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$CH_2OO + CO \rightarrow HCHO + CO_2$	3.6E-14	Vereecken et al. (2012)
G4141	StTrG	$CH_2OO + HCOOH \rightarrow 2\ HCOOH$	1.E-10	Welz et al. (2014)*
G4142	StTrG	$CH_2OO + HCHO \rightarrow 2\ LCARBON$	1.7E-12	Stone et al. (2014)*
G4143	StTrG	$CH_2OO + CH_3OH \rightarrow 2\ LCARBON$	5.E-12	Vereecken et al. (2012)*
G4144	StTrG	$CH_2OO + CH_3O_2 \rightarrow 2\ LCARBON$	5.E-12	Vereecken et al. (2012)*
G4145	StTrG	$CH_2OO + HO_2 \rightarrow LCARBON$	5.E-12	Vereecken et al. (2012)

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

#	labels	reaction	rate coefficient	reference
G4146	StTrG	$CH_2OO + O_3 \rightarrow HCHO + 2\ O_2$	`1.E-12`	Vereecken et al. (2014)
G4147	StTrG	$CH_2OO + CH_2OO \rightarrow 2\ HCHO + O_2$	`6.E-11`	Buras et al. (2014)
G4148	StTrGN	$HOCH_2O_2 + NO_2 \rightarrow HOCH_2O_2NO_2$	`k_NO2_CH3O2`	see note*
G4149	StTrGN	$HOCH_2O_2NO_2 \rightarrow HOCH_2O_2 + NO_2$	`k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))`	Barnes et al. (1985)*
G4150	StTrGN	$HOCH_2O_2NO_2 + OH \rightarrow HCOOH + NO_3 + H_2O$	`9.50E-13*EXP(-650./temp)*f_sOH`	see note*
G4151	StTrG	$CH_3 + O_2 \rightarrow CH_3O_2$	`k_3rd_iupac(temp,cair,7.0E-31,3.,1.8E-12,-1.1,0.33)`	Atkinson et al. (2006)
G4152	StTrG	$CH_3 + O_3 \rightarrow .956\ HCHO + .956\ H + .044\ CH_3O + O_2$	`5.1E-12*exp(-210./temp)`	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$CH_3 + O(^3P) \rightarrow .83\ HCHO + .83\ H + .17\ CO + .17\ H_2 + .17\ H$	`1.3E-10`	Atkinson et al. (2006)
G4154	StTrG	$CH_3O + O_3 \rightarrow CH_3O_2 + O_2$	`2.53E-14`	Albaladejo et al. (2002)*
G4155	StTrG	$CH_3O + O(^3P) \rightarrow .75\ CH_3 + .75\ O_2 + .25\ HCHO + .25\ OH$	`2.5E-11`	Baulch et al. (2005)
G4156	StTrG	$CH_3O_2 + O(^3P) \rightarrow CH_3O + O_2$	`4.3E-11`	Zellner et al. (1988)
G4157	StTrG	$HCHO + O(^3P) \rightarrow .7\ OH + .7\ CO + .3\ H + .3\ CO_2 + HO_2$	`3.4E-11*EXP(-1600./temp)`	Burkholder et al. (2015)
G4158	TrG	$CH_2OO^* \rightarrow .37\ CH_2OO + .47\ CO + .47\ H_2O + .16\ HO_2 + .16\ CO + .16\ OH$	`KDEC`	Atkinson et al. (2006)
G4159	TrGN	$HCN + OH \rightarrow H_2O + CN$	`k_3rd(temp,cair,4.28E-33,1.0,REAL(4.25E-13*EXP(-1150./temp),SP),1.0,0.8)`	Kleinböhl et al. (2006)
G4160a	TrGN	$HCN + O(^1D) \rightarrow O(^3P) + HCN$	`1.08E-10*EXP(105./temp)*0.15*EXP(200./temp)`	Strekowski et al. (2010)
G4160b	TrGN	$HCN + O(^1D) \rightarrow H + NCO$	`1.08E-10*EXP(105./temp)*0.68/2.`	Strekowski et al. (2010)*
G4160c	TrGN	$HCN + O(^1D) \rightarrow OH + CN$	`1.08E-10*EXP(105./temp)*(1.-(0.68/2.+0.15*EXP(200./temp)))`	Strekowski et al. (2010)*
G4161	TrGN	$HCN + O(^3P) \rightarrow H + NCO$	`1.0E-11*EXP(-4000./temp)`	Burkholder et al. (2015)*
G4162	TrGN	$CN + O_2 \rightarrow NCO + O(^3P)$	`1.2E-11*EXP(210./temp)*0.75`	Baulch et al. (2005)
G4163	TrGN	$CN + O_2 \rightarrow CO + NO$	`1.2E-11*EXP(210./temp)*0.25`	Baulch et al. (2005)
G4164	TrGN	$NCO + O_2 \rightarrow CO_2 + NO$	`7.E-15`	Becker et al. (2000)*
G42000	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	`1.49E-17*temp*temp*EXP(-499./temp)`	Atkinson et al. (2006)
G42001	TrGC	$C_2H_4 + O_3 \rightarrow HCHO + CH_2OO^*$	`9.1E-15*EXP(-2580./temp)`	Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G42002	TrGC	$C_2H_4 + OH \rightarrow HOCH_2CH_2O_2$	k_3rd_iupac(temp,cair,8.6E-29, 3.1,9.E-12,0.85,0.48)	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42003	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*EXP(700./temp)	Burkholder et al. (2015)
G42004a	TrGCN	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	2.55E-12*EXP(380./temp)*(1.-beta_ C2H5NO3)	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$C_2H_5O_2 + NO \rightarrow C_2H_5ONO_2$	2.55E-12*EXP(380./temp)*beta_ C2H5NO3	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42005	TrGCN	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	2.3E-12	Wallington et al. (2018)
G42006	TrGC	$C_2H_5O_2 \rightarrow .8\ CH_3CHO + .6\ HO_2 + .2\ C_2H_5OH$	2.*(7.6E-14*k_CH3O2)**(.5)*RO2	Sander et al. (2019), Atkinson et al. (2006)
G42007a	TrGC	$C_2H_5OOH + OH \rightarrow C_2H_5O_2 + H_2O$	k_ROOHRO	Sander et al. (2019)
G42007b	TrGC	$C_2H_5OOH + OH \rightarrow CH_3CHO + OH$	k_s*f_sOOH	Sander et al. (2019)
G42008a	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O) + H_2O$	4.4E-12*EXP(365./temp)*0.95	Atkinson et al. (2006)
G42008b	TrGC	$CH_3CHO + OH \rightarrow HCOCH_2O_2 + H_2O$	4.4E-12*EXP(365./temp)*0.05	Atkinson et al. (2006)
G42009	TrGCN	$CH_3CHO + NO_3 \rightarrow CH_3C(O) + HNO_3$	KNO3AL	Rickard and Pascoe (2009)
G42010	TrGC	$CH_3COOH + OH \rightarrow CH_3 + CO_2 + H_2O$	k_CH3CO2H_OH	Atkinson et al. (2006)*
G42011a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow OH + CH_3 + CO_2$	5.20E-13*EXP(980./temp)*1.507*0.61	Groß et al. (2014)
G42011b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	5.20E-13*EXP(980./temp)*1.507*0.23	Groß et al. (2014)
G42011c	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	5.20E-13*EXP(980./temp)*1.507*0.16	Groß et al. (2014)
G42012	TrGCN	$CH_3C(O)OO + NO \rightarrow CH_3 + CO_2 + NO_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001a)
G42013	TrGCN	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_CH3CO3_NO2	Burkholder et al. (2015)*
G42014	TrGCN	$CH_3C(O)OO + NO_3 \rightarrow CH_3 + NO_2 + CO_2$	4.E-12	Canosa-Mas et al. (1996)
G42017a	TrGC	$CH_3C(O)OO \rightarrow CH_3 + CO_2$	k1_RO2RCO3*0.9	Sander et al. (2019)
G42017b	TrGC	$CH_3C(O)OO \rightarrow CH_3COOH$	k1_RO2RCO3*0.1	Sander et al. (2019)
G42018	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	k_ROOHRO	Rickard and Pascoe (2009)*
G42020	TrGCN	$PAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	3.00E-14	Rickard and Pascoe (2009)
G42021	TrGCN	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_PAN_M	Burkholder et al. (2015)*
G42022a	TrGC	$C_2H_2 + OH \rightarrow GLYOX + OH$	k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,-2.,0.6)*0.71	Burkholder et al. (2015)*
G42022b	TrGC	$C_2H_2 + OH \rightarrow HCOOH + CO + HO_2$	k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,-2.,0.6)*0.29	Burkholder et al. (2015)*
G42023a	TrGC	$HOCH_2CHO + OH \rightarrow HOCH2CO + H_2O$	8.00E-12*0.80	Atkinson et al. (2006)
G42023b	TrGC	$HOCH_2CHO + OH \rightarrow HOCHCHO + H_2O$	8.00E-12*0.20	Atkinson et al. (2006)
G42024a	TrGC	$HOCH2CO + O_2 \rightarrow HOCH_2CO_3$	5.1E-12*(1.-1./(1+1.85E-18*cair))	Atkinson et al. (2006), Beyersdorf et al. (2010)*

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

#	labels	reaction	rate coefficient	reference
G42024b	TrGC	HOCH2CO + O_2 → OH + HCHO + CO_2	`5.1E-12*1./(1+1.85E-18*cair)`	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42025	TrGC	HOCHCHO → GLYOX + HO_2	`KDEC`	Sander et al. (2019)
G42026	TrGCN	$HOCH_2CHO$ + NO_3 → HOCH2CO + HNO_3	`KNO3AL`	Rickard and Pascoe (2009)
G42027a	TrGC	$HOCH_2CO_3$ → HCHO + CO_2 + HO_2	`k1_RO2RCO3*0.9`	Sander et al. (2019)
G42027b	TrGC	$HOCH_2CO_3$ → $HOCH_2CO_2H$	`k1_RO2RCO3*0.1`	Sander et al. (2019)
G42028a	TrGC	$HOCH_2CO_3$ + HO_2 → HCHO + HO_2 + OH + CO_2	`KAPHO2*r_CO3_OH`	Sander et al. (2019), Groß et al. (2014)
G42028b	TrGC	$HOCH_2CO_3$ + HO_2 → $HOCH_2CO_3H$	`KAPHO2*r_CO3_OOH`	Sander et al. (2019), Groß et al. (2014)
G42028c	TrGC	$HOCH_2CO_3$ + HO_2 → $HOCH_2CO_2H$ + O_3	`KAPHO2*r_CO3_O3`	Sander et al. (2019), Groß et al. (2014)
G42029	TrGCN	$HOCH_2CO_3$ + NO → NO_2 + HO_2 + HCHO + CO_2	`KAPNO`	Rickard and Pascoe (2009)
G42030	TrGCN	$HOCH_2CO_3$ + NO_2 → PHAN	`k_CH3CO3_NO2`	Rickard and Pascoe (2009)
G42031	TrGCN	$HOCH_2CO_3$ + NO_3 → NO_2 + HO_2 + HCHO + CO_2	`KRO2NO3*1.74`	Rickard and Pascoe (2009)
G42032	TrGC	$HOCH_2CO_2H$ + OH → .09 HCHO + .09 CO_2 + .91 $HCOCO_2H$ + HO_2 + H_2O	`k_CO2H+k_s*f_sOH*f_CO2H`	Sander et al. (2019)
G42033a	TrGC	$HOCH_2CO_3H$ + OH → $HOCH_2CO_3$ + H_2O	`k_ROOHRO`	Sander et al. (2019)
G42033b	TrGC	$HOCH_2CO_3H$ + OH → $HCOCO_3H$ + HO_2	`k_s*f_sOH*f_CO2H`	Sander et al. (2019)
G42034	TrGCN	PHAN → $HOCH_2CO_3$ + NO_2	`k_PAN_M`	Rickard and Pascoe (2009)
G42035	TrGCN	PHAN + OH → HCHO + CO + NO_2 + H_2O	`k_s*f_sOH*f_cpan+k_ROHRO`	Sander et al. (2019)
G42036	TrGC	GLYOX + OH → HCOCO + H_2O	`3.1E-12*EXP(340./temp)`	Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013)
G42037	TrGCN	GLYOX + NO_3 → HCOCO + HNO_3	`KNO3AL`	Rickard and Pascoe (2009)
G42038a	TrGC	HCOCO → CO + CO + HO_2	`7.E11*EXP(-3160./temp) +5.E-12*c(ind_O2)`	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	HCOCO → $HCOCO_3$	`5.E-12*c(ind_O2)*3.2*exp(-550./temp)`	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	HCOCO → OH + CO + CO_2	`5.E-12*c(ind_O2)*(1.-3.2*exp(-550./temp))`	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	$HCOCO_3$ → CO + HO_2 + CO_2	`k1_RO2RCO3*0.9`	Sander et al. (2019)
G42039b	TrGC	$HCOCO_3$ → $HCOCO_2H$	`k1_RO2RCO3*0.1`	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G42040	TrGC	$HCOCO_3 + HO_2 \rightarrow HO_2 + CO + CO_2 + OH$	KAPHO2	Feierabend et al. (2008), Sander et al. (2019)
G42041	TrGCN	$HCOCO_3 + NO \rightarrow HO_2 + CO + NO_2 + CO_2$	KAPNO	Rickard and Pascoe (2009)
G42042	TrGCN	$HCOCO_3 + NO_3 \rightarrow HO_2 + CO + NO_2 + CO_2$	KRO2NO3*1.74	Rickard and Pascoe (2009)
G42043	TrGCN	$HCOCO_3 + NO_2 \rightarrow HO_2 + CO + NO_3 + CO_2$	k_CH3CO3_NO2	Orlando and Tyndall (2001), Sander et al. (2019)
G42044	TrGC	$HCOCO_2H + OH \rightarrow CO + HO_2 + CO_2 + H_2O$	k_CO2H+k_t*f_O*f_CO2H	Sander et al. (2019)
G42045a	TrGC	$HCOCO_3H + OH \rightarrow HCOCO_3 + H_2O$	k_ROOHRO	Sander et al. (2019)
G42045b	TrGC	$HCOCO_3H + OH \rightarrow CO + CO_2 + H_2O + OH$	k_t*f_O*f_CO2H	Sander et al. (2019)
G42046	TrGC	$HOCH_2CH_2O_2 \rightarrow .6\ HOCH_2CH_2O + .2\ HOCH_2CHO + .2$ ETHGLY	2.*(7.8E-14*EXP(1000./temp) *k_CH3O2)**(.5)*RO2	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	$HOCH_2CH_2O_2 + NO \rightarrow .25\ HO_2 + .5\ HCHO + .75\ HOCH_2CH_2O + NO_2$	KRO2NO*(1.-alpha_AN(3,1,0,0,0, temp,cair))	Rickard and Pascoe (2009)*
G42048	TrGCN	$HOCH_2CH_2O_2 + NO \rightarrow$ ETHOHNO3	KRO2NO*alpha_AN(3,1,0,0,0,temp, cair)	Sander et al. (2019)
G42049a	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow$ HYETHO2H	1.53E-13*EXP(1300./temp) *(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G42049b	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow HOCH_2CH_2O + OH$	1.53E-13*EXP(1300./temp) *r_CHOHCH2O2_OH	Rickard and Pascoe (2009)
G42050	TrGCN	ETHOHNO3 + OH $\rightarrow .93\ NO_3$CH2CHO $+ .93\ HO_2 + .07\ HOCH_2CHO + .07\ NO_2 + H_2O$	k_s*(f_sOH*f_CH2ONO2+f_ONO2*f_ pCH2OH)+k_ROHRO	Sander et al. (2019)
G42051a	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CH_2O_2 + H_2O$	k_ROOHRO	Rickard and Pascoe (2009)*
G42051b	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CHO + OH + H_2O$	k_s*f_sOOH*f_pCH2OH	Sander et al. (2019)
G42051c	TrGC	HYETHO2H + OH $\rightarrow$ HOOCH2CHO $+ HO_2 + H_2O$	k_s*f_sOH*f_pCH2OH+k_ROHRO	Sander et al. (2019)
G42052a	TrGC	$HOCH_2CH_2O \rightarrow HO_2 + HOCH_2CHO$	6.00E-14*EXP(-550./temp) *C(ind_O2)	Rickard and Pascoe (2009)
G42052b	TrGC	$HOCH_2CH_2O \rightarrow HO_2 + HCHO + HCHO$	9.50E13*EXP(-5988./temp)	Rickard and Pascoe (2009)
G42053	TrGC	ETHGLY + OH $\rightarrow HOCH_2CHO + HO_2 + H_2O$	2.*k_s*f_sOH*f_pCH2OH+2.*k_ROHRO	Sander et al. (2019)
G42054	TrGC	$HCOCH_2O_2 \rightarrow .6\ HCHO + .6\ CO + .6\ HO_2 + .2$ GLYOX $+ .2\ HOCH_2CHO$	k1_RO2pORO2	Sander et al. (2019)
G42055a	TrGC	$HCOCH_2O_2 + HO_2 \rightarrow$ HOOCH2CHO	k_RO2_HO2(temp,2)*r_COCH2O2_OOH	Sander et al. (2019)
G42055b	TrGC	$HCOCH_2O_2 + HO_2 \rightarrow HCHO + CO + HO_2 + OH$	k_RO2_HO2(temp,2)*r_COCH2O2_OH	Sander et al. (2019)
G42056a	TrGCN	$HCOCH_2O_2 + NO \rightarrow NO_2 + HCHO + CO + HO_2$	KRO2NO*(1.-alpha_AN(3,1,1,0,0, temp,cair))	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G42056b	TrGCN	$HCOCH_2O_2$ + NO → NO_3CH2CHO	KRO2NO*alpha_AN(3,1,1,0,0,temp, cair)	Sander et al. (2019)
G42057	TrGCN	$HCOCH_2O_2$ + NO_3 → HCHO + CO + HO_2 + NO_2	KRO2NO3	Sander et al. (2019)
G42058a	TrGC	HOOCH2CHO + OH → $HCOCH_2O_2$	k_ROOHRO	Sander et al. (2019)
G42058b	TrGC	HOOCH2CHO + OH → HCHO + CO + OH	0.8*8.E-12	Sander et al. (2019)*
G42058c	TrGC	HOOCH2CHO + OH → GLYOX + OH	k_s*f_sOOH*f_CHO	Sander et al. (2019)
G42059	TrGCN	HOOCH2CHO + NO_3 → OH + HCHO + CO + HNO_3	KNO3AL	Rickard and Pascoe (2009)
G42060	TrGCN	$HOOCH_2CO_3$ + NO → NO_2 + OH + HCHO + CO_2	KAPNO	Sander et al. (2019)
G42061	TrGCN	$HOOCH_2CO_3$ + NO_3 → NO_2 + OH + HCHO + CO_2	KRO2NO3*1.74	Sander et al. (2019)
G42062a	TrGC	$HOOCH_2CO_3$ + HO_2 → 2 OH + HCHO + CO_2	KAPHO2*r_CO3_OH	Sander et al. (2019)
G42062b	TrGC	$HOOCH_2CO_3$ + HO_2 → HOOCH2CO3H	KAPHO2*r_CO3_OOH	Sander et al. (2019)
G42062c	TrGC	$HOOCH_2CO_3$ + HO_2 → HOOCH2CO2H + O_3	KAPHO2*r_CO3_O3	Sander et al. (2019)
G42063a	TrGC	$HOOCH_2CO_3$ → OH + HCHO + CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G42063b	TrGC	$HOOCH_2CO_3$ → HOOCH2CO2H	k1_RO2RCO3*0.1	Sander et al. (2019)
G42064a	TrGC	HOOCH2CO3H + OH → $HOOCH_2CO_3$ + H_2O	2.*k_ROOHRO	Sander et al. (2019)
G42064b	TrGC	HOOCH2CO3H + OH → $HCOCO_3H$ + OH + H_2O	k_s*f_sOOH*f_CO2H	Sander et al. (2019)
G42065	TrGC	HOOCH2CO2H + OH → $HCOCO_2H$ + OH + H_2O	k_s*f_sOOH*f_CO2H+k_CO2H	Sander et al. (2019)
G42066	TrGC	CH2CO + OH → .6 HCHO + .6 HO_2 + .6 CO + .4 HOOCH2CO2H	2.8E-12*exp(510./temp)	Baulch et al. (2005), Sander et al. (2019)
G42067a	TrGC	CH3CHOHOOH + OH → CH_3COOH + OH	(k_t*f_tOOH*f_tOH + k_ROHRO)	Sander et al. (2019)
G42067b	TrGC	CH3CHOHOOH + OH → CH3CHOHO2	k_ROOHRO	Sander et al. (2019)
G42068	TrGC	CH3CHOHO2 → CH_3CHO + HO_2	3.46E12*EXP(-12500./(1.98*temp))	Hermans et al. (2005), Sander et al. (2019)
G42069	TrGC	CH_3CHO + HO_2 → CH3CHOHO2	3.46E12*EXP(-12500./(1.98*temp)) /(6.34E26*EXP(-14700./ (1.98*temp)))	Hermans et al. (2005), Sander et al. (2019)
G42070	TrGC	CH3CHOHO2 + HO_2 → .5 CH3CHOHOOH + .3 CH_3COOH + .2 CH_3 + .2 HCOOH + .2 OH	5.6E-15*EXP(2300./temp)	Sander et al. (2019)
G42071	TrGC	CH3CHOHO2 → CH_3 + HCOOH + OH	k1_RO2sORO2	Sander et al. (2019)
G42072	TrGCN	CH3CHOHO2 + NO → CH_3 + HCOOH + OH + NO_2	KRO2NO	Sander et al. (2019)
G42073	TrGCN	$C_2H_5ONO_2$ + OH → CH_3CHO + H_2O + NO_2	6.7E-13*EXP(-395./temp)	Atkinson et al. (2006)
G42074a	TrGCN	NO_3CH2CHO + OH → GLYOX + NO_2 + H_2O	k_s*f_CH2ONO2*f_CHO	Paulot et al. (2009a), Sander et al. (2019)*
G42074b	TrGCN	NO_3CH2CHO + OH → NO_3CH2CO_3 + H_2O	k_t*f_O*f_CH2ONO2*3.	Paulot et al. (2009a), Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G42075	TrGCN	$NO_3CH2CO_3 + HO_2 \rightarrow HCHO + NO_2 + CO_2 + OH$	`KAPHO2`	Rickard and Pascoe (2009)*
G42076	TrGCN	$NO_3CH2CO_3 + NO \rightarrow HCHO + NO_2 + CO_2 + NO_2$	`KAPNO`	Rickard and Pascoe (2009)
G42077	TrGCN	$NO_3CH2CO_3 + NO_2 \rightarrow NO_3CH2CHO$	`k_CH3CO3_NO2`	Rickard and Pascoe (2009)
G42078	TrGCN	$NO_3CH2CO_3 \rightarrow HCHO + NO_2 + CO_2$	`k1_RO2RCO3`	Rickard and Pascoe (2009)*
G42079	TrGCN	$NO_3CH2CHO \rightarrow NO_3CH2CO_3 + NO_2$	`k_PAN_M`	Rickard and Pascoe (2009)
G42080	StTrGCN	$C_2H_5O_2 + NO_2 \rightarrow C_2H_5O_2NO_2$	`k_3rd_iupac(temp,cair,1.3E-29, 6.2,8.8E-12,0.0,0.31)`	Atkinson et al. (2006)
G42081	StTrGCN	$C_2H_5O_2NO_2 \rightarrow C_2H_5O_2 + NO_2$	`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	$C_2H_5O_2NO_2 + OH \rightarrow CH_3CHO + NO_3 + H_2O$	`9.50E-13*EXP(-650./temp)`	Sander et al. (2019)*
G42083a	TrGC	$CH_3C(O) + O_2 \rightarrow CH_3C(O)OO$	`5.1E-12*(1. - 1./(1.+ 9.4E-18*cair))`	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42083b	TrGC	$CH_3C(O) + O_2 \rightarrow OH + HCHO + CO$	`5.1E-12*1./(1.+9.4E-18*cair)`	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42084	TrGC	$C_2H_5OH + OH \rightarrow .95\ C_2H_5O_2 + .95\ HO_2 + .05\ HOCH_2CH_2O_2 + H_2O$	`3.0E-12*EXP(20./temp)`	Sander et al. (2019), Atkinson et al. (2006)
G42085a	TrGCN	$CH_3CN + OH \rightarrow NCCH_2O_2 + H_2O$	`8.1E-13*EXP(-1080./temp)*0.40`	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42085b	TrGCN	$CH_3CN + OH \rightarrow OH + CH_3C(O) + NO$	`8.1E-13*EXP(-1080./temp)*(1.-0.40)`	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$CH_3CN + O(^1D) \rightarrow O(^3P) + CH_3CN$	`2.54E-10*EXP(-24./temp) *0.0269*EXP(137./temp)`	Strekowski et al. (2010)
G42086b	TrGCN	$CH_3CN + O(^1D) \rightarrow 2\ H + CO + HCN$	`2.54E-10*EXP(-24./temp)*0.16`	Strekowski et al. (2010)*
G42086c	TrGCN	$CH_3CN + O(^1D) \rightarrow .5\ CH_3 + .5\ NCO + .5\ NCCH_2O_2 + .5\ OH$	`2.54E-10*EXP(-24./temp)*(1.-(0.16+ 0.0269*EXP(137./temp)))`	Strekowski et al. (2010)*
G42087	TrGCN	$NCCH_2O_2 + NO \rightarrow HCN + CO_2 + HO_2 + NO_2$	`KRO2NO`	see note*
G42088	TrGCN	$NCCH_2O_2 + HO_2 \rightarrow HCN + CO_2 + HO_2$	`k_RO2_HO2(temp,2)`	see note*
G42089a	TrGC	$CH_2CHOH + OH \rightarrow HCOOH + OH + HCHO$	`k_CH2CHOH_OH_HCOOH`	Sander et al. (2019), So et al. (2014)*
G42089b	TrGC	$CH_2CHOH + OH \rightarrow HOCH_2CHO + HO_2$	`k_CH2CHOH_OH_ALD`	Sander et al. (2019), So et al. (2014)
G42090	TrGC	$CH_2CHOH + HCOOH \rightarrow CH_3CHO + HCOOH$	`k_CH2CHOH_HCOOH`	Sander et al. (2019), da Silva (2010)*

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

#	labels	reaction	rate coefficient	reference
G42091	TrGC	$CH_3CHO + HCOOH \rightarrow CH_2CHOH + HCOOH$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G42092	TrGC	$HOOCCOOH + OH \rightarrow 2\ CO_2 + HO_2 + H_2O$	2.0 *k_co2h	see note*
G42093a	TrGC	$HOCH_2CHOHOH + OH \rightarrow HOCH_2CO_2H + HO_2 + H_2O$	k_t*f_toh*f_toh	see note*
G42093b	TrGC	$HOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + HO_2 + H_2O$	k_s*f_soh*f_pch2oh	see note*
G42093c	TrGC	$HOCH_2CHOHOH + OH \rightarrow HCOOH + HOCH_2O_2 + H_2O$	2.0 * k_rohro	see note*
G42093d	TrGC	$HOCH_2CHOHOH + OH \rightarrow HCHO + HCOOH + HO_2 + H_2O$	k_rohro	see note*
G42094a	TrGC	$CH_3CHOHOH + OH \rightarrow CH_3COOH + HO_2 + H_2O$	k_t*f_toh*f_toh	see note*
G42094b	TrGC	$CH_3CHOHOH + OH \rightarrow CH_3 + HCOOH + H_2O$	2.0 * k_rohro	see note*
G42095a	TrGC	$CHOHOHCOOH + OH \rightarrow HOOCCOOH + HO_2 + H_2O$	k_t*f_toh*f_toh*f_co2h	see note*
G42095b	TrGC	$CHOHOHCOOH + OH \rightarrow HCOOH + CO_2 + HO_2 + H_2O$	2.0 * k_rohro + k_co2h	see note*
G42096a	TrGC	$CHOHOHCHOHOH + OH \rightarrow 2\ HCOOH + HO_2 + H_2O$	4.0 * k_rohro	see note*
G42096b	TrGC	$CHOHOHCHOHOH + OH \rightarrow CHOHOHCOOH + HO_2 + H_2O$	2.0 * k_t*f_toh*f_toh*f_pch2oh	see note*
G42097a	TrGC	$CHOCHOHOH + OH \rightarrow HCOOH + CO + HO_2 + H_2O$	2.0 * k_rohro + k_t*f_o*f_pch2oh	see note*
G42097b	TrGC	$CHOCHOHOH + OH \rightarrow HCOCO_2H + HO_2 + H_2O$	k_t*f_toh*f_toh*f_cho	see note*
G42098a	TrGC	$HOOCH_2CHOHOH + OH \rightarrow HOOCH2CO2H + HO_2 + H_2O$	k_t*f_toh*f_toh*f_pch2oh	see note*
G42098b	TrGC	$HOOCH_2CHOHOH + OH \rightarrow HCOOH + HCHO + OH + H_2O$	2.0 * k_rohro	see note*
G42098c	TrGC	$HOOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + OH + H_2O$	k_s*f_pch2oh*f_sooh	see note*
G43000a	TrGC	$C_3H_8 + OH \rightarrow iC_3H_7O_2 + H_2O$	k_s	Sander et al. (2019)
G43000b	TrGC	$C_3H_8 + OH \rightarrow C_3H_7O_2 + H_2O$	2.*k_p	Sander et al. (2019)
G43001a	TrGC	$C_3H_6 + O_3 \rightarrow HCHO + .16\ CH3CHOHOOH + .50\ OH + .50\ HCOCH_2O_2 + .05\ CH2CO + .09\ CH_3OH + .09\ CO + .2\ CH_4 + .2\ CO_2$	5.5E-15*EXP(-1880./temp)*.57	Atkinson et al. (2006)*
G43001b	TrGC	$C_3H_6 + O_3 \rightarrow CH_3CHO + CH_2OO^*$	5.5E-15*EXP(-1880./temp)*.43	Atkinson et al. (2006)*
G43002	TrGC	$C_3H_6 + OH \rightarrow HYPROPO2$	k_3rd_iupac(temp,cair,8.6E-27, 3.5,3.E-11,1.,0.5)	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$C_3H_6 + NO_3 \rightarrow PRONO3BO2$	4.6E-13*EXP(-1155./temp)	Wallington et al. (2018)
G43004	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G43005a	TrGCN	$iC_3H_7O_2 + NO \rightarrow CH_3COCH_3 + HO_2 + NO_2$	2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,2,0,0,0,temp,cair))	Wallington et al. (2018)

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

#	labels	reaction	rate coefficient	reference
G43005b	TrGCN	$iC_3H_7O_2$ + NO → $iC_3H_7ONO_2$	`2.7E-12*EXP(360./temp)*alpha_AN(3,2,0,0,0,temp,cair)`	Wallington et al. (2018)
G43006	TrGC	$iC_3H_7O_2$ → .8 CH_3COCH_3 + .2 IPROPOL + .6 HO_2	`2.*(1.6E-12*EXP(-2200./temp)*k_CH3O2)**(.5)*RO2`	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	iC_3H_7OOH + OH → $iC_3H_7O_2$ + H_2O	`k_ROOHRO`	Sander et al. (2019)
G43007b	TrGC	iC_3H_7OOH + OH → CH_3COCH_3 + H_2O + OH	`k_t*f_tOOH`	Sander et al. (2019)
G43008	TrGC	$C_3H_7O_2$ + HO_2 → C_3H_7OOH	`1.9E-13*EXP(1300./temp)`	Atkinson (1997)*
G43009a	TrGCN	$C_3H_7O_2$ + NO → C_2H_5CHO + HO_2 + NO_2	`2.7E-12*EXP(360./temp)*(1.-alpha_AN(3,1,0,0,0,temp,cair))`	Wallington et al. (2018)
G43009b	TrGCN	$C_3H_7O_2$ + NO → $C_3H_7ONO_2$	`2.7E-12*EXP(360./temp)*alpha_AN(3,1,0,0,0,temp,cair)`	Wallington et al. (2018)
G43010	TrGC	$C_3H_7O_2$ → .8 CH_3COCH_3 + .2 NPROPOL + .6 HO_2	`2.*(k_CH3O2*3.E-13)**(.5)*RO2`	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43011	TrGC	CH_3COCH_3 + OH → $CH_3COCH_2O_2$ + H_2O	`(8.8E-12*EXP(-1320./temp)+1.7E-14*EXP(423./temp))`	Atkinson et al. (2006)*
G43012a	TrGC	$CH_3COCH_2O_2$ + HO_2 → $CH_3COCH_2O_2H$	`8.6E-13*EXP(700./temp)*r_COCH2O2_OOH`	Tyndall et al. (2001a), Sander et al. (2019)
G43012b	TrGC	$CH_3COCH_2O_2$ + HO_2 → OH + $CH_3C(O)$ + HCHO	`8.6E-13*EXP(700./temp)*r_COCH2O2_OH`	Tyndall et al. (2001a), Sander et al. (2019)
G43013a	TrGCN	$CH_3COCH_2O_2$ + NO → $CH_3C(O)$ + HCHO + NO_2	`2.9E-12*EXP(300./temp)*(1.-alpha_AN(4,1,1,0,0,temp,cair))`	Burkholder et al. (2015)
G43013b	TrGCN	$CH_3COCH_2O_2$ + NO → NOA	`2.9E-12*EXP(300./temp)*alpha_AN(4,1,1,0,0,temp,cair)`	Burkholder et al. (2015)
G43014	TrGC	$CH_3COCH_2O_2$ → .3 $CH_3C(O)$ + .3 HCHO + .5 MGLYOX + .2 CH_3COCH_2OH	`k1_RO2pORO2`	Orlando and Tyndall (2012)
G43015a	TrGC	$CH_3COCH_2O_2H$ + OH → $CH_3COCH_2O_2$ + H_2O	`k_ROOHRO`	see note*
G43015b	TrGC	$CH_3COCH_2O_2H$ + OH → MGLYOX + OH + H_2O	`k_s*f_sOOH*f_CO`	Sander et al. (2019)
G43016	TrGC	CH_3COCH_2OH + OH → MGLYOX + HO_2 + H_2O	`1.6E-12*EXP(305./temp)`	Atkinson et al. (2006)
G43017	TrGC	MGLYOX + OH → .4 CH_3 + .6 $CH_3C(O)$ + 1.4 CO + H_2O	`1.9E-12*EXP(575./temp)`	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$iC_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	`6.2E-13*EXP(-230./temp)`	Wallington et al. (2018)
G43021	TrGCN	$CH_3COCH_2O_2$ + NO_3 → $CH_3C(O)$ + HCHO + NO_2	`KRO2NO3`	Rickard and Pascoe (2009)
G43022	TrGC	HYPROPO2 → CH_3CHO + HCHO + HO_2	`k1_RO2sORO2`	Rickard and Pascoe (2009)
G43023a	TrGC	HYPROPO2 + HO_2 → HYPROPO2H	`k_RO2_HO2(temp,3)*(1.-r_CHOHCH2O2_OH)`	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43023b	TrGC	HYPROPO2 + HO_2 → CH_3CHO + HCHO + HO_2 + OH	k_RO2_HO2(temp,3)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)
G43024a	TrGCN	HYPROPO2 + NO → CH_3CHO + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(4,1,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G43024b	TrGCN	HYPROPO2 + NO → PROPOLNO3	KRO2NO*alpha_AN(4,1,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G43025	TrGCN	HYPROPO2 + NO_3 → CH_3CHO + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G43026a	TrGC	HYPROPO2H + OH → HYPROPO2	k_ROOHRO	Rickard and Pascoe (2009)
G43026b	TrGC	HYPROPO2H + OH → CH_3COCH_2OH + OH	(k_s*f_sOH*f_pCH2OH+k_t*f_ tOOH*f_pCH2OH)	Sander et al. (2019)
G43027	TrGCN	PRONO3BO2 + HO_2 → PR2O2HNO3	k_RO2_HO2(temp,3)	Rickard and Pascoe (2009)
G43028	TrGCN	PRONO3BO2 + NO → NOA + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G43029	TrGCN	PRONO3BO2 + NO_3 → NOA + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G43030a	TrGCN	PR2O2HNO3 + OH → PRONO3BO2	k_ROOHRO	Rickard and Pascoe (2009)
G43030b	TrGCN	PR2O2HNO3 + OH → NOA + OH	k_t*f_tOOH*f_CH2ONO2	Sander et al. (2019)
G43031	TrGCN	MGLYOX + NO_3 → $CH_3C(O)$ + CO + HNO_3	KNO3AL*2.4	Rickard and Pascoe (2009)
G43032	TrGCN	NOA + OH → MGLYOX + NO_2	(k_s*f_CO*f_ONO2+k_p*f_CO)	Sander et al. (2019)
G43033	TrGC	HOCH2COCHO + OH → .8609 HOCH2CO + .8609 CO + .1391 HCOCOCHO + .1391 HO_2	(1.9E-12*EXP(575./temp)+k_s*f_ sOH*f_CO)	Sander et al. (2019)
G43034	TrGCN	HOCH2COCHO + NO_3 → HOCH2CO + CO + HNO_3	KNO3AL*2.4	Sander et al. (2019)
G43035	TrGC	CH_3COCO_2H + OH → $CH_3C(O)$ + H_2O + CO_2	4.9E-14*EXP(276./temp)	Mellouki and Mu (2003), Sander et al. (2019)
G43036	TrGC	$HCOCOCH_2O_2$ → .6 HCOCO + .6 HCHO + .2 HCOCOCHO + .2 HOCH2COCHO	k1_RO2pORO2	Sander et al. (2019)
G43037	TrGCN	$HCOCOCH_2O_2$ + NO → HCOCO + HCHO + NO_2	KRO2NO	Sander et al. (2019)*
G43038a	TrGC	$HCOCOCH_2O_2$ + HO_2 → $HCOCOCH_2OOH$	k_RO2_HO2(temp,3)*r_COCH2O2_OOH	Sander et al. (2019)
G43038b	TrGC	$HCOCOCH_2O_2$ + HO_2 → HCOCO + HCHO + OH	k_RO2_HO2(temp,3)*r_COCH2O2_OH	Sander et al. (2019)
G43039	TrGCN	$HCOCOCH_2O_2$ + NO_3 → HCOCO + HCHO + NO_2	KRO2NO3	Sander et al. (2019)
G43040a	TrGC	$HCOCOCH_2OOH$ + OH → $HOOCH_2CO_3$ + CO + H_2O	k_t*f_CO*f_O	Sander et al. (2019)*
G43040b	TrGC	$HCOCOCH_2OOH$ + OH → HCOCOCHO + H_2O + OH	k_s*f_sOOH*f_CO	Sander et al. (2019)*
G43040c	TrGC	$HCOCOCH_2OOH$ + OH → $HCOCOCH_2O_2$ + H_2O	k_ROOHRO	Sander et al. (2019)
G43041	TrGCN	$HCOCOCH_2OOH$ + NO_3 → $HOOCH_2CO_3$ + CO + HNO_3	KNO3AL*2.4	Sander et al. (2019)
G43042	TrGC	HOCH2COCH2O2 → HCHO + HOCH2CO	k1_RO2pORO2	Sander et al. (2019)
G43043a	TrGC	HOCH2COCH2O2 + HO_2 → HOCH2COCH2OOH	k_RO2_HO2(temp,3)*r_COCH2O2_OOH	Sander et al. (2019)
G43043b	TrGC	HOCH2COCH2O2 + HO_2 → HCHO + HOCH2CO + OH	k_RO2_HO2(temp,3)*r_COCH2O2_OH	Sander et al. (2019)
G43044	TrGCN	HOCH2COCH2O2 + NO → HCHO + HOCH2CO + NO_2	KRO2NO	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G43045a	TrGC	HOCH2COCH2OOH + OH → HOCH2COCHO + OH	k_s*f_sOOH*f_CO	Sander et al. (2019)
G43045b	TrGC	HOCH2COCH2OOH + OH → HOCH2COCH2O2	k_ROOHRO	Sander et al. (2019)
G43045c	TrGC	HOCH2COCH2OOH + OH → $HCOCOCH_2OOH + HO_2$	1.60E-12*EXP(305./temp)	Sander et al. (2019)*
G43046	TrGC	CH3CHCO + OH → .72 CO + .72 CH_3CHO + .72 HO_2 + .21 CH_3COCO_2H + .07 CH_3CHO + .07 HO_2 + .07 CO_2	7.6E-11	Hatakeyama et al. (1985), Sander et al. (2019)
G43047	TrGCN	PROPOLNO3 + OH → $CH_3COCH_2OH + NO_2$	k_t*f_ONO2*f_pCH2OH+k_s*f_sOH*f_CH2ONO2	Sander et al. (2019)
G43048	TrGCN	$CH_3COCH_2O_2 + NO_2 \rightarrow CH_3COCH_2OONO_2$	2.3E-12*EXP(300./temp)	Tyndall et al. (2001a)*
G43049	TrGCN	$CH_3COCH_2OONO_2 \rightarrow CH_3COCH_2O_2 + NO_2$	1.9E16*EXP(-10830./temp)	Sehested et al. (1998)*
G43050	TrGCN	$CH_3COCH_2OONO_2$ + OH → MGLYOX + $NO_3 + H_2O$	9.50E-13*EXP(-650./temp)*f_CO	Sander et al. (2019)*
G43051a	TrGC	$C_3H_7OOH + OH \rightarrow C_3H_7O_2 + H_2O$	k_ROOHRO	Sander et al. (2019)
G43051b	TrGC	$C_3H_7OOH + OH \rightarrow C_2H_5CHO + H_2O + OH$	k_s*f_sOOH	Sander et al. (2019)
G43051c	TrGC	$C_3H_7OOH + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$	k_s*f_pCH2OH	Sander et al. (2019)*
G43052	TrGC	$C_2H_5CHO + OH \rightarrow C_2H_5CO_3 + H_2O$	4.9E-12*EXP(405./temp)	Atkinson et al. (2006)*
G43053	TrGCN	$C_2H_5CHO + NO_3 \rightarrow C_2H_5CO_3 + HNO_3$	6.3E-15	Atkinson et al. (2006)
G43054a	TrGC	$C_2H_5CO_3 \rightarrow C_2H_5O_2 + CO_2$	k1_RO2RCO3*0.9	Sander et al. (2019)
G43054b	TrGC	$C_2H_5CO_3 \rightarrow C_2H_5CO_2H$	k1_RO2RCO3*0.1	Sander et al. (2019)
G43055a	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5O_2 + CO_2 + OH$	KAPHO2*r_CO3_OH	Sander et al. (2019), Groß et al. (2014)
G43055b	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_3H$	KAPHO2*r_CO3_OOH	Sander et al. (2019), Groß et al. (2014)
G43055c	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_2H + O_3$	KAPHO2*r_CO3_O3	Sander et al. (2019), Groß et al. (2014)
G43056	TrGCN	$C_2H_5CO_3 + NO \rightarrow NO_2 + C_2H_5O_2 + CO_2$	KAPNO	Rickard and Pascoe (2009)
G43057	TrGCN	$C_2H_5CO_3 + NO_2$ → PPN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43058	TrGCN	PPN → $C_2H_5CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G43059	TrGC	$C_2H_5CO_2H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	k_CO2H+k_p+k_s*f_CO2H	Sander et al. (2019)*
G43060a	TrGC	$C_2H_5CO_3H + OH \rightarrow C_2H_5CO_3 + H_2O$	k_ROOHRO	Sander et al. (2019)
G43060b	TrGC	$C_2H_5CO_3H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	k_s*f_CO2H+k_p	Sander et al. (2019)*
G43061	TrGCN	PPN + OH → $CH_3CHO + CO_2 + NO_2 + H_2O$	k_s*f_cpan+k_p	Sander et al. (2019)*
G43062	TrGC	$CH_3COCO_3H + OH \rightarrow CH_3COCO_3 + H_2O$	k_ROOHRO	Sander et al. (2019)
G43063a	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3C(O) + CO_2 + OH$	KAPHO2*r_CO3_OH	Sander et al. (2019)
G43063b	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3COCO_3H$	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Sander et al. (2019)
G43064	TrGCN	$CH_3COCO_3 + NO \rightarrow CH_3C(O) + CO_2 + NO_2$	KAPNO	Sander et al. (2019)
G43065	TrGCN	$CH_3COCO_3 + NO_2 \rightarrow CH_3C(O) + CO_2 + NO_3$	k_CH3CO3_NO2	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G43066	TrGCN	$CH_3COCO_3 + NO_3 \rightarrow CH_3C(O)OO + CO_2 + NO_2$	KRO2NO3*1.74	Sander et al. (2019)
G43067	TrGC	$CH_3COCO_3 \rightarrow CH_3C(O)OO + CO_2$	k1_RO2RCO3	Sander et al. (2019)
G43068	TrGC	$HCOCOCHO + OH \rightarrow 3\ CO + HO_2$	2.*k_t*f_CO*f_O	Sander et al. (2019)
G43069	TrGC	$IPROPOL + OH \rightarrow CH_3COCH_3 + HO_2 + H_2O$	2.6E-12*EXP(200./temp)	Atkinson et al. (2006)
G43070a	TrGC	$NPROPOL + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$	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	$NPROPOL + OH \rightarrow HYPROPO2 + H_2O$	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	$CH_2CHCH_2OH + OH \rightarrow HCOOH + OH + CH_3CHO$	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G43072	TrGC	$CH_2CHCH_2OH + HCOOH \rightarrow C_2H_5CHO + HCOOH$	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G43073	TrGC	$C_2H_5CHO + HCOOH \rightarrow CH_2CHCH_2OH + HCOOH$	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G43074	TrGC	$HCOCOCH_2OOH + OH \rightarrow HCOCO + CO + HO_2 + OH$	k_s*f_sOOH*f_CO+k_ROOHRO	Sander et al. (2019)*
G43075a	TrGC	$CH_3COCHOHOH + OH \rightarrow CH_3C(O) + HCOOH + H_2O$	2.0 * k_rohro	see note*
G43075b	TrGC	$CH_3COCHOHOH + OH \rightarrow CH_3COCO_2H + H_2O$	k_t*f_toh*f_toh*f_co	see note*
G43202	TrGTerC	$HCOCH2CHO + OH \rightarrow HCOCH2CO3$	4.29E-11	Rickard and Pascoe (2009)
G43203	TrGTerCN	$HCOCH2CHO + NO_3 \rightarrow HCOCH2CO3 + HNO_3$	2.*KNO3AL*2.4	Rickard and Pascoe (2009)
G43204a	TrGTerC	$HCOCH2CO3 \rightarrow HCOCH_2O_2 + CO_2$	k1_RO2RCO3*0.9	Sander et al. (2019)
G43204b	TrGTerC	$HCOCH2CO3 \rightarrow HCOCH2CO2H$	k1_RO2RCO3*0.1	Sander et al. (2019)
G43205	TrGTerCN	$HCOCH2CO3 + NO \rightarrow HCOCH_2O_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43206	TrGTerCN	$HCOCH2CO3 + NO_2 \rightarrow C_3PAN2$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43207a	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH2CO3H$	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G43207b	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH2CO2H + O_3$	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G43207c	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH_2O_2 + CO_2 + OH$	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G43210	TrGTerCN	$C_3PAN2 \rightarrow HCOCH2CO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G43211	TrGTerCN	$C_3PAN2 + OH \rightarrow GLYOX + CO + NO_2$	2.10E-11	Rickard and Pascoe (2009)
G43212	TrGTerC	$HCOCH2CO2H + OH \rightarrow HCOCH_2O_2 + CO_2$	2.14E-11	Rickard and Pascoe (2009)
G43213a	TrGTerC	$HOC_2H_4CO_3 \rightarrow HOCH_2CH_2O_2 + CO_2$	k1_RO2RCO3*0.9	Sander et al. (2019)
G43213b	TrGTerC	$HOC_2H_4CO_3 \rightarrow HOC2H4CO2H$	k1_RO2RCO3*0.1	Sander et al. (2019)
G43214	TrGTerCN	$HOC_2H_4CO_3 + NO \rightarrow HOCH_2CH_2O_2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow HOC2H4CO3H$	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G43215b	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow HOCH_2CH_2O_2 + CO_2 + OH$	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43215c	TrGTerC	$HOC_2H_4CO_3 + HO_2 \rightarrow$ HOC2H4CO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G43218	TrGTerCN	$HOC_2H_4CO_3 + NO_2 \rightarrow C_3PAN1$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43219	TrGTerC	HOC2H4CO2H + OH $\rightarrow HOCH_2CH_2O_2 + CO_2$	1.39E-11	Rickard and Pascoe (2009)
G43220	TrGTerC	HOC2H4CO3H + OH $\rightarrow HOC_2H_4CO_3$	1.73E-11	Rickard and Pascoe (2009)
G43221	TrGTerCN	$C_3PAN1 \rightarrow HOC_2H_4CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G43222	TrGTerCN	$C_3PAN1 + OH \rightarrow HOCH_2CHO + CO + NO_2$	4.51E-12	Rickard and Pascoe (2009)
G43223	TrGTerC	HCOCH2CO3H + OH $\rightarrow HCOCH_2O_2 + CO_2 + H_2O$	2.49E-11	Rickard and Pascoe (2009)*
G43415	TrGAroC	C3DIALOOH + OH $\rightarrow$ HCOCOCHO + OH	1.44E-10	Rickard and Pascoe (2009)
G43418a	TrGAroC	C3DIALO2 + $HO_2 \rightarrow$ C3DIALOOH	k_RO2_HO2(temp,3)*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G43418b	TrGAroC	C3DIALO2 + $HO_2 \rightarrow$ GLYOX + CO + HO_2 + OH	k_RO2_HO2(temp,3)*r_CO3_OH	Rickard and Pascoe (2009)
G43419	TrGAroCN	C3DIALO2 + NO $\rightarrow$ GLYOX + CO + $HO_2 + NO_2$	KRO2NO	Rickard and Pascoe (2009)*
G43420	TrGAroCN	C3DIALO2 + $NO_3 \rightarrow$ GLYOX + CO + $HO_2 + NO_2$	KRO2NO3	Rickard and Pascoe (2009)*
G43421	TrGAroC	C3DIALO2 $\rightarrow$ GLYOX + CO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G43422a	TrGAroC	HCOCOHCO3 + $HO_2 \rightarrow$ GLYOX + $CO_2 + HO_2$ + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G43422b	TrGAroC	HCOCOHCO3 + $HO_2 \rightarrow$ HCOCOHCO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G43424	TrGAroCN	HCOCOHCO3 + NO $\rightarrow$ GLYOX + $CO_2 + HO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43425	TrGAroCN	HCOCOHCO3 + $NO_2 \rightarrow$ HCOCOHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43426	TrGAroCN	HCOCOHCO3 + $NO_3 \rightarrow$ GLYOX + $CO_2 + HO_2 + NO_2$	KRO2NO3*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	HCOCOHCO3 $\rightarrow$ GLYOX + $CO_2 + HO_2$	k1_RO2RCO3	Rickard and Pascoe (2009)
G43428	TrGAroC	METACETHO + OH $\rightarrow CH_3C(O) + CO_2$	9.82E-11	Rickard and Pascoe (2009)
G43442	TrGAroCN	HCOCOHPAN + OH $\rightarrow$ GLYOX + CO + NO_2	6.97E-11	Rickard and Pascoe (2009)
G43443	TrGAroCN	HCOCOHPAN $\rightarrow$ HCOCOHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	C32OH13CO + OH $\rightarrow$ HCOCOHCO3	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	HCOCOHCO3H + OH $\rightarrow$ HCOCOHCO3	7.33E-11	Rickard and Pascoe (2009)
G44000	TrGC	$C_4H_{10} + OH \rightarrow LC_4H_9O_2 + H_2O$	2.03E-17*temp*temp*EXP(78./temp)	Atkinson et al. (2006)*
G44001a	TrGC	$LC_4H_9O_2 \rightarrow C_3H_7CHO + HO_2$	(k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.1273	Rickard and Pascoe (2009), Sander et al. (2019)
G44001b	TrGC	$LC_4H_9O_2 \rightarrow .636$ MEK + .636 HO_2 + .364 CH_3CHO + .364 $C_2H_5O_2$	(k1_RO2pRO2*0.1273+k1_RO2sRO2*0.8727)*0.8727	Rickard and Pascoe (2009), Sander et al. (2019)*
G44002	TrGC	$LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44003a	TrGCN	$LC_4H_9O_2 + NO \rightarrow NO_2 + C_3H_7CHO + HO_2$	KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.1273	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44003b	TrGCN	$LC_4H_9O_2$ + NO → NO_2 + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 $C_2H_5O_2$	KRO2NO*(1.-(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair)))*0.8727	Rickard and Pascoe (2009), Sander et al. (2019)
G44003c	TrGCN	$LC_4H_9O_2$ + NO → LC4H9NO3	KRO2NO*(0.1273*alpha_AN(4,1,0,0,0,temp,cair)+0.8727*alpha_AN(4,2,0,0,0,temp,cair))	Rickard and Pascoe (2009)*
G44004a	TrGCN	$LC_4H_9O_2$ + NO_3 → NO_2 + C_3H_7CHO + HO_2	KRO2NO3*0.1273	Rickard and Pascoe (2009), Sander et al. (2019)
G44004b	TrGCN	$LC_4H_9O_2$ + NO_3 → NO_2 + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 $C_2H_5O_2$	KRO2NO3*0.8727	Rickard and Pascoe (2009), Sander et al. (2019)
G44005a	TrGC	LC_4H_9OOH + OH → $LC_4H_9O_2$ + H_2O	k_ROOHRO	Sander et al. (2019)
G44005b	TrGC	LC_4H_9OOH + OH → C_3H_7CHO + H_2O + OH	k_s*f_tOOH*f_alk*(k_p/(k_p+k_s))	Sander et al. (2019)
G44005c	TrGC	LC_4H_9OOH + OH → MEK + H_2O + OH	k_t*f_tOOH*f_alk*(k_s/(k_p+k_s))	Sander et al. (2019)
G44006a	TrGC	iC_4H_{10} + OH → $TC_4H_9O_2$ + H_2O	1.17E-17*temp*temp*EXP(213./temp)*k_t/(3.*k_p+k_t)	Atkinson (2003)
G44006b	TrGC	iC_4H_{10} + OH → $IC_4H_9O_2$ + H_2O	1.17E-17*temp*temp*EXP(213./temp)*3.*k_p/(3.*k_p+k_t)	Atkinson (2003)
G44007	TrGC	$TC_4H_9O_2$ → CH_3COCH_3 + CH_3	k1_RO2tRO2	Rickard and Pascoe (2009), Sander et al. (2019)
G44008	TrGC	$TC_4H_9O_2$ + HO_2 → TC_4H_9OOH	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44009a	TrGCN	$TC_4H_9O_2$ + NO → NO_2 + CH_3COCH_3 + CH_3	KRO2NO*(1.-alpha_AN(4,3,0,0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G44009b	TrGCN	$TC_4H_9O_2$ + NO → TC4H9NO3	KRO2NO*alpha_AN(4,3,0,0,0,temp,cair)	Rickard and Pascoe (2009)
G44010a	TrGC	TC_4H_9OOH + OH → $TC_4H_9O_2$ + H_2O	k_ROOHRO	Sander et al. (2019)
G44010b	TrGC	TC_4H_9OOH + OH → CH_3COCH_3 + HCHO + OH + H_2O	3.*k_p*f_tCH2OH	Sander et al. (2019)*
G44011	TrGCN	TC4H9NO3 + OH → CH_3COCH_3 + HCHO + NO_2 + H_2O	3.*k_p*f_CH2ONO2	Sander et al. (2019)*
G44012	TrGC	$IC_4H_9O_2$ → IPRCHO	k1_RO2sRO2	Rickard and Pascoe (2009), Sander et al. (2019)
G44013	TrGC	$IC_4H_9O_2$ + HO_2 → IC_4H_9OOH	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44014a	TrGCN	$IC_4H_9O_2$ + NO → NO_2 + IPRCHO	KRO2NO*(1.-alpha_AN(4,2,0,0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G44014b	TrGCN	$IC_4H_9O_2$ + NO → IC4H9NO3	KRO2NO*alpha_AN(4,2,0,0,0,temp,cair)	Rickard and Pascoe (2009)
G44015a	TrGC	IC_4H_9OOH + OH → $IC_4H_9O_2$ + H_2O	k_ROOHRO	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44015b	TrGC	IC_4H_9OOH + OH → IPRCHO + OH + H_2O	k_s*f_sOOH+2.*k_s+k_t*f_pCH2OH	Sander et al. (2019)*
G44016	TrGCN	IC4H9NO3 + OH → IPRCHO + NO_2 + H_2O	k_s*f_ONO2+2.*k_p+k_t*f_CH2ONO2	Sander et al. (2019)*
G44017	TrGC	MVK + O_3 → .87 MGLYOX + .5481 CO + .1392 HO_2 + .1392 OH + .3219 CH_2OO + .13 HCHO + .04680 OH + .04680 CO + .07280 $CH_3C(O)$ + .026 CH_3CHO + .026 CO_2 + .026 HCHO + .026 HO_2 + .02402 MGLYOX + .02402 H_2O_2 + .00718 CH_3COCO_2H	8.5E-16*EXP(-1520./temp)	Sander et al. (2019)
G44018	TrGC	MVK + OH → LHMVKABO2	2.6E-12*EXP(610./temp)	Sander et al. (2019), Atkinson et al. (2006)*
G44019	TrGC	MEK + OH → LMEKO2 + H_2O	1.5E-12*EXP(-90./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44020	TrGC	LMEKO2 + HO_2 → LMEKOOH	k_RO2_HO2(temp,4)	Sander et al. (2019)
G44021a	TrGCN	LMEKO2 + NO → .62 CH_3CHO + .62 $CH_3C(O)$ + .38 HCHO + .38 CO_2 + .38 $HOCH_2CH_2O_2$ + NO_2	KRO2NO*(1.-(.62*alpha_AN(4,2,1, 0,0,temp,cair)+.38*alpha_AN(4,1, 0,1,0,temp,cair)))	Sander et al. (2019)*
G44021b	TrGCN	LMEKO2 + NO → LMEKNO3	KRO2NO*(.62*alpha_AN(4,2,1,0,0, temp,cair)+.38*alpha_AN(4,1,0,1, 0,temp,cair))	Sander et al. (2019)
G44022a	TrGC	LMEKOOH + OH → LMEKO2 + H_2O	k_ROOHRO	Sander et al. (2019)
G44022b	TrGC	LMEKOOH + OH → .62 BIACET + .38 HCHO + .38 CO_2 + .38 $HOCH_2CH_2O_2$ + H_2O + OH	(.62*k_t*f_tOOH*f_CO+.38*k_s*f_ sOOH)	Sander et al. (2019)
G44023a	TrGCN	LC4H9NO3 + OH → MEK + NO_2 + H_2O	(k_t*f_ONO2*f_alk+k_p*f_alk+k_ s*f_CH2ONO2+k_p)*(k_s/(k_p+k_s))	Sander et al. (2019)*
G44023b	TrGCN	LC4H9NO3 + OH → C_3H_7CHO + NO_2 + H_2O	(k_p+k_s*(1.+f_CH2ONO2+f_ONO2) *f_alk)*(k_p/(k_p+k_s))	Sander et al. (2019)*
G44024	TrGCN	MPAN + OH → CH_3COCH_2OH + CO + NO_2	3.2E-11	Orlando et al. (2002)
G44025	TrGCN	MPAN → MACO3 + NO_2	k_PAN_M	see note*
G44026	TrGC	LMEKO2 → .538 HCHO + .538 CO_2 + .459 $HOCH_2CH_2O_2$ + .079 $C_2H_5O_2$ + .462 $CH_3C(O)$ + .462 CH_3CHO	(.62*k1_RO2sORO2+.38*k1_RO2pORO2)	Rickard and Pascoe (2009)*
G44027	TrGC	MACR + OH → .45 MACO3 + .55 MACRO2	8.E-12*EXP(380./temp)	Orlando et al. (1999b), Sander et al. (2019)
G44028	TrGC	MACR + O_3 → .5481 CO + .1392 HO_2 + .1392 OH + .3219 CH_2OO + .87 MGLYOX + .13 HCHO + .13 OH + .065 $HCOCOCH_2O_2$ + .065 CO + .065 $CH_3C(O)$	1.36E-15*EXP(-2112./temp)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44029	TrGCN	MACR + NO_3 → MACO3 + HNO_3	KNO3AL*2.0	Rickard and Pascoe (2009)
G44030a	TrGC	MACO3 → $CH_3C(O)$ + HCHO + CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G44030b	TrGC	MACO3 → MACO2H	k1_RO2RCO3*0.1	Sander et al. (2019)
G44031a	TrGC	MACO3 + HO_2 → MACO2 + OH	KAPHO2*r_CO3_OH	Sander et al. (2019)
G44031b	TrGC	MACO3 + HO_2 → MACO3H	KAPHO2*r_CO3_OOH	Sander et al. (2019)
G44031c	TrGC	MACO3 + HO_2 → MACO2H + O_3	KAPHO2*r_CO3_O3	Sander et al. (2019)
G44032	TrGCN	MACO3 + NO → MACO2 + NO_2	8.70E-12*EXP(290./temp)	Sander et al. (2019)
G44033	TrGCN	MACO3 + NO_2 → MPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44034	TrGCN	MACO3 + NO_3 → MACO2 + NO_2	KRO2NO3*1.74	Sander et al. (2019)
G44035	TrGC	MACRO2 → .7 CH_3COCH_2OH + .7 HCHO + .7 HO_2 + .3 MACROH	k1_RO2tORO2	Rickard and Pascoe (2009)*
G44036a	TrGC	MACRO2 + HO_2 → MACRO + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Sander et al. (2019)
G44036b	TrGC	MACRO2 + HO_2 → MACROOH	k_RO2_HO2(temp,4)*r_COCH2O2_OOH	Sander et al. (2019)
G44037a	TrGCN	MACRO2 + NO → MACRO + NO_2	KRO2NO*(1.-alpha_AN(6,3,1,0,0, temp,cair))	Sander et al. (2019)
G44037b	TrGCN	MACRO2 + NO → MACRNO3	KRO2NO*alpha_AN(6,3,1,0,0,temp, cair)	Sander et al. (2019)
G44038	TrGCN	MACRO2 + NO_3 → MACRO + NO_2	KRO2NO3	Sander et al. (2019)
G44039a	TrGC	MACROOH + OH → MACRO2	k_ROOHRO	Sander et al. (2019)
G44039b	TrGC	MACROOH + OH → CO + CH_3COCH_2OH + OH	k_t*f_O*f_tCH2OH*f_alk	Sander et al. (2019)
G44039c	TrGC	MACROOH + OH → CO + MGLYOX + HO_2	(k_s*f_sOH*f_pCH2OH + k_ROHRO)	Sander et al. (2019)
G44040	TrGC	MACROH + OH → CH_3COCH_2OH + CO + HO_2	k_t*f_O*f_tCH2OH*f_alk	Sander et al. (2019)
G44041	TrGC	MACRO → .885 CH_3COCH_2OH + .885 CO + .115 MGLYOX + .115 HCHO + HO_2	KDEC	Sander et al. (2019)
G44042	TrGC	MACO2H + OH → CH_3COCH_2OH + HO_2 + CO_2	((k_adt+k_adp)*a_CO2H+k_CO2H)	Sander et al. (2019)
G44043a	TrGC	MACO3H + OH → CH_3COCH_2OH + CO_2 + OH	(k_adt+k_adp)*a_CO2H	Sander et al. (2019)
G44043b	TrGC	MACO3H + OH → MACO3	k_ROOHRO	Sander et al. (2019)
G44044	TrGC	LHMVKABO2 → .024 CO2H3CHO + .072 MGLYOX + .072 HO_2 + .072 HCHO + .5280 $CH_3C(O)$ + .5280 $HOCH_2CHO$ + .176 BIACETOH + .2 HO12CO3C4	(.12*k1_RO2pORO2+.88*k1_RO2sORO2)	Sander et al. (2019)
G44045a	TrGC	LHMVKABO2 + HO_2 → OH + $HOCH_2CHO$ + $CH_3C(O)$	k_RO2_HO2(temp,4)*.88*r_COCH2O2_ OH	Sander et al. (2019)
G44045b	TrGC	LHMVKABO2 + HO_2 → LHMVKABOOH	k_RO2_HO2(temp,4)*(.12+.88*r_ COCH2O2_OOH)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44046a	TrGCN	LHMVKABO2 + NO → .12 MGLYOX + .12 HO_2 + .88 $HOCH_2CHO$ + .88 $CH_3C(O)$ + .12 HCHO + NO_2	`KRO2NO*(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	LHMVKABO2 + NO → MVKNO3	`KRO2NO*(.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	LHMVKABO2 + NO_3 → .12 MGLYOX + .12 HO_2 + .88 $HOCH_2CHO$ + .88 $CH_3C(O)$ + .12 HCHO + .12 HO_2 + NO_2	`KRO2NO3`	Sander et al. (2019)
G44048a	TrGC	LHMVKABOOH + OH → LHMVKABO2	`k_ROOHRO`	Sander et al. (2019)
G44048b	TrGC	LHMVKABOOH + OH → .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 → CO2H3CO3	`k_t*f_O*f_alk`	Sander et al. (2019)
G44049b	TrGC	CO2H3CHO + OH → $CH_3COCOCHO$ + HO_2 + H_2O	`k_t*f_CO*f_tOH*f_CHO`	Sander et al. (2019)
G44050	TrGCN	CO2H3CHO + NO_3 → CO2H3CO3 + HNO_3	`KNO3AL*4.0`	Rickard and Pascoe (2009)
G44051	TrGC	CO2H3CO3 → MGLYOX + HO_2 + CO_2	`k1_RO2RCO3`	Sander et al. (2019)
G44052a	TrGC	CO2H3CO3 + HO_2 → OH + MGLYOX + HO_2 + CO_2	`KAPHO2*r_CO3_OH`	Sander et al. (2019)
G44052b	TrGC	CO2H3CO3 + HO_2 → CO2H3CO2H + O_3	`KAPHO2*r_CO3_O3`	Sander et al. (2019)
G44052c	TrGC	CO2H3CO3 + HO_2 → CO2H3CO3H	`KAPHO2*r_CO3_OOH`	Sander et al. (2019)
G44053	TrGCN	CO2H3CO3 + NO → MGLYOX + HO_2 + NO_2 + CO_2	`KAPNO`	Sander et al. (2019)
G44054	TrGCN	CO2H3CO3 + NO_3 → MGLYOX + HO_2 + NO_2 + CO_2	`KRO2NO3*1.74`	Sander et al. (2019)
G44055a	TrGC	CO2H3CO3H + OH → CO2H3CO3	`k_ROOHRO`	Sander et al. (2019)
G44055b	TrGC	CO2H3CO3H + OH → $CH_3C(O)$ + CO + CO_2 + OH	`(k_t*f_CO2H*f_CO*f_tOH)`	Sander et al. (2019)
G44056	TrGC	CO2H3CO2H + OH → CH3COCOCO2H + HO_2	`k_t*f_CO2H*f_CO*f_tOH+k_CO2H`	Sander et al. (2019)
G44057a	TrGC	HO12CO3C4 + OH → BIACETOH + HO_2	`k_t*f_tOH*f_alk*f_CO`	Sander et al. (2019)
G44057b	TrGC	HO12CO3C4 + OH → CO2H3CHO + HO_2	`k_s*f_sOH*f_alk`	Sander et al. (2019)
G44058	TrGC	MACO2 → .65 CH_3 + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + CO_2	`KDEC`	Sander et al. (2019)
G44059	TrGC	LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 $CH_3C(O)$ + OH	`k_hsd`	Sander et al. (2019)
G44060	TrGC	MACRO2 → MGLYOX + HCHO + OH	`k_hsb`	Sander et al. (2019)
G44061a	TrGCN	MVKNO3 + OH → MGLYOX + CO_2 + HO_2 + NO_2 + H_2O	`k_s*f_sOOH*f_CH2ONO2+k_ROHRO`	Sander et al. (2019)*
G44061b	TrGCN	MVKNO3 + OH → BIACETOH + NO_2 + H_2O	`k_t*f_ONO2*f_CO*f_pCH2OH`	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G44062a	TrGCN	MACRNO3 + OH → CH_3COCH_2OH + CO_2 + NO_2 + H_2O	k_t*f_O*f_CH2ONO2	Sander et al. (2019)*
G44062b	TrGCN	MACRNO3 + OH → MGLYOX + CO + NO_2 + H_2O	k_ROHRO+k_s*f_sOOH*f_CH2ONO2	Sander et al. (2019)*
G44063	TrGC	MACRO2 → CH_3COCH_2OH + OH + CO	k_14hsal	Sander et al. (2019)
G44064	TrGC	EZCH3CO2CHCHO → .9 $CH_3COCHCO$ + .1 $CH_3C(O)$ + .01 GLYOX + .18 CO + .09 HO_2 + OH	k_15hs24vynal	Sander et al. (2019)
G44065	TrGC	EZCH3CO2CHCHO + HO_2→ $CH_3COOHCHCHO$	k_RO2_HO2(temp,4)	Sander et al. (2019)
G44066	TrGCN	EZCH3CO2CHCHO + NO → CH_3COCHO_2CHO + NO_2	KRO2NO	Sander et al. (2019)*
G44067	TrGCN	EZCH3CO2CHCHO + NO_3→ CH_3COCHO_2CHO + NO_2	KRO2NO3	Sander et al. (2019)
G44068	TrGC	EZCH3CO2CHCHO → CH_3COCHO_2CHO	k1_RO2sORO2	Sander et al. (2019)
G44069	TrGC	EZCHOCCH3CHO2 → $HCOCCH_3CO$ + OH	k_15hs24vynal	Sander et al. (2019)
G44070	TrGCN	EZCHOCCH3CHO2 + NO → $HCOCO_2CH_3CHO$ + NO_2	KRO2NO	Sander et al. (2019)*
G44071	TrGC	EZCHOCCH3CHO2 + HO_2→ $HCOCCH_3CHOOH$	k_RO2_HO2(temp,4)	Sander et al. (2019)
G44072	TrGCN	EZCHOCCH3CHO2 + NO_3→ $HCOCO_2CH_3CHO$ + NO_2	KRO2NO3	Sander et al. (2019)
G44073	TrGC	EZCHOCCH3CHO2 → $HCOCO_2CH_3CHO$	k1_RO2pORO2	Sander et al. (2019)
G44074	TrGC	$CH_3COOHCHCHO$ → CH_3COCHO_2CHO + OH	k_hydec	Sander et al. (2019)
G44075	TrGC	$HCOCCH_3CHOOH$ → $HCOCO_2CH_3CHO$ + OH	k_hydec	Sander et al. (2019)
G44076	TrGCN	CH_3COCHO_2CHO + NO → $CH_3C(O)$ + GLYOX + NO_2	KRO2NO	Sander et al. (2019)*
G44077	TrGCN	CH_3COCHO_2CHO + NO_3 → $CH_3C(O)$ + GLYOX + NO_2	KRO2NO3	Sander et al. (2019)
G44078	TrGC	CH_3COCHO_2CHO + HO_2 → $CH_3C(O)$ + GLYOX + OH	k_RO2_HO2(temp,4)	Sander et al. (2019)*
G44079	TrGC	CH_3COCHO_2CHO → $CH_3C(O)$ + GLYOX	k1_RO2sORO2	Sander et al. (2019)
G44080	TrGC	$HCOCO_2CH_3CHO$ → MGLYOX + CO + HO_2	k1_RO2tORO2	Sander et al. (2019)
G44081	TrGCN	$HCOCO_2CH_3CHO$ + NO → MGLYOX + CO + HO_2 + NO_2	KRO2NO	Sander et al. (2019)*
G44082	TrGC	$HCOCO_2CH_3CHO$ + HO_2 → MGLYOX + CO + HO_2 + OH	k_RO2_HO2(temp,4)	Sander et al. (2019)*
G44083	TrGCN	$HCOCO_2CH_3CHO$ + NO_3 → MGLYOX + CO + HO_2 + NO_2	KRO2NO3	Sander et al. (2019)
G44084	TrGC	$HCOCCH_3CO$ + OH → CO + MGLYOX + HO_2	1E-10*a_CHO	Hatakeyama et al. (1985), Sander et al. (2019)
G44085	TrGC	$CH_3COCHCO$ + OH → CO + MGLYOX + HO_2	7.6E-11*a_COCH3	Hatakeyama et al. (1985), Sander et al. (2019)*
G44086	TrGCN	LMEKNO3 + OH → .62 MGLYOX + .62 HCHO + .62 HO_2 + .62 NO_2 + .38 $CH_3C(O)$ + .38 $NO_3CH2CHO$	.62*(k_p*(f_CO+f_CH2ONO2)) +.38*(k_s*f_CH2ONO2*f_CO)	Sander et al. (2019)*
G44087	TrGC	MEPROPENE + OH → IBUTOLBO2	9.4E-12*EXP(505./temp)	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G44088a	TrGC	MEPROPENE + O_3 → CH_3COCH_3 + CH_2OO^*	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Sander et al. (2019)
G44088b	TrGC	MEPROPENE + O_3 → $CH_3COCH_2O_2$ + OH + HCHO	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Sander et al. (2019)
G44089	TrGCN	MEPROPENE + NO_3 → CH_3COCH_3 + HCHO + NO_2	3.4E-13	Atkinson et al. (2006), Sander et al. (2019)*
G44090	TrGC	IBUTOLBO2 → CH_3COCH_3 + HCHO + HO_2	k1_RO2tORO2	Sander et al. (2019)
G44091a	TrGC	IBUTOLBO2 + HO_2 → IBUTOLBOOH	k_RO2_HO2(temp,4)*r_COCH2O2_OOH	Sander et al. (2019)
G44091b	TrGC	IBUTOLBO2 + HO_2 → CH_3COCH_3 + HCHO + HO_2 + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Sander et al. (2019)
G44092a	TrGCN	IBUTOLBO2 + NO → CH_3COCH_3 + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,3,0,0,0, temp,cair))	Sander et al. (2019)
G44092b	TrGCN	IBUTOLBO2 + NO → IBUTOLBNO3	KRO2NO*alpha_AN(5,3,0,0,0,temp, cair)	Sander et al. (2019)
G44093	TrGCN	IBUTOLBO2 + NO_3 → CH_3COCH_3 + HCHO + HO_2 + NO_2	KRO2NO3	Sander et al. (2019)
G44094a	TrGC	IBUTOLBOOH + OH → IBUTOLBO2	k_ROOHRO	Sander et al. (2019)
G44094b	TrGC	IBUTOLBOOH + OH → CH_3COCH_3 + HCHO + HO_2	k_s*f_sOOH*f_pCH2OH	Sander et al. (2019)
G44095	TrGCN	IBUTOLBNO3 + OH → CH_3COCH_3 + HCHO + HO_2 + NO_2	3.*k_p	Sander et al. (2019)
G44096	TrGC	BUT1ENE + OH → LBUT1ENO2	6.6E-12*EXP(465./temp)	Atkinson et al. (2006)*
G44097a	TrGC	BUT1ENE + O_3 → HCHO + .5 C_2H_5CHO + .5 H_2O_2 + .5 CH_3CHO + .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_2H_5CHO + CH_2OO^*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Sander et al. (2019)*
G44098	TrGCN	BUT1ENE + NO_3 → C_2H_5CHO + HCHO + NO_2	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Sander et al. (2019)*
G44099	TrGC	LBUT1ENO2 → C_2H_5CHO + HCHO + HO_2	k1_RO2sORO2	Sander et al. (2019)
G44100a	TrGC	LBUT1ENO2 + HO_2 → LBUT1ENOOH	k_RO2_HO2(temp,4)*r_COCH2O2_OOH	Sander et al. (2019)
G44100b	TrGC	LBUT1ENO2 + HO_2 → C_2H_5CHO + HCHO + HO_2 + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Sander et al. (2019)
G44101a	TrGCN	LBUT1ENO2 + NO → C_2H_5CHO + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair))	Sander et al. (2019)
G44101b	TrGCN	LBUT1ENO2 + NO → LBUT1ENNO3	KRO2NO*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44102	TrGCN	LBUT1ENO2 + NO_3 → C_2H_5CHO + HCHO + HO_2 + NO_2	KRO2NO3	Sander et al. (2019)
G44103a	TrGC	LBUT1ENOOH + OH → LBUT1ENO2	k_ROOHRO	Sander et al. (2019)
G44103b	TrGC	LBUT1ENOOH + OH → $C_2H_5CO_3$ + HCHO + HO_2	k_t*f_tOOH*f_pCH2OH	Sander et al. (2019)*
G44104	TrGCN	LBUT1ENNO3 + OH → C_2H_5CHO + CO + HO_2 + NO_2	k_s*f_sOH*f_CH2ONO2	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_3CHO + .16 CH3CHOHOOH + .50 OH + .50 $HCOCH_2O_2$ + .05 CH2CO + .09 CH_3OH + .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_3CHO + 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_3CHO + .16 CH3CHOHOOH + .50 OH + .50 $HCOCH_2O_2$ + .05 CH2CO + .09 CH_3OH + .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_3CHO + 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_2H_5CHO + HCHO + HO_2	k1_RO2sORO2	Sander et al. (2019)
G44112a	TrGC	BUT2OLO2 + HO_2 → BUT2OLOOH	k_RO2_HO2(temp,4)*r_COCH2O2_OOH	Sander et al. (2019)
G44112b	TrGC	BUT2OLO2 + HO_2 → 2 CH_3CHO + HO_2 + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Sander et al. (2019)
G44113a	TrGCN	BUT2OLO2 + NO → 2 CH_3CHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair))	Sander et al. (2019)
G44113b	TrGCN	BUT2OLO2 + NO → BUT2OLNO3	KRO2NO*alpha_AN(5,2,0,0,0,temp, cair)	Sander et al. (2019)
G44114	TrGCN	BUT2OLO2 + NO_3 → 2 CH_3CHO + HO_2 + NO_2	KRO2NO3	Sander et al. (2019)
G44115a	TrGC	BUT2OLOOH + OH → BUT2OLO2	k_ROOHRO	Sander et al. (2019)
G44115b	TrGC	BUT2OLOOH + OH → LMEKOOH + HO_2	k_t*f_tOH*f_pCH2OH	Sander et al. (2019)
G44115c	TrGC	BUT2OLOOH + OH → BUT2OLO + OH	k_t*f_tOOH*f_pCH2OH	Sander et al. (2019)
G44116	TrGCN	BUT2OLNO3 + OH → LMEKNO3 + HO_2	k_t*f_tOH*f_CH2ONO2	Sander et al. (2019)
G44117	TrGC	BUT2OLO + OH → BIACET + HO_2	k_t*f_tOH*f_CO	Sander et al. (2019)
G44118	TrGC	IPRCHO + OH → IPRCO3 + H_2O	6.8E-12*EXP(410./temp)	Atkinson et al. (2006)
G44119	TrGCN	IPRCHO + NO_3 → IPRCO3 + HNO_3	1.67E-12*EXP(-1460./temp)	Atkinson et al. (2006)
G44120	TrGC	IPRCO3 → $iC_3H_7O_2$ + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G44121a	TrGC	IPRCO3 + HO_2 → PERIBUACID	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44121b	TrGC	IPRCO3 + HO_2 → $iC_3H_7O_2$ + CO_2 + OH	KAPHO2*(1.-r_CO3_OOH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44122	TrGCN	IPRCO3 + NO_2 → PIPN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44123	TrGCN	IPRCO3 + NO → $iC_3H_7O_2$ + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G44124a	TrGC	PERIBUACID + OH → IPRCO3 + H_2O	k_ROOHRO	Rickard and Pascoe (2009)
G44124b	TrGC	PERIBUACID + OH → CH_3COCH_3 + H_2O + CO_2	k_s*f_CO2H	Sander et al. (2019)*
G44125	TrGCN	PIPN → IPRCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	PIPN + OH → CH_3COCH_3 + CO_2 + NO_2	k_s*f_cpan	Sander et al. (2019)*
G44127	TrGC	MPROPENOL + OH → HCOOH + OH + CH_3COCH_3	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G44128	TrGC	MPROPENOL + HCOOH → IPRCHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44129	TrGC	IPRCHO + HCOOH → MPROPENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44130	TrGC	BUTENOL + OH → HCOOH + OH + C_2H_5CHO	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*
G44131	TrGC	BUTENOL + HCOOH → C_3H_7CHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44132	TrGC	C_3H_7CHO + HCOOH → BUTENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44133	TrGC	HVMK + OH → HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	HVMK + HCOOH → CO2C3CHO + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44135	TrGC	CO2C3CHO + HCOOH → HVMK + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44136	TrGC	HMAC + OH → HCOOH + OH + MGLYOX	8.8E-11	Sander et al. (2019), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	HMAC + HCOOH → IBUTDIAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G44138	TrGC	IBUTDIAL + HCOOH → HMAC + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G44139	TrGC	CO2C3CHO + OH → $CH_3COCH_2O_2$ + CO_2 + H_2O	k_t*f_O*f_alk+k_s*f_CHO*f_CO	Sander et al. (2019)*
G44140	TrGCN	CO2C3CHO + NO_3 → $CH_3COCH_2O_2$ + CO_2 + HNO_3	KNO3AL*4.0	Sander et al. (2019)*

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

#	labels	reaction	rate coefficient	reference
G44141	TrGC	IBUTDIAL + OH → CH_3CHO + CO + HO_2 + CO_2 + H_2O	2.*k_t*f_O*f_alk+k_t*f_CHO*f_CHO	Sander et al. (2019)*
G44142	TrGCN	IBUTDIAL + NO_3 → CH_3CHO + CO + HO_2 + CO_2 + HNO_3	2.*KNO3AL*4.0	Sander et al. (2019)*
G44200	TrGTerC	$CH_3COCOCH_2O_2$ → $CH_3C(O)$ + HCHO + CO	k1_RO2pORO2	Rickard and Pascoe (2009)
G44201	TrGTerC	$CH_3COCOCH_2O_2$ + HO_2 → $CH_3COCOCH_2OOH$	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44202	TrGTerCN	$CH_3COCOCH_2O_2$ + NO → $CH_3C(O)$ + HCHO + CO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44203a	TrGTerC	$CH_3COCOCH_2OOH$ + OH → $CH_3COCOCHO$ + OH	k_s*f_CO*f_sOOH	Rickard and Pascoe (2009)*
G44203b	TrGTerC	$CH_3COCOCH_2OOH$ + OH → $CH_3COCOCH_2O_2$	k_ROOHRO	Rickard and Pascoe (2009)
G44204	TrGTerC	C44O2 + HO_2 → C44OOH	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44205	TrGTerCN	C44O2 + NO → HCOCH2CHO + CO_2 + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O2 → HCOCH2CHO + CO_2 + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)
G44207	TrGTerC	C44OOH + OH → C44O2	7.46E-11	Rickard and Pascoe (2009)
G44208	TrGTerC	CHOC3COO2 → HCOCH2CO3 + HCHO	k1_RO2pORO2	Rickard and Pascoe (2009)
G44209	TrGTerC	CHOC3COO2 + HO_2 → C413COOOH	k_RO2_HO2(temp,4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	CHOC3COO2 + NO → HCOCH2CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44211	TrGTerC	C413COOOH + OH → CHOC3COO2	8.33E-11	Rickard and Pascoe (2009)
G44212	TrGTerC	C4CODIAL + OH → C312COCO3	3.39E-11	Rickard and Pascoe (2009)
G44213	TrGTerCN	C4CODIAL + NO_3 → C312COCO3 + HNO_3	2.*KNO3AL*4.0	Rickard and Pascoe (2009)
G44214	TrGTerC	C312COCO3 → $HCOCOCH_2O_2$ + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G44215a	TrGTerC	C312COCO3 + HO_2 → C312COCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G44215b	TrGTerC	C312COCO3 + HO_2 → $HCOCOCH_2O_2$ + CO_2 + OH	KAPHO2*(1.-r_CO3_OOH)	Rickard and Pascoe (2009)
G44216	TrGTerCN	C312COCO3 + NO_2 → C312COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44217	TrGTerCN	C312COCO3 + NO → $HCOCOCH_2O_2$ + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G44218	TrGTerC	C312COCO3H + OH → C312COCO3	1.63E-11	Rickard and Pascoe (2009)
G44219	TrGTerCN	C312COPAN → C312COCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G44220	TrGTerCN	C312COPAN + OH → HCOCOCHO + CO + NO_2	1.27E-11	Rickard and Pascoe (2009)
G44221	TrGTerC	$CH_3COCOCHO$ + OH → $CH_3C(O)$ + 2 CO	8.4E-13*EXP(830./temp)	Sander et al. (2019)*
G44222	TrGTerCN	$CH_3COCOCHO$ + NO_3 → $CH_3C(O)$ + 2 CO + HNO_3	KNO3AL*4.0	Rickard and Pascoe (2009)
G44223	TrGTerC	IBUTALOH + OH → IPRHOCO3	1.4E-11	Rickard and Pascoe (2009)
G44224a	TrGTerC	IPRHOCO3 + HO_2 → CH_3COCH_3 + CO_2 + HO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G44224b	TrGTerC	IPRHOCO3 + HO_2 → IPRHOCO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G44224c	TrGTerC	IPRHOCO3 + HO_2 → IPRHOCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G44225	TrGTerCN	IPRHOCO3 + NO → CH_3COCH_3 + CO_2 + HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G44226	TrGTerCN	IPRHOCO3 + NO_2 → C4PAN5	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44227	TrGTerCN	IPRHOCO3 + NO_3 → CH_3COCH_3 + CO_2 + HO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G44228a	TrGTerC	IPRHOCO3 → CH_3COCH_3 + CO_2 + HO_2	k1_RO2RCO3*0.7	Rickard and Pascoe (2009)
G44228b	TrGTerC	IPRHOCO3 → IPRHOCO2H	k1_RO2RCO3*0.3	Rickard and Pascoe (2009)
G44229	TrGTerC	IPRHOCO2H + OH → CH_3COCH_3 + CO_2 + HO_2 + H_2O	1.72E-12	Rickard and Pascoe (2009)
G44230	TrGTerC	OH + IPRHOCO3H → IPRHOCO3	4.80E-12	Rickard and Pascoe (2009)
G44231	TrGTerCN	C4PAN5 → IPRHOCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	C4PAN5 + OH → CH_3COCH_3 + CO + NO_2	4.75E-13	Rickard and Pascoe (2009)
G44233a	TrGTerC	MBOOO → IPRHOCO2H	1.60E-17*C(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009), Sander et al. (2019)
G44233b	TrGTerC	MBOOO → IBUTALOH + H_2O_2	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Sander et al. (2019)
G44234	TrGTerC	MBOOO + CO → IBUTALOH + CO_2	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	MBOOO + NO → IBUTALOH + NO_2	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	MBOOO + NO_2 → IBUTALOH + NO_3	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	MALANHY + OH → MALANHYO2	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	MALDIALOOH + OH → HOCOC4DIAL + OH	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	MALDIALOOH + OH → MALDIALO2	k_ROOHRO	Rickard and Pascoe (2009)
G44402	TrGAroCN	NC4DCO2H + OH → MALANHY + NO_2	k_ROOHRO	Rickard and Pascoe (2009)*
G44403	TrGAroC	CO14O3CO2H + OH → $HCOCH_2O_2$ + 2 CO_2	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	BZFUOOH + OH → BZFUO2	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	HOCOC4DIAL + OH → CO2C4DIAL + HO_2	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	MALDIALCO3 + HO_2 → MALDALCO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G44406b	TrGAroC	MALDIALCO3 + HO_2 → MALDALCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G44406c	TrGAroC	MALDIALCO3 + HO_2 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)*
G44407	TrGAroCN	MALDIALCO3 + NO → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
G44408	TrGAroCN	MALDIALCO3 + NO_2 → MALDIALPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO3 + NO_3 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44410	TrGAroC	MALDIALCO3 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO_3 → NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O_3 → .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H_2O_2 + .5 CO + .5 CO_2 + .5 $HCOCH_2O_2$ + .5 OH	2.20E-19	see note*
G44413	TrGAroC	BZFUONE + OH → BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH → NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH → MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH → C3DIALO2 + CO_2	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO_2 → C3DIALO2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO_2 → EPXDLCO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO_2 → EPXDLCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO → C3DIALO2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G44419	TrGAroCN	EPXDLCO3 + NO_2 → EPXDLPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44420	TrGAroCN	EPXDLCO3 + NO_3 → C3DIALO2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G44421	TrGAroC	EPXDLCO3 → C3DIALO2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G44422	TrGAroC	MALNHYOHCO + OH → CO + CO + CO + CO_2 + HO_2	5.68E-12	Rickard and Pascoe (2009)
G44423	TrGAroCN	MALDIAL + NO_3 → MALDIALCO3 + HNO_3	2.*KNO3AL*2.0	Rickard and Pascoe (2009)
G44424	TrGAroC	MALDIAL + O_3 → 1.0675 GLYOX + .125 HCHO + .1125 $HCOCO_2H$ + .0675 H_2O_2 + .82 HO_2 + .57 OH + 1.265 CO + .25 CO_2	2.00E-18	Rickard and Pascoe (2009)*
G44425	TrGAroC	MALDIAL + OH → .83 MALDIALCO3 + .17 MALDIALO2	5.20E-11	Rickard and Pascoe (2009)*
G44426	TrGAroC	MALANHYOOH + OH → MALNHYOHCO + OH	4.66E-11	Rickard and Pascoe (2009)
G44427	TrGAroCN	MALDIALPAN + OH → GLYOX + CO + CO + NO_2	3.70E-11	Rickard and Pascoe (2009)
G44428	TrGAroCN	MALDIALPAN → MALDIALCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G44429a	TrGAroC	MALANHYO2 + HO_2 → MALANHYOOH	k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44429b	TrGAroC	MALANHYO2 + HO_2 → HCOCOHCO3 + CO_2 + OH	k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCOHCO3 + CO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44431	TrGAroCN	MALANHYO2 + NO_3 → HCOCOHCO3 + CO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 → HCOCOHCO3 + CO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G44433	TrGAroC	EPXDLCO3H + OH → EPXDLCO3	2.62E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44434	TrGAroC	CO2C4DIAL + OH → CO + CO + CO + CO + HO_2	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	NBZFUO2 + HO_2 → NBZFUOOH	k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44435b	TrGAroCN	NBZFUO2 + HO_2 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G44436	TrGAroCN	NBZFUO2 + NO → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44437	TrGAroCN	NBZFUO2 + NO_3 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44438	TrGAroCN	NBZFUO2 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G44439	TrGAroC	MALDALCO2H + OH → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2	3.70E-11	Rickard and Pascoe (2009)*
G44440	TrGAroCN	EPXC4DIAL + NO_3 → EPXDLCO3 + HNO_3	2.*KNO3AL*4.0	Rickard and Pascoe (2009)
G44441	TrGAroC	EPXC4DIAL + OH → EPXDLCO3	4.32E-11	Rickard and Pascoe (2009)
G44442a	TrGAroC	MECOACETO2 + HO_2 → MECOACEOOH	k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44442b	TrGAroC	MECOACETO2 + HO_2 → $CH_3C(O)OO$ + HCHO + CO_2 + OH	k_RO2_HO2(temp,4)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G44443	TrGAroCN	MECOACETO2 + NO → $CH_3C(O)OO$ + HCHO + CO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44444	TrGAroCN	MECOACETO2 + NO_3 → $CH_3C(O)OO$ + HCHO + CO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44445	TrGAroC	MECOACETO2 → $CH_3C(O)OO$ + HCHO + CO_2	k1_RO2pORO2	Rickard and Pascoe (2009)*
G44446	TrGAroCN	CO14O3CHO + NO_3 → CO + $HCOCH_2O_2$ + CO_2 + HNO_3	KNO3AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	CO14O3CHO + OH → CO + $HCOCH_2O_2$ + CO_2	3.44E-11	Rickard and Pascoe (2009)
G44448	TrGAroCN	NBZFUONE + OH → BZFUCO + NO_2	1.16E-12	Rickard and Pascoe (2009)
G44449a	TrGAroC	BZFUO2 + HO_2 → BZFUOOH	k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44449b	TrGAroC	BZFUO2 + HO_2 → CO14O3CHO + HO_2 + OH	k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G44450	TrGAroCN	BZFUO2 + NO → CO14O3CHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44451	TrGAroCN	BZFUO2 + NO_3 → CO14O3CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44452	TrGAroC	BZFUO2 → CO14O3CHO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44453	TrGAroC	BZFUCO + OH → CO14O3CHO + HO_2	1.78E-11	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO_2 → MALDIALOOH	k_RO2_HO2(temp,4)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO_2 → GLYOX + GLYOX + HO_2 + OH	k_RO2_HO2(temp,4)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G44457	TrGAroCN	MALDIALO2 + NO → GLYOX + GLYOX + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G44458	TrGAroCN	MALDIALO2 + NO_3 → GLYOX + GLYOX + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44459	TrGAroC	MALDIALO2 → GLYOX + GLYOX + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH → HCOCOCHO + CO + NO_2	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN → EPXDLCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH → MECOACETO2	3.59E-12	Rickard and Pascoe (2009)
G45000	TrGC	C_5H_8 + O_3 → .3508 MACR + .01518 MACO2H + .2440 MVK + .7085 HCHO + .11 CH_2OO + .1275 C_3H_6 + .1575 $CH_3C(O)$ + .0510 CH_3 + .2625 HO_2 + .27 OH + .09482 H_2O_2 + .255 CO_2 + .522 CO + .07182 HCHO + .03618 $HCOCH_2O_2$ + .01782 CO + 0.05408 LCARBON	1.03E-14*EXP(-1995./temp)	Atkinson et al. (2006), Sander et al. (2019)
G45001	TrGC	C_5H_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_5H_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)
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)

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

#	labels	reaction	rate coefficient	reference
G45010b	TrGC	LDISOPACO2 $\rightarrow$ LZCODC23DBCOOH + HO_2	k_16hsz41 * (2./3.*f_HPAL + 1./3.)	Sander et al. (2019)
G45011	TrGC	LISOPACO2 $\rightarrow$ .9 LISOPACO + .1 ISOPAOH	k1_RO2LISOPACO2	Rickard and Pascoe (2009), Sander et al. (2019)
G45012	TrGC	LISOPACO2 + HO_2 $\rightarrow$ LISOPACOOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009)
G45013a	TrGCN	LISOPACO2 + NO $\rightarrow$ LISOPACO + NO_2	KRO2NO*(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 $\rightarrow$ LISOPACNO3	KRO2NO*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 $\rightarrow$ LISOPACO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45015	TrGC	LDISOPACO2 $\rightarrow$ .9 LISOPACO + .1 ISOPAOH	k1_RO2LISOPACO2	Rickard and Pascoe (2009), Sander et al. (2019)
G45016	TrGC	LDISOPACO2 + HO_2 $\rightarrow$ LISOPACOOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO $\rightarrow$ LISOPACO + NO_2	KRO2NO*(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 $\rightarrow$ LISOPACNO3	KRO2NO*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 $\rightarrow$ LISOPACO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH $\rightarrow$ LISOPACO2	k_ROOHRO	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_sOOH*f_allyl+ k_ROHRO)	Sander et al. (2019)
G45019d	TrGC	LISOPACOOH + OH $\rightarrow$ LIEPOX + OH	(k_adt+k_ads)*a_CH2OH*a_CH2OOH	Sander et al. (2019)*
G45020	TrGC	ISOPAOH + OH $\rightarrow$ LHC4ACCHO + HO_2	(k_adt+k_ads)*a_CH2OH*a_CH2OH+k_ s*f_sOH*f_allyl+k_ROHRO	Sander et al. (2019)
G45021	TrGCN	LISOPACNO3 + OH $\rightarrow$ LISOPACNO3O2	(k_adt+k_ads)*a_CH2ONO2*a_CH2OH	Sander et al. (2019)*
G45022	TrGC	ISOPBO2 $\rightarrow$ .8 MVK + .8 HCHO + .8 HO_2 + .2 ISOPBOH	k1_RO2ISOPBO2	Rickard and Pascoe (2009)
G45023a	TrGC	ISOPBO2 + HO_2 $\rightarrow$ ISOPBOOH	k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH)	Sander et al. (2019)
G45023b	TrGC	ISOPBO2 + HO_2 $\rightarrow$ MVK + HCHO + HO_2 + OH	k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH	Sander et al. (2019)
G45024a	TrGCN	ISOPBO2 + NO $\rightarrow$ MVK + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(6,3,0,0,0, temp,cair))	Lockwood et al. (2010), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45024b	TrGCN	ISOPBO2 + NO → ISOPBNO3	KRO2NO*alpha_AN(6,3,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45025	TrGCN	ISOPBO2 + NO_3 → MVK + .75 HCHO + .75 HO_2 + .25 CH_3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45026a	TrGC	ISOPBOOH + OH → LIEPOX + OH	(k_ads+k_adp)*a_CH2OOH	Paulot et al. (2009b), Sander et al. (2019)
G45026b	TrGC	ISOPBOOH + OH → ISOPBO2	k_ROOHRO	Sander et al. (2019)
G45026c	TrGC	ISOPBOOH + OH → MGLYOX + $HOCH_2CHO$	k_ROHRO+k_s*f_alk*f_sOH	Sander et al. (2019)
G45027	TrGC	ISOPBOOH + O_3 → .1368 MACROOH + .1368 H_2O_2 + .2280 HO_2 + .4332 CH_3COCH_2OH + .2280 CO_2 + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO_2 + .06880 OH + .2709 CO + .1591 CH_2OO	1.E-17	Sander et al. (2019)
G45028	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO_2 + .25 CH_3	k_s*f_alk*f_sOH+(k_adp+k_ads) *a_CH2OH	Sander et al. (2019)
G45029	TrGCN	ISOPBNO3 + OH → ISOPBDNO3O2	(k_adt+k_adp)*f_CH2ONO2	Sander et al. (2019)
G45030	TrGC	ISOPDO2 → .8 MACR + .8 HCHO + .8 HO_2 + .1 HCOC5 + .1 ISOPDOH	k1_RO2ISOPDO2	Rickard and Pascoe (2009)
G45031a	TrGC	ISOPDO2 + HO_2 → ISOPDOOH	k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH)	Sander et al. (2019)
G45031b	TrGC	ISOPDO2 + HO_2 → MACR + HCHO + HO_2 + OH	k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH	Sander et al. (2019)
G45032a	TrGCN	ISOPDO2 + NO → MACR + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(6,2,0,0,0, temp,cair))	Lockwood et al. (2010), Sander et al. (2019)
G45032b	TrGCN	ISOPDO2 + NO → ISOPDNO3	KRO2NO*alpha_AN(6,2,0,0,0,temp, cair)	Lockwood et al. (2010), Sander et al. (2019)
G45033	TrGCN	ISOPDO2 + NO_3 → MACR + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45034a	TrGC	ISOPDOOH + OH → LIEPOX + OH	(k_adt+k_adp)*a_CH2OOH	Paulot et al. (2009b), Sander et al. (2019)
G45034b	TrGC	ISOPDOOH + OH → ISOPDO2	k_ROOHRO	Sander et al. (2019)
G45034c	TrGC	ISOPDOOH + OH → HCOC5 + OH	k_t*f_tOOH*f_allyl*f_pCH2OH	Sander et al. (2019)
G45034d	TrGC	ISOPDOOH + OH → CH_3COCH_2OH + GLYOX + OH	k_s*f_pCH2OH*f_sOH	Sander et al. (2019)
G45035	TrGC	ISOPDOOH + O_3 → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO_2 + .2079 CO + .1221 CH_2OO	1.E-17	Sander et al. (2019)
G45036	TrGC	ISOPDOH + OH → HCOC5 + HO_2	2.*k_ROHRO+(k_t*f_tOH*f_allyl+k_ s*f_sOH)*f_pCH2OH+(k_adt+k_adp) *a_CH2OH	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45037	TrGCN	ISOPDNO3 + OH → ISOPBDNO3O2	(k_adp+k_ads)*a_CH2ONO2	Sander et al. (2019)*
G45038	TrGCN	NISOPO2 → .8 NC4CHO + .6 HO_2 + .2 LISOPACNO3	k1_RO2LISOPACO2	Rickard and Pascoe (2009)
G45039	TrGCN	NISOPO2 + HO_2 → NISOPOOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOPO2 + NO → NC4CHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOPO2 + NO_3 → NC4CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45042	TrGCN	NISOPOOH + OH → NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC4CHO + OH → LNISO3	(k_adt+k_ads)*a_CHO*a_CH2ONO2	Sander et al. (2019)*
G45044	TrGCN	NC4CHO + O_3 → .27 NOA + .027 $HCOCO_2H$ + .0162 GLYOX + .0162 H_2O_2 + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO_2 + 0.7705 HCHO + .4055 CO_2 + .73 GLYOX	2.40E-17	Sander et al. (2019)
G45045	TrGCN	NC4CHO + NO_3 → LNISO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO3 + HO_2 → LNISOOH	0.5*k_RO2_HO2(temp,5)+0.5*KAPHO2	Rickard and Pascoe (2009)
G45047	TrGCN	LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	0.5*KAPNO+0.5*KRO2NO	Rickard and Pascoe (2009)*
G45048	TrGCN	LNISO3 + NO_3 → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	KRO2NO3*1.37	Rickard and Pascoe (2009)
G45049	TrGCN	LNISOOH + OH → LNISO3	2.65E-11	Rickard and Pascoe (2009)
G45050a	TrGC	LHC4ACCHO + OH → LC578O2	(k_adtertprim+k_ads)*a_CHO*a_CH2OH	Sander et al. (2019)
G45050b	TrGC	LHC4ACCHO + OH → LHC4ACCO3	k_t*f_O	Sander et al. (2019)
G45050c	TrGC	LHC4ACCHO + OH → C4MDIAL + HO_2	k_s*f_sOH*f_allyl	Sander et al. (2019)
G45051	TrGC	LHC4ACCHO + O_3 → .2225 $CH_3C(O)$ + .89 CO + .0171875 $HOCH_2CO_2H$ + .075625 H_2O_2 + .0171875 $HCOCO_2H$ + .2775 CH_3COCH_2OH + .6675 HO_2 + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 $HOCH_2CHO$ + .5 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
G45052	TrGCN	LHC4ACCHO + NO_3 → LHC4ACCO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
G45053	TrGC	LC578O2 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2	k1_RO2tORO2	Rickard and Pascoe (2009)
G45054a	TrGC	LC578O2 + HO_2 → MGLYOX + $HOCH_2CHO$ + OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Rickard and Pascoe (2009)
G45054b	TrGC	LC578O2 + HO_2 → LC578OOH	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Rickard and Pascoe (2009)
G45055	TrGCN	LC578O2 + NO → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45056	TrGCN	LC578O2 + NO_3 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45057	TrGC	LC578O2 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 $HOCH_2CHO$ + .75 $HOCH_2CHO$ + HO_2 + OH	k_hsb	Sander et al. (2019)
G45058a	TrGC	LC578OOH + OH → LC578O2	k_ROOHRO	Sander et al. (2019)
G45058b	TrGC	LC578OOH + OH → C1ODC2OOHC4OD + HO_2	k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_pCH2OH*f_pCH2OH+k_s*f_sOH*f_pCH2OH	Sander et al. (2019)
G45059a	TrGC	LHC4ACCO3 → OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G45059b	TrGC	LHC4ACCO3 → LHC4ACCO2H	k1_RO2RCO3*0.1	Sander et al. (2019)
G45060a	TrGC	LHC4ACCO3 + HO_2 → 2 OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	KAPHO2*r_CO3_OH	Sander et al. (2019)
G45060b	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO3H	KAPHO2*r_CO3_OOH	Sander et al. (2019)
G45060c	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO2H + O_3	KAPHO2*r_CO3_O3	Sander et al. (2019)
G45061	TrGCN	LHC4ACCO3 + NO → .5 MACRO2 + .5 LHMVKABO2 + NO_2 + CO_2	KAPNO	Sander et al. (2019)
G45062	TrGCN	LHC4ACCO3 + NO_2 → LC5PAN1719	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45063	TrGCN	LHC4ACCO3 + NO_3 → .5 MACRO2 + .5 LHMVKABO2 + NO_2 + CO_2	KRO2NO3*1.74	Sander et al. (2019)
G45064a	TrGC	LHC4ACCO2H + OH → OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	2.52E-11	Sander et al. (2019)
G45064b	TrGC	LHC4ACCO3H + OH → LHC4ACCO3	2.88E-11	Rickard and Pascoe (2009)
G45065	TrGCN	LC5PAN1719 → LHC4ACCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45066	TrGCN	LC5PAN1719 + OH → .5 MACROH + .5 HO12CO3C4 + CO + NO_2	2.52E-11	Rickard and Pascoe (2009)
G45067	TrGC	HCOC5 + OH → C59O2	3.81E-11	Rickard and Pascoe (2009)
G45068	TrGC	HCOC5 + O_3 → BIACETOH + .335 H_2O_2 + .67 HCHO + .2079 CO + .1221 CH_2OO + .05280 OH	7.51E-16*EXP(-1521./temp)	Sander et al. (2019)
G45069	TrGC	C59O2 → CH_3COCH_2OH + HOCH2CO	k1_RO2tORO2	Sander et al. (2019)
G45070a	TrGC	C59O2 + HO_2 → OH + CH_3COCH_2OH + HOCH2CO	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Sander et al. (2019)
G45070b	TrGC	C59O2 + HO_2 → C59OOH	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Sander et al. (2019)
G45071	TrGCN	C59O2 + NO → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO	Sander et al. (2019)*
G45072	TrGCN	C59O2 + NO_3 → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO3	Sander et al. (2019)
G45073	TrGC	C59OOH + OH → C59O2	9.7E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45074	TrGC	LIEPOX + OH → DB1O2 + H_2O	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 → MVK + HCHO + OH	k_hsb	Sander et al. (2019)
G45076	TrGC	ISOPDO2 → MACR + HCHO + OH	k_hsd	Sander et al. (2019)
G45077a	TrGC	LZCODC23DBCOOH + OH → .6 C1ODC2O2C4OOH + .4 C1OOHC2O2C4OD	k_adt*a_CHO*a_CH2OOH	Sander et al. (2019)
G45077b	TrGC	LZCODC23DBCOOH + OH → .6 C1ODC3O2C4OOH + .4 C1OOHC3O2C4OD	k_ads*a_CHO*a_CH2OOH	Sander et al. (2019)
G45077c	TrGC	LZCODC23DBCOOH + OH → LZCO3HC23DBCOD	k_t*f_O*f_alk+k_ROOHRO	Sander et al. (2019)
G45077d	TrGC	LZCODC23DBCOOH + OH → C4MDIAL + OH	k_s*f_sOOH*f_allyl	Sander et al. (2019)
G45078	TrGC	LZCODC23DBCOOH + O_3 → .4672 OH + .2336 $HCOCOCH_2O_2$ + .2336 CO + .2336 $CH_3C(O)$ + .4672 HOOCH2CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH2CHO + .02765 H_2O_2 + .02592 CH_3OOH + .02592 CO_2 + .01037 HCOCO + .01555 CH_2OO + .01555 CO + .006908 $HOOCH_2CO_3$ + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 $HCOCOCH_2OOH$ + .2628 GLYOX + .0972 $CH_3COCH_2O_2H$ + .00972 $HCOCO_2H$ + .005832 GLYOX + .005832 H_2O_2 + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO_2 + .01458 HCOOH + .01458 CO	2.4E-17	Sander et al. (2019)
G45079	TrGC	C1OOHC2O2C4OD → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH	k1_RO2tORO2	Sander et al. (2019)
G45080	TrGCN	C1OOHC2O2C4OD + NO → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH + NO_2	KRO2NO	Sander et al. (2019)*
G45081a	TrGC	C1OOHC2O2C4OD + HO_2 → C1OOHC2OOHC4OD	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Sander et al. (2019)
G45081b	TrGC	C1OOHC2O2C4OD + HO_2 → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + 1.22 OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Sander et al. (2019)
G45082	TrGC	C1OOHC2O2C4OD → $CH_3COCH_2O_2H$ + GLYOX + OH	k_hsb	Sander et al. (2019)
G45083	TrGC	C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD	k_15hsdhb	Sander et al. (2019)
G45084a	TrGC	C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH	2.*k_s*f_sOOH*f_tCH2OH	Sander et al. (2019)
G45084b	TrGC	C1OOHC2OOHC4OD + OH → $CH_3COCH_2O_2H$ + 2 CO + 2 HO_2 + OH	k_t*f_tOH*f_pCH2OH*f_pCH2OH	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45084c	TrGC	C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD	k_ROOHRO	Sander et al. (2019)
G45085	TrGC	C1ODC2OOHC4OD + OH → CO2H3CHO + CO + H_2O + OH	k_t*f_O*f_tCH2OH+k_t*f_tOH*f_tOH*f_CHO	Sander et al. (2019)
G45086	TrGC	C1ODC3O2C4OOH → MGLYOX + HOOCH2CHO + HO_2	k1_RO2sORO2	Sander et al. (2019)
G45087	TrGCN	C1ODC3O2C4OOH + NO → MGLYOX + HOOCH2CHO + HO_2 + NO_2	KRO2NO	Sander et al. (2019)
G45088	TrGC	C1ODC3O2C4OOH + HO_2 → .5 $CH_3C(O)$ + .5 CO + .5 MGLYOX + .5 HO_2 + $HOOCH_2CO_3$	k_RO2_HO2(temp,5)	Sander et al. (2019)
G45089	TrGC	C1ODC3O2C4OOH → MGLYOX + OH + HOOCH2CHO	k_hsd	Sander et al. (2019)
G45090	TrGC	C1OOHC3O2C4OD → .625 MGLYOX + 2 CO + 1.625 HO_2 + .375 $CH_3C(O)$ + .375 CO_2 + OH	k_15hsdhb	Sander et al. (2019)
G45091	TrGC	LHC4ACCO3 → LZCO3HC23DBCOD + HO_2	k_16hs	Sander et al. (2019)
G45092a	TrGC	C4MDIAL + OH → C1ODC2O2C4OD	(k_adt+k_ads)*a_CHO*a_CHO	Sander et al. (2019)*
G45092b	TrGC	C4MDIAL + OH → LZCO3C23DBCOD	2.*k_t*f_O*f_alk	Sander et al. (2019)*
G45093	TrGCN	C4MDIAL + NO_3 → LZCO3C23DBCOD + HNO_3	KNO3AL*4.25*2.	Sander et al. (2019)*
G45094a	TrGC	C1ODC2O2C4OD + HO_2 → OH + MGLYOX + HOCHCHO	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Sander et al. (2019)
G45094b	TrGC	C1ODC2O2C4OD + HO_2 → C1ODC2OOHC4OD	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Sander et al. (2019)
G45095	TrGCN	C1ODC2O2C4OD + NO → NO_2 + MGLYOX + HOCHCHO	KRO2NO	Sander et al. (2019)*
G45096	TrGC	C1ODC2O2C4OD → MGLYOX + HOCHCHO	k1_RO2tORO2	Sander et al. (2019)
G45097a	TrGC	C1ODC2OOHC4OD + OH → MGLYOX + 2 CO	(2.*k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_CHO*f_pCH2OH)*.5	Sander et al. (2019)
G45097b	TrGC	C1ODC2OOHC4OD + OH → MGLYOX + 2 CO + OH	(2.*k_t*f_O*f_tCH2OH*f_alk+k_t*f_tOH*f_CHO*f_pCH2OH)*.5	Sander et al. (2019)
G45098	TrGCN	LISOPACNO3O2 + NO → .21 NOA + .21 $HOCH_2CHO$ + .21 HO_2 + .49 HO12CO3C4 + .49 HCHO + .49 NO_2 + .045 MVKNO3 + .045 HCHO + .255 CH_3COCH_2OH + .255 NO_3CH2CHO + .225 H_2O_2 + NO_2	KRO2NO	Sander et al. (2019)*
G45099	TrGCN	LISOPACNO3O2 → .21 NOA + .21 $HOCH_2CHO$ + .21 HO_2 + .49 HO12CO3C4 + .49 HCHO + .49 NO_2 + .045 MVKNO3 + .045 HCHO + .255 CH_3COCH_2OH + .255 NO_3CH2CHO + .225 H_2O_2	k1_RO2tORO2+k_RO2_HO2(temp,5)*c(ind_HO2)	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45100	TrGCN	ISOPBDNO3O2 + NO → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRNO3 + .14 MVKNO3 + .4 HCHO + .4 HO_2 + 1.6 NO_2	`KRO2NO`	Sander et al. (2019)*
G45101	TrGCN	ISOPBDNO3O2 → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRNO3 + .14 MVKNO3 + .4 HCHO + .4 HO_2 + .6 NO_2	`k1_RO2sORO2+k_RO2_HO2(temp,5)*c(ind_HO2)`	Sander et al. (2019)
G45102	TrGCN	LISOPACNO3 + O_3 → .8704 OH + .365 HO_2 + .73 MGLYOX + .4325 NO_3CH2CHO + .135 CH_3COCH_2OH + .0675 GLYOX + .4325 NO_2 + .0891 H_2O_2 + .135 NOA + .0675 HOCHCHO + .3866 $HOCH_2CHO$ + .0405 CH_3OH + .0405 CO + .0054 HOCH2CO	`2.8E-17`	Feierabend et al. (2008), Sander et al. (2019)
G45103	TrGC	DB1O2 → DB1O2	`k1_RO2sORO2`	Sander et al. (2019)
G45104a	TrGC	DB1O2 + HO_2 → DB1OOH	`k_RO2_HO2(temp,5)*(1.-r_CHOHCH2O2_OH)`	Sander et al. (2019)*
G45104b	TrGC	DB1O2 + HO_2 → DB1O2 + OH	`k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH`	Sander et al. (2019)
G45105a	TrGCN	DB1O2 + NO → DB1O2 + NO_2	`KRO2NO*(1.-alpha_AN(7,2,0,0,0,temp,cair))`	Sander et al. (2019)
G45105b	TrGCN	DB1O2 + NO → DB1NO3	`KRO2NO*alpha_AN(7,2,0,0,0,temp,cair)`	Sander et al. (2019)
G45106	TrGCN	DB1O2 + NO_3 → DB1O2 + NO_2	`KRO2NO3`	Sander et al. (2019)
G45107	TrGC	DB1O2 → DB1O2 + OH	`1.E4`	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 → DB1O2	`KDEC*0.72`	see note*
G45108b	TrGC	DB1O2 → .5 HVMK + .5 HMAC + HCHO + HO_2	`KDEC*0.28`	see note*
G45109	TrGC	DB1O2 → .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2	`k1_RO2sORO2`	Sander et al. (2019)
G45110a	TrGC	DB1O2 + HO_2 → DB2OOH	`k_RO2_HO2(temp,5)*(1.-r_CHOHCH2O2_OH)`	Sander et al. (2019)
G45110b	TrGC	DB1O2 + HO_2 → .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + OH	`k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH`	Sander et al. (2019)
G45111	TrGCN	DB1O2 + NO → .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + NO_2	`KRO2NO`	see note*
G45112	TrGCN	DB1O2 + NO_3 → .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + NO_2	`KRO2NO3`	Sander et al. (2019)
G45113	TrGC	DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH	`k_14hsal`	Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45114a	TrGC	DB1OOH + OH → DB1O2	k_ROOHRO	Sander et al. (2019)
G45114b	TrGC	DB1OOH + OH → HCOOH + HO_2 + CH_3COCHO_2CHO	k_adt	Sander et al. (2019)*
G45115	TrGC	DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH	4.67E-26*(temp)**(3.286) *EXP(4509./(1.987*temp))	Sander et al. (2019), da Silva (2010)*
G45116	TrGCN	DB1NO3 + OH → HCOOH + NO_2 + CH_3COCHO_2CHO	k_adt	Sander et al. (2019)*
G45117	TrGC	DB2OOH + OH → DB1O2	k_ROOHRO	Sander et al. (2019)*
G45118	TrGC	LISOPACOOH + O_3 → 1.3272 OH + .36986 HO_2 + .0432 H_2O_2 + .08422 CO + .2025 CH_3OOH + .01215 CH_2OO + .3704 HCHO + .00405 CH_3OH + .0405 CO_2 + .1825 HOCH2COCH2O2 + .365 MGLYOX + .3866 HOOCH2CHO + .135 CH_3COCH_2OH + .0675 GLYOX + .00324 HCOCO + .3866 $HOCH_2CHO$ + .135 $CH_3COCH_2O_2H$ + .0675 HOCHCHO + .0054 HOCH2CO	4.829E-16	Sander et al. (2019)
G45119a	TrGC	LZCO3HC23DBCOD + OH → .62 CO2H3CHO + .62 OH + .62 CO_2 + .38 MGLYOX + .38 $HCOCO_3H$ + .38 HO_2	k_adt*a_CHO*a_CO2H	Sander et al. (2019)
G45119b	TrGC	LZCO3HC23DBCOD + OH → .62 CH_3COCO_3H + 1.24 CO + 1.24 HO_2 + .38 MGLYOX + .38 HO_2 + .38 CO + .38 HO_2 + .38 OH + .38 CO_2	k_ads*a_CHO*a_CO2H	Sander et al. (2019)
G45120	TrGC	LISOPEFO2 → LISOPEFO	k1_RO2pORO2	Sander et al. (2019)
G45121a	TrGCN	LISOPEFO2 + NO → LISOPEFO + NO_2	KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Sander et al. (2019)
G45121b	TrGCN	LISOPEFO2 + NO → ISOPDNO3	KRO2NO*alpha_AN(6,1,0,0,0,temp, cair)	Sander et al. (2019)*
G45122a	TrGC	LISOPEFO2 + HO_2 → .7143 ISOPDOOH + .2857 ISOPBOOH	k_RO2_HO2(temp,5)*(1.-r_ CHOHCH2O2_OH)	Sander et al. (2019)
G45122b	TrGC	LISOPEFO2 + HO_2 → LISOPEFO + OH	k_RO2_HO2(temp,5)*r_CHOHCH2O2_OH	Sander et al. (2019)
G45123	TrGCN	LISOPEFO2 + NO_3 → LISOPEFO + NO_2	KRO2NO3	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)

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

#	labels	reaction	rate coefficient	reference
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_RO2sORO2	Sander et al. (2019)
G45131	TrGCN	L3METHYLFURANO2 + NO → C4MDIAL + HO_2 + NO_2	KRO2NO	Sander et al. (2019)*
G45132	TrGC	L3METHYLFURANO2 + HO_2 → C4MDIAL + HO_2	k_RO2_HO2(temp,5)	Sander et al. (2019)*
G45133	TrGC	LZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2	k1_RO2RCO3	Sander et al. (2019)
G45134a	TrGC	LZCO3C23DBCOD + HO_2 → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + OH	KAPHO2*r_CO3_OH	Sander et al. (2019)
G45134b	TrGC	LZCO3C23DBCOD + HO_2 → LZCO3HC23DBCOD	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Sander et al. (2019)*
G45135	TrGCN	LZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	KAPNO	Sander et al. (2019)
G45136	TrGCN	LZCO3C23DBCOD + NO_2 → LZCPANC23DBCOD	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45137	TrGCN	LZCO3C23DBCOD + NO_3 → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	KRO2NO3*1.74	Sander et al. (2019)
G45138	TrGCN	LZCPANC23DBCOD → LZCO3C23DBCOD + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	LZCPANC23DBCOD + OH → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	2.52E-11	Sander et al. (2019)*
G45200	TrGTerC	C511O2 → $CH_3C(O)$ + HCOCH2CHO	k1_RO2sORO2	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO → $CH_3C(O)$ + HCOCH2CHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45202a	TrGTerC	C511O2 + HO_2 → C511OOH	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G45202b	TrGTerC	C511O2 + HO_2 → $CH_3C(O)$ + HCOCH2CHO + OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)

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

#	labels	reaction	rate coefficient	reference
G45203	TrGTerC	C511OOH + OH → C511O2	7.49E-11	Rickard and Pascoe (2009)
G45204	TrGTerC	CO23C4CHO + OH → CO23C4CO3	6.65E-11	Rickard and Pascoe (2009)
G45205	TrGTerCN	CO23C4CHO + NO_3 → CO23C4CO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
G45206	TrGTerC	CO23C4CO3 → $CH_3COCOCH_2O_2$ + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G45207	TrGTerCN	CO23C4CO3 + NO → $CH_3COCOCH_2O_2$ + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
G45208	TrGTerCN	CO23C4CO3 + NO_2 → C5PAN9	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45209a	TrGTerC	CO23C4CO3 + HO_2 → CO23C4CO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G45209b	TrGTerC	CO23C4CO3 + HO_2 → $CH_3COCOCH_2O_2$ + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G45210	TrGTerCN	C5PAN9 → CO23C4CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45211	TrGTerCN	C5PAN9 + OH → $CH_3COCOCHO$ + CO + NO_2	3.12E-13	Rickard and Pascoe (2009)
G45212	TrGTerC	C512O2 → C513O2	k1_RO2pRO2	Rickard and Pascoe (2009)
G45213	TrGTerC	C512O2 + HO_2 → C512OOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009)
G45214	TrGTerCN	C512O2 + NO → C513O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45215	TrGTerC	C512OOH + OH → CO13C4CHO + OH	1.01E-10	Rickard and Pascoe (2009)
G45216	TrGTerC	C513O2 → GLYOX + $HOC_2H_4CO_3$	k1_RO2sORO2	Rickard and Pascoe (2009)
G45217	TrGTerCN	C513O2 + NO → GLYOX + $HOC_2H_4CO_3$ + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45218a	TrGTerC	C513O2 + HO_2 → C513OOH	k_RO2_HO2(temp,5)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G45218b	TrGTerC	C513O2 + HO_2 → GLYOX + $HOC_2H_4CO_3$ + OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45219	TrGTerC	CO13C4CHO + OH → CHOC3COCO3	1.33E-10	Rickard and Pascoe (2009)
G45220	TrGTerCN	CO13C4CHO + NO_3 → CHOC3COCO3 + HNO_3	2.*KNO3AL*5.5	Rickard and Pascoe (2009)
G45221	TrGTerC	C513OOH + OH → C513CO + OH	9.23E-11	Rickard and Pascoe (2009)
G45222	TrGTerC	CHOC3COCO3 → CHOC3COO2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G45223	TrGTerC	CHOC3COCO3 + HO_2 → CHOC3COOOH	KAPHO2	Rickard and Pascoe (2009)
G45224	TrGTerCN	CHOC3COCO3 + NO_2 → CHOC3COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45225	TrGTerCN	CHOC3COCO3 + NO → CHOC3COO2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
G45226	TrGTerC	C513CO + OH → $HOC_2H_4CO_3$ + CO + CO	2.64E-11	Rickard and Pascoe (2009)
G45227	TrGTerC	C514O2 + HO_2 → C514OOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009)
G45228a	TrGTerCN	C514O2 + NO → CO13C4CHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(7,2,0,1,0, temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G45228b	TrGTerCN	C514O2 + NO → C514NO3	KRO2NO*alpha_AN(7,2,0,1,0,temp, cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G45229	TrGTerCN	C514O2 + NO_3 → CO13C4CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45230	TrGTerC	C514O2 → CO13C4CHO + HO_2	k1_RO2sRO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45231	TrGTerC	C514OOH + OH → CO13C4CHO + OH	1.10E-10	Rickard and Pascoe (2009)
G45232	TrGTerCN	C514NO3 + OH → CO13C4CHO + NO_2	4.33E-11	Rickard and Pascoe (2009)
G45233	TrGTerC	CHOC3COOOH + OH → CHOC3COCO3	7.55E-11	Rickard and Pascoe (2009)
G45234	TrGTerCN	CHOC3COPAN → CHOC3COCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45235	TrGTerCN	CHOC3COPAN + OH → C4CODIAL + CO + NO_2	7.19E-11	Rickard and Pascoe (2009)
G45236	TrGTerC	MBO + OH → LMBOABO2	8.1E-12*EXP(610./temp)	Rickard and Pascoe (2009), Sander et al. (2019)*
G45237a	TrGTerC	MBO + O_3 → HCHO + .16 CH_3COCH_3 + .16 HO_2 + .16 CO + .16 OH + .84 MBOOO	1.0E-17*0.57	Rickard and Pascoe (2009), Sander et al. (2019)
G45237b	TrGTerC	MBO + O_3 → IBUTALOH + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 HO_2	1.0E-17*0.43	Rickard and Pascoe (2009), Sander et al. (2019)
G45238	TrGTerCN	MBO + NO_3 → LNMBOABO2	4.6E-14*EXP(-400./temp)	Rickard and Pascoe (2009), Sander et al. (2019)
G45239	TrGTerC	LMBOABO2 + HO_2 → LMBOABOOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009), Sander et al. (2019)
G45240a	TrGTerCN	LMBOABO2 + NO → LMBOABNO3	KRO2NO*(.67*alpha_AN(7,2,0,0,0, temp,cair)+.33*alpha_AN(7,1,0,0, 0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G45240b	TrGTerCN	LMBOABO2 + NO → $HOCH_2CHO$ + CH_3COCH_3 + HO_2 + NO_2	KRO2NO*(1.-(.67*alpha_AN(7,2,0, 0,0,temp,cair)+.33*alpha_AN(7,1, 0,0,0,temp,cair)))*.67	Rickard and Pascoe (2009), Sander et al. (2019)
G45240c	TrGTerCN	LMBOABO2 + NO → IBUTALOH + HCHO + HO_2 + NO_2	KRO2NO*(1.-(.67*alpha_AN(7,2,0, 0,0,temp,cair)+.33*alpha_AN(7,1, 0,0,0,temp,cair)))*.33	Rickard and Pascoe (2009), Sander et al. (2019)
G45241a	TrGTerC	LMBOABO2 → $HOCH_2CHO$ + CH_3COCH_3 + HO_2	k1_RO2sORO2*.67	Rickard and Pascoe (2009), Sander et al. (2019)
G45241b	TrGTerC	LMBOABO2 → IBUTALOH + HCHO + HO_2	k1_RO2pORO2*.33	Rickard and Pascoe (2009), Sander et al. (2019)
G45242a	TrGTerC	LMBOABOOH + OH → MBOACO	0.67*2.93E-11+.33*2.05E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45242b	TrGTerC	LMBOABOOH + OH → LMBOABO2	k_ROOHRO	Rickard and Pascoe (2009), Sander et al. (2019)
G45243	TrGTerCN	LMBOABNO3 + OH → MBOACO + NO_2	0.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45244	TrGTerC	MBOACO + OH → MBOCOCO + HO_2	3.79E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45245	TrGTerC	MBOCOCO + OH → CO + IPRHOCO3	1.38E-11	Rickard and Pascoe (2009)
G45246	TrGTerCN	LNMBOABO2 + HO_2 → LNMBOABOOH	k_RO2_HO2(temp,5)	Rickard and Pascoe (2009), Sander et al. (2019)
G45247	TrGTerCN	LNMBOABO2 + NO → .65 NO_3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Sander et al. (2019)*
G45248	TrGTerCN	LNMBOABO2 + NO_3 → .65 NO_3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Sander et al. (2019)
G45249	TrGTerCN	LNMBOABO2 → .65 NO_3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2	k1_RO2sORO2	Rickard and Pascoe (2009), Sander et al. (2019)
G45250a	TrGTerCN	LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBCO	0.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45250b	TrGTerCN	LNMBOABOOH + OH → LNMBOABO2	k_ROOHRO	Rickard and Pascoe (2009), Sander et al. (2019)
G45251	TrGTerCN	NMBOBCO + OH → NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45252a	TrGTerCN	NC4OHCO3 + HO_2 → IBUTALOH + CO_2 + NO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45252b	TrGTerCN	NC4OHCO3 + HO_2 → NC4OHCO3H	KAPHO2*(r_CO3_O3+r_CO3_OOH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45253	TrGTerCN	NC4OHCO3 + NO → IBUTALOH + CO_2 + NO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G45254	TrGTerCN	NC4OHCO3 + NO_2 → NC4OHCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45255	TrGTerCN	NC4OHCO3 + NO_3 → IBUTALOH + CO_2 + NO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45256	TrGTerCN	NC4OHCO3 → IBUTALOH + CO_2 + NO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G45257	TrGTerCN	NC4OHCO3H + OH → NC4OHCO3	4.50E-12	Rickard and Pascoe (2009)
G45258	TrGTerCN	NC4OHCPAN + OH → IBUTALOH + CO + NO_2 + NO_2	1.27E-12	Rickard and Pascoe (2009)
G45259	TrGTerCN	NC4OHCPAN → NC4OHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45260	TrGTerCN	C4MCONO3OH + OH → CH_3COCH_3 + HCHO + CO_2 + NO_2	1.23E-12	Rickard and Pascoe (2009), Sander et al. (2019)
G45400	TrGAroCN	NC4MDCO2HN + OH → MMALANHY + NO_2	k_ROOHRO	Rickard and Pascoe (2009)*
G45401	TrGAroCN	C54CO + NO_3 → 3 CO + $CH_3C(O)OO$ + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	C54CO + OH → 3 CO + $CH_3C(O)OO$	1.72E-11	Rickard and Pascoe (2009)
G45403a	TrGAroCN	NTLFUO2 + HO_2 → NTLFUOOH	k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	NTLFUO2 + HO_2 → ACCOMECHO + NO_2 + OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45404	TrGAroCN	NTLFUO2 + NO → ACCOMECHO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45405	TrGAroCN	NTLFUO2 + NO_3 → ACCOMECHO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G45406	TrGAroCN	NTLFUO2 → ACCOMECHO + NO_2	k1_RO2tORO2	Rickard and Pascoe (2009)*
G45407	TrGAroC	C5134CO2OH + OH → C54CO + HO_2	7.48E-11	Rickard and Pascoe (2009)
G45408	TrGAroCN	C5COO2NO2 + OH → MGLYOX + CO + CO + NO_2	5.43E-11	Rickard and Pascoe (2009)
G45409	TrGAroCN	C5COO2NO2 → C5CO14O2 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
G45410	TrGAroC	C5DIALOOH + OH → C5DIALCO + OH	7.52E-11	Rickard and Pascoe (2009)
G45411a	TrGAroC	C4CO2DBCO3 + HO_2 → C4CO2DCO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G45411b	TrGAroC	C4CO2DBCO3 + HO_2 → HO_2 + CO + HCOCOCHO + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G45412	TrGAroCN	C4CO2DBCO3 + NO → HO_2 + CO + HCOCOCHO + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G45413	TrGAroCN	C4CO2DBCO3 + NO_2 → C4CO2DBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45414	TrGAroCN	C4CO2DBCO3 + NO_3 → HO_2 + CO + HCOCOCHO + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45415	TrGAroC	C4CO2DBCO3 → HO_2 + CO + HCOCOCHO + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G45416	TrGAroC	MMALANHY + OH → MMALANHYO2	1.50E-12	Rickard and Pascoe (2009)
G45421a	TrGAroC	MMALANHYO2 + HO_2 → MMALNHYOOH	k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45421b	TrGAroC	MMALANHYO2 + HO_2 → CO2H3CO3 + CO_2 + OH	k_RO2_HO2(temp,5)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G45422	TrGAroCN	MMALANHYO2 + NO → CO2H3CO3 + CO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45423	TrGAroCN	MMALANHYO2 + NO_3 → CO2H3CO3 + CO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G45424	TrGAroC	MMALANHYO2 → CO2H3CO3 + CO_2	k1_RO2tORO2	Rickard and Pascoe (2009)*
G45428	TrGAroCN	C4CO2DBPAN + OH → HCOCOCHO + CO_2 + CO + NO_2	2.74E-11	Rickard and Pascoe (2009)
G45429	TrGAroCN	C4CO2DBPAN → C4CO2DBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	C5CO14O2 + HO_2 → .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)*
G45430b	TrGAroC	C5CO14O2 + HO_2 → C5CO14OH + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G45430c	TrGAroC	C5CO14O2 + HO_2 → C5CO14OOH	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G45431	TrGAroCN	C5CO14O2 + NO → .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
G45432	TrGAroCN	C5CO14O2 + NO_2 → C5COO2NO2	k_CH3CO3_NO2	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45433	TrGAroCN	C5CO14O2 + NO_3 → .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	C5CO14O2 → .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G45436	TrGAroC	C5CO14OH + OH → .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	C5DICARB + NO_3 → C5CO14O2 + HNO_3	KNO3AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	C5DICARB + O_3 → .5338 GLYOX + .063 CH_3CHO + .348 $CH_3C(O)OO$ + .918 CO + .57 OH + .473 HO_2 + .0563 CH_3COCO_2H + .5338 MGLYOX + .676 H_2O_2 + .063 HCHO + .0563 $HCOCO_2H$ + .2465 CO_2	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	C5DICARB + OH → .48 C5CO14O2 + .52 C5DICARBO2	6.2E-11	Rickard and Pascoe (2009)
G45444	TrGAroC	MC3ODBCO2H + OH → .35 GLYOX + .35 CH_3 + .35 CO + .35 CO_2 + .65 MMALANHY + .65 HO_2	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	TLFUONE + NO_3 → NTLFUO2	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	TLFUONE + O_3 → .5 CO + .5 OH + .5 MECOACETO2 + .3125 C24O3CCO2H + .1875 ACCOMECHO + .1875 H_2O_2	8.00E-19	see note*
G45453	TrGAroC	TLFUONE + OH → TLFUO2	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	ACCOMECO3 + HO_2 → ACCOMECO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	ACCOMECO3 + HO_2 → MECOACETO2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G45455	TrGAroCN	ACCOMECO3 + NO → MECOACETO2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	ACCOMECO3 + NO_2 → ACCOMEPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45457	TrGAroCN	ACCOMECO3 + NO_3 → MECOACETO2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	ACCOMECO3 → MECOACETO2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G45459	TrGAroC	C4CO2DCO3H + OH → C4CO2DBCO3	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	ACCOMECHO + NO_3 → ACCOMECO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	ACCOMECHO + OH → ACCOMECO3	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	MMALNHYOOH + OH → MMALANHYO2	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	C5DICAROOH + OH → C5134CO2OH + OH	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	C5DICAROOH + OH → C5DICARBO2	k_ROOHRO	Rickard and Pascoe (2009)
G45468	TrGAroC	C24O3CCO2H + OH → MECOACETO2 + CO_2	8.76E-13	Rickard and Pascoe (2009)
G45469	TrGAroCN	NTLFUOOH + OH → NTLFUO2	4.44E-12	Rickard and Pascoe (2009)
G45470	TrGAroCN	ACCOMEPAN + OH → METACETHO + CO + CO + NO_2	1.00E-14	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45471	TrGAroCN	ACCOMEPAN → ACCOMECO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45476a	TrGAroC	TLFUO2 + HO_2 → TLFUOOH	k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G45476b	TrGAroC	TLFUO2 + HO_2 → ACCOMECHO + HO_2 + OH	k_RO2_HO2(temp,5)*(r_COCH2O2_OH+r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)*
G45477	TrGAroCN	TLFUO2 + NO → ACCOMECHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45478	TrGAroCN	TLFUO2 + NO_3 → ACCOMECHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G45479	TrGAroC	TLFUO2 → ACCOMECHO + HO_2	k1_RO2tORO2	Rickard and Pascoe (2009)*
G45480	TrGAroC	C5CO14OOH + OH → C5CO14O2	3.59E-12	Rickard and Pascoe (2009)
G45483	TrGAroC	TLFUOOH + OH → TLFUO2	2.53E-11	Rickard and Pascoe (2009)
G45485	TrGAroC	ACCOMECO3H + OH → ACCOMECO3	3.59E-12	Rickard and Pascoe (2009)
G45486a	TrGAroC	C5DIALO2 + HO_2 → C5DIALOOH	k_RO2_HO2(temp,5)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G45486b	TrGAroC	C5DIALO2 + HO_2 → MALDIAL + CO + HO_2 + OH	k_RO2_HO2(temp,5)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G45487	TrGAroCN	C5DIALO2 + NO → MALDIAL + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45488	TrGAroCN	C5DIALO2 + NO_3 → MALDIAL + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G45489	TrGAroC	C5DIALO2 → MALDIAL + CO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G45490a	TrGAroC	C5DICARBO2 + HO_2 → C5DICAROOH	k_RO2_HO2(temp,5)*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G45491b	TrGAroC	C5DICARBO2 + HO_2 → MGLYOX + GLYOX + HO_2 + OH	k_RO2_HO2(temp,5)*r_CO3_OH	Rickard and Pascoe (2009)*
G45492	TrGAroCN	C5DICARBO2 + NO → MGLYOX + GLYOX + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45493	TrGAroCN	C5DICARBO2 + NO_3 → MGLYOX + GLYOX + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G45494	TrGAroC	C5DICARBO2 → MGLYOX + GLYOX + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G46200a	TrGTerC	CO235C6O2 + HO_2 → CO235C6OOH	k_RO2_HO2(temp,6)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G46200b	TrGTerC	CO235C6O2 + HO_2 → CO23C4CO3 + HCHO + OH	k_RO2_HO2(temp,6)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G46201	TrGTerCN	CO235C6O2 + NO → CO23C4CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46202	TrGTerC	CO235C6O2 → CO23C4CO3 + HCHO	k1_RO2pORO2	Rickard and Pascoe (2009)
G46203	TrGTerC	CO235C6OOH + OH → CO235C6O2	1.01E-11	Rickard and Pascoe (2009)
G46204	TrGTerC	C614O2 → CO23C4CHO + HCHO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46205a	TrGTerCN	C614O2 + NO → CO23C4CHO + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(9,2,0,1,0,temp,cair))	Rickard and Pascoe (2009)
G46205b	TrGTerCN	C614O2 + NO → C614NO3	KRO2NO*alpha_AN(9,2,0,1,0,temp,cair)	Rickard and Pascoe (2009)
G46206a	TrGTerC	C614O2 + HO_2 → C614OOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G46206b	TrGTerC	C614O2 + HO_2 → CO23C4CHO + HCHO + HO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G46207	TrGTerCN	C614NO3 + OH → C614CO + NO_2	7.11E-12	Rickard and Pascoe (2009)
G46208	TrGTerC	C614OOH + OH → C614CO + OH	8.69E-11	Rickard and Pascoe (2009)
G46209	TrGTerC	C614CO + OH → CO235C5CHO + HO_2	3.22E-12	Rickard and Pascoe (2009)
G46210	TrGTerC	CO235C5CHO + OH → CO23C4CO3 + CO	1.33E-11	Rickard and Pascoe (2009)
G46211	TrGTerCN	CO235C5CHO + NO_3 → CO23C4CO3 + CO + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
G46400	TrGAroC	PHENOOH + OH → PHENO2	1.16E-10	Rickard and Pascoe (2009)
G46401	TrGAroC	C6CO4DB + OH → CO + CO + HO_2 + CO + HCOCOCHO	7.70E-11	Rickard and Pascoe (2009)
G46402	TrGAroC	C5CO2DCO3H + OH → C5CO2DBCO3	3.60E-11	Rickard and Pascoe (2009)
G46403	TrGAroCN	NDNPHENOOH + OH → NDNPHENO2	k_ROOHRO	Rickard and Pascoe (2009)
G46404a	TrGAroC	C615CO2O2 + HO_2 → C615CO2OOH	k_RO2_HO2(temp,6)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G46404b	TrGAroC	C615CO2O2 + HO_2 → C5DICARB + CO + HO_2 + OH	k_RO2_HO2(temp,6)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G46405	TrGAroCN	C615CO2O2 + NO → C5DICARB + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46406	TrGAroCN	C615CO2O2 + NO_3 → C5DICARB + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46407	TrGAroC	C615CO2O2 → C5DICARB + CO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G46408	TrGAroCN	BZEMUCPAN + OH → MALDIAL + CO + CO_2 + NO_2	4.05E-11	Rickard and Pascoe (2009)
G46409	TrGAroCN	BZEMUCPAN → BZEMUCCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G46410	TrGAroCN	BZBIPERNO3 + OH → BZOBIPEROH + NO_2	7.30E-11	Rickard and Pascoe (2009)
G46411	TrGAroCN	HOC6H4NO2 + NO_3 → NPHEN1O + HNO_3	9.00E-14	Rickard and Pascoe (2009)
G46412	TrGAroCN	HOC6H4NO2 + OH → NPHEN1O	9.00E-13	Rickard and Pascoe (2009)
G46413a	TrGAroCN	NDNPHENO2 + HO_2 → NDNPHENOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46413b	TrGAroCN	NDNPHENO2 + HO_2 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46414	TrGAroCN	NDNPHENO2 + NO → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46415	TrGAroCN	NDNPHENO2 + NO_3 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46416	TrGAroCN	NDNPHENO2 → NC4DCO2H + HNO_3 + CO + CO + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46417	TrGAroC	PBZQCO + OH → C5CO2OHCO3	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	CATECHOL + NO_3 → CATEC1O + HNO_3	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	CATECHOL + O_3 → MALDALCO2H + $HCOCO_2H$ + HO_2 + OH	9.2E-18	Rickard and Pascoe (2009)
G46420	TrGAroC	CATECHOL + OH → CATEC1O	1.0E-10	Rickard and Pascoe (2009)
G46421	TrGAroC	C5COOHCO3H + OH → C5CO2OHCO3	8.01E-11	Rickard and Pascoe (2009)
G46422	TrGAroCN	NCATECHOL + NO_3 → NNCATECO2	2.60E-12	Rickard and Pascoe (2009)
G46423	TrGAroCN	NCATECHOL + OH → NCATECO2	3.47E-12	Rickard and Pascoe (2009)
G46424a	TrGAroC	C5CO2OHCO3 + HO_2 → C5COOHCO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G46424b	TrGAroC	C5CO2OHCO3 + HO_2 → HOCOC4DIAL + HO_2 + CO + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G46425	TrGAroCN	C5CO2OHCO3 + NO → HOCOC4DIAL + HO_2 + CO + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G46426	TrGAroCN	C5CO2OHCO3 + NO_2 → C5CO2OHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G46427	TrGAroCN	C5CO2OHCO3 + NO_3 → HOCOC4DIAL + HO_2 + CO + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G46428	TrGAroC	C5CO2OHCO3 → HOCOC4DIAL + HO_2 + CO + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G46429	TrGAroCN	BZEPOXMUC + NO_3 → BZEMUCCO3 + HNO_3	2.*KNO3AL*2.75	Rickard and Pascoe (2009)
G46430	TrGAroC	BZEPOXMUC + O_3 → EPXC4DIAL + .125 HCHO + .1125 $HCOCO_2H$ + .0675 GLYOX + .0675 H_2O_2 + .82 HO_2 + .57 OH + 1.265 CO + .25 CO_2	2.00E-18	Rickard and Pascoe (2009)*
G46431	TrGAroC	BZEPOXMUC + OH → .31 BZEMUCCO3 + .69 BZEMUCO2	6.08E-11	Rickard and Pascoe (2009)
G46432a	TrGAroCN	NCATECO2 + HO_2 → NCATECOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	NCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46433	TrGAroCN	NCATECO2 + NO → NC4DCO2H + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46434	TrGAroCN	NCATECO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46435	TrGAroCN	NCATECO2 → NC4DCO2H + $HCOCO_2H$ + HO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46436	TrGAroCN	NPHEN1OOH + OH → NPHEN1O2	9.00E-13	Rickard and Pascoe (2009)
G46437a	TrGAroCN	NPHENO2 + HO_2 → NPHENOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46437b	TrGAroCN	NPHENO2 + HO_2 → MALDALCO2H + GLYOX + NO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46438	TrGAroCN	NPHENO2 + NO → MALDALCO2H + GLYOX + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46439	TrGAroCN	NPHENO2 + NO_3 → MALDALCO2H + GLYOX + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46440	TrGAroCN	NPHENO2 → MALDALCO2H + GLYOX + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46441	TrGAroC	BENZENE + OH → .352 BZBIPERO2 + .118 BZEPOXMUC + .118 HO_2 + .53 PHENOL + .53 HO_2	2.3E-12*EXP(-190./temp)	Rickard and Pascoe (2009)*
G46442	TrGAroCN	C5CO2OHPAN + OH → HOCOC4DIAL + CO + CO + NO_2	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	C5CO2OHPAN → C5CO2OHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G46444	TrGAroCN	CATEC1O + NO_2 → NCATECHOL	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
G46445	TrGAroC	CATEC1O + O_3 → CATEC1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46446	TrGAroC	BZEMUCCO + OH → EPXDLCO3 + GLYOX	9.20E-11	Rickard and Pascoe (2009)
G46447a	TrGAroCN	NNCATECO2 + HO_2 → NNCATECOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46447b	TrGAroCN	NNCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46448	TrGAroCN	NNCATECO2 + NO → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46449	TrGAroCN	NNCATECO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46450	TrGAroCN	NNCATECO2 → NC4DCO2H + $HCOCO_2H$ + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46451	TrGAroC	BZEMUCCO2H + OH → C5DIALO2 + CO_2	4.06E-11	Rickard and Pascoe (2009)
G46452	TrGAroCN	NNCATECOOH + OH → NNCATECO2	k_ROOHRO	Rickard and Pascoe (2009)
G46453	TrGAroCN	NPHEN1O + NO_2 → DNPHEN	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)

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

#	labels	reaction	rate coefficient	reference
G46454	TrGAroCN	NPHEN1O + O_3 → NPHEN1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46455	TrGAroCN	DNPHEN + NO_3 → NDNPHENO2	2.25E-15	Rickard and Pascoe (2009)
G46456	TrGAroCN	DNPHEN + OH → DNPHENO2	3.00E-14	Rickard and Pascoe (2009)
G46457	TrGAroCN	PHENOL + NO_3 → .742 C6H5O + .742 HNO_3 + .258 NPHENO2	3.8E-12	Rickard and Pascoe (2009)*
G46458	TrGAroC	PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 HO_2 + .14 PHENO2	4.7E-13*EXP(1220./temp)	Rickard and Pascoe (2009)*
G46459	TrGAroCN	PBZQONE + NO_3 → NBZQO2	3.00E-13	Rickard and Pascoe (2009)
G46460	TrGAroC	PBZQONE + OH → PBZQO2	4.6E-12	Rickard and Pascoe (2009)
G46461a	TrGAroC	PHENO2 + HO_2 → PHENOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46461b	TrGAroC	PHENO2 + HO_2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46462	TrGAroCN	PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46463	TrGAroCN	PHENO2 + NO_3 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46464	TrGAroC	PHENO2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46465	TrGAroC	C615CO2OOH + OH → C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
G46466a	TrGAroC	C5CO2DBCO3 + HO_2 → C5CO2DCO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBCO3 + HO_2 → $CH_3C(O)$ + HCOCOCHO + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBCO3 + NO → $CH_3C(O)$ + HCOCOCHO + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBCO3 + NO_2 → C5CO2DBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBCO3 + NO_3 → $CH_3C(O)$ + HCOCOCHO + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBCO3 → $CH_3C(O)$ + HCOCOCHO + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G46471	TrGAroCN	NPHEN1O2 + HO_2 → NPHEN1OOH	k_RO2_HO2(temp,6)	Rickard and Pascoe (2009)
G46472a	TrGAroCN	NPHEN1O2 + NO → NPHEN1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G46472b	TrGAroCN	NPHEN1O2 + NO_2 → NPHEN1O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G46473	TrGAroCN	NPHEN1O2 + NO_3 → NPHEN1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G46474	TrGAroCN	NPHEN1O2 → NPHEN1O	k1_RO2sRO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46475	TrGAroCN	NPHENOOH + OH → NPHENO2	1.07E-10	Rickard and Pascoe (2009)
G46476	TrGAroCN	C6H5O + NO_2 → HOC6H4NO2	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O_3 → C6H5O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46478	TrGAroCN	NCATECOOH + OH → NCATECO2	k_ROOHRO	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH → PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)
G46480a	TrGAroC	PBZQO2 + HO_2 → PBZQOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G46480b	TrGAroC	PBZQO2 + HO_2 → C5CO2OHCO3 + OH	k_RO2_HO2(temp,6)*(r_CHOHCH2O2_OH+r_COCH2O2_OH)	Rickard and Pascoe (2009)*
G46481	TrGAroCN	PBZQO2 + NO → C5CO2OHCO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46482	TrGAroCN	PBZQO2 + NO_3 → C5CO2OHCO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46483	TrGAroC	PBZQO2 → C5CO2OHCO3	k1_RO2sORO2	Rickard and Pascoe (2009)*
G46484	TrGAroC	BZOBIPEROH + OH → MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	DNPHENO2 + HO_2 → DNPHENOOH	k_RO2_HO2(temp,6)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G46485b	TrGAroCN	DNPHENO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	k_RO2_HO2(temp,6)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G46486	TrGAroCN	DNPHENO2 + NO → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46487	TrGAroCN	DNPHENO2 + NO_3 → NC4DCO2H + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46488	TrGAroCN	DNPHENO2 → NC4DCO2H + $HCOCO_2H$ + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G46489	TrGAroC	BZBIPEROOH + OH → BZOBIPEROH + OH	9.77E-11	Rickard and Pascoe (2009)
G46490a	TrGAroC	BZEMUCO2 + HO_2 → BZEMUCOOH	k_RO2_HO2(temp,6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	BZEMUCO2 + HO_2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + OH	k_RO2_HO2(temp,6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	BZEMUCO2 + NO → BZEMUCNO3	KRO2NO*alpha_AN(10,2,0,1,0,temp,cair)	Rickard and Pascoe (2009)
G46491b	TrGAroCN	BZEMUCO2 + NO → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + NO_2	KRO2NO*(1.-alpha_AN(10,2,0,1,0,temp,cair))	Rickard and Pascoe (2009)*
G46492	TrGAroCN	BZEMUCO2 + NO_3 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + NO_2	KRO2NO3	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46493	TrGAroC	BZEMUCO2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO	k1_RO2sORO2	Rickard and Pascoe (2009)*
G46494	TrGAroCN	C5CO2DBPAN + OH → HCOCOCHO + CH_3CHO + CO_2 + NO_2	3.28E-11	Rickard and Pascoe (2009)
G46495	TrGAroCN	C5CO2DBPAN → C5CO2DBCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	NBZQOOH + OH → NBZQO2	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	CATEC1OOH + OH → CATEC1O2	k_ROOHRO	Rickard and Pascoe (2009)
G46498	TrGAroC	C6125CO + OH → C5CO14O2 + CO	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	NBZQO2 + HO_2 → NBZQOOH	k_RO2_HO2(temp,6)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G46499b	TrGAroCN	NBZQO2 + HO_2 → C6CO4DB + NO_2 + OH	k_RO2_HO2(temp,6)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G46500	TrGAroCN	NBZQO2 + NO → C6CO4DB + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46501	TrGAroCN	NBZQO2 + NO_3 → C6CO4DB + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G46502	TrGAroCN	NBZQO2 → C6CO4DB + NO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G46503	TrGAroCN	DNPHENOOH + OH → DNPHENO2	k_ROOHRO	Rickard and Pascoe (2009)
G46504	TrGAroC	CATEC1O2 + HO_2 → CATEC1OOH	k_RO2_HO2(temp,6)	Rickard and Pascoe (2009)
G46505a	TrGAroCN	CATEC1O2 + NO → CATEC1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G46505b	TrGAroCN	CATEC1O2 + NO_2 → CATEC1O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G46506	TrGAroCN	CATEC1O2 + NO_3 → CATEC1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G46507	TrGAroC	CATEC1O2 → CATEC1O	k1_RO2sORO2	Rickard and Pascoe (2009)
G46508	TrGAroC	BZEMUCCO3H + OH → BZEMUCCO3	4.37E-11	Rickard and Pascoe (2009)
G46509	TrGAroC	C6H5OOH + OH → C6H5O2	3.60E-12	Rickard and Pascoe (2009)
G46510	TrGAroC	BZEMUCOOH + OH → BZEMUCCO + OH	1.31E-10	Rickard and Pascoe (2009)
G46511a	TrGAroC	BZEMUCCO3 + HO_2 → BZEMUCCO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G46511b	TrGAroC	BZEMUCCO3 + HO_2 → BZEMUCCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G46511c	TrGAroC	BZEMUCCO3 + HO_2 → C5DIALO2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G46512	TrGAroCN	BZEMUCCO3 + NO → C5DIALO2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G46513	TrGAroCN	BZEMUCCO3 + NO_2 → BZEMUCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G46514	TrGAroCN	BZEMUCCO3 + NO_3 → C5DIALO2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G46515	TrGAroC	BZEMUCCO3 → C5DIALO2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G46516	TrGAroC	C6H5O2 + HO_2 → C6H5OOH	k_RO2_HO2(temp,6)	Rickard and Pascoe (2009)
G46517	TrGAroCN	C6H5O2 + NO → C6H5O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G46518	TrGAroCN	C6H5O2 + NO_3 → C6H5O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G46519	TrGAroC	C6H5O2 → C6H5O	k1_RO2sRO2	Rickard and Pascoe (2009)
G46520	TrGAroCN	C6H5O2 + NO_2 → C6H5O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)

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

#	labels	reaction	rate coefficient	reference
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO_2	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	BZBIPERO2 + HO_2 → BZBIPEROOH	k_RO2_HO2(temp,6)*(1.-r_BIPERO2_OH)	Rickard and Pascoe (2009)
G46522b	TrGAroC	BZBIPERO2 + HO_2 → OH + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	k_RO2_HO2(temp,6)*r_BIPERO2_OH	Rickard and Pascoe (2009), Birdsall et al. (2010)*
G46523a	TrGAroCN	BZBIPERO2 + NO → BZBIPERNO3	KRO2NO*alpha_AN(9,2,0,0,1,temp,cair)	Rickard and Pascoe (2009)
G46523b	TrGAroCN	BZBIPERO2 + NO → NO_2 + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	KRO2NO*(1.-alpha_AN(9,2,0,0,1,temp,cair))	Rickard and Pascoe (2009)*
G46524	TrGAroCN	BZBIPERO2 + NO_3 → NO_2 + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	KRO2NO3	Rickard and Pascoe (2009)*
G46525	TrGAroC	BZBIPERO2 → GLYOX + HO_2 + BZFUONE	k1_RO2sORO2	Rickard and Pascoe (2009)*
G47200	TrGTerCN	CO235C6CHO + NO_3 → CO235C6CO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	CO235C6CO3 + HO_2 → C235C6CO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO_2 → CO235C6O2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G47203	TrGTerCN	CO235C6CO3 + NO → CO235C6O2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G47204	TrGTerCN	CO235C6CO3 + NO_2 → C7PAN3	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G47205	TrGTerC	CO235C6CO3 → CO235C6O2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G47206	TrGTerC	C235C6CO3H + OH → CO235C6CO3	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	C7PAN3 + OH → CO235C5CHO + CO + NO_2	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	C7PAN3 → CO235C6CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G47209a	TrGTerC	C716O2 + HO_2 → C716OOH	k_RO2_HO2(temp,7)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G47209b	TrGTerC	C716O2 + HO_2 → CO13C4CHO + $CH_3C(O)$ + OH	k_RO2_HO2(temp,7)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G47210	TrGTerCN	C716O2 + NO → CO13C4CHO + $CH_3C(O)$ + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47211	TrGTerC	C716O2 → CO13C4CHO + $CH_3C(O)$	k1_RO2sORO2	Rickard and Pascoe (2009)
G47212	TrGTerC	C716OOH + OH → CO235C6CHO + OH	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	C721O2 + HO_2 → C721OOH	k_RO2_HO2(temp,7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	C721O2 + NO → C722O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47215	TrGTerC	C721O2 → C722O2	k1_RO2pRO2	Rickard and Pascoe (2009)
G47216	TrGTerC	C721OOH + OH → C721O2	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	C722O2 + HO_2 → C722OOH	k_RO2_HO2(temp,7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	C722O2 + NO → CH_3COCH_3 + C44O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47219	TrGTerC	C722O2 → CH_3COCH_3 + C44O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G47220	TrGTerC	C722OOH + OH → C722O2	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	ROO6R3O2 → ROO6R5O2	5.68E10*EXP(-8745./temp)	Vereecken and Peeters (2012)
G47222	TrGTerCN	ROO6R3O2 + NO → ROO6R3O + NO_2	KRO2NO	Vereecken and Peeters (2012)*
G47223	TrGTerC	ROO6R3O2 + HO_2 → 7 LCARBON	k_RO2_HO2(temp,7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	ROO6R3O2 → ROO6R3O	k1_RO2sRO2	Vereecken and Peeters (2012)
G47225	TrGTerC	ROO6R3O → 7 LCARBON + HO_2	5.7E10*EXP(-2949./temp)	Vereecken and Peeters (2012)*
G47226	TrGTerC	ROO6R5O2 → 7 LCARBON + OH	9.17E10*EXP(-8706./temp)	Vereecken and Peeters (2012)*
G47400	TrGAroC	TOLUENE + OH → .07 C6H5CH2O2 + .18 CRESOL + .18 HO_2 + .65 TLBIPERO2 + .10 TLEPOXMUC + .10 HO_2	1.8E-12*EXP(340./temp)	Rickard and Pascoe (2009)*
G47401	TrGAroC	C6H5CH2O2 + HO_2 → C6H5CH2OOH	1.5E-13*EXP(1310./temp)	Rickard and Pascoe (2009)
G47402a	TrGAroCN	C6H5CH2O2 + NO → C6H5CH2NO3	KRO2NO*alpha_AN(7,1,0,0,0,temp, cair)	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	C6H5CH2O2 + NO → BENZAL + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(7,1,0,0,0, temp,cair))	Rickard and Pascoe (2009)*
G47403	TrGAroCN	C6H5CH2O2 + NO_3 → BENZAL + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47404	TrGAroC	C6H5CH2O2 → BENZAL + HO_2	2.*(k_CH3O2*2.4E-14*EXP(1620./ temp))**(0.5)*RO2	Rickard and Pascoe (2009)*
G47405	TrGAroCN	CRESOL + NO_3 → .103 CRESO2 + .103 HNO_3 + .506 NCRESO2 + .391 TOL1O + .391 HNO_3	1.4E-11	Rickard and Pascoe (2009)*
G47406	TrGAroC	CRESOL + OH → .2 CRESO2 + .727 MCATECHOL + .727 HO_2 + .073 TOL1O	4.65E-11	Rickard and Pascoe (2009)*
G47407a	TrGAroC	TLBIPERO2 + HO_2 → TLBIPEROOH	k_RO2_HO2(temp,7)*(1.-r_BIPERO2_ OH)	Rickard and Pascoe (2009)
G47407b	TrGAroC	TLBIPERO2 + HO_2 → OH + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k_RO2_HO2(temp,7)*r_BIPERO2_OH	Rickard and Pascoe (2009), 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	KRO2NO*(1.-alpha_AN(11,2,0,0,1, temp,cair))	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	TLBIPERO2 + NO → TLBIPERNO3	KRO2NO*alpha_AN(11,2,0,0,1, temp,cair)	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47409	TrGAroCN	TLBIPERO2 + NO_3 → NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KRO2NO3	Rickard and Pascoe (2009)*
G47410	TrGAroC	TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k1_RO2sORO2	Rickard and Pascoe (2009)*
G47411	TrGAroCN	TLEPOXMUC + NO_3 → TLEMUCCO3 + HNO_3	KNO3AL*2.75	Rickard and Pascoe (2009)
G47412	TrGAroC	TLEPOXMUC + O_3 → EPXC4DIAL + .125 CH_3CHO + .695 $CH_3C(O)$ + .57 CO + .57 OH + .125 HO_2 + .1125 CH_3COCO_2H + .0675 MGLYOX + .0675 H_2O_2 + .25 CO_2	5.00E-18	Rickard and Pascoe (2009)*
G47413	TrGAroC	TLEPOXMUC + OH → .31 TLEMUCCO3 + .69 TLEMUCO2	7.99E-11	Rickard and Pascoe (2009)*
G47414	TrGAroC	C6H5CH2OOH + OH → BENZAL + OH	2.05E-11	Rickard and Pascoe (2009)
G47415	TrGAroCN	C6H5CH2NO3 + OH → BENZAL + NO_2	6.03E-12	Rickard and Pascoe (2009)
G47416	TrGAroCN	BENZAL + NO_3 → C6H5CO3 + HNO_3	2.40E-15	Rickard and Pascoe (2009)
G47417	TrGAroC	BENZAL + OH → C6H5CO3	5.9E-12*EXP(225./temp)	Rickard and Pascoe (2009)
G47418a	TrGAroC	CRESO2 + HO_2 → CRESOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO2 + HO_2 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO2 + NO → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO2 + NO_3 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47421	TrGAroC	CRESO2 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO2 + HO_2 → NCRESOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO2 + HO_2 → C5CO14OH + GLYOX + NO_2 + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO2 + NO → C5CO14OH + GLYOX + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO2 + NO_3 → C5CO14OH + GLYOX + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO2 → C5CO14OH + GLYOX + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47426	TrGAroCN	TOL1O + NO_2 → TOL1OHNO2	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O_3 → OXYL1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47428	TrGAroCN	MCATECHOL + NO_3 → MCATEC1O + HNO_3	1.7E-10*1.0	Rickard and Pascoe (2009)
G47429	TrGAroC	MCATECHOL + O_3 → MC3ODBCO2H + $HCOCO_2H$ + HO_2 + OH	2.8E-17	Rickard and Pascoe (2009)*
G47430	TrGAroC	MCATECHOL + OH → MCATEC1O	2.0E-10*1.0	Rickard and Pascoe (2009)
G47431	TrGAroC	TLBIPEROOH + OH → TLOBIPEROH + OH	9.64E-11	Rickard and Pascoe (2009)
G47432	TrGAroCN	TLBIPERNO3 + OH → TLOBIPEROH + NO_2	7.16E-11	Rickard and Pascoe (2009)
G47433	TrGAroC	TLOBIPEROH + OH → C5CO14O2 + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO3 + HO_2 → C615CO2O2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO3 + HO_2 → TLEMUCCO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO3 + HO_2 → TLEMUCCO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO3 + NO → C615CO2O2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO3 + NO_2 → TLEMUCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO3 + NO_3 → C615CO2O2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G47438	TrGAroC	TLEMUCCO3 → C615CO2O2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G47439a	TrGAroC	TLEMUCO2 + HO_2 → TLEMUCOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G47439b	TrGAroC	TLEMUCO2 + HO_2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH	k_RO2_HO2(temp,7)*(r_CHOHCH2O2_OH+r_COCH2O2_OH)	Rickard and Pascoe (2009)*
G47440a	TrGAroCN	TLEMUCO2 + NO → TLEMUCNO3	KRO2NO*alpha_AN(11,2,1,0,0, temp,cair)	Rickard and Pascoe (2009)
G47440b	TrGAroCN	TLEMUCO2 + NO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + NO_2	KRO2NO*(1.-alpha_AN(11,2,1,0,0, temp,cair))	Rickard and Pascoe (2009)*
G47441	TrGAroCN	TLEMUCO2 + NO_3 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47442	TrGAroC	TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
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	KAPNO	Rickard and Pascoe (2009)
G47445	TrGAroCN	C6H5CO3 + NO_2 → PBZN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47446	TrGAroCN	C6H5CO3 + NO_3 → C6H5O2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G47447	TrGAroC	C6H5CO3 → C6H5O2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G47448	TrGAroC	CRESOOH + OH → CRESO2	1.15E-10	Rickard and Pascoe (2009)
G47449	TrGAroCN	NCRESOOH + OH → NCRESO2	1.07E-10	Rickard and Pascoe (2009)
G47450	TrGAroCN	TOL1OHNO2 + NO_3 → NCRES1O + HNO_3	3.13E-13*1.0	Rickard and Pascoe (2009)
G47451	TrGAroCN	TOL1OHNO2 + OH → NCRES1O	2.8E-12	Rickard and Pascoe (2009)
G47452	TrGAroC	OXYL1O2 + HO_2 → OXYL1OOH	k_RO2_HO2(temp,7)	Rickard and Pascoe (2009)
G47453	TrGAroCN	OXYL1O2 + NO → TOL1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G47454	TrGAroCN	OXYL1O2 + NO_2 → TOL1O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G47455	TrGAroCN	OXYL1O2 + NO_3 → TOL1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G47456	TrGAroC	OXYL1O2 → TOL1O	k1_RO2sRO2	Rickard and Pascoe (2009)
G47457	TrGAroCN	MCATEC1O + NO_2 → MNCATECH	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
G47458	TrGAroC	MCATEC1O + O_3 → MCATEC1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47459	TrGAroC	TLEMUCCO2H + OH → C615CO2O2 + CO_2	5.98E-11	Rickard and Pascoe (2009)
G47460	TrGAroC	TLEMUCCO3H + OH → TLEMUCCO3	6.29E-11	Rickard and Pascoe (2009)
G47461	TrGAroCN	TLEMUCPAN + OH → C5DICARB + CO + CO_2 + NO_2	5.96E-11	Rickard and Pascoe (2009)
G47462	TrGAroCN	TLEMUCPAN → TLEMUCCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G47463	TrGAroC	TLEMUCOOH + OH → TLEMUCCO + OH	7.04E-11	Rickard and Pascoe (2009)
G47464	TrGAroCN	TLEMUCNO3 + OH → TLEMUCCO + NO_2	3.06E-11	Rickard and Pascoe (2009)
G47465	TrGAroC	TLEMUCCO + OH → $CH_3C(O)$ + EPXC4DIAL + CO	4.06E-11	Rickard and Pascoe (2009)
G47466	TrGAroC	C6H5CO3H + OH → C6H5CO3	4.66E-12	Rickard and Pascoe (2009)
G47467	TrGAroC	PHCOOH + OH → C6H5O2 + CO_2	1.10E-12	Rickard and Pascoe (2009)
G47468	TrGAroCN	PBZN + OH → C6H5OOH + CO + NO_2	1.06E-12	Rickard and Pascoe (2009)
G47469	TrGAroCN	PBZN → C6H5CO3 + NO_2	k_PAN_M*0.67	Rickard and Pascoe (2009)
G47470	TrGAroCN	PTLQONE + NO_3 → NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
G47471	TrGAroC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard and Pascoe (2009)
G47472	TrGAroCN	NCRES1O + NO_2 → DNCRES	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O_3 → NCRES1O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47474	TrGAroC	OXYL1OOH + OH → OXYL1O2	4.65E-11	Rickard and Pascoe (2009)
G47475	TrGAroCN	MNCATECH + NO_3 → MNNCATECO2	5.03E-12	Rickard and Pascoe (2009)
G47476	TrGAroCN	MNCATECH + OH → MNCATECO2	6.83E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47477	TrGAroC	MCATEC1O2 + HO_2 → MCATEC1OOH	k_RO2_HO2(temp,7)	Rickard and Pascoe (2009)
G47478	TrGAroCN	MCATEC1O2 + NO → MCATEC1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G47479	TrGAroCN	MCATEC1O2 + NO_2 → MCATEC1O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO_3 → MCATEC1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G47481	TrGAroC	MCATEC1O2 → MCATEC1O	k1_RO2sORO2	Rickard and Pascoe (2009)
G47482a	TrGAroCN	NPTLQO2 + HO_2 → NPTLQOOH	k_RO2_HO2(temp,7)*(1.-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO_2 → C7CO4DB + NO_2 + OH	k_RO2_HO2(temp,7)*r_COCH2O2_OH	Rickard and Pascoe (2009)*
G47483	TrGAroCN	NPTLQO2 + NO → C7CO4DB + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47484	TrGAroCN	NPTLQO2 + NO_3 → C7CO4DB + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47485	TrGAroCN	NPTLQO2 → C7CO4DB + NO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G47486a	TrGAroC	PTLQO2 + HO_2 → PTLQOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH-r_COCH2O2_OH)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO_2 → C6CO2OHCO3 + OH	k_RO2_HO2(temp,7)*(r_CHOHCH2O2_OH+r_COCH2O2_OH)	Rickard and Pascoe (2009)*
G47487	TrGAroCN	PTLQO2 + NO → C6CO2OHCO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47488	TrGAroCN	PTLQO2 + NO_3 → C6CO2OHCO3 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47489	TrGAroC	PTLQO2 → C6CO2OHCO3	k1_RO2sORO2	Rickard and Pascoe (2009)*
G47490	TrGAroCN	DNCRES + NO_3 → NDNCRESO2	7.83E-15	Rickard and Pascoe (2009)
G47491	TrGAroCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard and Pascoe (2009)
G47492	TrGAroCN	NCRES1O2 + HO_2 → NCRES1OOH	k_RO2_HO2(temp,7)	Rickard and Pascoe (2009)
G47493	TrGAroCN	NCRES1O2 + NO → NCRES1O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G47494	TrGAroCN	NCRES1O2 + NO_2 → NCRES1O + NO_3	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G47495	TrGAroCN	NCRES1O2 + NO_3 → NCRES1O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G47496	TrGAroCN	NCRES1O2 → NCRES1O	k1_RO2sRO2	Rickard and Pascoe (2009)
G47497a	TrGAroCN	MNNCATECO2 + HO_2 → MNNCATCOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47497b	TrGAroCN	MNNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47498	TrGAroCN	MNNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47499	TrGAroCN	MNNCATECO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47500	TrGAroCN	MNNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47501a	TrGAroCN	MNCATECO2 + HO_2 → MNCATECOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47501b	TrGAroCN	MNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47502	TrGAroCN	MNCATECO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47503	TrGAroCN	MNCATECO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47504	TrGAroCN	MNCATECO2 → NC4MDCO2HN + $HCOCO_2H$ + HO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G47505	TrGAroC	MCATEC1OOH + OH → MCATEC1O2	2.05E-10	Rickard and Pascoe (2009)
G47506	TrGAroCN	NPTLQOOH + OH → NPTLQO2	8.56E-11	Rickard and Pascoe (2009)
G47507	TrGAroC	PTLQOOH + OH → PTLQCO + OH	1.42E-10	Rickard and Pascoe (2009)
G47508	TrGAroC	PTLQCO + OH → C6CO2OHCO3	7.95E-11	Rickard and Pascoe (2009)
G47509a	TrGAroCN	NDNCRESO2 + HO_2 → NDNCRESOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47509b	TrGAroCN	NDNCRESO2 + HO_2 → NC4MDCO2HN + HNO_3 + 2 CO + NO_2 + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47510	TrGAroCN	NDNCRESO2 + NO → NC4MDCO2HN + HNO_3 + 2 CO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47511	TrGAroCN	NDNCRESO2 + NO_3 → NC4MDCO2HN + HNO_3 + 2 CO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47512	TrGAroCN	NDNCRESO2 → NC4MDCO2HN + HNO_3 + 2 CO + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G47513a	TrGAroCN	DNCRESO2 + HO_2 → DNCRESOOH	k_RO2_HO2(temp,7)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G47513b	TrGAroCN	DNCRESO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	k_RO2_HO2(temp,7)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G47514	TrGAroCN	DNCRESO2 + NO → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G47515	TrGAroCN	DNCRESO2 + NO_3 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G47516	TrGAroCN	DNCRESO2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2	k1_RO2ISOPDO2	Rickard and Pascoe (2009)*
G47517	TrGAroCN	NCRES1OOH + OH → NCRES1O2	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	MNNCATCOOH + OH → MNNCATECO2	k_ROOHRO	Rickard and Pascoe (2009)
G47519	TrGAroCN	MNCATECOOH + OH → MNCATECO2	k_ROOHRO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47520	TrGAroC	C7CO4DB + OH → CO + CO + $CH_3C(O)$ + HCOCOCHO	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	C6CO2OHCO3 + HO_2 → C5134CO2OH + HO_2 + CO + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G47521b	TrGAroC	C6CO2OHCO3 + HO_2 → C6COOHCO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G47522	TrGAroCN	C6CO2OHCO3 + NO → C5134CO2OH + HO_2 + CO + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G47523	TrGAroCN	C6CO2OHCO3 + NO_2 → C6CO2OHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G47524	TrGAroCN	C6CO2OHCO3 + NO_3 → C5134CO2OH + HO_2 + CO + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	C6CO2OHCO3 → C5134CO2OH + HO_2 + CO + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G47526	TrGAroCN	NDNCRESOOH + OH → NDNCRESO2	k_ROOHRO	Rickard and Pascoe (2009)
G47527	TrGAroCN	DNCRESOOH + OH → DNCRESO2	k_ROOHRO	Rickard and Pascoe (2009)
G47528	TrGAroC	C6COOHCO3H + OH → C6CO2OHCO3	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	C6CO2OHPAN + OH → C5134CO2OH + CO + CO + NO_2	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	C6CO2OHPAN → C6CO2OHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	C85O2 → C86O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G48201	TrGTerC	C85O2 + HO_2 → C85OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	C85O2 + NO → C86O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G48203	TrGTerC	C85OOH + OH → C85O2	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	C86O2 → C511O2 + CH_3COCH_3	k1_RO2tRO2	Rickard and Pascoe (2009)
G48205	TrGTerCN	C86O2 + NO → C511O2 + CH_3COCH_3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G48206	TrGTerC	C86O2 + HO_2 → C86OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48207	TrGTerC	C86OOH + OH → C86O2	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	C811O2 → C812O2	k1_RO2pRO2	Rickard and Pascoe (2009)
G48209	TrGTerC	C811O2 + HO_2 → 8 LCARBON	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48210	TrGTerCN	C811O2 + NO → C812O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G48211	TrGTerC	C812O2 → C813O2	k1_RO2tORO2	Rickard and Pascoe (2009)
G48212	TrGTerCN	C812O2 + NO → C813O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G48213	TrGTerC	C812O2 + HO_2 → C812OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48214	TrGTerC	C812OOH + OH → C812O2	1.09E-11	Rickard and Pascoe (2009)
G48215	TrGTerC	C813O2 → CH_3COCH_3 + C512O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G48216	TrGTerCN	C813O2 + NO → CH_3COCH_3 + C512O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G48217	TrGTerC	C813O2 + HO_2 → C813OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48218	TrGTerC	C813OOH + OH → C813O2	1.86E-11	Rickard and Pascoe (2009)
G48219	TrGTerCN	C721CHO + NO_3 → C721CO3 + HNO_3	KNO3AL*8.5	Rickard and Pascoe (2009)
G48220	TrGTerC	C721CHO + OH → C721CO3	2.63E-11	Rickard and Pascoe (2009)
G48221a	TrGTerC	C721CO3 + HO_2 → C721CO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G48221b	TrGTerC	C721CO3 + HO_2 → C721O2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G48221c	TrGTerC	C721CO3 + HO_2 → NORPINIC + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G48222	TrGTerCN	C721CO3 + NO → C721O2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)*
G48223	TrGTerCN	C721CO3 + NO_2 → C721PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G48224	TrGTerCN	C721CO3 + NO_3 → C721O2 + CO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	C721CO3 → C721O2 + CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G48226	TrGTerC	C721CO3 → NORPINIC	k1_RO2RCO3*0.1	Sander et al. (2019)
G48227	TrGTerC	C721CO3H + OH → C721CO3	9.65E-12	Rickard and Pascoe (2009)
G48228	TrGTerC	NORPINIC + OH → C721O2 + CO_2	6.57E-12	Rickard and Pascoe (2009)
G48229	TrGTerCN	C721PAN + OH → C721OOH + CO + NO_2	2.96E-12	Rickard and Pascoe (2009)
G48230	TrGTerCN	C721PAN → C721CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G48231	TrGTerC	C8BC + OH → C8BCO2	3.04E-12	Rickard and Pascoe (2009)
G48232	TrGTerC	C8BCO2 + HO_2 → C8BCOOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48233a	TrGTerCN	C8BCO2 + NO → C89O2 + NO_2	KRO2NO*(1.-alpha_AN(8,2,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	C8BCO2 + NO → C8BCNO3	KRO2NO*alpha_AN(8,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48234	TrGTerC	C8BCO2 → C89O2	k1_RO2sRO2	Rickard and Pascoe (2009)
G48235	TrGTerC	C8BCOOH + OH → C8BCCO + OH	1.62E-11	Rickard and Pascoe (2009)
G48236	TrGTerCN	C8BCNO3 + OH → C8BCCO + NO_2	1.84E-12	Rickard and Pascoe (2009)
G48237	TrGTerC	C8BCCO + OH → C89O2	3.94E-12	Rickard and Pascoe (2009)
G48238	TrGTerC	C89O2 + HO_2 → C89OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48239a	TrGTerCN	C89O2 + NO → C810O2 + NO_2	KRO2NO*(1.-alpha_AN(7,2,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G48239b	TrGTerCN	C89O2 + NO → C89NO3	KRO2NO*alpha_AN(7,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48240	TrGTerCN	C89O2 + NO_3 → C810O2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G48241	TrGTerC	C89O2 → C810O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G48242	TrGTerC	C89OOH + OH → C89O2	3.61E-11	Rickard and Pascoe (2009)
G48243	TrGTerCN	C89NO3 + OH → CH_3COCH_3 + CO13C4CHO + NO_2	2.56E-11	Rickard and Pascoe (2009)
G48244	TrGTerC	C810O2 + HO_2 → C810OOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48245a	TrGTerCN	C810O2 + NO → CH_3COCH_3 + C514O2 + NO_2	KRO2NO*(1.-alpha_AN(10,3,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G48245b	TrGTerCN	C810O2 + NO → C810NO3	KRO2NO*alpha_AN(10,3,0,0,0, temp,cair)	Rickard and Pascoe (2009)
G48246	TrGTerCN	C810O2 + NO_3 → CH_3COCH_3 + C514O2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G48247	TrGTerC	C810O2 → CH_3COCH_3 + C514O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G48248	TrGTerC	C810OOH + OH → C810O2	8.35E-11	Rickard and Pascoe (2009)
G48249	TrGTerCN	C810NO3 + OH → CH_3COCH_3 + CO13C4CHO + NO_2	4.96E-11	Rickard and Pascoe (2009)
G48400a	TrGAroC	LXYL + OH → TLEPOXMUC + HO_2 + LCARBON	0.401E-11	Rickard and Pascoe (2009)*
G48400b	TrGAroC	LXYL + OH → C6H5CH2O2 + LCARBON	0.101E-11	Rickard and Pascoe (2009)*
G48400c	TrGAroC	LXYL + OH → CRESOL + LCARBON	0.261E-11	Rickard and Pascoe (2009)*
G48400d	TrGAroC	LXYL + OH → TLBIPERO2 + HO_2 + LCARBON	0.932E-11	Rickard and Pascoe (2009)*
G48401	TrGAroCN	LXYL + NO_3 → C6H5CH2O2 + HNO_3 + LCARBON	3.9E-16	Rickard and Pascoe (2009)*
G48402	TrGAroC	EBENZ + OH → .10 TLEPOXMUC + .07 C6H5CH2O2 + .18 CRESOL + .65 TLBIPERO2 + .28 HO_2 + LCARBON	7.00E-12	Rickard and Pascoe (2009)*
G48403	TrGAroCN	EBENZ + NO_3 → C6H5CH2O2 + HNO_3 + LCARBON	1.20E-16	Rickard and Pascoe (2009)*
G48404	TrGAroCN	STYRENE + NO_3 → NSTYRENO2	1.50E-12	Rickard and Pascoe (2009)
G48405	TrGAroC	STYRENE + O_3 → .545 HCHO + .1 BENZENE + .28 C6H5O2 + .56 CO + .36 OH + .28 HO_2 + .075 PHCOOH + .545 BENZAL + .09 H_2O_2 + .075 HCOOH + .2 CO_2	1.70E-17	Rickard and Pascoe (2009)*
G48406	TrGAroC	STYRENE + OH → STYRENO2	5.80E-11	Rickard and Pascoe (2009)
G48407	TrGAroCN	NSTYRENO2 + HO_2 → NSTYRENOOH	k_RO2_HO2(temp,8)	Rickard and Pascoe (2009)
G48408	TrGAroCN	NSTYRENO2 + NO → NO_2 + NO_2 + HCHO + BENZAL	KRO2NO	Rickard and Pascoe (2009)*
G48409	TrGAroCN	NSTYRENO2 + NO_3 → NO_2 + NO_2 + HCHO + BENZAL	KRO2NO3	Rickard and Pascoe (2009)*
G48410	TrGAroCN	NSTYRENO2 → NO_2 + HCHO + BENZAL	k1_RO2sRO2	Rickard and Pascoe (2009)*
G48411	TrGAroCN	NSTYRENOOH + OH → NSTYRENO2	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	STYRENO2 + HO_2 → STYRENOOH	k_RO2_HO2(temp,8)*(1.-r_ CHOHCH2O2_OH)	Rickard and Pascoe (2009)
G48412b	TrGAroC	STYRENO2 + HO_2 → HO_2 + OH + HCHO + BENZAL	k_RO2_HO2(temp,8)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009)*
G48413	TrGAroCN	STYRENO2 + NO → NO_2 + HO_2 + HCHO + BENZAL	KRO2NO	Rickard and Pascoe (2009)*
G48414	TrGAroCN	STYRENO2 + NO_3 → NO_2 + HO_2 + HCHO + BENZAL	KRO2NO3	Rickard and Pascoe (2009)*
G48415	TrGAroC	STYRENO2 → HO_2 + HCHO + BENZAL	k1_RO2sRO2	Rickard and Pascoe (2009)*
G48416	TrGAroC	STYRENOOH + OH → STYRENO2	6.16E-11	Rickard and Pascoe (2009)
G49200	TrGTerC	C96O2 → C97O2	k1_RO2pRO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49201	TrGTerC	C96O2 + HO_2 → C96OOH	k_RO2_HO2(temp,9)	Rickard and Pascoe (2009)
G49202a	TrGTerCN	C96O2 + NO → C97O2 + NO_2	KRO2NO*(1.-alpha_AN(10,1,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G49202b	TrGTerCN	C96O2 + NO → C96NO3	KRO2NO*alpha_AN(10,1,0,0,0, temp,cair)	Rickard and Pascoe (2009)
G49203	TrGTerCN	C96NO3 + OH → NORPINAL + NO_2	2.88E-12	Rickard and Pascoe (2009)
G49204a	TrGTerC	C96OOH + OH → C96O2	k_ROOHRO	Rickard and Pascoe (2009)
G49205b	TrGTerC	C96OOH + OH → NORPINAL + OH	1.30E-11	Rickard and Pascoe (2009)
G49206	TrGTerC	C97O2 → C98O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G49207	TrGTerCN	C97O2 + NO → C98O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G49208a	TrGTerC	C97O2 + HO_2 → C97OOH	k_RO2_HO2(temp,9)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G49208b	TrGTerC	C97O2 + HO_2 → C98O2 + OH	k_RO2_HO2(temp,9)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G49209	TrGTerC	C97OOH + OH → C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 → C614O2 + CH_3COCH_3	k1_RO2tRO2	Rickard and Pascoe (2009)
G49211a	TrGTerCN	C98O2 + NO → C614O2 + CH_3COCH_3 + NO_2	KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G49211b	TrGTerCN	C98O2 + NO → 9 LCARBON + LNITROGEN	KRO2NO*alpha_AN(12,3,0,0,0, temp,cair)	Rickard and Pascoe (2009)
G49212	TrGTerC	C98O2 + HO_2 → C98OOH	k_RO2_HO2(temp,9)	Rickard and Pascoe (2009)
G49213	TrGTerC	C98OOH + OH → C98O2	2.05E-11	Rickard and Pascoe (2009)
G49214	TrGTerC	NORPINAL + OH → C85CO3	2.64E-11	Rickard and Pascoe (2009)
G49215	TrGTerCN	NORPINAL + NO_3 → C85CO3 + HNO_3	KNO3AL*8.5	Rickard and Pascoe (2009)
G49216	TrGTerC	C85CO3 → C85O2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G49217	TrGTerCN	C85CO3 + NO → C85O2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G49218	TrGTerCN	C85CO3 + NO_2 → C9PAN2	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G49219a	TrGTerC	C85CO3 + HO_2 → C85CO3H	KAPHO2*(r_CO3_OOH+r_CO3_O3)	Rickard and Pascoe (2009)
G49219b	TrGTerC	C85CO3 + HO_2 → C85O2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G49220	TrGTerCN	C9PAN2 → C85CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G49221	TrGTerCN	C9PAN2 + OH → C85OOH + CO + NO_2	6.60E-12	Rickard and Pascoe (2009)
G49222	TrGTerC	C85CO3H + OH → C85CO3	1.02E-11	Rickard and Pascoe (2009)
G49223a	TrGTerC	C89CO3 → .8 C811CO3 + .2 C89O2 + .2 CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G49223b	TrGTerC	C89CO3 → C89CO2H	k1_RO2RCO3*0.1	Sander et al. (2019)
G49224a	TrGTerC	C89CO3 + HO_2 → C89CO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49224b	TrGTerC	C89CO3 + HO_2 → C89CO2H + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G49224c	TrGTerC	C89CO3 + HO_2 → .80 C811CO3 + .20 C89O2 + .2 CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G49225	TrGTerCN	C89CO3 + NO_2 → C89PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G49226	TrGTerCN	C89CO3 + NO → .8 C811CO3 + .2 C89O2 + .2 CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G49227	TrGTerC	C89CO2H + OH → .8 C811CO3 + .2 C89O2 + .2 CO_2	2.69E-11	Rickard and Pascoe (2009)
G49228	TrGTerC	C89CO3H + OH → C89CO3	3.00E-11	Rickard and Pascoe (2009)
G49229	TrGTerCN	C89PAN → C89CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G49230	TrGTerCN	C89PAN + OH → CH_3COCH_3 + CO13C4CHO + CO + NO_2	2.52E-11	Rickard and Pascoe (2009)
G49231a	TrGTerC	C811CO3 → C811O2 + CO_2	k1_RO2RCO3*0.9	Sander et al. (2019)
G49231b	TrGTerC	C811CO3 → PINIC	k1_RO2RCO3*0.1	Sander et al. (2019)
G49232a	TrGTerC	C811CO3 + HO_2 → C811CO3H	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G49232b	TrGTerC	C811CO3 + HO_2 → PINIC + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G49232c	TrGTerC	C811CO3 + HO_2 → C811O2 + CO_2 + OH	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G49233	TrGTerCN	C811CO3 + NO → C811O2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G49234	TrGTerCN	C811CO3 + NO_2 → C811PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G49235	TrGTerC	PINIC + OH → C811O2 + CO_2	7.29E-12	Rickard and Pascoe (2009)
G49236	TrGTerC	NOPINONE + OH → NOPINDO2	1.55E-11	Capouet et al. (2008), Rickard and Pascoe (2009)
G49237a	TrGTerC	NOPINDO2 + HO_2 → NOPINDOOH	k_RO2_HO2(temp,9)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G49237b	TrGTerC	NOPINDO2 + HO_2 → C89CO3 + OH	k_RO2_HO2(temp,9)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G49238	TrGTerCN	NOPINDO2 + NO → C89CO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G49239	TrGTerC	NOPINDO2 → C89CO3	k1_RO2pORO2	Rickard and Pascoe (2009)
G49240	TrGTerC	NOPINDOOH → NOPINDCO	2.63E-11	Rickard and Pascoe (2009)
G49241	TrGTerC	NOPINDCO + OH → C89CO3	3.07E-12	Rickard and Pascoe (2009)
G49242	TrGTerC	NOPINOO → NOPINONE + H_2O_2	6.00E-18*c(ind_H2O)	Rickard and Pascoe (2009)
G49243	TrGTerC	NOPINOO + CO → NOPINONE + CO_2	1.2E-15	Rickard and Pascoe (2009)
G49244	TrGTerCN	NOPINOO + NO → NOPINONE + NO_2	1.E-14	Rickard and Pascoe (2009)
G49245	TrGTerCN	NOPINOO + NO_2 → NOPINONE + NO_3	1.E-15	Rickard and Pascoe (2009)
G49246	TrGTerC	NORPINENOL + OH → HCOOH + OH + C86O2	k_CH2CHOH_OH_HCOOH	Sander et al. (2019), So et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
G49247	TrGTerC	NORPINENOL + HCOOH → NORPINAL + HCOOH	k_CH2CHOH_HCOOH	Sander et al. (2019), da Silva (2010)*
G49248	TrGTerC	NORPINAL + HCOOH → NORPINENOL + HCOOH	k_ALD_HCOOH	Sander et al. (2019), da Silva (2010)*
G49249	TrGTerC	C811CO3H + OH → C811CO3	1.04E-11	Rickard and Pascoe (2009)
G49250	TrGTerCN	C811PAN → C811CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	C811PAN + OH → C721CHO + CO + NO_2	6.77E-12	Rickard and Pascoe (2009)
G49400a	TrGAroC	LTMB + OH → TLEPOXMUC + HO_2 + 2 LCARBON	0.827E-11	Rickard and Pascoe (2009)*
G49400b	TrGAroC	LTMB + OH → C6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard and Pascoe (2009)*
G49400c	TrGAroC	LTMB + OH → CRESOL + 2 LCARBON	0.141E-11	Rickard and Pascoe (2009)*
G49400d	TrGAroC	LTMB + OH → TLBIPERO2 + HO_2 + 2 LCARBON	2.917E-11	Rickard and Pascoe (2009)*
G49401	TrGAroCN	LTMB + NO_3 → C6H5CH2O2 + HNO_3 + 2 LCARBON	1.52E-15	Rickard and Pascoe (2009)*
G40200	TrGTerC	APINENE + OH → .75 LAPINABO2 + .15 MENTHEN6ONE + .15 HO_2 + .10 ROO6R1O2	1.2E-11*EXP(440./temp)	Atkinson et al. (2006)*
G40201a	TrGTerCN	LAPINABO2 + NO → PINAL + HO_2 + NO_2	KRO2NO*(1.-(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair)))	Rickard and Pascoe (2009), Sander et al. (2019)
G40201b	TrGTerCN	LAPINABO2 + NO → LAPINABNO3	KRO2NO*(.65*alpha_AN(11,3,0,0,0,temp,cair)+.35*alpha_AN(11,2,0,0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40202a	TrGTerC	LAPINABO2 + HO_2 → LAPINABOOH	k_RO2_HO2(temp,10)*(1.-r_CHOHCH2O2_OH)	Rickard and Pascoe (2009), Sander et al. (2019)
G40202b	TrGTerC	LAPINABO2 + HO_2 → PINAL + HO_2 + OH	k_RO2_HO2(temp,10)*r_CHOHCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40203	TrGTerC	LAPINABO2 → PINAL + HO_2	RO2*(0.65*k1_RO2tORO2+.35*k1_RO2sORO2)	Rickard and Pascoe (2009)*
G40204	TrGTerC	LAPINABOOH + OH → .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard and Pascoe (2009)*
G40205	TrGTerCN	LAPINABNO3 + OH → .35 PINAL + .65 C96CO3 + NO_2	4.29E-12	Rickard and Pascoe (2009)*
G40206	TrGTerC	MENTHEN6ONE + OH → OHMENTHEN6ONEO2	6.46E-11	Vereecken et al. (2007)*
G40207	TrGTerCN	OHMENTHEN6ONEO2 + NO → 2OHMENTHEN6ONE + HO_2 + NO_2	KRO2NO	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO_2 → 2OHMENTHEN6ONE	k_RO2_HO2(temp,10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 → 2OHMENTHEN6ONE + HO_2	k1_RO2tORO2	Vereecken et al. (2007)
G40210	TrGTerC	2OHMENTHEN6ONE + OH → 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH → .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./temp)	Wallington et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G40212	TrGTerCN	PINAL + NO_3 → C96CO3 + HNO_3	2.0E-14	Wallington et al. (2018)*
G40213a	TrGTerC	C96CO3 → C96O2 + CO_2	k1_RO2RCO3*0.9	Rickard and Pascoe (2009)
G40213b	TrGTerC	C96CO3 → PINONIC	k1_RO2RCO3*0.1	Rickard and Pascoe (2009)
G40214a	TrGTerC	C96CO3 + HO_2 → PERPINONIC	KAPHO2*r_CO3_OOH	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO_2 → PINONIC + O_3	KAPHO2*r_CO3_O3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO_2 → C96O2 + OH + CO_2	KAPHO2*r_CO3_OH	Rickard and Pascoe (2009)
G40215	TrGTerCN	C96CO3 + NO_2 → C10PAN2	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G40216	TrGTerCN	C96CO3 + NO → C96O2 + NO_2 + CO_2	KAPNO	Rickard and Pascoe (2009)
G40217	TrGTerCN	C96CO3 + NO_3 → C96O2 + NO_2 + CO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G40218	TrGTerCN	C10PAN2 → C96CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G40219	TrGTerCN	C10PAN2 + OH → NORPINAL + CO + NO_2	3.66E-12	Rickard and Pascoe (2009)
G40220	TrGTerC	PINONIC + OH → C96O2 + CO_2	6.65E-12	Rickard and Pascoe (2009)
G40221	TrGTerC	PERPINONIC + OH → C96CO3	9.73E-12	Rickard and Pascoe (2009)
G40222	TrGTerC	PINALO2 + HO_2 → PINALOOH	k_RO2_HO2(temp,10)	Rickard and Pascoe (2009)
G40223a	TrGTerCN	PINALO2 + NO → C106O2 + NO_2	KRO2NO*(1.-alpha_AN(12,3,0,1,0, temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40223b	TrGTerCN	PINALO2 + NO → PINALNO3	KRO2NO*alpha_AN(12,3,0,1,0, temp,cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40224	TrGTerC	PINALO2 → C106O2	k1_RO2tRO2	Rickard and Pascoe (2009)
G40225	TrGTerC	PINALOOH + OH → PINALO2	2.75E-11	Rickard and Pascoe (2009)
G40226	TrGTerCN	PINALNO3 + OH → CO235C6CHO + CH_3COCH_3 + NO_2	2.25E-11	Rickard and Pascoe (2009)
G40227	TrGTerC	C106O2 + HO_2 → C106OOH	k_RO2_HO2(temp,10)	Rickard and Pascoe (2009)
G40228a	TrGTerCN	C106O2 + NO → C716O2 + CH_3COCH_3 + NO_2	KRO2NO*0.875*(1.-alpha_AN(13,3,0, 0,0,temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40228b	TrGTerCN	C106O2 + NO → C106NO3	KRO2NO*0.875*alpha_AN(13,3,0,0, 0,temp,cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40229	TrGTerC	C106O2 → C716O2 + CH_3COCH_3	k1_RO2tRO2	Rickard and Pascoe (2009)
G40230	TrGTerC	C106OOH + OH → C106O2	8.01E-11	Rickard and Pascoe (2009)
G40231	TrGTerCN	C106NO3 + OH → CO235C6CHO + CH_3COCH_3 + NO_2	7.03E-11	Rickard and Pascoe (2009)
G40232	TrGTerC	APINENE + O_3 → .09 APINBOO + .08 PINONIC + .77 OH + .33 NORPINAL + .33 CO + .33 HO_2 + .06 APINAOO + .44 C109O2	8.05E-16*EXP(-640./temp)	Wallington et al. (2018)*
G40233	TrGTerC	APINAOO → PINAL + H_2O_2	1.00E-17*c(ind_H2O)	Rickard and Pascoe (2009)
G40234	TrGTerC	APINAOO + CO → PINAL + CO_2	1.20E-15	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40235	TrGTerCN	APINAOO + NO → PINAL + NO_2	1.00E-14	Rickard and Pascoe (2009)
G40236	TrGTerCN	APINAOO + NO_2 → PINAL + NO_3	1.00E-15	Rickard and Pascoe (2009)
G40237a	TrGTerC	APINBOO → PINONIC	1.00E-17*c(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009)
G40237b	TrGTerC	APINBOO → PINAL + H_2O_2	1.00E-17*c(ind_H2O)*0.77	Rickard and Pascoe (2009)
G40238	TrGTerC	APINBOO + CO → PINAL + CO_2	1.20E-15	Rickard and Pascoe (2009)
G40239	TrGTerCN	APINBOO + NO → PINAL + NO_2	1.00E-14	Rickard and Pascoe (2009)
G40240	TrGTerCN	APINBOO + NO_2 → PINAL + NO_3	1.00E-15	Rickard and Pascoe (2009)
G40241	TrGTerC	C109O2 → C89CO3 + HCHO	k1_RO2pORO2	Rickard and Pascoe (2009)
G40242	TrGTerCN	C109O2 + NO → C89CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G40243a	TrGTerC	C109O2 + HO_2 → C109OOH	k_RO2_HO2(temp,10)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G40243b	TrGTerC	C109O2 + HO_2 → C89CO3 + HCHO + OH	k_RO2_HO2(temp,10)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40244	TrGTerC	C109OOH + OH → C109CO + OH	5.47E-11	Rickard and Pascoe (2009)
G40245	TrGTerC	C109CO + OH → C89CO3 + CO	5.47E-11	Rickard and Pascoe (2009)
G40246	TrGTerCN	APINENE + NO_3 → LNAPINABO2	1.2E-12*EXP(490./temp)	Wallington et al. (2018)*
G40247	TrGTerCN	LNAPINABO2 → PINAL + NO_2	(0.65*k1_RO2tRO2 + 0.35*k1_ RO2sRO2)	Rickard and Pascoe (2009)
G40248	TrGTerCN	LNAPINABO2 + NO → PINAL + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G40249	TrGTerCN	LNAPINABO2 + HO_2 → LNAPINABOOH	k_RO2_HO2(temp,10)	Rickard and Pascoe (2009)
G40250	TrGTerCN	LNAPINABO2 + NO_3 → PINAL + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G40251	TrGTerCN	LNAPINABOOH + OH → LNAPINABO2	(.65*6.87E-12+.35*1.23E-11)	Rickard and Pascoe (2009)
G40252a	TrGTerC	BPINENE + OH → BPINAO2	1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40252b	TrGTerC	BPINENE + OH → ROO6R1O2	1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068)	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO_2 → BPINAOOH	k_RO2_HO2(temp,10)*r_COCH2O2_OOH	Rickard and Pascoe (2009), Sander et al. (2019)
G40253b	TrGTerC	BPINAO2 + HO_2 → NOPINONE + HCHO + HO_2 + OH	k_RO2_HO2(temp,10)*r_COCH2O2_OH	Rickard and Pascoe (2009), Sander et al. (2019)
G40254a	TrGTerCN	BPINAO2 + NO → NOPINONE + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(11,3,0,0,0, temp,cair))	Rickard and Pascoe (2009), Sander et al. (2019)
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KRO2NO*alpha_AN(11,3,0,0,0, temp,cair)	Rickard and Pascoe (2009), Sander et al. (2019)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO_2	k1_RO2tORO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40256	TrGTerC	BPINAOOH + OH → BPINAO2	1.33E-11	Rickard and Pascoe (2009)
G40257	TrGTerCN	BPINANO3 + OH → NOPINONE + HCHO + NO_2	4.70E-12	Rickard and Pascoe (2009)
G40258a	TrGTerCN	ROO6R1O2 + NO → ROO6R3O2 + CH_3COCH_3 + NO_2	KRO2NO*(1.-alpha_AN(13,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO → ROO6R1NO3	KRO2NO*alpha_AN(13,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40259	TrGTerC	ROO6R1O2 + HO_2 → 10 LCARBON	k_RO2_HO2(temp,10)	Vereecken and Peeters (2012)*
G40260	TrGTerC	ROO6R1O2 → ROO6R3O2 + CH_3COCH_3	k1_RO2tORO2	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO → RO6R3O2 + NO_2	KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO → RO6R1NO3	KRO2NO*alpha_AN(12,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO_2 → 10 LCARBON	k_RO2_HO2(temp,10)	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 → RO6R3O2	k1_RO2sORO2	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO → 9 LCARBON + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40264b	TrGTerCN	RO6R3O2 + NO → 10 LCARBON + LNITROGEN	KRO2NO*alpha_AN(12,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO_2 → 10 LCARBON	k_RO2_HO2(temp,10)	Vereecken and Peeters (2012)
G40266	TrGTerC	RO6R3O2 → 9 LCARBON + HCHO + HO_2	k1_RO2sRO2	Vereecken and Peeters (2012)*
G40267a	TrGTerC	BPINENE + O_3 → NOPINONE + .63 CO + .37 CH_2OO + .16 OH + .16 HO_2	1.35E-15*EXP(-1270./temp) *.051/(1.-.027)	Wallington et al. (2018)*
G40267b	TrGTerC	BPINENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./temp) *.368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267c	TrGTerC	BPINENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40267d	TrGTerC	BPINENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40268	TrGTerCN	BPINENE + NO_3 → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40269	TrGTerCN	LNBPINABO2 + HO_2 → LNBPINABOOH	k_RO2_HO2(temp,10)	Rickard and Pascoe (2009)
G40270	TrGTerCN	LNBPINABO2 + NO → NOPINONE + HCHO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G40271	TrGTerCN	LNBPINABO2 + NO_3 → NOPINONE + HCHO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G40272a	TrGTerCN	LNBPINABO2 → NOPINONE + HCHO + NO_2	k1_RO2tRO2*0.7	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G40272b	TrGTerCN	LNBPINABO2 → BPINANO3	k1_RO2tRO2*0.3	Rickard and Pascoe (2009)
G40273	TrGTerCN	LNBPINABOOH + OH → LNBPINABO2	9.58E-12	Rickard and Pascoe (2009)
G40274	TrGTerCN	ROO6R1NO3 + OH → ROO6R3O2 + CH_3COCH_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 → APINAOO	3.7E-17*.50*.12	Atkinson and Arey (2003)
G40280e	TrGC	CARENE + O_3 → OH + C109O2	3.7E-17*.50*(.22+.66)	Atkinson and Arey (2003)
G40281	TrGCN	CARENE + NO_3 → LNAPINABO2	9.1E-12	Atkinson and Arey (2003)
G40282a	TrGTerC	SABINENE + OH → BPINAO2	1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40282b	TrGTerC	SABINENE + OH → ROO6R1O2	1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40283a	TrGTerC	SABINENE + O_3 → NOPINONE + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 HO_2	1.35E-15*EXP(-1270./temp) *.051/(1.-.027)	Wallington et al. (2018)*
G40283b	TrGTerC	SABINENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./temp) *.368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283c	TrGTerC	SABINENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40283d	TrGTerC	SABINENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40284	TrGTerCN	SABINENE + NO_3 → LNBPINABO2	2.51E-12	Wallington et al. (2018)*

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

#	labels	reaction	rate coefficient	reference
G40285a	TrGTerC	CAMPHENE + OH → BPINAO2	1.47E-11*EXP(467./temp) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40285b	TrGTerC	CAMPHENE + OH → ROO6R1O2	1.47E-11*EXP(467./temp) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40286a	TrGTerC	CAMPHENE + O_3 → NOPINONE + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 HO_2	1.35E-15*EXP(-1270./temp) *.051/(1.-.027)	Wallington et al. (2018)*
G40286b	TrGTerC	CAMPHENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./temp) *.368/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286c	TrGTerC	CAMPHENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./temp) *.283/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40286d	TrGTerC	CAMPHENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./temp) *(.104+.167)/(1.-.027)	Nguyen et al. (2009), Wallington et al. (2018)
G40287	TrGTerCN	CAMPHENE + NO_3 → LNBPINABO2	2.51E-12	Wallington et al. (2018)*
G40400	TrGAroC	LHAROM + OH → .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + .18 HO_2 + 4 LCARBON	5.67E-11	Rickard and Pascoe (2009)*
G40401	TrGAroCN	LHAROM + NO_3 → C6H5CH2O2 + HNO_3 + 4 LCARBON	2.60E-15	Rickard and Pascoe (2009)*
G6100	UpStTrGCl	Cl + O_3 → ClO + O_2	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + $O(^3P)$ → Cl + O_2	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Burkholder et al. (2015)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(2.16E-27*EXP(8537./temp))	Burkholder et al. (2015)*
G6200	StGCl	Cl + H_2 → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO_2 → HCl + O_2	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO_2 → ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → .94 Cl + .94 HO_2 + .06 HCl + .06 O_2	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	ClO + HO_2 → HOCl + O_2	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)*
G6205	StTrGCl	HCl + OH → Cl + H_2O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl + OH → ClO + H_2O	3.0E-12*EXP(-500./temp)	Burkholder et al. (2015)
G6300	UpStTrGClN	ClO + NO → NO_2 + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G6301	StTrGClN	$ClO + NO_2 \rightarrow ClNO_3$	`k_3rd_iupac(temp,cair,1.6E-31, 3.4,7.E-11,0.,0.4)`	Atkinson et al. (2007)
G6302	TrGClN	$ClNO_3 \rightarrow ClO + NO_2$	`6.918E-7*EXP(-10909./temp)*cair`	Anderson and Fahey (1990)
G6303	StGClN	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	`4.5E-12*EXP(-900./temp)`	Atkinson et al. (2007)
G6304	StTrGClN	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	`6.2E-12*EXP(145./temp)`	Atkinson et al. (2007)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3$	`6.6E-12*EXP(-1240./temp)`	Atkinson et al. (2006)
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	`8.1E-11*EXP(-34./temp)`	Atkinson et al. (2006)
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	`5.9E-11`	Atkinson et al. (2006)*
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	`1.8E-12*EXP(-600./temp)`	Burkholder et al. (2015)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow$ LCARBON $+ ClO + 3\ Cl$	`3.3E-10`	Burkholder et al. (2015)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow 0.1\ CH_3Cl + 0.1\ O(^3P) + 0.46\ ClO + 0.35\ Cl + 0.09\ H + 0.9$ LCARBON $+ 0.09$ LCHLORINE	`1.65E-10`	Burkholder et al. (2015)
G6406	StGCl	$CH_3Cl + OH \rightarrow$ LCARBON $+ H_2O + Cl$	`1.96E-12*EXP(-1200./temp)`	Burkholder et al. (2015)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow 2$ LCARBON $+ OH + 3\ Cl$	`3.25E-10`	Burkholder et al. (2015)
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow 2$ LCARBON $+ H_2O + 3\ Cl$	`1.64E-12*EXP(-1520./temp)`	Burkholder et al. (2015)
G6409	TrGCCl	$Cl + C_2H_4 \rightarrow HOCH_2CH_2O_2 + HCl$	`k_3rd_iupac(temp,cair,1.85E-29, 3.3,6.0E-10,0.0,0.4)`	Atkinson et al. (2006)*
G6410	TrGCCl	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)$	`8.0e-11`	Atkinson et al. (2006)
G6411	TrGCCl	$C_2H_2 + Cl \rightarrow$ LCARBON $+ CH_3 + HCl$	`k_3rd_iupac(temp,cair,6.1e-30, 3.0,2.0e-10,0.,0.6)`	Atkinson et al. (2006)
G6412	TrGCCl	$C_2H_6 + Cl \rightarrow C_2H_5O_2 + HCl$	`8.3E-11*EXP(-100./temp)`	Atkinson et al. (2006)
G6413	StTrGClN	$Cl + CH_3ONO_2 \rightarrow HCl + HCHO + NO_2$	`1.3E-11*EXP(-1200./temp)`	Burkholder et al. (2015)
G6414	StTrGClN	$Cl + CH_3ONO \rightarrow HCl + HCHO + NO$	`2.1E-12`	Sokolov et al. (1999)
G6415	StTrGCl	$Cl + CH_3O_2 \rightarrow .5\ ClO + .5\ CH_3O + .5\ HCl + .5\ CH_2OO$	`1.6E-10`	Burkholder et al. (2015)
G6416	TrGCClN	$Cl + CH_3CN \rightarrow NCCH_2O_2 + HCl$	`1.6E-11*EXP(-2104./temp)`	Tyndall et al. (1996), Tyndall et al. (2001b), Sander et al. (2019)
G6500	StGClF	$CF_2Cl_2 + O(^1D) \rightarrow$ LCARBON $+ 2$ LFLUORINE $+ ClO + Cl$	`1.4E-10`	Burkholder et al. (2015)
G6501	StGClF	$CFCl_3 + O(^1D) \rightarrow$ LCARBON $+$ LFLUORINE $+ ClO + 2\ Cl$	`2.3E-10`	Burkholder et al. (2015)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	`1.7E-11*EXP(-800./temp)`	Atkinson et al. (2007)
G7101	StGBr	$BrO + O(^3P) \rightarrow Br + O_2$	`1.9E-11*EXP(230./temp)`	Atkinson et al. (2007)
G7102a	StTrGBr	$BrO + BrO \rightarrow 2\ Br + O_2$	`2.7E-12`	Atkinson et al. (2007)
G7102b	StTrGBr	$BrO + BrO \rightarrow Br_2 + O_2$	`2.9E-14*EXP(840./temp)`	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr + O_2$	7.7E-12*EXP(-450./temp)	Atkinson et al. (2007)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr + O_2$	4.5E-12*EXP(500./temp)	Atkinson et al. (2007)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	6.7E-12*EXP(155./temp)	Atkinson et al. (2007)
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGBrN	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	$BrO + NO \rightarrow Br + NO_2$	8.7E-12*EXP(260./temp)	Atkinson et al. (2007)
G7302	StTrGBrN	$BrO + NO_2 \rightarrow BrNO_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$BrNO_3 \rightarrow BrO + NO_2$	k_BrO_NO2/(5.44E-9*EXP(14192./temp)*1.E6*R_gas*temp/(atm2Pa*N_A))	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	7.7E-12*EXP(-580./temp)	Atkinson et al. (2006)
G7401	TrGBr	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	2.6E-12*EXP(-1600./temp)	Kondo and Benson (1984)
G7402	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + CH_2OO$	2.42E-14*EXP(1617./temp)	Shallcross et al. (2015)
G7403	StTrGBr	$CH_3Br + OH \rightarrow LCARBON + H_2O + Br$	1.42E-12*EXP(-1150./temp)	Burkholder et al. (2015)
G7404	TrGBrC	$Br + C_2H_4 \rightarrow HOCH_2CH_2O_2 + HBr$	2.8E-13*EXP(224./temp)/(1.+1.13E24*EXP(-3200./temp)/C(ind_O2))	Atkinson et al. (2006)*
G7405	TrGBrC	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)$	1.8e-11*EXP(-460./temp)	Atkinson et al. (2006)
G7406	TrGBrC	$Br + C_2H_2 \rightarrow LCARBON + CH_3O_2 + HBr$	6.35e-15*EXP(440./temp)	Atkinson et al. (2006)
G7407	TrGBr	$CHBr_3 + OH \rightarrow LCARBON + H_2O + 3\ Br$	9.0E-13*EXP(-360./temp)	Burkholder et al. (2015)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow LCARBON + H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	Burkholder et al. (2015)*
G7600	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	3.32E-15	Manion et al. (2015)
G7601	TrGBrCl	$Br + Cl_2 \rightarrow BrCl + Cl$	1.10E-15	Dolson and Leone (1987)
G7602	TrGBrCl	$Br_2 + Cl \rightarrow BrCl + Br$	2.3E-10*EXP(135./temp)	Bedjanian et al. (1998)
G7603a	StTrGBrCl	$BrO + ClO \rightarrow Br + OClO$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGBrCl	$BrO + ClO \rightarrow Br + Cl + O_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGBrCl	$BrO + ClO \rightarrow BrCl + O_2$	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G7604	TrGBrCl	$BrCl + Cl \rightarrow Br + Cl_2$	1.45E-11	Clyne and Cruse (1972)
G7605	TrGBrCl	$CHCl_2Br + OH \rightarrow LCARBON + 2\ Cl + H_2O + Br$	2.0E-12*EXP(-840./temp)	see note*
G7606	TrGBrCl	$CHClBr_2 + OH \rightarrow LCARBON + Cl + H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	see note*
G7607	TrGBrCl	$CH_2ClBr + OH \rightarrow LCARBON + Cl + H_2O + Br$	2.1E-12*EXP(-880./temp)	Burkholder et al. (2015)*
G8100	TrGI	$I + O_3 \rightarrow IO + O_2$	2.1E-11*EXP(-830./temp)	Atkinson et al. (2007)
G8102	TrGI	$OIO + OIO \rightarrow I(part)$	5.E-11	von Glasow et al. (2002)*
G8103	TrGI	$IO + IO \rightarrow .38\ OIO + 1.62\ I + .62\ O_2$	5.4E-11*EXP(180./temp)	Atkinson et al. (2007)*

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

#	labels	reaction	rate coefficient	reference
G8200	TrGI	$I + HO_2 \rightarrow HI + O_2$	`1.5E-11*EXP(-1090./temp)`	Atkinson et al. (2007)
G8201	TrGI	$IO + HO_2 \rightarrow HOI + O_2$	`1.4E-11*EXP(540./temp)`	Atkinson et al. (2007)
G8202	TrGI	$HI + OH \rightarrow I + H_2O$	`1.6E-11*EXP(440./temp)`	Atkinson et al. (2007)
G8203	TrGI	$OIO + OH \rightarrow HIO_3$	`2.2E-10*EXP(243./temp)`	Plane et al. (2006)
G8204	TrGI	$I_2 + OH \rightarrow HOI + I$	`2.1E-10`	Atkinson et al. (2007)
G8205	TrGI	$HOI + OH \rightarrow IO + H_2O$	`5.0E-12`	Riffault et al. (2005)
G8300	TrGIN	$I + NO_2 \rightarrow INO_2$	`k_I_NO2`	Atkinson et al. (2007)*
G8301	TrGIN	$I + NO_3 \rightarrow IO + NO_2$	`1.E-10`	Dillon et al. (2008)
G8302	TrGIN	$IO + NO \rightarrow I + NO_2$	`7.15E-12*EXP(300./temp)`	Atkinson et al. (2007)
G8303	TrGIN	$IO + NO_2 \rightarrow INO_3$	`k_3rd_iupac(temp,cair,7.7E-31, 5.,1.6E-11,0.,0.4)`	Atkinson et al. (2007)
G8304	TrGIN	$OIO + NO \rightarrow NO_2 + IO$	`1.1E-12*EXP(542./temp)`	Atkinson et al. (2007)
G8305	TrGIN	$INO_2 \rightarrow I + NO_2$	`k_I_NO2/(3.7E-7*EXP(9568./temp) *1.E6*R_gas*temp/(atm2Pa*N_A))`	van den Bergh and Troe (1976), Atkinson et al. (2007)*
G8306	TrGIN	$INO_3 \rightarrow IO + NO_2$	`2.1e15*EXP(-13670./temp)`	Kaltsoyannis and Plane (2008)
G8307	TrGIN	$I_2 + NO_3 \rightarrow I + INO_3$	`1.5E-12`	Atkinson et al. (2007)
G8308	TrGIN	$IO + NO_3 \rightarrow OIO + NO_2$	`9.E-12`	Dillon et al. (2008)
G8309	TrGIN	$I + INO_3 \rightarrow I_2 + NO_3$	`9.1E-11*EXP(-146./temp)`	Kaltsoyannis and Plane (2008)
G8400	TrGCI	$CH_3CHICH_3 + OH \rightarrow 2\ LCARBON + CH_3O_2 + I$	`1.22E-12`	Carl and Crowley (2001)
G8401	TrGI	$CH_3O_2 + IO \rightarrow .4\ I + .6\ OIO + HCHO + HO_2$	`2.E-12`	Dillon et al. (2006b), Bale et al. (2005)*
G8402	TrGIN	$CH_3I + NO_3 \rightarrow HNO_3 + HCHO + IO$	`3.4E-17`	Wayne et al. (1991)*
G8600	TrGClI	$IO + ClO \rightarrow .2\ ICl + .25\ Cl + .55\ OClO + .8\ I + .45\ O_2$	`4.7E-12*EXP(280./temp)`	Atkinson et al. (2007)
G8700	TrGBrI	$I + BrO \rightarrow IO + Br$	`1.2E-11`	Burkholder et al. (2015)
G8701	TrGBrI	$IO + BrO \rightarrow Br + .8\ OIO + .2\ I + .2\ O_2$	`1.5E-11*EXP(510./temp)`	Atkinson et al. (2007)*
G8702	TrGBrI	$IBr + OH \rightarrow .84\ HOI + .84\ Br + .16\ HOBr + .16\ I$	`1.4E-10`	Riffault et al. (2005)
G8703	TrGBrI	$IO + Br \rightarrow I + BrO$	`2.3E-11`	Bedjanian et al. (1997)
G8704	TrGBrI	$I_2 + Br \rightarrow IBr + I$	`1.2E-10`	Bedjanian et al. (1997)
G9200	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	`k_3rd(temp,cair,3.3E-31,4.3, 1.6E-12,0.,0.6)`	Burkholder et al. (2015)
G9400a	TrGCS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2004)*
G9400b	TrGCS	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`	Atkinson et al. (2004)*
G9401	TrGCNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2004)
G9402	TrGCS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)*

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

#	labels	reaction	rate coefficient	reference
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3$	1.8E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	5.E-11	Barone et al. (1995)
G9408	StTrGS	$CH_2OO + SO_2 \rightarrow H_2SO_4 + HCHO$	k_CH2OO_SO2	Welz et al. (2012), Stone et al. (2014)*
G9409	TrGTerCS	$NOPINOO + SO_2 \rightarrow NOPINONE + H_2SO_4$	7.E-14	Rickard and Pascoe (2009)
G9410	TrGTerCS	$APINAOO + SO_2 \rightarrow PINAL + H_2SO_4$	7.00E-14	Rickard and Pascoe (2009)
G9411	TrGTerCS	$APINBOO + SO_2 \rightarrow PINAL + H_2SO_4$	7.00E-14	Rickard and Pascoe (2009)
G9412	TrGTerCS	$MBOOO + SO_2 \rightarrow IBUTALOH + H_2SO_4$	7.00E-14	Rickard and Pascoe (2009)
G9600	TrGCClS	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	3.3E-10	Atkinson et al. (2004)
G9700	TrGBrCS	$DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGBrCS	$DMS + BrO \rightarrow DMSO + Br$	4.4E-13	Ingham et al. (1999)
G9800	TrGCIS	$DMS + IO \rightarrow DMSO + I$	3.2E-13*EXP(-925./temp)	Dillon et al. (2006a)
G10100	TrGHg	$Hg + O_3 \rightarrow HgO + O_2$	3.0E-20	Hall (1995)
G10200	TrGHg	$Hg + OH \rightarrow HgO + H$	3.55E-14*EXP(294./temp)	Pal and Ariya (2004)
G10201	TrGHg	$Hg + H_2O_2 \rightarrow HgO + H_2O$	8.5E-19	Tokos et al. (1998)*
G10600	TrGClHg	$Hg + Cl \rightarrow HgCl$	1.0E-11	Ariya et al. (2002)
G10601	TrGClHg	$Hg + Cl_2 \rightarrow HgCl_2$	2.6E-18	Ariya et al. (2002)
G10700	TrGBrHg	$Hg + Br \rightarrow HgBr$	3.0E-13	Donohoue et al. (2006)
G10701	TrGBrHg	$HgBr + Br \rightarrow HgBr_2$	2.5E-10*(temp/298.)**(-0.57)	Goodsite et al. (2004)
G10702	TrGBrHg	$Hg + Br_2 \rightarrow HgBr_2$	9.0E-17	Ariya et al. (2002)
G10703	TrGBrHg	$Hg + BrO \rightarrow HgO + Br$	1.0E-15	Raofie and Ariya (2003)
G10704	TrGBrHg	$HgBr + BrO \rightarrow BrHgOBr$	3.0E-12	Calvert and Lindberg (2003)
G10705	TrGBrClHg	$HgCl + BrO \rightarrow ClHgOBr$	3.0E-12	Calvert and Lindberg (2003)
G10706	TrGBrClHg	$HgBr + Cl \rightarrow ClHgBr$	3.0E-12	Calvert and Lindberg (2003)
G10707	TrGBrClHg	$HgCl + Br \rightarrow ClHgBr$	3.0E-12	Calvert and Lindberg (2003)

General notes

Three-body reactions

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

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

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

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

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_c^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}}))^2}\right)} \quad (4)$$

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:

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

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

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

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

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\mathrm{ratio}}} \times f_c^{\left(\frac{1}{1+(\log_{10}(k_{\mathrm{ratio}})/N)^2}\right)} \quad (9)$$

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 $\mathrm{cm^{-3}s^{-1}}$	
k_p	$4.49 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-320\,\mathrm{K}/T)$
k_s	$4.50 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(253\,\mathrm{K}/T)$
k_t	$2.12 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(696\,\mathrm{K}/T)$
k_ROHRO	$2.1 \times 10^{-18} \times (T/\mathrm{K})^2 \exp(-85\,\mathrm{K}/T)$
k_CO2H	$0.7 \times k_{\mathrm{CH_3CO_2H+OH}}$
k_ROOHRO	$0.6 \times k_{\mathrm{CH_3OOH+OH}}$
f_alk	1.23
f_sOH	3.44
f_tOH	2.68
f_sOOH	8.
f_tOOH	8.
f_ONO2	0.04
f_CH2ONO2	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 $\mathrm{cm^{-3}s^{-1}}$	
k_adp	$4.5 \times 10^{-12} \times (T/300\,\mathrm{K})^{-0.85}$
k_ads	$1/4 \times (1.1 \times 10^{-11} \times \exp(485\,\mathrm{K}/T) + 1.0 \times 10^{-11} \times \exp(553\,\mathrm{K}/T))$
k_adt	$1.922 \times 10^{-11} \times \exp(450\,\mathrm{K}/T) - k_{\mathrm{ads}}$
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_CH2ONO2	0.64

RO_2 self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as decribed by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{1\mathrm{st}} = 2 \times \sqrt{k_{\mathrm{self}} \times \texttt{k\_CH3O2}} \times [\mathrm{RO_2}]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, k_CH3O2 = second-order rate coefficient of the self reaction of CH_3O_2, and $[RO_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

G1002a: The path leading to 2 O(^{3}P) + O_2 results in a null cycle regarding odd oxygen and is neglected.

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

G2117: Converted to Kc [molec-1 cm3]= Kp*R*T/NA, where R is 82.05736 [cm3atmK1mol1].

G2118: Assuming fast equilibrium.

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

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

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

G3206: The rate coefficient is: `k_HNO3_OH = 1.32E-14 * EXP(527/temp) + 1 / ( 1 / (7.39E-32 * EXP(453/temp)*cair) + 1 / (9.73E-17 * EXP(1910/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 OH + 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 CH_3CHO+NO_3 assumed.

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

G4116: Same value as for PAN + OH.

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

G4127: Same as for CH3O2 + NO3 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 $CH_2OO + NO_2$ (G4138) multiplied by the factor from Ouyang et al. (2013).

G4136: Average of two measurements.

G4137: Upper limit.

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

G4141: $HOOCH_2OCHO$ 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 NO_2+CH_3O_2.

G4149: Barnes et al. (1985) estimated a decomposition rate equal to that of $CH_3O_2NO_2$.

G4150: Value for $CH_3O_2NO_2$ + OH, H-abstraction enhanced by the HO-group by f_sOH.

G4154: Products assumed to be $CH_3O_2 + O_2$ (could also be HCHO + O_2 + OH).

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

G4160c: The NH + CO channel is also significant but neglected here.

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

G4164: Upper limit. Dominant pathway under atmospheric conditions.

G42001: The product distribution is from Rickard and Pascoe (2009), after substitution of the energized Criegee intermediate, 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_CH3CO3_NO2 = k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)`.

G42018: The rate coefficient is the same as for the CH_3 channel in G4107 (CH_3OOH+OH).

G42021: The rate coefficient is `k_PAN_M = k_CH3CO3_NO2/9.0E-29*EXP(-14000./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 $HOCH_2CH_2O$ in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + HO_2.

G42051a: Same as for the CH_3O_2 channel in G4107: CH_3OOH+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.E-11 molec/cm3/s by Paulot et al. (2009a).

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

G42075: $NO_3CH_2CO_2H$ and $NO_3CH_2CO_3H$ neglected.

G42078: $NO_3CH_2CO_2H$ neglected.

G42082: Same rate constant as for PAN + OH.

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

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

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

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

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

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

G42087: HCOCN is produced but replaced here by its likely oxidation products (HCN + CO_2) as studied by Tyndall et al. (2001b). The rate constant for a typical RO_2 + NO reaction is used.

G42088: $NCCH_2OOH$ is produced but replaced here by its likely oxidation products (HCN + CO_2) as studied by Tyndall et al. (2001b). The rate constant for a typical RO_2 + HO_2 reaction is used.

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

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

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

G42092: approximated OH reaction for oxalic acid

G42093a: SAR for H-abstraction by OH

G42093b: SAR for H-abstraction by OH, assuming that -CHOHOH has an effect like -CH2OH

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 -CH2OOH has the same effect as -CH2OH

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 RO_2 + HO_2 reaction from Atkinson (1997) is used here.

G43008: The value for the generic RO_2 + 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 (CH_3OOH + 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 $CH_3O_2NO_2$ + OH, H-abstraction enhanced by the CH_3CO-group by f_CO.

G43051c: Products approximated with C_2H_5CHO + 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 $\rightarrow$ GLYOX + CO + HO2

G43420: KDEC C3DIALO $\rightarrow$ GLYOX + CO + HO2

G43421: Permutation reaction (minor channels removed).

G44000: The $LC_4H_9O_2$ composition ($nC_4H_9O_2$:$sC_4H_9O_2$ ratio) is assumed to be equal to the ratio of the production rates at 298K: k_p/(k_p+k_s) = 0.1273 and k_s/(k_p+k_s) = 0.8727.

G44001b: $sC_4H_9O_2$ products are substituted with 0.636 MEK + HO_2 and 0.364 CH_3CHO + $C_2H_5O_2$ at 1 bar and 298 K.

G44003c: The alkyl nitrate yield is the weighted average yield for the two isomers forming from $nC_4H_9O_2$ and $sC_4H_9O_2$.

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

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

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

G44016: Products assumed to be only from H-abstraction from a secondary C bearing the $-ONO_2$ group.

G44018: LHMVKABO2 is 0.12 HMVKAO2 + 0.88 HMVKBO2.

G44019: LMEKO2 represents 0.62 MEKBO2 + 0.38 MEKAO2.

G44021a: The products of MEKAO are substituted with HCHO + CO_2 + $HOCH_2CH_2O_2$.

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

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

G44025: Same value as for PAN.

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

G44035: Rate constant replaced with the one of beta hydroxy RO_2.

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

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

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

G44062a: Simplified products.

G44062b: Simplified products.

G44066: Alkyl nitrate formation neglected.

G44070: Alkyl nitrate formation neglected.

G44076: Alkyl nitrate formation neglected.

G44078: Other channel neglected.

G44081: Alkyl nitrate formation neglected.

G44082: Other channel neglected.

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

G44086: Simplified product distribution.

G44089: The nitrated RO_2 is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO2 isomers mostly C_2H_5CHO.

G44097a: Branching ratios according to Rickard et al. (1999). CH_3CHO_2CHO is replaced with its major products CH_3CHO + CO + HO_2.

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

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

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH3CHOOA products as from C_3H_6 + O_3 reaction.

G44107: The nitrated RO_2 is replaced by its products upon reaction with NO.

G44110: The nitrated RO_2 is replaced by its products upon reaction with NO.

G44124b: Skipping intermediate steps mostly leading to acetone.

G44126: Skipping intermediate steps mostly leading to acetone.

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

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

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

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

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

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

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

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

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

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

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

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

G44139: Simplified oxidation.

G44140: Simplified oxidation.

G44141: Simplified oxidation.

G44142: Simplified oxidation.

G44202: Alkyl nitrate formation neglected.

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

G44205: Alkyl nitrate formation neglected.

G44210: Alkyl nitrate formation neglected.

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

G44402: KDEC NC4DCO2→ MALANHY + NO2

G44406c: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

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

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

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

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

G44421: Only major channel.

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

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCO3

G44431: KDEC MALANHYO → HCOCOHCO3

G44432: Only major channel. KDEC MALANHYO → HCOCOHCO3

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

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

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

G44439: KDEC MALDIALCO2 → 0.6 MALANHY + HO2 + 0.4 GLYOX + 0.4 CO + 0.4 CO2

G44443: KDEC MECOACETO → CH3CO3 + HCHO

G44444: KDEC MECOACETO → CH3CO3 + HCHO

G44445: KDEC MECOACETO → CH3CO3 + HCHO

G44450: KDEC BZFUO → CO14O3CHO + HO2

G44451: KDEC BZFUO → CO14O3CHO + HO2

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

G44457: KDEC MALDIALO → GLYOX + GLYOX + HO2

G44458: KDEC MALDIALO → GLYOX + GLYOX + HO2

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

G44461: KBPAN → k_PAN_M

G45019d: Delta-1 and delta-2 LIEPOX are not considered and replaced by beta-LIEPOX formed by ISOPBOOH 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 HMAC (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting from the ring opening after H-abstraction). The rate constant is from Paulot et al. (2009b) and adjusted based on Bates et al. (2014) that determined the single rate constants for the cis- and trans- beta isomer.

G45080: Alkyl nitrate formation neglected.

G45092a: C4MDIAL = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with NO_3 but only one isomer product considered.

G45095: Alkyl nitrate formation neglected.

G45098: Alkyl nitrate formation neglected.

G45100: Alkyl nitrate formation neglected.

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

G45107: OH production here is to take into account the hydroperoxidic function formed by the shift of the enolic hydrogen and not present in DB2O2. This approximation leads to spurious HO_2 production.

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

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

G45111: Alkyl nitrate formation neglected.

G45114b: Here, formic acid is mechanistically produced by the OH-addition to the vinyl alcohol which, upon RO_2-to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with O_2 forming $HCOOH + HO_2$. Along $CH_3COCHOOHCHO$ should be produced but not in the mechanism. Only CH_3COCHO_2CHO. The rate constant is consistent with predictions by Ganzeveld et al. (2006) for ENOL. OH-addition to the OH-bearing carbon is considered the dominant channel as it is already for the ENOL (Ganzeveld et al., 2006).

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

G45116: As for DB1OOH + OH.

G45117: Additional sinks for DB2OOH are neglected.

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

G45128: Rate constant by Liljegren and Stevens (2013). A lumped RO_2 that upon conversion to RO yields 100% 2-methyl-butenedial (C4MDIAL) although Aschmann et al. (2014) quantified a 38% yield of the Z/E mixture.

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

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

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

G45139: LZCPANC23DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO2 = 0.67 MBOAO2 + 0.33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2 → MMALANHY + NO2

G45404: KDEC NTLFUO → ACCOMECHO + NO2

G45405: KDEC NTLFUO → ACCOMECHO + NO2

G45406: KDEC NTLFUO → ACCOMECHO

G45409: KBPAN → k_PAN_M(renaming)

G45413: KFPAN → k_CH3CO3_NO2 (renaming)

G45422: KDEC MMALANHYO→CO2H3CO3

G45423: KDEC MMALANHYO→CO2H3CO3

G45424: KDEC MMALANHYO→CO2H3CO3 and Only major channel.

G45429: KBPAN → k_PAN_M (renamed)

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

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

G45432: KFPAN →k_CH3CO3_NO2 (renaming)

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

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

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

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

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

G45456: KFPAN →k_CH3CO3_NO2 (renaming)

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

G45477: KDEC NTLFUO → ACCOMECHO + NO2

G45478: KDEC NTLFUO → ACCOMECHO + NO2

G45479: KDEC NTLFUO → ACCOMECHO + NO2

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

G45487: KDEC C5DIALO →MALDIAL

G45488: KDEC C5DIALO →MALDIAL

G45489: KDEC C5DIALO →MALDIAL

G45491b: Reactions with KRO2HO2.

G45492: MGLYOX + GLYOX + HO2 from KDEC substitution

G45493: MGLYOX + GLYOX + HO2 from KDEC substitution

G45494: Permutation reaction (minor channels removed).

G46201: Alkyl nitrate formation neglected.

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

G46405: KDEC C615CO2O → C5DICARB + CO + HO2

G46406: KDEC C615CO2O → C5DICARB + CO + HO2

G46407: Only major channel.

G46413b: Reactions with KRO2HO2 and KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2.

G46414: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46415: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46416: KDEC NDNPHENO → NC4DCO2H + HNO3 + CO + CO + NO2

G46418: KDEC CATECOOA → MALDALCO2H + HCOCO2H + HO2 + OH

G46426: KFPAN →k_CH3CO3_NO2

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

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

G46433: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46434: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

G46435: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

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

G46438: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46439: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46440: KDEC NPHENO → MALDALCO2H + GLYOX + NO2

G46441: Merged equations.

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

G46448: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46449: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46450: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

G46457: Merged equations.

G46458: Merged equations.

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

G46462: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

G46463: KDEC PHENO → 0.71 MALDALCO2H + 0.71 GLYOX + 0.29 PBZQONE + HO2

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

G46468: KFPAN →k_CH3CO3_NO2

G46472b: new channel

G46476: HOC6H4NO2 is a nitro-phenol

G46480b: Reactions with KRO2HO2 and KDEC PBZQO →C5CO2OHCO3

G46481: KDEC PBZQO →C5CO2OHCO3

G46482: KDEC PBZQO →C5CO2OHCO3

G46483: KDEC PBZQO →C5CO2OHCO3 and Only major channel.

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

G46486: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46487: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

G46488: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

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

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

G46492: KDEC BZEMUCO → 0.5 EPXC4DIAL + 0.5 GLYOX + 0.5 HO2 + 0.5 C3DIALO2 + 0.5 C32OH13CO

G46493: KDEC BZEMUCO → 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 → C6CO4DB + NO2.

G46500: KDEC NBZQO → C6CO4DB + NO2

G46501: KDEC NBZQO → C6CO4DB + NO2

G46502: KDEC NBZQO → C6CO4DB + NO2

G46505b: New channel.

G46515: Only major channel.

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

G46523b: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46524: KDEC BZBIPERO → GLYOX + HO2 + 0.5 BZFUONE + 0.5 BZFUONE

G46525: KDEC BZBIPERO → 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 → 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 → 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 → 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 → 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 → 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 → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE.

G47419: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

G47420: KDEC CRESO → 0.68 C5CO14OH + 0.68 GLYOX + HO2 + 0.32 PTLQONE

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

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

G47423: KDEC NCRESO → C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO → C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

G47429: KDEC MCATECOOA → MC3ODBCO2H + HCOCO2H + HO2 + OH

G47436: KFPAN →k_CH3CO3_NO2

G47438: Only major channel.

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

G47440b: KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

G47441: KDEC TLEMUCO→ 0.5 C3DIALO2 + 0.5 CO2H3CHO + 0.5 EPXC4DIAL + 0.5 MGLYOX + 0.5 HO2

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

G47445: KFPAN →k_CH3CO3_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

G47482b: Reactions with KRO2HO2 and KDEC NPTLQO → C7CO4DB + NO2

G47483: KDEC NPTLQO → C7CO4DB + NO2

G47484: KDEC NPTLQO → C7CO4DB + NO2

G47485: KDEC NPTLQO → C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO → C6CO2OHCO3

G47487: KDEC PTLQO → C6CO2OHCO3

G47488: KDEC PTLQO → C6CO2OHCO3

G47489: Only major channel. KDEC PTLQO → C6CO2OHCO3.

G47494: New channel.

G47497b: Reactions with KRO2HO2 and KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47498: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

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

G47502: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

G47509b: Reactions with KRO2HO2 and KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47510: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47511: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

G47512: KDEC NDNCRESO → NC4MDCO2H + HNO3 + CO + CO + NO2

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

G47514: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO → 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 (1.36E-11*0.24 + 2.31E-11*0.29 + 1.43E-11*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 (1.36E-11*0.05 + 2.31E-11*0.04 + 1.43E-11*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 (1.36E-11*0.16 + 2.31E-11*0.17 + 1.43E-11*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 (1.36E-11*0.55 + 2.31E-11*0.50 + 1.43E-11*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=(4.10E-16+2.60E-16+5.00E-16)/3 = 3.9E-16.

G48402: merged under same rate constant

G48403: Same products as for toluene

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

G48408: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

G48409: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

G48410: KDEC NSTYRENEO → NO2 + HCHO + BENZAL

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

G48413: KDEC STYRENO → HO2 + HCHO + BENZAL

G48414: KDEC STYRENO → HO2 + HCHO + BENZAL

G48415: KDEC STYRENO → HO2 + HCHO + BENZAL

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

G49246: Only this channel considered as the intermediate radical is likely more stable than $CHCH(OH)_2$.Instead of the (lacking) carbonyl a product of further degradation is assumed.

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

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

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to (3.27E-11*0.21 + 3.25E-11*0.30 + 5.67E-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 (3.27E-11*0.06 + 3.25E-11*0.06 + 5.67E-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 (3.27E-11*0.03 + 3.25E-11*0.03 + 5.67E-11*.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 (3.27E-11*0.70 + 3.25E-11*0.61 + 5.67E-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)E-15/3=1.52E-15.

G40200: Products from Vereecken et al. (2007). LAPINABO2 = 0.65 APINAO2 + 0.35 APINBO2

G40203: Weighted average for isomers A and B, `k = 0.33*9.20E-14+0.67*8.80E-13`.

G40204: Weighted average for isomers A and B, `k = 0.35*1.83E-11+0.65*3.28E-11`.

G40205: Weighted average for isomers A and B, `k = 0.35*5.50E-12+0.65*3.64E-12`.

G40206: SAR-estimated rate constant, `(kads+kadt)*acoch3 = 6.46E-11` where `kads = 3.0E-11`, `kadt = 5.5E-11`, `acoch3 = 0.76`

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard and Pascoe (2009).

G40212: Products from Rickard and Pascoe (2009).

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

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard and Pascoe (2009).

G40248: Alkyl nitrate formation neglected.

G40252a: Products from Vereecken and Peeters (2012).

G40252b: Products from Vereecken and Peeters (2012).

G40259: ROO6R1OOH is produced but no sink for it.

G40262: RO6R1OOH is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

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

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for RO6R1NO3 in G4085.

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

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

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

G40282a: Products from Vereecken and Peeters (2012).

G40282b: Products from Vereecken and Peeters (2012).

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

G40284: Products from Rickard and Pascoe (2009).

G40285a: Products from Vereecken and Peeters (2012).

G40285b: Products from Vereecken and Peeters (2012).

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

G40287: Products from Rickard and Pascoe (2009).

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

`G40401`: Same products as for toluene.

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

`G6204`: At low temperatures, there may be a minor reaction channel leading to O_3+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

`G6402`: The initial products are probably HCl and CH_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

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

`G7302`: The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

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

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

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

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

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

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

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

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

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

`G8300`: The rate coefficient is: `k_I_NO2 = k_3rd_iupac(temp,cair,3.E-31,1.,6.6E-11,0.,0.63)`.

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

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

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

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

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

$$\begin{array}{rcl}
\mathrm{DMS + OH} & \rightarrow & \mathrm{CH_3SCH_2} \\
\mathrm{CH_3SCH_2 + O_2} & \rightarrow & \mathrm{CH_3SCH_2OO} \\
\mathrm{CH_3SCH_2OO + NO} & \rightarrow & \mathrm{CH_3SCH_2O + NO_2} \\
\mathrm{CH_3SCH_2O} & \rightarrow & \mathrm{CH_3S + HCHO} \\
\mathrm{CH_3S + O_3} & \rightarrow & \mathrm{CH_3SO} \\
\mathrm{CH_3SO + O_3} & \rightarrow & \mathrm{CH_3SO_2} \\
\hline
\mathrm{DMS + OH + NO + 2O_3} & \rightarrow & \mathrm{CH_3SO_2 + HCHO + NO_2}
\end{array}$$

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

$$\mathrm{DMS + OH + O_3 \rightarrow CH_3SO_2 + HCHO}$$

.

`G9400b`: For the addition path, the rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

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

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

`G10201`: Upper limit.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J (gas)				
J0001	UpGJ	$O(^3P) \rightarrow O^+ + e^-$	`jx(ip_Op_em) +jx(ip_se_Op_em)`	Fuller-Rowell (1993)
J0002a	UpGJ	$O_2 \rightarrow O_2^+ + e^-$	`jx(ip_O2p_em) +jx(ip_se_O2_b1)`	Fuller-Rowell (1993)
J0002b	UpGJ	$O_2 \rightarrow O^+ + O(^3P) + e^-$	`jx(ip_Op_O_em) +jx(ip_se_O2_b2)`	Fuller-Rowell (1993)
J0003a	UpGJN	$N_2 \rightarrow N_2^+ + e^-$	`jx(ip_N2p_em) +jx(ip_se_N2_b1)`	Fuller-Rowell (1993)
J0003b	UpGJN	$N_2 \rightarrow N^+ + N + e^-$	`jx(ip_Np_N_em) +jx(ip_se_N2_b2)`	Fuller-Rowell (1993)
J0003c	UpGJN	$N_2 \rightarrow N^+ + N(^2D) + e^-$	`jx(ip_Np_N2D_em)+jx(ip_se_N2_b3)`	Fuller-Rowell (1993)
J0003d	UpGJN	$N_2 \rightarrow N + N(^2D)$	`jx(ip_N_N2D_em) +jx(ip_se_N2_b4)`	Fuller-Rowell (1993)
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	`jx(ip_O2)`	Sander et al. (2014)
J1000b	UpGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^1D)$	`jx(ip_O3PO1D)`	Sander et al. (2014)
J1000c	UpGJ	$O_2 + h\nu \rightarrow O_2^+ + e^-$	`jx(ip_O2_b1)`	Sander et al. (2014)
J1000d	UpGJ	$O_2 + h\nu \rightarrow O^+ + O(^3P) + e^-$	`jx(ip_O2_b2)`	Sander et al. (2014)
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	`jx(ip_O1D)`	Sander et al. (2014)
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	`jx(ip_O3P)`	Sander et al. (2014)
J1002	UpGJ	$O(^3P) + h\nu \rightarrow O^+ + e^-$	`jx(ip_O3Pp)`	Sander et al. (2014)
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	`jx(ip_H2O)`	Sander et al. (2014)
J2100b	UpGJ	$H_2O + h\nu \rightarrow H_2 + O(^1D)$	`jx(ip_H2O1D)`	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	`jx(ip_H2O2)`	Sander et al. (2014)
J3000a	UpGJN	$N_2 + h\nu \rightarrow N_2^+ + e^-$	`jx(ip_N2_b1)`	Sander et al. (2014)
J3000b	UpGJN	$N_2 + h\nu \rightarrow N^+ + N + e^-$	`jx(ip_N2_b2)`	Sander et al. (2014)
J3000c	UpGJN	$N_2 + h\nu \rightarrow N^+ + N(^2D) + e^-$	`jx(ip_N2_b3)`	Sander et al. (2014)
J3000d	UpGJN	$N_2 + h\nu \rightarrow N + N(^2D)$	`jx(ip_NN2D)`	Sander et al. (2014)
J3100	UpStGJN	$N_2O + h\nu \rightarrow O(^1D) + N_2$	`jx(ip_N2O)`	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	`jx(ip_NO2)`	Sander et al. (2014)
J3102a	UpStGJN	$NO + h\nu \rightarrow N + O(^3P)$	`jx(ip_NO)`	Sander et al. (2014)
J3102b	UpGJN	$NO + h\nu \rightarrow NO^+ + e^-$	`jx(ip_NOp)`	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	`jx(ip_NO2O)`	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	`jx(ip_NOO2)`	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	`jx(ip_N2O5)`	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow NO + OH$	`jx(ip_HONO)`	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	`jx(ip_HNO3)`	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	`jx(ip_HNO4)`	Sander et al. (2014)
J41000	StTrGJ	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	`jx(ip_CH3OOH)`	Sander et al. (2014)
J41001a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	`jx(ip_COH2)`	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41001b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	Sander et al. (2014)
J41002	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	jx(ip_CO2)	Sander et al. (2014)
J41003	StGJ	$CH_4 + h\nu \rightarrow .42\ CH_3 + .42\ H + .6912\ H_2 + .0864\ HCHO + .0864\ O(^3P) + .1584\ OH + .1584\ HO_2 + .2112\ CO_2 + .1824\ CO + .024\ H_2O + .10\ LCARBON$	jx(ip_CH4)	Sander et al. (2014)*
J41004	StTrGJN	$CH_3ONO + h\nu \rightarrow CH_3O + NO$	jx(ip_CH3ONO)	Sander et al. (2014)
J41005	StTrGJN	$CH_3ONO_2 + h\nu \rightarrow CH_3O + NO_2$	jx(ip_CH3NO3)	Sander et al. (2014)
J41006	StTrGJN	$CH_3O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ CH_3O_2 + .333\ NO_3 + .333\ CH_3O$	jx(ip_CH3O2NO2)	Sander et al. (2014)*
J41007	StTrGJ	$HOCH_2OOH + h\nu \rightarrow HCOOH + OH + HO_2$	jx(ip_CH3OOH)	Sander et al. (2014)
J41008	StTrGJ	$CH_3O_2 + h\nu \rightarrow HCHO + OH$	jx(ip_CH3O2)	Sander et al. (2014)
J41009	StTrGJ	$HCOOH + h\nu \rightarrow CO + HO_2 + OH$	jx(ip_HCOOH)	Sander et al. (2014)
J41010	StTrGJN	$HOCH_2O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ HOCH_2O_2 + .333\ NO_3 + .333\ HCOOH + .333\ HO_2$	jx(ip_CH3O2NO2)	Sander et al. (2014)
J42000	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)
J42001a	TrGJC	$CH_3CHO + h\nu \rightarrow CH_3 + HO_2 + CO$	jx(ip_CH3CHO)	Sander et al. (2014)
J42001b	TrGJC	$CH_3CHO + h\nu \rightarrow CH_2CHOH$	jx(ip_CH3CHO2VINY)	Clubb et al. (2012)
J42002	TrGJC	$CH_3C(O)OOH + h\nu \rightarrow CH_3 + OH + CO_2$	jx(ip_CH3CO3H)	Sander et al. (2014)
J42004	TrGJCN	$PAN + h\nu \rightarrow .7\ CH_3C(O) + .7\ NO_2 + .3\ CH_3 + .3\ CO_2 + .3\ NO_3$	jx(ip_PAN)	Sander et al. (2014)*
J42005a	TrGJC	$HOCH_2CHO + h\nu \rightarrow HCHO + 2\ HO_2 + CO$	jx(ip_HOCH2CHO)*0.83	Sander et al. (2014)*
J42005b	TrGJC	$HOCH_2CHO + h\nu \rightarrow OH + HCOCH_2O_2$	jx(ip_HOCH2CHO)*0.07	Sander et al. (2014)*
J42005c	TrGJC	$HOCH_2CHO + h\nu \rightarrow CH_3OH + CO$	jx(ip_HOCH2CHO)*0.10	Sander et al. (2014)*
J42006	TrGJC	$HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J42007	TrGJCN	$PHAN + h\nu \rightarrow .7\ HOCH2CO + .7\ NO_2 + .3\ HCHO + .3\ HO_2 + .3\ CO_2 + .3\ NO_3$	jx(ip_PAN)	see note*
J42008	TrGJC	$GLYOX + h\nu \rightarrow 2\ CO + 2\ HO_2$	jx(ip_GLYOX)	Sander et al. (2014)
J42009	TrGJC	$HCOCO_2H + h\nu \rightarrow 2\ HO_2 + CO + CO_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J42010	TrGJC	$HCOCO_3H + h\nu \rightarrow HO_2 + CO + OH + CO_2$	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J42011	TrGJC	$HYETHO2H + h\nu \rightarrow HOCH_2CH_2O + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J42012	TrGJCN	$ETHOHNO3 + h\nu \rightarrow HO_2 + 2\ HCHO + NO_2$	j_IC3H7NO3	Rickard and Pascoe (2009)
J42013	TrGJC	$HOOCH2CO3H + h\nu \rightarrow OH + HCHO + CO_2 + OH$	2.*jx(ip_CH3OOH)	Sander et al. (2019)
J42014	TrGC	$HOOCH2CO2H + h\nu \rightarrow OH + HCHO + HO_2 + CO_2$	jx(ip_CH3OOH)	Sander et al. (2019)
J42015	TrGC	$CH2CO + h\nu \rightarrow .4\ CO_2 + .8\ H + .34\ CO + .34\ OH + .34\ HO_2 + .16\ HCHO + .16\ O(^3P) + .1\ HCOOH + CO$	j_ketene*0.36	Sander et al. (2019)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42016	TrGC	CH3CHOHOOH + hν $\rightarrow$ CH_3 + HCOOH + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J42017	TrGJCN	NO_3CH2CHO + hν $\rightarrow$ HO_2 + CO + HCHO + NO_2	(jx(ip_C2H5NO3)+jx(ip_CH3CHO)) *(jx(ip_NOA)+1E-10)/(0.59*j_ IC3H7NO3+jx(ip_CH3COCH3)+1E-10)	Sander et al. (2019)*
J42018	TrGJC	HOOCH2CHO + hν $\rightarrow$ OH + HCHO + CO + HO_2	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Sander et al. (2019)
J42019	TrGJCN	$C_2H_5ONO_2$ + hν $\rightarrow$ CH_3CHO + HO_2 + NO_2	jx(ip_C2H5NO3)	Sander et al. (2019)
J42020	TrGJCN	NO_3CH2CHO + hν $\rightarrow$ .7 NO_3CH2CO_3 + .7 NO_2 + .3 HCHO + .3 NO_2 + .3 CO_2 + .3 NO_3	jx(ip_PAN)	Sander et al. (2019)*
J42021	StTrGJCN	$C_2H_5O_2NO_2$ + hν $\rightarrow$ .667 NO_2 + .667 $C_2H_5O_2$ + .333 NO_3 + .333 CH_3CHO + .333 HO_2	jx(ip_CH3O2NO2)	Sander et al. (2019)*
J42022	TrGJC	HOOCCOOH + hν $\rightarrow$ CO_2 + .72 HCOOH + .28 CO + .28 H_2O	jx(ip_HOOCCOOH)	Yamamoto and Back (1985)
J43000	TrGJC	iC_3H_7OOH + hν $\rightarrow$ CH_3COCH_3 + HO_2 + OH	jx(ip_CH3OOH)	von Kuhlmann (2001)
J43001	TrGJC	CH_3COCH_3 + hν $\rightarrow$ $CH_3C(O)$ + CH_3	jx(ip_CH3COCH3)	Sander et al. (2014)
J43002	TrGJC	CH_3COCH_2OH + hν $\rightarrow$ .5 $CH_3C(O)$ + .5 HCHO + .5 HO_2 + .5 HOCH2CO + .5 CH_3	j_ACETOL	Sander et al. (2014)*
J43003	TrGJC	MGLYOX + hν $\rightarrow$ $CH_3C(O)$ + CO + HO_2	jx(ip_MGLYOX)	Sander et al. (2014)
J43004	TrGJC	$CH_3COCH_2O_2H$ + hν $\rightarrow$ $CH_3C(O)$ + HCHO + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J43005	TrGJC	HOCH2COCH2OOH + hν $\rightarrow$ HOCH2CO + HCHO + OH	jx(ip_CH3OOH)+j_ACETOL	Sander et al. (2019)
J43006	TrGJCN	i$C_3H_7ONO_2$ + hν $\rightarrow$ CH_3COCH_3 + NO_2 + HO_2	j_IC3H7NO3	von Kuhlmann et al. (2003)*
J43007	TrGJCN	NOA + hν $\rightarrow$ $CH_3C(O)$ + HCHO + NO_2	jx(ip_NOA)	Barnes et al. (1993)
J43009	TrGJC	HYPROPO2H + hν $\rightarrow$ CH_3CHO + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J43010	TrGJCN	PR2O2HNO3 + hν $\rightarrow$ NOA + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J43011	TrGJC	HOCH2COCHO + hν $\rightarrow$ HOCH2CO + CO + HO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J43012	TrGJC	$HCOCOCH_2OOH$ + hν $\rightarrow$ HCOCO + HCHO + OH	jx(ip_CH3OOH)+j_ACETOL	Sander et al. (2019)
J43013	TrGJC	$HCOCOCH_2OOH$ + hν $\rightarrow$ $HOOCH_2CO_3$ + CO + HO_2	jx(ip_MGLYOX)	Sander et al. (2019)
J43014	TrGJTerC	HCOCH2CHO + hν $\rightarrow$ $HCOCH_2O_2$ + HO_2 + CO	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J43015	TrGJTerC	HCOCH2CO2H + hν $\rightarrow$ $HCOCH_2O_2$ + CO_2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J43016	TrGJTerC	HOC2H4CO3H + hν $\rightarrow$ $HOCH_2CH_2O_2$ + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J43017	TrGJC	HCOCOCHO + hν $\rightarrow$ HCOCO + HO_2 + CO	2.*jx(ip_MGLYOX)	Sander et al. (2019)
J43018	TrGJC	CH_3COCO_2H + hν $\rightarrow$ .32 CH_3CHO + .16 CH_2CHOH + .54 CO_2 + .38 $CH_3C(O)$ + .38 HO_2 + .38 CO_2 + .07 CH_3COOH + .07 CO + .05 $CH_3C(O)$ + .05 CO + .05 OH	jx(ip_CH3COCO2H)	Sander et al. (2019)*
J43019	TrGC	CH_3COCO_3H + hν $\rightarrow$ $CH_3C(O)$ + OH + CO_2	jx(ip_MGLYOX)+jx(ip_CH3OOH)	Sander et al. (2019)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43020	TrGC	CH3CHCO + hν $\rightarrow$ C_2H_4 + CO	j_ketene*0.36*2.	Sander et al. (2019)
J43021	TrGCN	PROPOLNO3 + hν $\rightarrow$ $HOCH_2CHO$ + HCHO + HO_2 + NO_2	j_IC3H7NO3	Sander et al. (2019)
J43022	TrGCN	$CH_3COCH_2OONO_2$ + hν $\rightarrow$ $CH_3C(O)$ + HCHO + NO_3	jx(ip_CH3O2NO2)+jx(ip_CH3COCH3)	Sander et al. (2019)
J43023	TrGJC	C_3H_7OOH + hν $\rightarrow$ C_2H_5CHO + HO_2 + OH	jx(ip_CH3OOH)	von Kuhlmann (2001)
J43024	TrGJCN	$C_3H_7ONO_2$ + hν $\rightarrow$ C_2H_5CHO + NO_2 + HO_2	0.59*j_IC3H7NO3	see note*
J43025a	TrGJC	C_2H_5CHO + hν $\rightarrow$ $C_2H_5O_2$ + HO_2 + CO	jx(ip_C2H5CHO2HCO)	see note*
J43025b	TrGJC	C_2H_5CHO + hν $\rightarrow$ CH_2CHCH_2OH	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Sander et al. (2019)*
J43026	TrGJCN	PPN + hν $\rightarrow$ .7 $C_2H_5CO_3$ + .7 NO_2 + .3 $C_2H_5O_2$ + .3 CO_2 + .3 NO_3	jx(ip_PAN)	Sander et al. (2014)
J43027	TrGJC	$C_2H_5CO_3H$ + hν $\rightarrow$ $C_2H_5O_2$ + CO_2 + OH	jx(ip_CH3OOH)	von Kuhlmann (2001)
J43028a	TrGJC	$HCOCOCH_2OOH$ + hν $\rightarrow$ $HOOCH_2CO_3$ + CO + HO_2	jx(ip_MGLYOX)	Sander et al. (2019)
J43028b	TrGJC	$HCOCOCH_2OOH$ + hν $\rightarrow$ HCOCO + HCHO + OH	jx(ip_HOCH2CHO)+jx(ip_CH3OOH)	Sander et al. (2019)
J43200	TrGJTerC	HCOCH2CO3H + hν $\rightarrow$ $HCOCH_2O_2$ + CO_2 + OH	jx(ip_HOCH2CHO)+jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J43400	TrGJAroC	C3DIALOOH + hν $\rightarrow$ GLYOX + CO + HO_2 + OH	jx(ip_HOCH2CHO)*2.+jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J43401	TrGJAroC	C32OH13CO + hν $\rightarrow$ GLYOX + HO_2 + HO_2 + CO	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J43402	TrGJAroC	HCOCOHCO3H + hν $\rightarrow$ GLYOX + HO_2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44000a	TrGJC	LC_4H_9OOH + hν $\rightarrow$ OH + C_3H_7CHO + HO_2	jx(ip_CH3OOH)*(k_p/(k_p+k_s))	Rickard and Pascoe (2009), Sander et al. (2019)
J44000b	TrGJC	LC_4H_9OOH + hν $\rightarrow$ OH + .636 MEK + .636 HO_2 + .364 CH_3CHO + .364 $C_2H_5O_2$	jx(ip_CH3OOH)*(k_s/(k_p+k_s))	Rickard and Pascoe (2009), Sander et al. (2019)
J44001	TrGJC	MVK + hν $\rightarrow$ .5 C_3H_6 + .5 $CH_3C(O)$ + .5 HCHO + CO + .5 HO_2	jx(ip_MVK)	Sander et al. (2014)
J44002	TrGJC	MEK + hν $\rightarrow$ $CH_3C(O)$ + $C_2H_5O_2$	0.42*jx(ip_CHOH)	von Kuhlmann et al. (2003)
J44003	TrGJC	LMEKOOH + hν $\rightarrow$ .62 $CH_3C(O)$ + .62 CH_3CHO + .38 HCHO + .38 CO_2 + .38 $HOCH_2CH_2O_2$ + OH	jx(ip_CH3OOH)+0.42*jx(ip_CHOH)	Sander et al. (2019)
J44004	TrGJC	BIACET + hν $\rightarrow$ 2 $CH_3C(O)$	2.15*jx(ip_MGLYOX)	see note*
J44005a	TrGJCN	LC4H9NO3 + hν $\rightarrow$ NO_2 + C_3H_7CHO + HO_2	j_IC3H7NO3*(k_p/(k_p+k_s))	see note*
J44005b	TrGJCN	LC4H9NO3 + hν $\rightarrow$ NO_2 + MEK + HO_2	j_IC3H7NO3*(k_s/(k_p+k_s))	see note*
J44006	TrGJCN	MPAN + hν $\rightarrow$ .7 MACO3 + .7 NO_2 + .3 MACO2 + .3 NO_3	jx(ip_PAN)	see note*
J44007a	TrGJC	CO2H3CO3H + hν $\rightarrow$ MGLYOX + HO_2 + OH + CO_2	jx(ip_CH3OOH)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44007b	TrGJC	CO2H3CO3H + hν → $CH_3C(O)$ + HO_2 + $HCOCO_3H$	j_ACETOL	Rickard and Pascoe (2009)
J44008	TrGJC	MACR + hν → .5 MACO3 + .5 $CH_3C(O)$ + .5 HCHO + .5 CO + HO_2	jx(ip_MACR)	Sander et al. (2014)
J44009	TrGJC	MACROOH + hν → MACRO + OH	jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)	Sander et al. (2019)*
J44010	TrGJC	MACROH + hν → CH_3COCH_2OH + CO + HO_2 + HO_2	2.77*jx(ip_HOCH2CHO)	see note*
J44011	TrGJC	MACO3H + hν → MACO2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44012	TrGJC	LHMVKABOOH + hν → .12 MGLYOX + .12 HO_2 + .88 $CH_3C(O)$ + .88 $HOCH_2CHO$ + .12 HCHO + OH	jx(ip_CH3OOH)+j_ACETOL	Sander et al. (2019)
J44013	TrGJC	CO2H3CHO + hν → MGLYOX + CO + HO_2 + HO_2	jx(ip_HOCH2CHO)+j_ACETOL	Sander et al. (2019)
J44014	TrGJC	HO12CO3C4 + hν → $CH_3C(O)$ + $HOCH_2CHO$ + HO_2	j_ACETOL	Rickard and Pascoe (2009)
J44015	TrGJC	BIACETOH + hν → $CH_3C(O)$ + HOCH2CO	2.15*jx(ip_MGLYOX)	see note*
J44016	TrGC	$HCOCCH_3CO$ + hν → .5 OH + .5 CH_3CHO + CO + .5 CH3CHCO + .5 CO	j_ketene	Sander et al. (2019)
J44017a	TrGC	$CH_3COCHCO$ + hν → .0192 CH_3COCO_2H + .1848 H_2O_2 + .2208 MGLYOX + .36 OH + .36 CO + .56 $CH_3C(O)$ + .2 CH_3CHO + .2 CO_2 + .2 HCHO + .2 HO_2 + CO	j_ketene*0.5	Sander et al. (2019),Rickard and Pascoe (2009)*
J44017b	TrGC	$CH_3COCHCO$ + hν → CH3CHCO + CO	j_ketene*0.5	Sander et al. (2019)
J44018a	TrGJC	$CH_3COCOCHO$ + hν → $CH_3C(O)$ + 2 CO + HO_2	jx(ip_MGLYOX)	Sander et al. (2019)
J44018b	TrGJC	$CH_3COCOCHO$ + hν → HCOCO + $CH_3C(O)$	2.15*jx(ip_MGLYOX)	Sander et al. (2019)
J44019	TrGJC	CH3COCOCO2H + hν → $CH_3C(O)$ + CO + CO_2 + HO_2	3.15*jx(ip_MGLYOX)	Sander et al. (2019)
J44020a	TrGJTerC	$CH_3COCOCH_2OOH$ + hν → $CH_3C(O)$ + OH + HCHO + CO	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J44020b	TrGJTerC	$CH_3COCOCH_2OOH$ + hν → $CH_3C(O)$ + HCOCO	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44021	TrGJTerC	C44OOH + hν → HCOCH2CHO + CO_2 + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44022	TrGJTerC	C413COOOH + hν → HCOCH2CO3 + HCHO + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)+j_ACETOL	Rickard and Pascoe (2009)
J44023a	TrGJTerC	C4CODIAL + hν → $HCOCOCH_2O_2$ + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44023b	TrGJTerC	C4CODIAL + hν → HCOCH2CO3 + HO_2 + CO	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44024	TrGJTerC	C312COCO3H + hν → $HCOCOCH_2O_2$ + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44025	TrGJCN	LMEKNO3 + hν → .62 $CH_3C(O)$ + .62 CH_3CHO + .38 HCHO + .38 CO_2 + .38 $HOCH_2CH_2O_2$ + NO_2	jx(ip_MEKNO3)	Barnes et al. (1993), Sander et al. (2019)*
J44026	TrGJCN	MVKNO3 + hν → $CH_3C(O)$ + $HOCH_2CHO$ + NO_2	jx(ip_MEKNO3)	Barnes et al. (1993), Sander et al. (2019)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44027	TrGJCN	MACRNO3 + hν $\rightarrow$ CH_3COCH_2OH + CO + HO_2 + NO_2	(2.84*j_IC3H7NO3+jx(ip_CH3CHO)) *(jx(ip_MEKNO3)+1E-10)/(j_ IC3H7NO3+0.42*jx(ip_CHOH)+1E-10)	Müller et al. (2014), Sander et al. (2019)*
J44028	TrGJCN	TC4H9NO3 + hν $\rightarrow$ CH_3COCH_3 + CH_3 + NO_2	2.84*j_IC3H7NO3	Sander et al. (2019)
J44029	TrGJC	TC_4H_9OOH + hν $\rightarrow$ CH_3COCH_3 + CH_3 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44030	TrGJCN	IBUTOLBNO3 + hν $\rightarrow$ CH_3COCH_3 + HCHO + HO_2 + NO_2	2.84*j_IC3H7NO3	Sander et al. (2019)
J44031	TrGJC	IBUTOLBOOH + hν $\rightarrow$ CH_3COCH_3 + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44032	TrGJC	LBUT1ENOOH + hν $\rightarrow$ C_2H_5CHO + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44033	TrGJCN	LBUT1ENNO3 + hν $\rightarrow$ C_2H_5CHO + HCHO + HO_2 + NO_2	j_IC3H7NO3	Sander et al. (2019)
J44034	TrGJC	BUT2OLOOH + hν $\rightarrow$ 2 CH_3CHO + HO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44035	TrGJCN	BUT2OLNO3 + hν $\rightarrow$ 2 CH_3CHO + HO_2 + NO_2	j_IC3H7NO3	Sander et al. (2019)
J44036	TrGJC	BUT2OLO + hν $\rightarrow$ $CH_3C(O)$ + HOCH2CO	j_ACETOL	Sander et al. (2019)
J44037a	TrGJC	C_3H_7CHO + hν $\rightarrow$ $C_3H_7O_2$ + CO + HO_2	jx(ip_C3H7CHO2HCO)	Sander et al. (2019)
J44037b	TrGJC	C_3H_7CHO + hν $\rightarrow$ C_2H_4 + CH_2CHOH	jx(ip_C3H7CHO2VINY)	Sander et al. (2019)*
J44038	TrGJC	IPRCHO + hν $\rightarrow$ $iC_3H_7O_2$ + CO + HO_2	jx(ip_IPRCHO2HCO)	Sander et al. (2019)
J44039	TrGJCN	IC4H9NO3 + hν $\rightarrow$ IPRCHO + NO_2	j_IC3H7NO3	Sander et al. (2019)
J44040	TrGJC	IC_4H_9OOH + hν $\rightarrow$ IPRCHO + HO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44041	TrGJC	PERIBUACID + hν $\rightarrow$ $iC_3H_7O_2$ + CO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J44042	TrGJCN	PIPN + hν $\rightarrow$ .7 IPRCO3 + .7 NO_2 + .3 $iC_3H_7O_2$ + .3 CO_2 + .3 NO_3	jx(ip_PAN)	Sander et al. (2019), Sander et al. (2014)
J44043	TrGJC	HVMK + hν $\rightarrow$ MGLYOX + CO + 2 OH	jx(ip_PeDIONE24)	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	HMAC + hν $\rightarrow$ $HCOCCH_3CO$ + 2 OH	jx(ip_PeDIONE24)	Sander et al. (2019), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	CO2C3CHO + hν $\rightarrow$ $CH_3COCH_2O_2$ + HO_2 + CO	jx(ip_C2H5CHO2HCO)	Rickard and Pascoe (2009)
J44045b	TrGJC	CO2C3CHO + hν $\rightarrow$ HVMK	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Sander et al. (2019)
J44046a	TrGJC	IBUTDIAL + hν $\rightarrow$ CH_3CHO + CO + HO_2 + CO_2 + H_2O	jx(ip_C2H5CHO2HCO)*2.	see note*
J44046b	TrGJC	IBUTDIAL + hν $\rightarrow$ HMAC	jx(ip_C2H5CHO2ENOL)*2.	Andrews et al. (2012), Sander et al. (2019)
J44200	TrGJTerC	IBUTALOH + hν $\rightarrow$ CH_3COCH_3 + HO_2 + HO_2 + CO	j_ACETOL	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44201	TrGJTerC	IPRHOCO3H + hν $\rightarrow$ CH_3COCH_3 + HO_2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44400a	TrGJAroC	MALDIALOOH + hν $\rightarrow$ C32OH13CO + CO + OH + HO_2	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J44400b	TrGJAroC	MALDIALOOH + hν $\rightarrow$ GLYOX + GLYOX + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J44401	TrGJAroC	BZFUOOH + hν $\rightarrow$ CO14O3CHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J44402	TrGJAroC	HOCOC4DIAL + hν $\rightarrow$ HCOCOHCO3 + HO_2 + CO	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44403	TrGJAroCN	NBZFUOOH + hν $\rightarrow$ .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	MALDALCO3H + hν $\rightarrow$ $HCOCO_3H$ + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J44404b	TrGJAroC	MALDALCO3H + hν $\rightarrow$ .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J44405	TrGJAroC	EPXDLCO2H + hν $\rightarrow$ C3DIALO2 + CO_2 + HO_2	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44406	TrGJAroC	MALDIAL + hν $\rightarrow$ .4 BZFUONE + .6 MALDIALCO3 + .6 HO_2	jx(ip_NO2)*0.14	Rickard and Pascoe (2009)
J44407	TrGJAroC	MALANHYOOH + hν $\rightarrow$ HCOCOHCO3 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J44408	TrGJAroC	EPXDLCO3H + hν $\rightarrow$ C3DIALO2 + OH + CO_2	jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J44409	TrGJAroC	CO2C4DIAL + hν $\rightarrow$ CO + CO + HO_2 + HO_2 + CO + CO	jx(ip_MGLYOX)*2.	Rickard and Pascoe (2009)
J44410	TrGJAroC	MALDALCO2H + hν $\rightarrow$ $HCOCO_2H$ + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J44411	TrGJAroC	EPXC4DIAL + hν $\rightarrow$ C3DIALO2 + CO + HO_2	2.77*jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J44412	TrGJAroC	CO14O3CHO + hν $\rightarrow$ HO_2 + CO + $HCOCH_2O_2$ + CO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J44414	TrGJAroC	MECOACEOOH + hν $\rightarrow$ $CH_3C(O)$ + HCHO + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J45002	TrGJC	LISOPACOOH + hν $\rightarrow$ LISOPACO + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45003	TrGJCN	LISOPACNO3 + hν $\rightarrow$ LISOPACO + NO_2	0.59*j_IC3H7NO3	see note*
J45004	TrGJC	ISOPBOOH + hν $\rightarrow$ MVK + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45005	TrGJCN	ISOPBNO3 + hν $\rightarrow$ MVK + HCHO + HO_2 + NO_2	2.84*j_IC3H7NO3	see note*
J45006	TrGJC	ISOPDOOH + hν $\rightarrow$ MACR + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45007	TrGJCN	ISOPDNO3 + hν $\rightarrow$ MACR + HCHO + HO_2 + NO_2	j_IC3H7NO3	see note*
J45008	TrGJCN	NISOPOOH + hν $\rightarrow$ NC4CHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45009	TrGJCN	NC4CHO + hν $\rightarrow$ LHC4ACCO3 + NO_2	(.59*j_IC3H7NO3+jx(ip_MACR))*(jx(ip_MEKNO3)+1E-10)/(j_IC3H7NO3+0.42*jx(ip_CHOH)+1E-10)	Müller et al. (2014), Sander et al. (2019)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45010	TrGJCN	LNISOOH + hν $\rightarrow$ NOA + OH + .5 HOCHCHO + .5 CO + .5 HO_2 + .5 CO_2	`jx(ip_CH3OOH)`	Taraborrelli et al. (2009), Sander et al. (2019)
J45011	TrGJC	LHC4ACCHO + hν $\rightarrow$ .5 LHC4ACCO3 + .5 HO_2 + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2	`jx(ip_MACR)`	Sander et al. (2019)
J45012	TrGJC	LC578OOH + hν $\rightarrow$ .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + OH	`jx(ip_CH3OOH)+ 2.77*jx(ip_HOCH2CHO)`	Sander et al. (2019)
J45013	TrGJC	LHC4ACCO3H + hν $\rightarrow$ OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO_2	`j_HPALD`	Sander et al. (2019)
J45014	TrGJCN	LC5PAN1719 + hν $\rightarrow$ .7 LHC4ACCO3 + .7 NO_2 + .15 MACRO2 + .15 LHMVKABO2 + .3 CO_2 + .3 NO_3	`jx(ip_PAN)`	Sander et al. (2019)
J45015	TrGJC	HCOC5 + hν $\rightarrow$ .65 CH_3 + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + HOCH2CO	`0.5*jx(ip_MVK)`	Sander et al. (2019)*
J45016	TrGJC	C59OOH + hν $\rightarrow$ CH_3COCH_2OH + HOCH2CO + OH	`j_ACETOL+jx(ip_CH3OOH)`	Sander et al. (2019)
J45017	TrGJTerC	C511OOH + hν $\rightarrow$ $CH_3C(O)$ + HCOCH2CHO + OH	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J45018a	TrGJTerC	CO23C4CHO + hν $\rightarrow$ $CH_3COCOCH_2O_2$ + HO_2 + CO	`jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J45018b	TrGJTerC	CO23C4CHO + hν $\rightarrow$ $CH_3C(O)$ + HCOCH2CO3	`2.15*jx(ip_MGLYOX)`	Rickard and Pascoe (2009)
J45019	TrGJTerC	CO23C4CO3H + hν $\rightarrow$ $CH_3COCOCH_2O_2$ + CO_2 + OH	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J45020	TrGJTerC	C512OOH + hν $\rightarrow$ C513O2 + OH	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J45021	TrGJTerC	CO13C4CHO + hν $\rightarrow$ CHOC3COO2 + CO + HO_2	`jx(ip_HOCH2CHO)*2.`	Rickard and Pascoe (2009)
J45022	TrGJTerC	C513OOH + hν $\rightarrow$ GLYOX + $HOC_2H_4CO_3$ + OH	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J45023	TrGJTerC	C513CO + hν $\rightarrow$ $HOC_2H_4CO_3$ + HO_2 + CO + CO	`jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)`	Rickard and Pascoe (2009)
J45024	TrGJTerC	C514OOH + hν $\rightarrow$ CO13C4CHO + HO_2 + OH	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)*2.`	Rickard and Pascoe (2009)
J45025	TrGJTerCN	C514NO3 + hν $\rightarrow$ CO13C4CHO + HO_2 + NO_2	`j_IC3H7NO3+jx(ip_HOCH2CHO)*2.`	Rickard and Pascoe (2009)
J45026a	TrGJC	LZCODC23DBCOOH + hν $\rightarrow$ OH + CO + HVMK + OH	`j_HPALD*0.6*0.5`	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	LZCODC23DBCOOH + hν $\rightarrow$ OH + CO + $CH_3C(O)$ + $HOCH_2CHO$	`j_HPALD*0.6*0.5`	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	LZCODC23DBCOOH + hν $\rightarrow$ OH + CO + HMAC + OH	`j_HPALD*0.4*0.5`	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	LZCODC23DBCOOH + hν $\rightarrow$ OH + CO + CO + CH_3COCH_2OH + HO_2	`j_HPALD*0.4*0.5`	Sander et al. (2019), Jenkin et al. (2015), Peeters et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45027	TrGJC	LZCO3HC23DBCOD + hν $\rightarrow$ .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO_2	j_HPALD	Sander et al. (2019)
J45028a	TrGJC	C1OOHC2OOHC4OD + hν $\rightarrow$ $CH_3COCH_2O_2H$ + OH + 2 CO + HO_2	2.77*jx(ip_HOCH2CHO)	Sander et al. (2019)
J45028b	TrGJC	C1OOHC2OOHC4OD + hν $\rightarrow$ .5 $CH_3COCH_2O_2H$ + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH	2.*jx(ip_CH3OOH)	Sander et al. (2019)
J45029	TrGC	DB1OOH + hν $\rightarrow$ DB1O2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J45030	TrGC	DB2OOH + hν $\rightarrow$ .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J45031a	TrGJC	C1ODC2OOHC4OD + hν $\rightarrow$ MGLYOX + HOCHCHO + OH	jx(ip_CH3OOH)	Sander et al. (2019)
J45031b	TrGJC	C1ODC2OOHC4OD + hν $\rightarrow$ CO2H3CHO + CO + HO_2 + OH	2.*2.77*jx(ip_HOCH2CHO)	Sander et al. (2019)
J45032	TrGJC	C4MDIAL + hν $\rightarrow$ .5 $CH_3COCHCO$ + .5 $HCOCCH_3CO$ + CO + HO_2 + OH	jx(ip_NO2)*0.1*0.5	Sander et al. (2019)*
J45033	TrGCN	DB1NO3 + hν $\rightarrow$ DB1O2 + NO_2	j_IC3H7NO3	Sander et al. (2019)
J45034	TrGJTerC	CHOC3COOOH + hν $\rightarrow$ CHOC3COO2 + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +j_ACETOL	Rickard and Pascoe (2009)
J45200a	TrGJTerC	LMBOABOOH + hν $\rightarrow$ $HOCH_2CHO$ + CH_3COCH_3 + HO_2 + OH	jx(ip_CH3OOH)*.67	Rickard and Pascoe (2009), Sander et al. (2019)
J45200b	TrGJTerC	LMBOABOOH + hν $\rightarrow$ IBUTALOH + HCHO + HO_2 + OH	jx(ip_CH3OOH)*.33	Rickard and Pascoe (2009), Sander et al. (2019)
J45201	TrGJTerC	MBOACO + hν $\rightarrow$ HCHO + HO_2 + IPRHOCO3	j_ACETOL	Rickard and Pascoe (2009)
J45202	TrGJTerC	MBOCOCO + hν $\rightarrow$ CO + HO_2 + IPRHOCO3	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45203a	TrGJTerCN	LNMBOABOOH + hν $\rightarrow$ NO_3CH2CHO + CH_3COCH_3 + HO_2 + OH	jx(ip_CH3OOH)*.65	Rickard and Pascoe (2009), Sander et al. (2019)
J45203b	TrGJTerCN	LNMBOABOOH + hν $\rightarrow$ IBUTALOH + HCHO + NO_2 + OH	jx(ip_CH3OOH)*.35	Rickard and Pascoe (2009), Sander et al. (2019)
J45204	TrGJTerCN	NC4OHCO3H + hν $\rightarrow$ IBUTALOH + CO_2 + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45400	TrGJAroC	C54CO + hν $\rightarrow$ HO_2 + CO + CO + CO + $CH_3C(O)$	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX) *2.	Rickard and Pascoe (2009)
J45401	TrGJAroC	C5134CO2OH + hν $\rightarrow$ $CH_3COCOCHO$ + HO_2 + CO + HO_2	jx(ip_HOCH2CHO)+2.15*jx(ip_ MGLYOX)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45402	TrGJAroC	C5DIALOOH + hν $\rightarrow$ MALDIAL + CO + HO_2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)*
J45406	TrGJAroC	C5CO14OH + hν $\rightarrow$ $CH_3C(O)$ + $HCOCO_2H$ + HO_2 + CO	jx(ip_MVK)	Rickard and Pascoe (2009)
J45407	TrGJAroC	C5DICARB + hν $\rightarrow$ .6 C5CO14O2 + .6 HO_2 + .4 TLFUONE	jx(ip_NO2)*0.2	Rickard and Pascoe (2009)*
J45408	TrGJAroC	MC3ODBCO2H + hν $\rightarrow$ CH_3COCO_2H + HO_2 + CO + HO_2 + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J45409	TrGJAroC	ACCOMECHO + hν $\rightarrow$ MECOACETO2 + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45410	TrGJAroC	MMALNHYOOH + hν $\rightarrow$ CO2H3CO3 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J45411	TrGJAroC	C5DICAROOH + hν $\rightarrow$ MGLYOX + GLYOX + HO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +j_ACETOL	Rickard and Pascoe (2009)*
J45412	TrGJAroCN	NTLFUOOH + hν $\rightarrow$ ACCOMECHO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J45414	TrGJAroC	C5CO14OOH + hν $\rightarrow$ .83 MALANHY + .83 CH_3 + .17 MGLYOX + .17 HO_2 + .17 CO + .17 CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J45415	TrGJAroC	TLFUOOH + hν $\rightarrow$ ACCOMECHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J45417	TrGJAroC	ACCOMECO3H + hν $\rightarrow$ MECOACETO2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J45418	TrGJAroC	C5DIALCO + hν $\rightarrow$ MALDIALCO3 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46200	TrGJTerCN	C614NO3 + hν $\rightarrow$ CO23C4CHO + HCHO + HO_2 + NO_2	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46201	TrGJTerC	C614OOH + hν $\rightarrow$ CO23C4CHO + HCHO + HO_2 + OH	jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46202	TrGJTerC	CO235C5CHO + hν $\rightarrow$ CO23C4CO3 + CO + HO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46203	TrGJTerC	CO235C6OOH + hν $\rightarrow$ CO23C4CO3 + HCHO + OH	jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46400	TrGJAroC	PHENOOH + hν $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46401	TrGJAroC	C6CO4DB + hν $\rightarrow$ C4CO2DBCO3 + HO_2 + CO	jx(ip_MGLYOX)*2.	Rickard and Pascoe (2009)
J46402	TrGJAroC	C5CO2DCO3H + hν $\rightarrow$ $CH_3C(O)$ + HCOCOCHO + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46403	TrGJAroCN	NDNPHENOOH + hν $\rightarrow$ NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	BZBIPERNO3 + hν $\rightarrow$ GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + NO_2	j_IC3H7NO3	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	HOC6H4NO2 + hν $\rightarrow$ HONO + CPDKETENE	jx(ip_HOC6H4NO2)	Chen et al. (2011)*
J46406	TrGJAroC	CPDKETENE + hν $\rightarrow$ CO_2 + CO + 2 HO_2 + MALDIAL	j_ketene	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46407	TrGJAroC	C5COOHCO3H + hν $\rightarrow$ HOCOC4DIAL + HO_2 + CO + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46408	TrGJAroC	BZEPOXMUC + hν $\rightarrow$ .5 C5DIALO2 + 1.5 HO_2 + 1.5 CO + .5 MALDIAL	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)
J46409	TrGJAroCN	NPHEN1OOH + hν $\rightarrow$ NPHEN1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46410	TrGJAroC	BZEMUCCO + hν $\rightarrow$ HCOCOHCO3 + C3DIALO2	jx(ip_HOCH2CHO)*2.+j_ACETOL	Rickard and Pascoe (2009)
J46411	TrGJAroC	BZEMUCCO2H + hν $\rightarrow$ C5DIALO2 + CO_2 + HO_2	jx(ip_MACR)	Rickard and Pascoe (2009)
J46412	TrGJAroCN	NNCATECOOH + hν $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46413	TrGJAroC	C615CO2OOH + hν $\rightarrow$ C5DICARB + CO + HO_2 + OH	jx(ip_MVK)+jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46414	TrGJAroCN	NPHENOOH + hν $\rightarrow$ MALDALCO2H + GLYOX + OH + NO_2	j_IC3H7NO3 + jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46415	TrGJAroCN	NCATECOOH + hν $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46416	TrGJAroC	PBZQOOH + hν $\rightarrow$ C5CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46417	TrGJAroC	BZOBIPEROH + hν $\rightarrow$ MALDIALCO3 + GLYOX + HO_2	j_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	BZBIPEROOH + hν $\rightarrow$ GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	NBZQOOH + hν $\rightarrow$ C6CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46420	TrGJAroC	CATEC1OOH + hν $\rightarrow$ CATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46421	TrGJAroC	C6125CO + hν $\rightarrow$ C5CO14O2 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_MVK)	Rickard and Pascoe (2009)
J46422	TrGJAroCN	DNPHENOOH + hν $\rightarrow$ NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46423	TrGJAroC	BZEMUCCO3H + hν $\rightarrow$ C5DIALO2 + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46424	TrGJAroC	C6H5OOH + hν $\rightarrow$ C6H5O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46425	TrGJAroC	BZEMUCOOH + hν $\rightarrow$ .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)*
J46427	TrGJAroCN	BZEMUCNO3 + hν $\rightarrow$ EPXC4DIAL + NO_2 + GLYOX + HO_2	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J46428	TrGJAroCN	DNPHEN + hν $\rightarrow$ HONO + NCPDKETENE	jx(ip_HOC6H4NO2)	Sander et al. (2019)
J46429	TrGJAroCN	NCPDKETENE + hν $\rightarrow$ CO_2 + CO + 2 HO_2 + NC4DCO2H	j_ketene	see note*
J47200	TrGJTerC	CO235C6CHO + hν $\rightarrow$ CHOC3COCO3 + $CH_3C(O)$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47201	TrGJTerC	C235C6CO3H + hν $\rightarrow$ CO235C6O2 + CO_2 + OH	jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47202	TrGJTerC	C716OOH + hν $\rightarrow$ CO13C4CHO + $CH_3C(O)$ + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J47203	TrGJTerC	C721OOH + hν $\rightarrow$ C722O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47204	TrGJTerC	C722OOH + hν $\rightarrow$ CH_3COCH_3 + C44O2 + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J47400	TrGJAroC	TLEPOXMUC + hν $\rightarrow$ .5 C615CO2O2 + HO_2 + CO + .5 EPXC4DIAL + .5 $CH_3C(O)$	`4.E3*jx(ip_MVK)*0.1`	Rickard and Pascoe (2009)
J47401	TrGJAroC	C6H5CH2OOH + hν $\rightarrow$ BENZAL + HO_2 + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J47402	TrGJAroCN	C6H5CH2NO3 + hν $\rightarrow$ BENZAL + HO_2 + NO_2	`0.59*j_IC3H7NO3`	Rickard and Pascoe (2009)*
J47403	TrGJAroC	BENZAL + hν $\rightarrow$ HO_2 + CO + C6H5O2	`jx(ip_BENZAL)`	Wallington et al. (2018)
J47404	TrGJAroC	TLBIPEROOH + hν $\rightarrow$ .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J47405	TrGJAroCN	TLBIPERNO3 + hν $\rightarrow$ .6 GLYOX + .4 MGLYOX + HO_2 + .2 C4MDIAL + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO_2	`j_IC3H7NO3`	Rickard and Pascoe (2009)*
J47406	TrGJAroC	TLOBIPEROH + hν $\rightarrow$ C5CO14O2 + GLYOX + HO_2	`j_ACETOL`	Rickard and Pascoe (2009)
J47407	TrGJAroC	CRESOOH + hν $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J47408a	TrGJAroCN	NCRESOOH + hν $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH + NO_2	`j_IC3H7NO3`	Rickard and Pascoe (2009)*
J47408b	TrGJAroCN	NCRESOOH + hν $\rightarrow$ C5CO14OH + GLYOX + NO_2 + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	TOL1OHNO2 + hν $\rightarrow$ HONO + MCPDKETENE	`jx(ip_HOPh3Me2NO2)`	see note*
J47410	TrGJAroC	TLEMUCCO2H + hν $\rightarrow$ C615CO2O2 + CO_2 + HO_2	`jx(ip_MACR)`	Rickard and Pascoe (2009)
J47411	TrGJAroC	TLEMUCCO3H + hν $\rightarrow$ C615CO2O2 + CO_2 + OH	`jx(ip_CH3OOH)+jx(ip_MACR)`	Rickard and Pascoe (2009)
J47412	TrGJAroC	TLEMUCOOH + hν $\rightarrow$ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH	`jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)+j_ACETOL`	Rickard and Pascoe (2009)*
J47413	TrGJAroCN	TLEMUCNO3 + hν $\rightarrow$ EPXC4DIAL + NO_2 + $CH_3C(O)$ + CO + HO_2	`2.77*jx(ip_HOCH2CHO)+j_ACETOL`	Rickard and Pascoe (2009)
J47414	TrGJAroC	TLEMUCCO + hν $\rightarrow$ $CH_3C(O)$ + EPXC4DIAL + CO + HO_2	`2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)`	Rickard and Pascoe (2009)
J47415	TrGJAroC	C6H5CO3H + hν $\rightarrow$ C6H5O2 + CO_2 + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J47416	TrGJAroC	OXYL1OOH + hν $\rightarrow$ TOL1O + OH	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J47417	TrGJAroCN	MNCATECH + hν $\rightarrow$ HONO + MCPDKETENE	`jx(ip_HOPh3Me2NO2)`	see note*
J47418	TrGJAroC	MCPDKETENE + hν $\rightarrow$ CO_2 + CO + 2 HO_2 + C4MDIAL	`j_ketene`	see note*
J47419	TrGJAroCN	DNCRES + hν $\rightarrow$ HONO + MNCPDKETENE	`jx(ip_HOPh3Me2NO2)`	see note*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47420	TrGJAroCN	MNCPDKETENE + hν $\rightarrow$ CO_2 + CO + 2 HO_2 + NC4MDCO2HN	j_ketene	see note*
J47421	TrGJAroC	MCATEC1OOH + hν $\rightarrow$ MCATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47422	TrGJAroCN	NPTLQOOH + hν $\rightarrow$ C7CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47423	TrGJAroC	PTLQOOH + hν $\rightarrow$ C6CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47424	TrGJAroCN	NCRES1OOH + hν $\rightarrow$ NCRES1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47425	TrGJAroCN	MNNCATCOOH + hν $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47426	TrGJAroCN	MNCATECOOH + hν $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47427	TrGJAroC	C7CO4DB + hν $\rightarrow$ C5CO2DBCO3 + HO_2 + CO	jx(ip_MGLYOX)*2.	Rickard and Pascoe (2009)
J47428	TrGJAroCN	NDNCRESOOH + hν $\rightarrow$ NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47429	TrGJAroCN	DNCRESOOH + hν $\rightarrow$ NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47430	TrGJAroC	C6COOHCO3H + hν $\rightarrow$ C5134CO2OH + HO_2 + CO + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48200	TrGJTerC	C86OOH + hν $\rightarrow$ C511O2 + CH_3COCH_3 + OH	jx(ip_CH3OOH)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48201	TrGJTerC	C812OOH + hν $\rightarrow$ C813O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48202	TrGJTerC	C813OOH + hν $\rightarrow$ CH_3COCH_3 + C512O2 + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J48203	TrGJTerC	C721CHO + hν $\rightarrow$ C721O2 + CO + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48204	TrGJTerC	C721CO3H + hν $\rightarrow$ C721O2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48205	TrGJTerC	C8BCOOH + hν $\rightarrow$ C89O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48206	TrGJTerC	C89OOH + hν $\rightarrow$ C810O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48207	TrGJTerCN	C89NO3 + hν $\rightarrow$ C810O2 + NO_2	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48208	TrGJTerC	C810OOH + hν $\rightarrow$ CH_3COCH_3 + C514O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48209	TrGJTerCN	C810NO3 + hν $\rightarrow$ CH_3COCH_3 + C514O2 + NO_2	2.84*j_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48210	TrGJTerCN	C8BCNO3 + hν $\rightarrow$ C89O2 + NO_2	j_IC3H7NO3	Rickard and Pascoe (2009)
J48211	TrGJTerC	C85OOH + hν $\rightarrow$ C86O2 + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J48400	TrGJAroC	STYRENOOH + hν $\rightarrow$ HO_2 + HCHO + BENZAL + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J49200	TrGJTerC	C96OOH + hν $\rightarrow$ C97O2 + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J49201	TrGJTerC	C97OOH + hν $\rightarrow$ C98O2 + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J49202	TrGJTerC	C98OOH + hν $\rightarrow$ C614O2 + CH_3COCH_3 + OH	(jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX))	Rickard and Pascoe (2009)
J49203a	TrGJTerC	NORPINAL + hν $\rightarrow$ C85O2 + CO + HO_2	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009), Sander et al. (2019)
J49203b	TrGJTerC	NORPINAL + hν $\rightarrow$ NORPINENOL	jx(ip_PINAL2ENOL)	Sander et al. (2019), Andrews et al. (2012)
J49204	TrGJTerC	C85CO3H + hν $\rightarrow$ C85O2 + CO_2 + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J49205	TrGJTerC	C89CO2H + hν $\rightarrow$ .8 C811CO3 + .2 C89O2 + .2 CO_2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49206	TrGJTerC	C89CO3H + hν $\rightarrow$ .8 C811CO3 + .2 C89O2 + .2 CO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49207	TrGJTerC	C811CO3H + hν $\rightarrow$ C811O2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J49208	TrGJTerC	NOPINDOOH + hν $\rightarrow$ C89CO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40200	TrGJTerC	LAPINABOOH + hν $\rightarrow$ PINAL + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40201	TrGJTerC	MENTHEN6ONE + hν $\rightarrow$ RO6R1O2 + OH	jx(ip_CH3OOH)	Vereecken et al. (2007)
J40202	TrGJTerC	2OHMENTHEN6ONE + hν $\rightarrow$ 10 LCARBON + OH	jx(ip_CH3OOH)	Vereecken et al. (2007)
J40203a	TrGJTerC	PINAL + hν $\rightarrow$ C96O2 + CO + HO_2	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009)
J40203b	TrGJTerC	PINAL + hν $\rightarrow$ PINEOL	jx(ip_PINAL2ENOL)	Sander et al. (2019), Andrews et al. (2012)*
J40204	TrGJTerC	PERPINONIC + hν $\rightarrow$ C96O2 + CO_2 + OH	jx(ip_CH3OOH)+j_ACETOL	Rickard and Pascoe (2009)
J40205	TrGJTerC	PINALOOH + hν $\rightarrow$ C106O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40206	TrGJTerCN	PINALNO3 + hν $\rightarrow$ C106O2 + NO_2	j_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40207	TrGJTerC	C106OOH + hν $\rightarrow$ C716O2 + CH_3COCH_3 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40208	TrGJTerCN	C106NO3 + hν $\rightarrow$ C716O2 + CH_3COCH_3 + NO_2	j_IC3H7NO3+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40209	TrGJTerC	C109OOH + hν $\rightarrow$ C89CO3 + HCHO + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40210	TrGJTerC	C109CO + hν $\rightarrow$ C89CO3 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40211	TrGJTerCN	LNAPINABOOH + hν $\rightarrow$ PINAL + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40212	TrGJTerC	BPINAOOH + hν $\rightarrow$ NOPINONE + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40213	TrGJTerCN	LNBPINABOOH + hν $\rightarrow$ NOPINONE + HCHO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40214	TrGJTerCN	ROO6R1NO3 + hν $\rightarrow$ ROO6R3O2 + CH_3COCH_3 + NO_2	2.84*j_IC3H7NO3+jx(ip_CH3OOH)	Sander et al. (2019)
J40215	TrGJTerCN	RO6R1NO3 + hν $\rightarrow$ 9 LCARBON + HCHO + HO_2 + NO_2	2.84*j_IC3H7NO3	Sander et al. (2019)
J6000	StTrGJCl	Cl_2 + hν $\rightarrow$ Cl + Cl	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	Cl_2O_2 + hν $\rightarrow$ 2 Cl	jx(ip_Cl2O2)	Sander et al. (2014)
J6101	StTrGJCl	OClO + hν $\rightarrow$ ClO + O(^{3}P)	jx(ip_OClO)	Sander et al. (2014)
J6200	StGJCl	HCl + hν $\rightarrow$ Cl + H	jx(ip_HCl)	Sander et al. (2014)
J6201	StTrGJCl	HOCl + hν $\rightarrow$ OH + Cl	jx(ip_HOCl)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6300	TrGJClN	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	jx(ip_ClNO2)	Sander et al. (2014)
J6301a	StTrGJClN	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	jx(ip_ClNO3)	Sander et al. (2014)
J6301b	StTrGJClN	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	jx(ip_ClONO2)	Sander et al. (2014)
J6400	StGJCl	$CH_3Cl + h\nu \rightarrow Cl + CH_3$	jx(ip_CH3Cl)	Sander et al. (2014)
J6401	StGJCl	$CCl_4 + h\nu \rightarrow$ LCARBON + 4 Cl	jx(ip_CCl4)	Sander et al. (2014)
J6402	StGJCCl	$CH_3CCl_3 + h\nu \rightarrow$ 2 LCARBON + 3 Cl	jx(ip_CH3CCl3)	Sander et al. (2014)
J6500	StGJClF	$CFCl_3 + h\nu \rightarrow$ LCARBON + LFLUORINE + 3 Cl	jx(ip_CFCl3)	Sander et al. (2014)*
J6501	StGJClF	$CF_2Cl_2 + h\nu \rightarrow$ LCARBON + 2 LFLUORINE + 2 Cl	jx(ip_CF2Cl2)	Sander et al. (2014)*
J7000	StTrGJBr	$Br_2 + h\nu \rightarrow Br + Br$	jx(ip_Br2)	Sander et al. (2014)
J7100	StTrGJBr	$BrO + h\nu \rightarrow Br + O(^3P)$	jx(ip_BrO)	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_BrNO2)	Sander et al. (2014)
J7301	StTrGJBrN	$BrNO_3 + h\nu \rightarrow .85\ Br + .85\ NO_3 + .15\ BrO + .15\ NO_2$	jx(ip_BrNO3)	Sander et al. (2014)*
J7400	StGJBr	$CH_3Br + h\nu \rightarrow Br + CH_3$	jx(ip_CH3Br)	Sander et al. (2014)
J7401	TrGJBr	$CH_2Br_2 + h\nu \rightarrow$ 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)
J7500	StGJBrF	$CF_3Br + h\nu \rightarrow$ LCARBON + 3 LFLUORINE + Br	jx(ip_CF3Br)	Sander et al. (2014)
J7600	StTrGJBrCl	$BrCl + h\nu \rightarrow Br + Cl$	jx(ip_BrCl)	Sander et al. (2014)
J7601	StGJBrClF	$CF_2ClBr + h\nu \rightarrow$ LCARBON + 2 LFLUORINE + Br + Cl	jx(ip_CF2ClBr)	Sander et al. (2014)
J7602	TrGJBrCl	$CH_2ClBr + h\nu \rightarrow$ LCARBON + Br + Cl	jx(ip_CH2ClBr)	Sander et al. (2014)
J7603	TrGJBrCl	$CHCl_2Br + h\nu \rightarrow$ LCARBON + Br + 2 Cl	jx(ip_CHCl2Br)	Sander et al. (2014)
J7604	TrGJBrCl	$CHClBr_2 + h\nu \rightarrow$ LCARBON + 2 Br + Cl	jx(ip_CHClBr2)	Sander et al. (2014)
J8000	TrGJI	$I_2 + h\nu \rightarrow I + I$	jx(ip_I2)	Sander et al. (2014)
J8100	TrGJI	$IO + h\nu \rightarrow I + O(^3P)$	jx(ip_IO)	Sander et al. (2014)
J8200	TrGJI	$HOI + h\nu \rightarrow I + OH$	jx(ip_HOI)	Sander et al. (2014)
J8300	TrGJIN	$INO_2 + h\nu \rightarrow I + NO_2$	jx(ip_INO2)	Sander et al. (2014)
J8301	TrGJIN	$INO_3 + h\nu \rightarrow I + NO_3$	jx(ip_INO3)	Sander et al. (2014)
J8400	TrGJI	$CH_2I_2 + h\nu \rightarrow 2\ I + 2\ HO_2 + CO$	jx(ip_CH2I2)	Sander et al. (2014)
J8401	TrGJI	$CH_3I + h\nu \rightarrow I + CH_3$	jx(ip_CH3I)	Sander et al. (2014)
J8402	TrGJCI	$CH_3CHICH_3 + h\nu \rightarrow$ 2 LCARBON + I + CH_3	jx(ip_C3H7I)	Sander et al. (2014)
J8403	TrGJClI	$CH_2ClI + h\nu \rightarrow I + Cl + 2\ HO_2 + CO$	jx(ip_CH2ClI)	Sander et al. (2014)
J8600	TrGJClI	$ICl + h\nu \rightarrow I + Cl$	jx(ip_ICl)	Sander et al. (2014)
J8700	TrGJBrI	$IBr + h\nu \rightarrow I + Br$	jx(ip_IBr)	Sander et al. (2014)
PH (aqueous)				

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH2100_a01	TrAa01ScJ	$H_2O_2(aq) + h\nu \rightarrow 2\ OH(aq)$	2.33*xaer(01)*jx(ip_H2O2)	see note*
PH3200_a01	TrAa01JN	$NO_3^-(aq) + h\nu \rightarrow NO_2(aq) + OH(aq) + OH^-(aq)$	xaer(01)*jx(ip_NO2) * 1.4E-4	see note*
PH4100_a01	TrAa01ScJ	$HOCH_2OOH(aq) + h\nu \rightarrow HCOOH(aq) + OH(aq) + HO_2(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	Sander et al. (2014)
PH4101_a01	TrAa01ScJ	$CH_3OOH(aq) + h\nu \rightarrow HCHO(aq) + OH(aq) + HO_2(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	Sander et al. (2014)
PH4200_a01	TrAa01ScJC	$C2H5OOH(aq) + h\nu \rightarrow CH_3CHO(aq) + HO_2(aq) + OH(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	von Kuhlmann (2001)*
PH4201_a01	TrAa01ScJC	$HOOCH2CO2H(aq) + h\nu \rightarrow HCHO(aq) + CO_2(aq) + HO_2(aq) + OH(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
PH4202_a01	TrAa01ScJC	$CH_2OOHCO_2^-(aq) + h\nu \rightarrow CHOHOOCOO_2^-(aq) + OH(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	see note*
PH4203_a01	TrAa01ScJC	$CH_3C(O)OOH(aq) + h\nu \rightarrow CH_3OO(aq) + CO_2(aq) + OH(aq)$	2.33*xaer(01)*jx(ip_CH3CO3H)	Sander et al. (2014)
PH4204_a01	TrAa01ScJC	$HOCH_2CO_3H(aq) + h\nu \rightarrow HCHO(aq) + OH(aq) + HO_2(aq) + CO_2(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	Rickard and Pascoe (2009)
PH4205_a01	TrAa01ScJC	$CH_3CHO(aq) + h\nu \rightarrow CH_3OO(aq) + HO_2(aq) + CO(aq)$	2.33*xaer(01)*jx(ip_CH3CHO)	Sander et al. (2014)
PH4206_a01	TrAa01ScJC	$CH_2OOHCHO(aq) + h\nu \rightarrow OH(aq) + HCHO(aq) + CO(aq) + HO_2(aq)$	2.33*xaer(01)*(jx(ip_CH3OOH) +jx(ip_HOCH2CHO))	Sander et al. (2019)
PH4207a_a01	TrAa01ScJC	$CH_2OHCHO(aq) + h\nu \rightarrow HCHO(aq) + 2\ HO_2(aq) + CO(aq)$	2.33*xaer(01)*jx(ip_HOCH2CHO) *0.83	Sander et al. (2014)*
PH4207b_a01	TrAa01ScJC	$CH_2OHCHO(aq) + h\nu \rightarrow OH(aq) + .6\ HCHO(aq) + .6\ CO(aq) + .6\ HO_2(aq) + .2\ GLYOX(aq) + .2\ CH_2OHCHO(aq)$	2.33*xaer(01)*jx(ip_HOCH2CHO) *0.07	Sander et al. (2014)*
PH4207c_a01	TrAa01ScJC	$CH_2OHCHO(aq) + h\nu \rightarrow CH_3OH(aq) + CO(aq)$	2.33*xaer(01)*jx(ip_HOCH2CHO) *0.10	Sander et al. (2014)*
PH4208_a01	TrAa01ScJC	$CHOCOOH(aq) + h\nu \rightarrow 2\ HO_2(aq) + CO(aq) + CO_2(aq)$	2.33*xaer(01)*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
PH4209_a01	TrAa01ScJC	$GLYOX(aq) + h\nu \rightarrow 2\ CO(aq) + 2\ HO_2(aq)$	2.33*xaer(01)*jx(ip_GLYOX)	Sander et al. (2014)
PH4210a_a01	TrAa01ScJC	$HOOCCOOH(aq) + h\nu \rightarrow CO_2(aq) + HCOOH(aq)$	2.33*xaer(01)*0.72*jx(ip_ HOOCCOOH)	Yamamoto and Back (1985)
PH4210b_a01	TrAa01ScJC	$HOOCCOOH(aq) + h\nu \rightarrow CO_2(aq) + CO(aq) + H_2O(aq)$	2.33*xaer(01)*0.28*jx(ip_ HOOCCOOH)	Yamamoto and Back (1985)
PH4211_a01	TrAa01ScJC	$CHOCHOHOH(aq) + h\nu \rightarrow HCOOH(aq) + 2\ HO_2(aq) + CO(aq)$	2.33*xaer(01)*jx(ip_HOCH2CHO)	Sander et al. (2014)*
PH4300_a01	TrAa01ScJC	$CH_3COCH_2O_2H(aq) + h\nu \rightarrow CH_3COOO(aq) + HCHO(aq) + OH(aq)$	2.33*xaer(01)*(jx(ip_CH3OOH) +0.65*0.11*jx(ip_CHOH))	see note*
PH4301_a01	TrAa01ScJC	$iC_3H_7OOH(aq) + h\nu \rightarrow CH_3COCH_3(aq) + HO_2(aq) + OH(aq)$	2.33*xaer(01)*jx(ip_CH3OOH)	see note*
PH4302_a01	TrAa01ScJC	$CH_3COCH_2OH(aq) + h\nu \rightarrow .5\ OH(aq) + .5\ HCHO(aq) + .5\ CO(aq) + .5\ HCHO(aq) + .5\ HO_2(aq) + .5\ CH_2OHCO3(aq) + .5\ CH_3OO(aq)$	2.33*xaer(01)*0.65*0.11*jx(ip_ CHOH)	Sander et al. (2014)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
PH4303_a01	TrAa01ScJC	$CH_3C(O)CHO(aq) + h\nu \rightarrow OH(aq) + HCHO(aq) + CO(aq) + CO(aq) + HO_2(aq)$	2.33*xaer(01)*jx(ip_MGLYOX)	Sander et al. (2014)*
PH10200_a01	TrAa01JHg	$Hg(OH)_2(aq) + h\nu \rightarrow Hg(aq)$	xaer(01)*6E-5*jx(ip_NO2)	see note*
PH11200_a01	TrAa01JFe	$FeOH^{2+}(aq) + h\nu \rightarrow Fe^{2+}(aq) + OH(aq)$	xaer(01)*4.51E-3*0.312	Herrmann et al. (2000)
PH11201_a01	TrAa01JFe	$Fe(OH)_2^+(aq) + h\nu \rightarrow Fe^{2+}(aq) + OH(aq) + OH^-(aq)$	xaer(01)*5.77E-3*0.255	Herrmann et al. (2000)
PH11800_a01	TrAa01JFeS	$FeSO_4^+(aq) + h\nu \rightarrow Fe^{2+}(aq) + SO_4^-(aq)$	xaer(01)*6.43E-3*7.9E-3	Herrmann et al. (2000)

General notes

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

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:
j(11) → jx(ip_COH2)
j(12) → jx(ip_CHOH)
j(15) → jx(ip_HOCH2CHO)
j(18) → jx(ip_MACR)
j(22) → jx(ip_ACETOL)
j(23)+j(24) → jx(ip_MVK)
j(31)+j(32)+j(33) → jx(ip_GLYOX)
j(34) → jx(ip_MGLYOX)
j(41) → jx(ip_CH3OOH)
j(53) → j(isopropyl nitrate)
j(54) → j(isopropyl nitrate)
j(55) → j(isopropyl nitrate)
j(56)+j(57) → jx(ip_NOA)

Specific notes

J41003: CH_3- and CH_2-channels are considered only and with their branching ratios being 0.42 and 0.48, respectively (Gans et al., 2011). CH-production is neglected. CH_2 is assumed to react only with O2 yielding 1.44 H_2 + 0.18 HCHO + 0.18 $O(^3P)$ + 0.33 OH + 0.33 HO_2 + 0.44 CO_2 + 0.38 CO + 0.05 H_2O as assumed in the WACCM model by J. Orlando (Doug Kinnison, pers. comm. with D. Taraborrelli).

J41006: product distribution as for HNO4

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

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

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

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

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

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

J42020: It is assumed that $j(NO_3CH2CHO)$ is the same as j(PAN).

J42021: In analogy to what is assumed for $CH_3O_2NO_2$ photolysis as in (Sander et al., 2014).

J43002: Following von Kuhlmann et al. (2003), we use $j(CH_3COCH_2OH)$ = 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 $J(iC_3H_7ONO_2)$ = 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 $J(C_3H_7ONO_2) = 0.59 \times J(iC_3H_7ONO_2)$, consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

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

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

J43400: 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 and Pascoe, 2009).

J44005a: It is assumed that J(LC4H9NO3) is the same as $J(iC_3H_7ONO_2)$.

J44005b: It is assumed that J(LC4H9NO3) is the same as $J(iC_3H_7ONO_2)$.

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

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

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

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

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

J44025: J values only for the secondary nitrate.

J44026: Like for LMEKNO3 photolysis

J44027: 2.84*J_IC3H7NO3 like for other tertiary alkyl nitrates (see J4505). Enhancement of J according to Müller et al. (2014).

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

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: KDEC MALDIALO → GLYOX + GLYOX + HO2

J44401: KDEC BZFUO → CO14O3CHO + HO2

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

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

J44407: KDEC MALANHYO → HCOCOHCO3

J44414: KDEC MECOACETO → CH3CO3 + HCHO

J45003: It is assumed that J(LISOPACNO3) = 0.59 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45005: It is assumed that J(ISOPBNO3) = 2.84 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J45007: It is assumed that J(ISOPDNO3) is the same as J($iC_3H_7ONO_2$).

J45009: 0.59*J_IC3H7NO3 like for other primary alkyl nitrates (see J4503). Enhancement of J according to Müller et al. (2014).

J45015: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that J(HCOC5) is half as large as J(MVK). With exeption of HOCH2CO the products of MACO2 decomposition without CO_2.

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

J45402: KDEC C5DIALO → MALDIAL + CO + HO2

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

J45410: KDEC MMALANHYO → CO2H3CO3

J45411: KDEC C5DICARBO → MGLYOX + GLYOX + HO2

J45412: KDEC NTLFUO → ACCOMECHO + NO2

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

J45415: KDEC TLFUO → ACCOMECHO + HO2

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

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

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

J46405: new channel created for nitrophenol decomposition

J46406: new channel created for nitrophenol decomposition

J46412: KDEC NNCATECO → NC4DCO2H + HCOCO2H + NO2

J46415: KDEC NCATECO → NC4DCO2H + HCOCO2H + HO2

J46416: KDEC PBZQO → C5CO2OHCO3

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

J46419: KDEC NBZQO → C6CO4DB + NO2

J46422: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

J46425: KDEC BZEMUCO → 0.5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

J46429: new channel

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

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

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

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

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

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

J47408b: KDEC NCRESO → C5CO14OH + GLYOX + NO2

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

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

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

J47418: new channel

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

J47420: new channel

J47422: KDEC NPTLQO → C7CO4DB + NO2

J47423: KDEC PTLQO → C6CO2OHCO3

J47425: KDEC MNNCATECO → NC4MDCO2H + HCOCO2H + NO2

J47426: KDEC MNCATECO → NC4MDCO2H + HCOCO2H + HO2

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

J47429: KDEC DNCRESO → NC4MDCO2H + HCOCO2H + NO2

J48400: KDEC STYRENO → HO2 + HCHO + BENZAL

J40203b: Substituted vinyl alcohol in analogy to CH_3CHO photolysis.

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

J6501: Even though the elementary reaction probably produces only 1 Cl atom (as for $CFCl_3$), it is assumed here that eventually all Cl atoms are released in secondary reactions.

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

PH2100_a01: 2.33 times the gas-phase value

PH3200_a01: Scaled to $J(NO_2)$ so that its lifetime is about 10.5 days, as suggested by Zellner et al. (1990).

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

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

PH4202_a01: assumed to be the same as C2H5OOH + hv

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

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

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

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

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

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

PH4302_a01: Following von Kuhlmann et al. (2003), we use $j(CH_3COCH_2OH)$ = `0.11*jx(ip_CHOH)`. As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a). CH3CO reacts with O2 to form OH + HCHO + CO. HOCH2CO reacts with O2 to form HOCH2CO3

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

PH10200_a01: Scaled to $J(NO_2)$ so that it produces about 3.0×10^{-7}.

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

#	labels	reaction	rate coefficient	reference
H10000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	k_exf(01,ind_O2)	see general notes*
H10000b_a01	TrAa01Sc	$O_2(aq) \rightarrow O_2$	k_exb(01,ind_O2)	see general notes*
H10001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	k_exf(01,ind_O3)	see general notes*
H10001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	k_exb(01,ind_O3)	see general notes*
H21000f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	k_exf(01,ind_OH)	see general notes*
H21000b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	k_exb(01,ind_OH)	see general notes*
H21001f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	k_exf(01,ind_HO2)	see general notes*
H21001b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	k_exb(01,ind_HO2)	see general notes*
H21002f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	k_exf(01,ind_H2O2)	see general notes*
H21002b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	k_exb(01,ind_H2O2)	see general notes*
H31000f_a01	TrAa01ScN	$NO \rightarrow NO(aq)$	k_exf(01,ind_NO)	see general notes*
H31000b_a01	TrAa01ScN	$NO(aq) \rightarrow NO$	k_exb(01,ind_NO)	see general notes*
H31001f_a01	TrAa01ScN	$NO_2 \rightarrow NO_2(aq)$	k_exf(01,ind_NO2)	see general notes*
H31001b_a01	TrAa01ScN	$NO_2(aq) \rightarrow NO_2$	k_exb(01,ind_NO2)	see general notes*
H31002f_a01	TrAa01ScN	$NO_3 \rightarrow NO_3(aq)$	k_exf(01,ind_NO3)	see general notes*
H31002b_a01	TrAa01ScN	$NO_3(aq) \rightarrow NO_3$	k_exb(01,ind_NO3)	see general notes*
H32000f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(aq)$	k_exf(01,ind_NH3)	see general notes*
H32000b_a01	TrAa01MblScScmN	$NH_3(aq) \rightarrow NH_3$	k_exb(01,ind_NH3)	see general notes*
H32001_a01	TrAa01MblScScmN	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	k_exf_N2O5(01)*C(ind_H2O_a01)	Behnke et al. (1994), Behnke et al. (1997)
H32002f_a01	TrAa01ScN	$HONO \rightarrow HONO(aq)$	k_exf(01,ind_HONO)	see general notes*
H32002b_a01	TrAa01ScN	$HONO(aq) \rightarrow HONO$	k_exb(01,ind_HONO)	see general notes*
H32003f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(aq)$	k_exf(01,ind_HNO3)	see general notes*
H32003b_a01	TrAa01MblScScmN	$HNO_3(aq) \rightarrow HNO_3$	k_exb(01,ind_HNO3)	see general notes*
H32004f_a01	TrAa01ScN	$HNO_4 \rightarrow HNO_4(aq)$	k_exf(01,ind_HNO4)	see general notes*
H32004b_a01	TrAa01ScN	$HNO_4(aq) \rightarrow HNO_4$	k_exb(01,ind_HNO4)	see general notes*
H41000f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	k_exf(01,ind_CO2)	see general notes*
H41000b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	k_exb(01,ind_CO2)	see general notes*
H41001f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	k_exf(01,ind_HCHO)	see general notes*
H41001b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	k_exb(01,ind_HCHO)	see general notes*
H41002f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	k_exf(01,ind_CH3O2)	see general notes*
H41002b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	k_exb(01,ind_CH3O2)	see general notes*
H41003f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	k_exf(01,ind_HCOOH)	see general notes*
H41003b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	k_exb(01,ind_HCOOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H41004f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	k_exf(01,ind_CH3OOH)	see general notes*
H41004b_a01	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	k_exb(01,ind_CH3OOH)	see general notes*
H41005f_a01	TrAa01Sc	$CH_3OH \rightarrow CH_3OH(aq)$	k_exf(01,ind_CH3OH)	see general notes*
H41005b_a01	TrAa01Sc	$CH_3OH(aq) \rightarrow CH_3OH$	k_exb(01,ind_CH3OH)	see general notes*
H41006f_a01	TrAa01Sc	$HOCH_2OH \rightarrow HOCH_2OH(aq)$	k_exf(01,ind_HOCH2OH)	see general notes*
H41006b_a01	TrAa01Sc	$HOCH_2OH(aq) \rightarrow HOCH_2OH$	k_exb(01,ind_HOCH2OH)	see general notes*
H41007f_a01	TrAa01Sc	$HOCH_2OOH \rightarrow HOCH_2OOH(aq)$	k_exf(01,ind_HOCH2OOH)	see general notes*
H41007b_a01	TrAa01Sc	$HOCH_2OOH(aq) \rightarrow HOCH_2OOH$	k_exb(01,ind_HOCH2OOH)	see general notes*
H41008f_a01	TrAa01Sc	$CO \rightarrow CO(aq)$	k_exf(01,ind_CO)	see general notes*
H41008b_a01	TrAa01Sc	$CO(aq) \rightarrow CO$	k_exb(01,ind_CO)	see general notes*
H42000f_a01	TrAa01ScScmC	$CH_3COOH \rightarrow CH_3COOH(aq)$	k_exf(01,ind_CH3CO2H)	see general notes*
H42000b_a01	TrAa01ScScmC	$CH_3COOH(aq) \rightarrow CH_3COOH$	k_exb(01,ind_CH3CO2H)	see general notes*
H42001f_a01	TrAa01ScC	$CH_3CHO \rightarrow CH_3CHO(aq)$	k_exf(01,ind_CH3CHO)	see general notes*
H42001b_a01	TrAa01ScC	$CH_3CHO(aq) \rightarrow CH_3CHO$	k_exb(01,ind_CH3CHO)	see general notes*
H42002f_a01	TrAa01ScCN	$PAN \rightarrow PAN(aq)$	k_exf(01,ind_PAN)	see general notes*
H42002b_a01	TrAa01ScCN	$PAN(aq) \rightarrow PAN$	k_exb(01,ind_PAN)	see general notes*
H42003f_a01	TrAa01ScC	$C_2H_5OH \rightarrow CH_3CH_2OH(aq)$	k_exf(01,ind_C2H5OH)	see general notes*
H42003b_a01	TrAa01ScC	$CH_3CH_2OH(aq) \rightarrow C_2H_5OH$	k_exb(01,ind_C2H5OH)	see general notes*
H42004f_a01	TrAa01ScC	$ETHGLY \rightarrow ETHGLY(aq)$	k_exf(01,ind_ETHGLY)	see general notes*
H42004b_a01	TrAa01ScC	$ETHGLY(aq) \rightarrow ETHGLY$	k_exb(01,ind_ETHGLY)	see general notes*
H42006f_a01	TrAa01ScC	$CH_3C(O)OO \rightarrow CH_3COOO(aq)$	k_exf(01,ind_CH3CO3)	see general notes*
H42006b_a01	TrAa01ScC	$CH_3COOO(aq) \rightarrow CH_3C(O)OO$	k_exb(01,ind_CH3CO3)	see general notes*
H42007f_a01	TrAa01ScC	$HOCH_2CHO \rightarrow CH_2OHCHO(aq)$	k_exf(01,ind_HOCH2CHO)	see general notes*
H42007b_a01	TrAa01ScC	$CH_2OHCHO(aq) \rightarrow HOCH_2CHO$	k_exb(01,ind_HOCH2CHO)	see general notes*
H42008f_a01	TrAa01ScC	$GLYOX \rightarrow GLYOX(aq)$	k_exf(01,ind_GLYOX)	see general notes*
H42008b_a01	TrAa01ScC	$GLYOX(aq) \rightarrow GLYOX$	k_exb(01,ind_GLYOX)	see general notes*
H42009f_a01	TrAa01ScC	$CH_3C(O)OOH \rightarrow CH_3C(O)OOH(aq)$	k_exf(01,ind_CH3CO3H)	see general notes*
H42009b_a01	TrAa01ScC	$CH_3C(O)OOH(aq) \rightarrow CH_3C(O)OOH$	k_exb(01,ind_CH3CO3H)	see general notes*
H42010f_a01	TrAa01ScC	$HOCH_2CO_3H \rightarrow HOCH_2CO_3H(aq)$	k_exf(01,ind_HOCH2CO3H)	see general notes*
H42010b_a01	TrAa01ScC	$HOCH_2CO_3H(aq) \rightarrow HOCH_2CO_3H$	k_exb(01,ind_HOCH2CO3H)	see general notes*
H42011f_a01	TrAa01ScC	$C_2H_5OOH \rightarrow$ C2H5OOH(aq)	k_exf(01,ind_C2H5OOH)	see general notes*
H42011b_a01	TrAa01ScC	C2H5OOH(aq) $\rightarrow C_2H_5OOH$	k_exb(01,ind_C2H5OOH)	see general notes*
H42012f_a01	TrAa01ScC	$HOOCCOOH \rightarrow HOOCCOOH(aq)$	k_exf(01,ind_HOOCCOOH)	see general notes*
H42012b_a01	TrAa01ScC	$HOOCCOOH(aq) \rightarrow HOOCCOOH$	k_exb(01,ind_HOOCCOOH)	see general notes*
H42013f_a01	TrAa01ScC	HOOCH2CO2H $\rightarrow$ HOOCH2CO2H(aq)	k_exf(01,ind_HOOCH2CO2H)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H42013b_a01	TrAa01ScC	HOOCH2CO2H(aq) → HOOCH2CO2H	k_exb(01,ind_HOOCH2CO2H)	see general notes*
H42014f_a01	TrAa01ScC	$HOCH_2CO_2H$ → $HOCH_2CO_2H$(aq)	k_exf(01,ind_HOCH2CO2H)	see general notes*
H42014b_a01	TrAa01ScC	$HOCH_2CO_2H$(aq) → $HOCH_2CO_2H$	k_exb(01,ind_HOCH2CO2H)	see general notes*
H42015f_a01	TrAa01ScC	$HCOCO_2H$ → CHOCOOH(aq)	k_exf(01,ind_HCOCO2H)	see general notes*
H42015b_a01	TrAa01ScC	CHOCOOH(aq) → $HCOCO_2H$	k_exb(01,ind_HCOCO2H)	see general notes*
H42017f_a01	TrAa01ScCN	$C_2H_5ONO_2$ → $C_2H_5ONO_2$(aq)	k_exf(01,ind_C2H5NO3)	see general notes*
H42017b_a01	TrAa01ScCN	$C_2H_5ONO_2$(aq) → $C_2H_5ONO_2$	k_exb(01,ind_C2H5NO3)	see general notes*
H42018f_a01	TrAa01ScCN	CH_3CN → CH_3CN(aq)	k_exf(01,ind_CH3CN)	see general notes*
H42018b_a01	TrAa01ScCN	CH_3CN(aq) → CH_3CN	k_exb(01,ind_CH3CN)	see general notes*
H42019f_a01	TrAa01ScC	$HOCH_2CHOHOH$ → $CH_2OHCHOHOH$(aq)	k_exf(01,ind_HOCH2CHOHOH)	see general notes*
H42019b_a01	TrAa01ScC	$CH_2OHCHOHOH$(aq) → $HOCH_2CHOHOH$	k_exb(01,ind_HOCH2CHOHOH)	see general notes*
H42020f_a01	TrAa01ScC	$CH_3CHOHOH$ → $CH_3CHOHOH$(aq)	k_exf(01,ind_CH3CHOHOH)	see general notes*
H42020b_a01	TrAa01ScC	$CH_3CHOHOH$(aq) → $CH_3CHOHOH$	k_exb(01,ind_CH3CHOHOH)	see general notes*
H42021f_a01	TrAa01ScC	CHOHOHCOOH → CHOOHOHCOOH(aq)	k_exf(01,ind_CHOHOHCOOH)	see general notes*
H42021b_a01	TrAa01ScC	CHOOHOHCOOH(aq) → CHOHOHCOOH	k_exb(01,ind_CHOHOHCOOH)	see general notes*
H42022f_a01	TrAa01ScC	CHOHOHCHOHOH → CHOHOHCHOHOH(aq)	k_exf(01,ind_CHOHOHCHOHOH)	see general notes*
H42022b_a01	TrAa01ScC	CHOHOHCHOHOH(aq) → CHOHOHCHOHOH	k_exb(01,ind_CHOHOHCHOHOH)	see general notes*
H42023f_a01	TrAa01ScC	HOOCH2CHO → $CH_2OOHCHO$(aq)	k_exf(01,ind_HOOCH2CHO)	see general notes*
H42023b_a01	TrAa01ScC	$CH_2OOHCHO$(aq) → HOOCH2CHO	k_exb(01,ind_HOOCH2CHO)	see general notes*
H42024f_a01	TrAa01ScC	CHOCHOHOH → CHOCHOHOH(aq)	k_exf(01,ind_CHOCHOHOH)	see general notes*
H42024b_a01	TrAa01ScC	CHOCHOHOH(aq) → CHOCHOHOH	k_exb(01,ind_CHOCHOHOH)	see general notes*
H42025f_a01	TrAa01ScC	$HOOCH_2CHOHOH$ → $HOOCH_2CHOHOH$(aq)	k_exf(01,ind_HOOCH2CHOHOH)	see general notes*
H42025b_a01	TrAa01ScC	$HOOCH_2CHOHOH$(aq) → $HOOCH_2CHOHOH$	k_exb(01,ind_HOOCH2CHOHOH)	see general notes*
H42026f_a01	TrAa01ScC	CH2CO → CH2CO(aq)	k_exf(01,ind_CH2CO)	see general notes*
H42026b_a01	TrAa01ScC	CH2CO(aq) → CH2CO	k_exb(01,ind_CH2CO)	see general notes*
H42027f_a01	TrAa01ScC	CH3CHOHOOH → CH3CHOHOOH(aq)	k_exf(01,ind_CH3CHOHOOH)	see general notes*
H42027b_a01	TrAa01ScC	CH3CHOHOOH(aq) → CH3CHOHOOH	k_exb(01,ind_CH3CHOHOOH)	see general notes*
H42028f_a01	TrAa01ScCN	ETHOHNO3 → ETHOHNO3(aq)	k_exf(01,ind_ETHOHNO3)	see general notes*
H42028b_a01	TrAa01ScCN	ETHOHNO3(aq) → ETHOHNO3	k_exb(01,ind_ETHOHNO3)	see general notes*
H42029f_a01	TrAa01ScC	$HCOCO_3H$ → $HCOCO_3H$(aq)	k_exf(01,ind_HCOCO3H)	see general notes*
H42029b_a01	TrAa01ScC	$HCOCO_3H$(aq) → $HCOCO_3H$	k_exb(01,ind_HCOCO3H)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H42030f_a01	TrAa01ScC	HOOCH2CO3H → HOOCH2CO3H(aq)	`k_exf(01,ind_HOOCH2CO3H)`	see general notes*
H42030b_a01	TrAa01ScC	HOOCH2CO3H(aq) → HOOCH2CO3H	`k_exb(01,ind_HOOCH2CO3H)`	see general notes*
H42031f_a01	TrAa01ScC	HYETHO2H → HYETHO2H(aq)	`k_exf(01,ind_HYETHO2H)`	see general notes*
H42031b_a01	TrAa01ScC	HYETHO2H(aq) → HYETHO2H	`k_exb(01,ind_HYETHO2H)`	see general notes*
H42032f_a01	TrAa01ScCN	PHAN → PHAN(aq)	`k_exf(01,ind_PHAN)`	see general notes*
H42032b_a01	TrAa01ScCN	PHAN(aq) → PHAN	`k_exb(01,ind_PHAN)`	see general notes*
H43000f_a01	TrAa01ScC	CH_3COCH_3 → CH_3COCH_3(aq)	`k_exf(01,ind_CH3COCH3)`	see general notes*
H43000b_a01	TrAa01ScC	CH_3COCH_3(aq) → CH_3COCH_3	`k_exb(01,ind_CH3COCH3)`	see general notes*
H43001f_a01	TrAa01ScC	MGLYOX → $CH_3C(O)CHO$(aq)	`k_exf(01,ind_MGLYOX)`	see general notes*
H43001b_a01	TrAa01ScC	$CH_3C(O)CHO$(aq) → MGLYOX	`k_exb(01,ind_MGLYOX)`	see general notes*
H43002f_a01	TrAa01ScC	CH_3COCO_2H → $CH_3COCOOH$(aq)	`k_exf(01,ind_CH3COCO2H)`	see general notes*
H43002b_a01	TrAa01ScC	$CH_3COCOOH$(aq) → CH_3COCO_2H	`k_exb(01,ind_CH3COCO2H)`	see general notes*
H43003f_a01	TrAa01ScC	$CH_3COCHOHOH$ → $CH_3COCHOHOH$(aq)	`k_exf(01,ind_CH3COCHOHOH)`	see general notes*
H43003b_a01	TrAa01ScC	$CH_3COCHOHOH$(aq) → $CH_3COCHOHOH$	`k_exb(01,ind_CH3COCHOHOH)`	see general notes*
H43005f_a01	TrAa01ScC	IPROPOL → IPROPOL(aq)	`k_exf(01,ind_IPROPOL)`	see general notes*
H43005b_a01	TrAa01ScC	IPROPOL(aq) → IPROPOL	`k_exb(01,ind_IPROPOL)`	see general notes*
H43006f_a01	TrAa01ScC	$CH_3COCH_2O_2H$ → $CH_3COCH_2O_2H$(aq)	`k_exf(01,ind_HYPERACET)`	see general notes*
H43006b_a01	TrAa01ScC	$CH_3COCH_2O_2H$(aq) → $CH_3COCH_2O_2H$	`k_exb(01,ind_HYPERACET)`	see general notes*
H43007f_a01	TrAa01ScC	iC_3H_7OOH → iC_3H_7OOH(aq)	`k_exf(01,ind_IC3H7OOH)`	see general notes*
H43007b_a01	TrAa01ScC	iC_3H_7OOH(aq) → iC_3H_7OOH	`k_exb(01,ind_IC3H7OOH)`	see general notes*
H43008f_a01	TrAa01ScC	$HCOCOCH_2OOH$ → $HCOCOCH_2OOH$(aq)	`k_exf(01,ind_ALCOCH2OOH)`	see general notes*
H43008b_a01	TrAa01ScC	$HCOCOCH_2OOH$(aq) → $HCOCOCH_2OOH$	`k_exb(01,ind_ALCOCH2OOH)`	see general notes*
H43009f_a01	TrAa01ScC	C32OH13CO → C32OH13CO(aq)	`k_exf(01,ind_C32OH13CO)`	see general notes*
H43009b_a01	TrAa01ScC	C32OH13CO(aq) → C32OH13CO	`k_exb(01,ind_C32OH13CO)`	see general notes*
H43010f_a01	TrAa01ScC	HCOCOCHO → HCOCOCHO(aq)	`k_exf(01,ind_C33CO)`	see general notes*
H43010b_a01	TrAa01ScC	HCOCOCHO(aq) → HCOCOCHO	`k_exb(01,ind_C33CO)`	see general notes*
H43011f_a01	TrAa01ScC	C3DIALOOH → C3DIALOOH(aq)	`k_exf(01,ind_C3DIALOOH)`	see general notes*
H43011b_a01	TrAa01ScC	C3DIALOOH(aq) → C3DIALOOH	`k_exb(01,ind_C3DIALOOH)`	see general notes*
H43012f_a01	TrAa01ScCN	C_3PAN1 → C_3PAN1(aq)	`k_exf(01,ind_C3PAN1)`	see general notes*
H43012b_a01	TrAa01ScCN	C_3PAN1(aq) → C_3PAN1	`k_exb(01,ind_C3PAN1)`	see general notes*
H43013f_a01	TrAa01ScCN	C_3PAN2 → C_3PAN2(aq)	`k_exf(01,ind_C3PAN2)`	see general notes*
H43013b_a01	TrAa01ScCN	C_3PAN2(aq) → C_3PAN2	`k_exb(01,ind_C3PAN2)`	see general notes*
H43014f_a01	TrAa01ScC	CH3CHCO → CH3CHCO(aq)	`k_exf(01,ind_CH3CHCO)`	see general notes*
H43014b_a01	TrAa01ScC	CH3CHCO(aq) → CH3CHCO	`k_exb(01,ind_CH3CHCO)`	see general notes*

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

#	labels	reaction	rate coefficient	reference
H43015f_a01	TrAa01ScCN	$CH_3COCH_2OONO_2 \rightarrow CH_3COCH_2OONO_2(aq)$	k_exf(01,ind_CH3COCH2O2NO2)	see general notes*
H43015b_a01	TrAa01ScCN	$CH_3COCH_2OONO_2(aq) \rightarrow CH_3COCH_2OONO_2$	k_exb(01,ind_CH3COCH2O2NO2)	see general notes*
H43016f_a01	TrAa01ScC	$CH_3COCO_3H \rightarrow CH_3COCO_3H(aq)$	k_exf(01,ind_CH3COCO3H)	see general notes*
H43016b_a01	TrAa01ScC	$CH_3COCO_3H(aq) \rightarrow CH_3COCO_3H$	k_exb(01,ind_CH3COCO3H)	see general notes*
H43017f_a01	TrAa01ScC	HCOCH2CHO → HCOCH2CHO(aq)	k_exf(01,ind_HCOCH2CHO)	see general notes*
H43017b_a01	TrAa01ScC	HCOCH2CHO(aq) → HCOCH2CHO	k_exb(01,ind_HCOCH2CHO)	see general notes*
H43018f_a01	TrAa01ScC	HCOCH2CO2H → HCOCH2CO2H(aq)	k_exf(01,ind_HCOCH2CO2H)	see general notes*
H43018b_a01	TrAa01ScC	HCOCH2CO2H(aq) → HCOCH2CO2H	k_exb(01,ind_HCOCH2CO2H)	see general notes*
H43019f_a01	TrAa01ScC	HCOCH2CO3H → HCOCH2CO3H(aq)	k_exf(01,ind_HCOCH2CO3H)	see general notes*
H43019b_a01	TrAa01ScC	HCOCH2CO3H(aq) → HCOCH2CO3H	k_exb(01,ind_HCOCH2CO3H)	see general notes*
H43020f_a01	TrAa01ScC	$HCOCOCH_2OOH \rightarrow HCOCOCH_2OOH(aq)$	k_exf(01,ind_HCOCOCH2OOH)	see general notes*
H43020b_a01	TrAa01ScC	$HCOCOCH_2OOH(aq) \rightarrow HCOCOCH_2OOH$	k_exb(01,ind_HCOCOCH2OOH)	see general notes*
H43021f_a01	TrAa01ScC	HCOCOHCO3H → HCOCOHCO3H(aq)	k_exf(01,ind_HCOCOHCO3H)	see general notes*
H43021b_a01	TrAa01ScC	HCOCOHCO3H(aq) → HCOCOHCO3H	k_exb(01,ind_HCOCOHCO3H)	see general notes*
H43022f_a01	TrAa01ScCN	HCOCOHPAN → HCOCOHPAN(aq)	k_exf(01,ind_HCOCOHPAN)	see general notes*
H43022b_a01	TrAa01ScCN	HCOCOHPAN(aq) → HCOCOHPAN	k_exb(01,ind_HCOCOHPAN)	see general notes*
H43023f_a01	TrAa01ScC	HOC2H4CO2H → HOC2H4CO2H(aq)	k_exf(01,ind_HOC2H4CO2H)	see general notes*
H43023b_a01	TrAa01ScC	HOC2H4CO2H(aq) → HOC2H4CO2H	k_exb(01,ind_HOC2H4CO2H)	see general notes*
H43024f_a01	TrAa01ScC	HOC2H4CO3H → HOC2H4CO3H(aq)	k_exf(01,ind_HOC2H4CO3H)	see general notes*
H43024b_a01	TrAa01ScC	HOC2H4CO3H(aq) → HOC2H4CO3H	k_exb(01,ind_HOC2H4CO3H)	see general notes*
H43025f_a01	TrAa01ScC	HOCH2COCH2OOH → HOCH2COCH2OOH(aq)	k_exf(01,ind_HOCH2COCH2OOH)	see general notes*
H43025b_a01	TrAa01ScC	HOCH2COCH2OOH(aq) → HOCH2COCH2OOH	k_exb(01,ind_HOCH2COCH2OOH)	see general notes*
H43026f_a01	TrAa01ScC	HOCH2COCHO → HOCH2COCHO(aq)	k_exf(01,ind_HOCH2COCHO)	see general notes*
H43026b_a01	TrAa01ScC	HOCH2COCHO(aq) → HOCH2COCHO	k_exb(01,ind_HOCH2COCHO)	see general notes*
H43027f_a01	TrAa01ScC	HYPROPO2H → HYPROPO2H(aq)	k_exf(01,ind_HYPROPO2H)	see general notes*
H43027b_a01	TrAa01ScC	HYPROPO2H(aq) → HYPROPO2H	k_exb(01,ind_HYPROPO2H)	see general notes*
H43028f_a01	TrAa01ScC	METACETHO → METACETHO(aq)	k_exf(01,ind_METACETHO)	see general notes*
H43028b_a01	TrAa01ScC	METACETHO(aq) → METACETHO	k_exb(01,ind_METACETHO)	see general notes*
H43029f_a01	TrAa01ScCN	NOA → NOA(aq)	k_exf(01,ind_NOA)	see general notes*
H43029b_a01	TrAa01ScCN	NOA(aq) → NOA	k_exb(01,ind_NOA)	see general notes*
H43030f_a01	TrAa01ScCN	PR2O2HNO3 → PR2O2HNO3(aq)	k_exf(01,ind_PR2O2HNO3)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H43030b_a01	TrAa01ScCN	PR2O2HNO3(aq) → PR2O2HNO3	k_exb(01,ind_PR2O2HNO3)	see general notes*
H43031f_a01	TrAa01ScCN	PROPOLNO3 → PROPOLNO3(aq)	k_exf(01,ind_PROPOLNO3)	see general notes*
H43031b_a01	TrAa01ScCN	PROPOLNO3(aq) → PROPOLNO3	k_exb(01,ind_PROPOLNO3)	see general notes*
H43032f_a01	TrAa01ScC	CH_3COCH_2OH → CH_3COCH_2OH(aq)	k_exf(01,ind_ACETOL)	see general notes*
H43032b_a01	TrAa01ScC	CH_3COCH_2OH(aq) → CH_3COCH_2OH	k_exb(01,ind_ACETOL)	see general notes*
H44000f_a01	TrAa01ScC	MACR → MACR(aq)	k_exf(01,ind_MACR)	see general notes*
H44000b_a01	TrAa01ScC	MACR(aq) → MACR	k_exb(01,ind_MACR)	see general notes*
H44001f_a01	TrAa01ScC	MVK → MVK(aq)	k_exf(01,ind_MVK)	see general notes*
H44001b_a01	TrAa01ScC	MVK(aq) → MVK	k_exb(01,ind_MVK)	see general notes*
H44002f_a01	TrAa01ScC	$CH_3COCOCH_2O_2$ → $CH_3COCOCH_2O_2$(aq)	k_exf(01,ind_BIACETO2)	see general notes*
H44002b_a01	TrAa01ScC	$CH_3COCOCH_2O_2$(aq) → $CH_3COCOCH_2O_2$	k_exb(01,ind_BIACETO2)	see general notes*
H44003f_a01	TrAa01ScC	BIACETOH → BIACETOH(aq)	k_exf(01,ind_BIACETOH)	see general notes*
H44003b_a01	TrAa01ScC	BIACETOH(aq) → BIACETOH	k_exb(01,ind_BIACETOH)	see general notes*
H44004f_a01	TrAa01ScC	$CH_3COCOCH_2OOH$ → $CH_3COCOCH_2OOH$(aq)	k_exf(01,ind_BIACETOOH)	see general notes*
H44004b_a01	TrAa01ScC	$CH_3COCOCH_2OOH$(aq) → $CH_3COCOCH_2OOH$	k_exb(01,ind_BIACETOOH)	see general notes*
H44005f_a01	TrAa01ScC	BUT2OLO → BUT2OLO(aq)	k_exf(01,ind_BUT2OLO)	see general notes*
H44005b_a01	TrAa01ScC	BUT2OLO(aq) → BUT2OLO	k_exb(01,ind_BUT2OLO)	see general notes*
H44006f_a01	TrAa01ScC	BUT2OLOOH → BUT2OLOOH(aq)	k_exf(01,ind_BUT2OLOOH)	see general notes*
H44006b_a01	TrAa01ScC	BUT2OLOOH(aq) → BUT2OLOOH	k_exb(01,ind_BUT2OLOOH)	see general notes*
H44007f_a01	TrAa01ScC	BZFUCO → BZFUCO(aq)	k_exf(01,ind_BZFUCO)	see general notes*
H44007b_a01	TrAa01ScC	BZFUCO(aq) → BZFUCO	k_exb(01,ind_BZFUCO)	see general notes*
H44008f_a01	TrAa01ScC	BZFUOOH → BZFUOOH(aq)	k_exf(01,ind_BZFUOOH)	see general notes*
H44008b_a01	TrAa01ScC	BZFUOOH(aq) → BZFUOOH	k_exb(01,ind_BZFUOOH)	see general notes*
H44009f_a01	TrAa01ScC	C312COCO3H → C312COCO3H(aq)	k_exf(01,ind_C312COCO3H)	see general notes*
H44009b_a01	TrAa01ScC	C312COCO3H(aq) → C312COCO3H	k_exb(01,ind_C312COCO3H)	see general notes*
H44010f_a01	TrAa01ScCN	C312COPAN → C312COPAN(aq)	k_exf(01,ind_C312COPAN)	see general notes*
H44010b_a01	TrAa01ScCN	C312COPAN(aq) → C312COPAN	k_exb(01,ind_C312COPAN)	see general notes*
H44011f_a01	TrAa01ScC	C413COOOH → C413COOOH(aq)	k_exf(01,ind_C413COOOH)	see general notes*
H44011b_a01	TrAa01ScC	C413COOOH(aq) → C413COOOH	k_exb(01,ind_C413COOOH)	see general notes*
H44012f_a01	TrAa01ScC	C44OOH → C44OOH(aq)	k_exf(01,ind_C44OOH)	see general notes*
H44012b_a01	TrAa01ScC	C44OOH(aq) → C44OOH	k_exb(01,ind_C44OOH)	see general notes*
H44013f_a01	TrAa01ScC	C4CODIAL → C4CODIAL(aq)	k_exf(01,ind_C4CODIAL)	see general notes*
H44013b_a01	TrAa01ScC	C4CODIAL(aq) → C4CODIAL	k_exb(01,ind_C4CODIAL)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H44014f_a01	TrAa01ScCN	C4PAN5 → C4PAN5(aq)	k_exf(01,ind_C4PAN5)	see general notes*
H44014b_a01	TrAa01ScCN	C4PAN5(aq) → C4PAN5	k_exb(01,ind_C4PAN5)	see general notes*
H44015f_a01	TrAa01ScC	$CH_3COCHCO$ → $CH_3COCHCO(aq)$	k_exf(01,ind_CH3COCHCO)	see general notes*
H44015b_a01	TrAa01ScC	$CH_3COCHCO(aq)$ → $CH_3COCHCO$	k_exb(01,ind_CH3COCHCO)	see general notes*
H44016f_a01	TrAa01ScC	CH3COCOCO2H → CH3COCOCO2H(aq)	k_exf(01,ind_CH3COCOCO2H)	see general notes*
H44016b_a01	TrAa01ScC	CH3COCOCO2H(aq) → CH3COCOCO2H	k_exb(01,ind_CH3COCOCO2H)	see general notes*
H44017f_a01	TrAa01ScC	$CH_3COOHCHCHO$ → $CH_3COOHCHCHO(aq)$	k_exf(01,ind_CH3COOHCHCHO)	see general notes*
H44017b_a01	TrAa01ScC	$CH_3COOHCHCHO(aq)$ → $CH_3COOHCHCHO$	k_exb(01,ind_CH3COOHCHCHO)	see general notes*
H44018f_a01	TrAa01ScC	CHOC3COO2 → CHOC3COO2(aq)	k_exf(01,ind_CHOC3COO2)	see general notes*
H44018b_a01	TrAa01ScC	CHOC3COO2(aq) → CHOC3COO2	k_exb(01,ind_CHOC3COO2)	see general notes*
H44019f_a01	TrAa01ScC	CO14O3CHO → CO14O3CHO(aq)	k_exf(01,ind_CO14O3CHO)	see general notes*
H44019b_a01	TrAa01ScC	CO14O3CHO(aq) → CO14O3CHO	k_exb(01,ind_CO14O3CHO)	see general notes*
H44020f_a01	TrAa01ScC	CO14O3CO2H → CO14O3CO2H(aq)	k_exf(01,ind_CO14O3CO2H)	see general notes*
H44020b_a01	TrAa01ScC	CO14O3CO2H(aq) → CO14O3CO2H	k_exb(01,ind_CO14O3CO2H)	see general notes*
H44021f_a01	TrAa01ScC	$CH_3COCOCHO$ → $CH_3COCOCHO(aq)$	k_exf(01,ind_CO23C3CHO)	see general notes*
H44021b_a01	TrAa01ScC	$CH_3COCOCHO(aq)$ → $CH_3COCOCHO$	k_exb(01,ind_CO23C3CHO)	see general notes*
H44022f_a01	TrAa01ScC	CO2C3CHO → CO2C3CHO(aq)	k_exf(01,ind_CO2C3CHO)	see general notes*
H44022b_a01	TrAa01ScC	CO2C3CHO(aq) → CO2C3CHO	k_exb(01,ind_CO2C3CHO)	see general notes*
H44023f_a01	TrAa01ScC	CO2C4DIAL → CO2C4DIAL(aq)	k_exf(01,ind_CO2C4DIAL)	see general notes*
H44023b_a01	TrAa01ScC	CO2C4DIAL(aq) → CO2C4DIAL	k_exb(01,ind_CO2C4DIAL)	see general notes*
H44024f_a01	TrAa01ScC	CO2H3CHO → CO2H3CHO(aq)	k_exf(01,ind_CO2H3CHO)	see general notes*
H44024b_a01	TrAa01ScC	CO2H3CHO(aq) → CO2H3CHO	k_exb(01,ind_CO2H3CHO)	see general notes*
H44025f_a01	TrAa01ScC	CO2H3CO2H → CO2H3CO2H(aq)	k_exf(01,ind_CO2H3CO2H)	see general notes*
H44025b_a01	TrAa01ScC	CO2H3CO2H(aq) → CO2H3CO2H	k_exb(01,ind_CO2H3CO2H)	see general notes*
H44026f_a01	TrAa01ScC	CO2H3CO3H → CO2H3CO3H(aq)	k_exf(01,ind_CO2H3CO3H)	see general notes*
H44026b_a01	TrAa01ScC	CO2H3CO3H(aq) → CO2H3CO3H	k_exb(01,ind_CO2H3CO3H)	see general notes*
H44027f_a01	TrAa01ScC	EPXC4DIAL → EPXC4DIAL(aq)	k_exf(01,ind_EPXC4DIAL)	see general notes*
H44027b_a01	TrAa01ScC	EPXC4DIAL(aq) → EPXC4DIAL	k_exb(01,ind_EPXC4DIAL)	see general notes*
H44028f_a01	TrAa01ScC	EPXDLCO2H → EPXDLCO2H(aq)	k_exf(01,ind_EPXDLCO2H)	see general notes*
H44028b_a01	TrAa01ScC	EPXDLCO2H(aq) → EPXDLCO2H	k_exb(01,ind_EPXDLCO2H)	see general notes*
H44029f_a01	TrAa01ScC	EPXDLCO3H → EPXDLCO3H(aq)	k_exf(01,ind_EPXDLCO3H)	see general notes*
H44029b_a01	TrAa01ScC	EPXDLCO3H(aq) → EPXDLCO3H	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	$HCOCCH_3CHOOH \rightarrow HCOCCH_3CHOOH(aq)$	k_exf(01,ind_HCOCCH3CHOOH)	see general notes*
H44030b_a01	TrAa01ScC	$HCOCCH_3CHOOH(aq) \rightarrow HCOCCH_3CHOOH$	k_exb(01,ind_HCOCCH3CHOOH)	see general notes*
H44031f_a01	TrAa01ScC	$HCOCCH_3CO \rightarrow HCOCCH_3CO(aq)$	k_exf(01,ind_HCOCCH3CO)	see general notes*
H44031b_a01	TrAa01ScC	$HCOCCH_3CO(aq) \rightarrow HCOCCH_3CO$	k_exb(01,ind_HCOCCH3CO)	see general notes*
H44032f_a01	TrAa01ScC	HMAC → HMAC(aq)	k_exf(01,ind_HMAC)	see general notes*
H44032b_a01	TrAa01ScC	HMAC(aq) → HMAC	k_exb(01,ind_HMAC)	see general notes*
H44033f_a01	TrAa01ScC	HO12CO3C4 → HO12CO3C4(aq)	k_exf(01,ind_HO12CO3C4)	see general notes*
H44033b_a01	TrAa01ScC	HO12CO3C4(aq) → HO12CO3C4	k_exb(01,ind_HO12CO3C4)	see general notes*
H44034f_a01	TrAa01ScC	HOCOC4DIAL → HOCOC4DIAL(aq)	k_exf(01,ind_HOCOC4DIAL)	see general notes*
H44034b_a01	TrAa01ScC	HOCOC4DIAL(aq) → HOCOC4DIAL	k_exb(01,ind_HOCOC4DIAL)	see general notes*
H44035f_a01	TrAa01ScC	HVMK → HVMK(aq)	k_exf(01,ind_HVMK)	see general notes*
H44035b_a01	TrAa01ScC	HVMK(aq) → HVMK	k_exb(01,ind_HVMK)	see general notes*
H44036f_a01	TrAa01ScC	IBUTALOH → IBUTALOH(aq)	k_exf(01,ind_IBUTALOH)	see general notes*
H44036b_a01	TrAa01ScC	IBUTALOH(aq) → IBUTALOH	k_exb(01,ind_IBUTALOH)	see general notes*
H44037f_a01	TrAa01ScC	IBUTDIAL → IBUTDIAL(aq)	k_exf(01,ind_IBUTDIAL)	see general notes*
H44037b_a01	TrAa01ScC	IBUTDIAL(aq) → IBUTDIAL	k_exb(01,ind_IBUTDIAL)	see general notes*
H44038f_a01	TrAa01ScC	IBUTOLBOOH → IBUTOLBOOH(aq)	k_exf(01,ind_IBUTOLBOOH)	see general notes*
H44038b_a01	TrAa01ScC	IBUTOLBOOH(aq) → IBUTOLBOOH	k_exb(01,ind_IBUTOLBOOH)	see general notes*
H44039f_a01	TrAa01ScC	IPRHOCO2H → IPRHOCO2H(aq)	k_exf(01,ind_IPRHOCO2H)	see general notes*
H44039b_a01	TrAa01ScC	IPRHOCO2H(aq) → IPRHOCO2H	k_exb(01,ind_IPRHOCO2H)	see general notes*
H44040f_a01	TrAa01ScC	IPRHOCO3H → IPRHOCO3H(aq)	k_exf(01,ind_IPRHOCO3H)	see general notes*
H44040b_a01	TrAa01ScC	IPRHOCO3H(aq) → IPRHOCO3H	k_exb(01,ind_IPRHOCO3H)	see general notes*
H44041f_a01	TrAa01ScC	LBUT1ENOOH → LBUT1ENOOH(aq)	k_exf(01,ind_LBUT1ENOOH)	see general notes*
H44041b_a01	TrAa01ScC	LBUT1ENOOH(aq) → LBUT1ENOOH	k_exb(01,ind_LBUT1ENOOH)	see general notes*
H44042f_a01	TrAa01ScC	LHMVKABOOH → LHMVKABOOH(aq)	k_exf(01,ind_LHMVKABOOH)	see general notes*
H44042b_a01	TrAa01ScC	LHMVKABOOH(aq) → LHMVKABOOH	k_exb(01,ind_LHMVKABOOH)	see general notes*
H44043f_a01	TrAa01ScC	LMEKOOH → LMEKOOH(aq)	k_exf(01,ind_LMEKOOH)	see general notes*
H44043b_a01	TrAa01ScC	LMEKOOH(aq) → LMEKOOH	k_exb(01,ind_LMEKOOH)	see general notes*
H44044f_a01	TrAa01ScC	MACO2H → MACO2H(aq)	k_exf(01,ind_MACO2H)	see general notes*
H44044b_a01	TrAa01ScC	MACO2H(aq) → MACO2H	k_exb(01,ind_MACO2H)	see general notes*
H44045f_a01	TrAa01ScC	MACO3H → MACO3H(aq)	k_exf(01,ind_MACO3H)	see general notes*
H44045b_a01	TrAa01ScC	MACO3H(aq) → MACO3H	k_exb(01,ind_MACO3H)	see general notes*
H44046f_a01	TrAa01ScC	MACROH → MACROH(aq)	k_exf(01,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) → MACROH	k_exb(01,ind_MACROH)	see general notes*
H44047f_a01	TrAa01ScC	MACROOH → MACROOH(aq)	k_exf(01,ind_MACROOH)	see general notes*
H44047b_a01	TrAa01ScC	MACROOH(aq) → MACROOH	k_exb(01,ind_MACROOH)	see general notes*
H44048f_a01	TrAa01ScC	MALANHYOOH → MALANHYOOH(aq)	k_exf(01,ind_MALANHYOOH)	see general notes*
H44048b_a01	TrAa01ScC	MALANHYOOH(aq) → MALANHYOOH	k_exb(01,ind_MALANHYOOH)	see general notes*
H44049f_a01	TrAa01ScC	MALDALCO2H → MALDALCO2H(aq)	k_exf(01,ind_MALDALCO2H)	see general notes*
H44049b_a01	TrAa01ScC	MALDALCO2H(aq) → MALDALCO2H	k_exb(01,ind_MALDALCO2H)	see general notes*
H44050f_a01	TrAa01ScC	MALDALCO3H → MALDALCO3H(aq)	k_exf(01,ind_MALDALCO3H)	see general notes*
H44050b_a01	TrAa01ScC	MALDALCO3H(aq) → MALDALCO3H	k_exb(01,ind_MALDALCO3H)	see general notes*
H44051f_a01	TrAa01ScC	MALDIAL → MALDIAL(aq)	k_exf(01,ind_MALDIAL)	see general notes*
H44051b_a01	TrAa01ScC	MALDIAL(aq) → MALDIAL	k_exb(01,ind_MALDIAL)	see general notes*
H44052f_a01	TrAa01ScC	MALDIALOOH → MALDIALOOH(aq)	k_exf(01,ind_MALDIALOOH)	see general notes*
H44052b_a01	TrAa01ScC	MALDIALOOH(aq) → MALDIALOOH	k_exb(01,ind_MALDIALOOH)	see general notes*
H44053f_a01	TrAa01ScC	MALNHYOHCO → MALNHYOHCO(aq)	k_exf(01,ind_MALNHYOHCO)	see general notes*
H44053b_a01	TrAa01ScC	MALNHYOHCO(aq) → MALNHYOHCO	k_exb(01,ind_MALNHYOHCO)	see general notes*
H44054f_a01	TrAa01ScC	MECOACEOOH → MECOACEOOH(aq)	k_exf(01,ind_MECOACEOOH)	see general notes*
H44054b_a01	TrAa01ScC	MECOACEOOH(aq) → MECOACEOOH	k_exb(01,ind_MECOACEOOH)	see general notes*
H44055f_a01	TrAa01ScCN	MVKNO3 → MVKNO3(aq)	k_exf(01,ind_MVKNO3)	see general notes*
H44055b_a01	TrAa01ScCN	MVKNO3(aq) → MVKNO3	k_exb(01,ind_MVKNO3)	see general notes*
H44056f_a01	TrAa01ScCN	NBZFUOOH → NBZFUOOH(aq)	k_exf(01,ind_NBZFUOOH)	see general notes*
H44056b_a01	TrAa01ScCN	NBZFUOOH(aq) → NBZFUOOH	k_exb(01,ind_NBZFUOOH)	see general notes*
H44057f_a01	TrAa01ScCN	NC4DCO2H → NC4DCO2H(aq)	k_exf(01,ind_NC4DCO2H)	see general notes*
H44057b_a01	TrAa01ScCN	NC4DCO2H(aq) → NC4DCO2H	k_exb(01,ind_NC4DCO2H)	see general notes*
H45000f_a01	TrAa01ScC	ACCOMECHO → ACCOMECHO(aq)	k_exf(01,ind_ACCOMECHO)	see general notes*
H45000b_a01	TrAa01ScC	ACCOMECHO(aq) → ACCOMECHO	k_exb(01,ind_ACCOMECHO)	see general notes*
H45001f_a01	TrAa01ScC	ACCOMECO3H → ACCOMECO3H(aq)	k_exf(01,ind_ACCOMECO3H)	see general notes*
H45001b_a01	TrAa01ScC	ACCOMECO3H(aq) → ACCOMECO3H	k_exb(01,ind_ACCOMECO3H)	see general notes*
H45002f_a01	TrAa01ScC	C1ODC2O2C4OOH → C1ODC2O2C4OOH(aq)	k_exf(01,ind_C1ODC2O2C4OOH)	see general notes*
H45002b_a01	TrAa01ScC	C1ODC2O2C4OOH(aq) → C1ODC2O2C4OOH	k_exb(01,ind_C1ODC2O2C4OOH)	see general notes*
H45003f_a01	TrAa01ScC	C1ODC2OOHC4OD → C1ODC2OOHC4OD(aq)	k_exf(01,ind_C1ODC2OOHC4OD)	see general notes*
H45003b_a01	TrAa01ScC	C1ODC2OOHC4OD(aq) → 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	C1ODC3O2C4OOH → C1ODC3O2C4OOH(aq)	k_exf(01,ind_C1ODC3O2C4OOH)	see general notes*
H45004b_a01	TrAa01ScC	C1ODC3O2C4OOH(aq) → C1ODC3O2C4OOH	k_exb(01,ind_C1ODC3O2C4OOH)	see general notes*
H45005f_a01	TrAa01ScC	C1OOHC2OOHC4OD → C1OOHC2OOHC4OD(aq)	k_exf(01,ind_C1OOHC2OOHC4OD)	see general notes*
H45005b_a01	TrAa01ScC	C1OOHC2OOHC4OD(aq) → C1OOHC2OOHC4OD	k_exb(01,ind_C1OOHC2OOHC4OD)	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) → C59OOH	k_exb(01,ind_C59OOH)	see general notes*
H45020f_a01	TrAa01ScC	C5CO14OH → C5CO14OH(aq)	k_exf(01,ind_C5CO14OH)	see general notes*
H45020b_a01	TrAa01ScC	C5CO14OH(aq) → C5CO14OH	k_exb(01,ind_C5CO14OH)	see general notes*
H45021f_a01	TrAa01ScC	C5CO14OOH → C5CO14OOH(aq)	k_exf(01,ind_C5CO14OOH)	see general notes*
H45021b_a01	TrAa01ScC	C5CO14OOH(aq) → C5CO14OOH	k_exb(01,ind_C5CO14OOH)	see general notes*
H45022f_a01	TrAa01ScC	C5DIALCO → C5DIALCO(aq)	k_exf(01,ind_C5DIALCO)	see general notes*
H45022b_a01	TrAa01ScC	C5DIALCO(aq) → C5DIALCO	k_exb(01,ind_C5DIALCO)	see general notes*
H45023f_a01	TrAa01ScC	C5DIALOOH → C5DIALOOH(aq)	k_exf(01,ind_C5DIALOOH)	see general notes*
H45023b_a01	TrAa01ScC	C5DIALOOH(aq) → C5DIALOOH	k_exb(01,ind_C5DIALOOH)	see general notes*
H45024f_a01	TrAa01ScC	C5DICARB → C5DICARB(aq)	k_exf(01,ind_C5DICARB)	see general notes*
H45024b_a01	TrAa01ScC	C5DICARB(aq) → C5DICARB	k_exb(01,ind_C5DICARB)	see general notes*
H45025f_a01	TrAa01ScC	C5DICAROOH → C5DICAROOH(aq)	k_exf(01,ind_C5DICAROOH)	see general notes*
H45025b_a01	TrAa01ScC	C5DICAROOH(aq) → C5DICAROOH	k_exb(01,ind_C5DICAROOH)	see general notes*
H45026f_a01	TrAa01ScCN	C5PAN9 → C5PAN9(aq)	k_exf(01,ind_C5PAN9)	see general notes*
H45026b_a01	TrAa01ScCN	C5PAN9(aq) → C5PAN9	k_exb(01,ind_C5PAN9)	see general notes*
H45027f_a01	TrAa01ScC	CHOC3COOOH → CHOC3COOOH(aq)	k_exf(01,ind_CHOC3COOOH)	see general notes*
H45027b_a01	TrAa01ScC	CHOC3COOOH(aq) → CHOC3COOOH	k_exb(01,ind_CHOC3COOOH)	see general notes*
H45028f_a01	TrAa01ScCN	CHOC3COPAN → CHOC3COPAN(aq)	k_exf(01,ind_CHOC3COPAN)	see general notes*
H45028b_a01	TrAa01ScCN	CHOC3COPAN(aq) → CHOC3COPAN	k_exb(01,ind_CHOC3COPAN)	see general notes*
H45029f_a01	TrAa01ScC	CO13C4CHO → CO13C4CHO(aq)	k_exf(01,ind_CO13C4CHO)	see general notes*
H45029b_a01	TrAa01ScC	CO13C4CHO(aq) → CO13C4CHO	k_exb(01,ind_CO13C4CHO)	see general notes*
H45030f_a01	TrAa01ScC	CO23C4CHO → CO23C4CHO(aq)	k_exf(01,ind_CO23C4CHO)	see general notes*
H45030b_a01	TrAa01ScC	CO23C4CHO(aq) → CO23C4CHO	k_exb(01,ind_CO23C4CHO)	see general notes*
H45031f_a01	TrAa01ScC	CO23C4CO3H → CO23C4CO3H(aq)	k_exf(01,ind_CO23C4CO3H)	see general notes*
H45031b_a01	TrAa01ScC	CO23C4CO3H(aq) → CO23C4CO3H	k_exb(01,ind_CO23C4CO3H)	see general notes*
H45032f_a01	TrAa01ScCN	DB1NO3 → DB1NO3(aq)	k_exf(01,ind_DB1NO3)	see general notes*
H45032b_a01	TrAa01ScCN	DB1NO3(aq) → DB1NO3	k_exb(01,ind_DB1NO3)	see general notes*
H45033f_a01	TrAa01ScC	DB1OOH → DB1OOH(aq)	k_exf(01,ind_DB1OOH)	see general notes*
H45033b_a01	TrAa01ScC	DB1OOH(aq) → DB1OOH	k_exb(01,ind_DB1OOH)	see general notes*
H45034f_a01	TrAa01ScC	DB2OOH → DB2OOH(aq)	k_exf(01,ind_DB2OOH)	see general notes*
H45034b_a01	TrAa01ScC	DB2OOH(aq) → DB2OOH	k_exb(01,ind_DB2OOH)	see general notes*
H45035f_a01	TrAa01ScC	ISOPAOH → ISOPAOH(aq)	k_exf(01,ind_ISOPAOH)	see general notes*
H45035b_a01	TrAa01ScC	ISOPAOH(aq) → ISOPAOH	k_exb(01,ind_ISOPAOH)	see general notes*
H45036f_a01	TrAa01ScCN	ISOPBNO3 → ISOPBNO3(aq)	k_exf(01,ind_ISOPBNO3)	see general notes*
H45036b_a01	TrAa01ScCN	ISOPBNO3(aq) → 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 → ISOPBOH(aq)	k_exf(01,ind_ISOPBOH)	see general notes*
H45037b_a01	TrAa01ScC	ISOPBOH(aq) → ISOPBOH	k_exb(01,ind_ISOPBOH)	see general notes*
H45038f_a01	TrAa01ScC	ISOPBOOH → ISOPBOOH(aq)	k_exf(01,ind_ISOPBOOH)	see general notes*
H45038b_a01	TrAa01ScC	ISOPBOOH(aq) → ISOPBOOH	k_exb(01,ind_ISOPBOOH)	see general notes*
H45039f_a01	TrAa01ScCN	ISOPDNO3 → ISOPDNO3(aq)	k_exf(01,ind_ISOPDNO3)	see general notes*
H45039b_a01	TrAa01ScCN	ISOPDNO3(aq) → ISOPDNO3	k_exb(01,ind_ISOPDNO3)	see general notes*
H45040f_a01	TrAa01ScC	ISOPDOH → ISOPDOH(aq)	k_exf(01,ind_ISOPDOH)	see general notes*
H45040b_a01	TrAa01ScC	ISOPDOH(aq) → ISOPDOH	k_exb(01,ind_ISOPDOH)	see general notes*
H45041f_a01	TrAa01ScC	ISOPDOOH → ISOPDOOH(aq)	k_exf(01,ind_ISOPDOOH)	see general notes*
H45041b_a01	TrAa01ScC	ISOPDOOH(aq) → ISOPDOOH	k_exb(01,ind_ISOPDOOH)	see general notes*
H45042f_a01	TrAa01ScC	LC578OOH → LC578OOH(aq)	k_exf(01,ind_LC578OOH)	see general notes*
H45042b_a01	TrAa01ScC	LC578OOH(aq) → LC578OOH	k_exb(01,ind_LC578OOH)	see general notes*
H45043f_a01	TrAa01ScCN	LC5PAN1719 → LC5PAN1719(aq)	k_exf(01,ind_LC5PAN1719)	see general notes*
H45043b_a01	TrAa01ScCN	LC5PAN1719(aq) → LC5PAN1719	k_exb(01,ind_LC5PAN1719)	see general notes*
H45044f_a01	TrAa01ScC	LHC4ACCHO → LHC4ACCHO(aq)	k_exf(01,ind_LHC4ACCHO)	see general notes*
H45044b_a01	TrAa01ScC	LHC4ACCHO(aq) → LHC4ACCHO	k_exb(01,ind_LHC4ACCHO)	see general notes*
H45045f_a01	TrAa01ScC	LHC4ACCO2H → LHC4ACCO2H(aq)	k_exf(01,ind_LHC4ACCO2H)	see general notes*
H45045b_a01	TrAa01ScC	LHC4ACCO2H(aq) → LHC4ACCO2H	k_exb(01,ind_LHC4ACCO2H)	see general notes*
H45046f_a01	TrAa01ScC	LHC4ACCO3H → LHC4ACCO3H(aq)	k_exf(01,ind_LHC4ACCO3H)	see general notes*
H45046b_a01	TrAa01ScC	LHC4ACCO3H(aq) → LHC4ACCO3H	k_exb(01,ind_LHC4ACCO3H)	see general notes*
H45047f_a01	TrAa01ScC	LIEPOX → LIEPOX(aq)	k_exf(01,ind_LIEPOX)	see general notes*
H45047b_a01	TrAa01ScC	LIEPOX(aq) → LIEPOX	k_exb(01,ind_LIEPOX)	see general notes*
H45048f_a01	TrAa01ScCN	LISOPACNO3 → LISOPACNO3(aq)	k_exf(01,ind_LISOPACNO3)	see general notes*
H45048b_a01	TrAa01ScCN	LISOPACNO3(aq) → LISOPACNO3	k_exb(01,ind_LISOPACNO3)	see general notes*
H45049f_a01	TrAa01ScC	LISOPACOOH → LISOPACOOH(aq)	k_exf(01,ind_LISOPACOOH)	see general notes*
H45049b_a01	TrAa01ScC	LISOPACOOH(aq) → LISOPACOOH	k_exb(01,ind_LISOPACOOH)	see general notes*
H45050f_a01	TrAa01ScCN	LMBOABNO3 → LMBOABNO3(aq)	k_exf(01,ind_LMBOABNO3)	see general notes*
H45050b_a01	TrAa01ScCN	LMBOABNO3(aq) → LMBOABNO3	k_exb(01,ind_LMBOABNO3)	see general notes*
H45051f_a01	TrAa01ScC	LMBOABOOH → LMBOABOOH(aq)	k_exf(01,ind_LMBOABOOH)	see general notes*
H45051b_a01	TrAa01ScC	LMBOABOOH(aq) → LMBOABOOH	k_exb(01,ind_LMBOABOOH)	see general notes*
H45052f_a01	TrAa01ScCN	LNMBOABOOH → LNMBOABOOH(aq)	k_exf(01,ind_LNMBOABOOH)	see general notes*
H45052b_a01	TrAa01ScCN	LNMBOABOOH(aq) → LNMBOABOOH	k_exb(01,ind_LNMBOABOOH)	see general notes*
H45053f_a01	TrAa01ScC	MBO → MBO(aq)	k_exf(01,ind_MBO)	see general notes*
H45053b_a01	TrAa01ScC	MBO(aq) → MBO	k_exb(01,ind_MBO)	see general notes*
H45054f_a01	TrAa01ScC	MBOACO → 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) → MBOACO	k_exb(01,ind_MBOACO)	see general notes*
H45055f_a01	TrAa01ScC	MBOCOCO → MBOCOCO(aq)	k_exf(01,ind_MBOCOCO)	see general notes*
H45055b_a01	TrAa01ScC	MBOCOCO(aq) → MBOCOCO	k_exb(01,ind_MBOCOCO)	see general notes*
H45056f_a01	TrAa01ScC	MC3ODBCO2H → MC3ODBCO2H(aq)	k_exf(01,ind_MC3ODBCO2H)	see general notes*
H45056b_a01	TrAa01ScC	MC3ODBCO2H(aq) → MC3ODBCO2H	k_exb(01,ind_MC3ODBCO2H)	see general notes*
H45057f_a01	TrAa01ScC	3METHYLFURAN → 3METHYLFURAN(aq)	k_exf(01,ind_ME3FURAN)	see general notes*
H45057b_a01	TrAa01ScC	3METHYLFURAN(aq) → 3METHYLFURAN	k_exb(01,ind_ME3FURAN)	see general notes*
H45058f_a01	TrAa01ScC	MMALNHYOOH → MMALNHYOOH(aq)	k_exf(01,ind_MMALNHYOOH)	see general notes*
H45058b_a01	TrAa01ScC	MMALNHYOOH(aq) → MMALNHYOOH	k_exb(01,ind_MMALNHYOOH)	see general notes*
H45059f_a01	TrAa01ScCN	NC4MDCO2HN → NC4MDCO2HN(aq)	k_exf(01,ind_NC4MDCO2H)	see general notes*
H45059b_a01	TrAa01ScCN	NC4MDCO2HN(aq) → NC4MDCO2HN	k_exb(01,ind_NC4MDCO2H)	see general notes*
H45060f_a01	TrAa01ScCN	NC4OHCO3H → NC4OHCO3H(aq)	k_exf(01,ind_NC4OHCO3H)	see general notes*
H45060b_a01	TrAa01ScCN	NC4OHCO3H(aq) → NC4OHCO3H	k_exb(01,ind_NC4OHCO3H)	see general notes*
H45061f_a01	TrAa01ScCN	NC4OHCPAN → NC4OHCPAN(aq)	k_exf(01,ind_NC4OHCPAN)	see general notes*
H45061b_a01	TrAa01ScCN	NC4OHCPAN(aq) → NC4OHCPAN	k_exb(01,ind_NC4OHCPAN)	see general notes*
H45062f_a01	TrAa01ScCN	NISOPOOH → NISOPOOH(aq)	k_exf(01,ind_NISOPOOH)	see general notes*
H45062b_a01	TrAa01ScCN	NISOPOOH(aq) → NISOPOOH	k_exb(01,ind_NISOPOOH)	see general notes*
H45063f_a01	TrAa01ScCN	NMBOBCO → NMBOBCO(aq)	k_exf(01,ind_NMBOBCO)	see general notes*
H45063b_a01	TrAa01ScCN	NMBOBCO(aq) → NMBOBCO	k_exb(01,ind_NMBOBCO)	see general notes*
H45064f_a01	TrAa01ScCN	NTLFUOOH → NTLFUOOH(aq)	k_exf(01,ind_NTLFUOOH)	see general notes*
H45064b_a01	TrAa01ScCN	NTLFUOOH(aq) → NTLFUOOH	k_exb(01,ind_NTLFUOOH)	see general notes*
H45065f_a01	TrAa01ScC	TLFUOOH → TLFUOOH(aq)	k_exf(01,ind_TLFUOOH)	see general notes*
H45065b_a01	TrAa01ScC	TLFUOOH(aq) → TLFUOOH	k_exb(01,ind_TLFUOOH)	see general notes*
H45066f_a01	TrAa01ScC	LZCO3HC23DBCOD → LZCO3HC23DBCOD(aq)	k_exf(01,ind_LZCO3HC23DBCOD)	see general notes*
H45066b_a01	TrAa01ScC	LZCO3HC23DBCOD(aq) → LZCO3HC23DBCOD	k_exb(01,ind_LZCO3HC23DBCOD)	see general notes*
H45067f_a01	TrAa01ScC	C4MDIAL → C4MDIAL(aq)	k_exf(01,ind_C4MDIAL)	see general notes*
H45067b_a01	TrAa01ScC	C4MDIAL(aq) → C4MDIAL	k_exb(01,ind_C4MDIAL)	see general notes*
H46000f_a01	TrAa01ScCN	BZBIPERNO3 → BZBIPERNO3(aq)	k_exf(01,ind_BZBIPERNO3)	see general notes*
H46000b_a01	TrAa01ScCN	BZBIPERNO3(aq) → BZBIPERNO3	k_exb(01,ind_BZBIPERNO3)	see general notes*
H46001f_a01	TrAa01ScC	BZBIPEROOH → BZBIPEROOH(aq)	k_exf(01,ind_BZBIPEROOH)	see general notes*
H46001b_a01	TrAa01ScC	BZBIPEROOH(aq) → 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 → BZEMUCCO(aq)	k_exf(01,ind_BZEMUCCO)	see general notes*
H46002b_a01	TrAa01ScC	BZEMUCCO(aq) → BZEMUCCO	k_exb(01,ind_BZEMUCCO)	see general notes*
H46003f_a01	TrAa01ScC	BZEMUCCO2H → BZEMUCCO2H(aq)	k_exf(01,ind_BZEMUCCO2H)	see general notes*
H46003b_a01	TrAa01ScC	BZEMUCCO2H(aq) → BZEMUCCO2H	k_exb(01,ind_BZEMUCCO2H)	see general notes*
H46004f_a01	TrAa01ScC	BZEMUCCO3H → BZEMUCCO3H(aq)	k_exf(01,ind_BZEMUCCO3H)	see general notes*
H46004b_a01	TrAa01ScC	BZEMUCCO3H(aq) → BZEMUCCO3H	k_exb(01,ind_BZEMUCCO3H)	see general notes*
H46005f_a01	TrAa01ScCN	BZEMUCNO3 → BZEMUCNO3(aq)	k_exf(01,ind_BZEMUCNO3)	see general notes*
H46005b_a01	TrAa01ScCN	BZEMUCNO3(aq) → BZEMUCNO3	k_exb(01,ind_BZEMUCNO3)	see general notes*
H46006f_a01	TrAa01ScC	BZEMUCOOH → BZEMUCOOH(aq)	k_exf(01,ind_BZEMUCOOH)	see general notes*
H46006b_a01	TrAa01ScC	BZEMUCOOH(aq) → BZEMUCOOH	k_exb(01,ind_BZEMUCOOH)	see general notes*
H46007f_a01	TrAa01ScC	BZEPOXMUC → BZEPOXMUC(aq)	k_exf(01,ind_BZEPOXMUC)	see general notes*
H46007b_a01	TrAa01ScC	BZEPOXMUC(aq) → BZEPOXMUC	k_exb(01,ind_BZEPOXMUC)	see general notes*
H46008f_a01	TrAa01ScC	BZOBIPEROH → BZOBIPEROH(aq)	k_exf(01,ind_BZOBIPEROH)	see general notes*
H46008b_a01	TrAa01ScC	BZOBIPEROH(aq) → BZOBIPEROH	k_exb(01,ind_BZOBIPEROH)	see general notes*
H46009f_a01	TrAa01ScCN	C5CO2DBPAN → C5CO2DBPAN(aq)	k_exf(01,ind_C5CO2DBPAN)	see general notes*
H46009b_a01	TrAa01ScCN	C5CO2DBPAN(aq) → C5CO2DBPAN	k_exb(01,ind_C5CO2DBPAN)	see general notes*
H46010f_a01	TrAa01ScC	C5CO2DCO3H → C5CO2DCO3H(aq)	k_exf(01,ind_C5CO2DCO3H)	see general notes*
H46010b_a01	TrAa01ScC	C5CO2DCO3H(aq) → C5CO2DCO3H	k_exb(01,ind_C5CO2DCO3H)	see general notes*
H46011f_a01	TrAa01ScCN	C5CO2OHPAN → C5CO2OHPAN(aq)	k_exf(01,ind_C5CO2OHPAN)	see general notes*
H46011b_a01	TrAa01ScCN	C5CO2OHPAN(aq) → C5CO2OHPAN	k_exb(01,ind_C5CO2OHPAN)	see general notes*
H46012f_a01	TrAa01ScC	C5COOHCO3H → C5COOHCO3H(aq)	k_exf(01,ind_C5COOHCO3H)	see general notes*
H46012b_a01	TrAa01ScC	C5COOHCO3H(aq) → C5COOHCO3H	k_exb(01,ind_C5COOHCO3H)	see general notes*
H46013f_a01	TrAa01ScC	C6125CO → C6125CO(aq)	k_exf(01,ind_C6125CO)	see general notes*
H46013b_a01	TrAa01ScC	C6125CO(aq) → C6125CO	k_exb(01,ind_C6125CO)	see general notes*
H46014f_a01	TrAa01ScC	C614CO → C614CO(aq)	k_exf(01,ind_C614CO)	see general notes*
H46014b_a01	TrAa01ScC	C614CO(aq) → C614CO	k_exb(01,ind_C614CO)	see general notes*
H46015f_a01	TrAa01ScCN	C614NO3 → C614NO3(aq)	k_exf(01,ind_C614NO3)	see general notes*
H46015b_a01	TrAa01ScCN	C614NO3(aq) → C614NO3	k_exb(01,ind_C614NO3)	see general notes*
H46016f_a01	TrAa01ScC	C614OOH → C614OOH(aq)	k_exf(01,ind_C614OOH)	see general notes*
H46016b_a01	TrAa01ScC	C614OOH(aq) → C614OOH	k_exb(01,ind_C614OOH)	see general notes*
H46017f_a01	TrAa01ScC	C615CO2OOH → C615CO2OOH(aq)	k_exf(01,ind_C615CO2OOH)	see general notes*
H46017b_a01	TrAa01ScC	C615CO2OOH(aq) → C615CO2OOH	k_exb(01,ind_C615CO2OOH)	see general notes*
H46018f_a01	TrAa01ScC	C6CO4DB → C6CO4DB(aq)	k_exf(01,ind_C6CO4DB)	see general notes*
H46018b_a01	TrAa01ScC	C6CO4DB(aq) → C6CO4DB	k_exb(01,ind_C6CO4DB)	see general notes*
H46019f_a01	TrAa01ScC	C6H5O → 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	C6H5O(aq) → C6H5O	k_exb(01,ind_C6H5O)	see general notes*
H46020f_a01	TrAa01ScC	C6H5OOH → C6H5OOH(aq)	k_exf(01,ind_C6H5OOH)	see general notes*
H46020b_a01	TrAa01ScC	C6H5OOH(aq) → C6H5OOH	k_exb(01,ind_C6H5OOH)	see general notes*
H46021f_a01	TrAa01ScC	CATEC1O → CATEC1O(aq)	k_exf(01,ind_CATEC1O)	see general notes*
H46021b_a01	TrAa01ScC	CATEC1O(aq) → CATEC1O	k_exb(01,ind_CATEC1O)	see general notes*
H46022f_a01	TrAa01ScC	CATEC1OOH → CATEC1OOH(aq)	k_exf(01,ind_CATEC1OOH)	see general notes*
H46022b_a01	TrAa01ScC	CATEC1OOH(aq) → CATEC1OOH	k_exb(01,ind_CATEC1OOH)	see general notes*
H46023f_a01	TrAa01ScC	CATECHOL → CATECHOL(aq)	k_exf(01,ind_CATECHOL)	see general notes*
H46023b_a01	TrAa01ScC	CATECHOL(aq) → CATECHOL	k_exb(01,ind_CATECHOL)	see general notes*
H46024f_a01	TrAa01ScC	CO235C5CHO → CO235C5CHO(aq)	k_exf(01,ind_CO235C5CHO)	see general notes*
H46024b_a01	TrAa01ScC	CO235C5CHO(aq) → CO235C5CHO	k_exb(01,ind_CO235C5CHO)	see general notes*
H46025f_a01	TrAa01ScC	CO235C6OOH → CO235C6OOH(aq)	k_exf(01,ind_CO235C6OOH)	see general notes*
H46025b_a01	TrAa01ScC	CO235C6OOH(aq) → CO235C6OOH	k_exb(01,ind_CO235C6OOH)	see general notes*
H46026f_a01	TrAa01ScCN	DNPHEN → DNPHEN(aq)	k_exf(01,ind_DNPHEN)	see general notes*
H46026b_a01	TrAa01ScCN	DNPHEN(aq) → DNPHEN	k_exb(01,ind_DNPHEN)	see general notes*
H46027f_a01	TrAa01ScCN	DNPHENOOH → DNPHENOOH(aq)	k_exf(01,ind_DNPHENOOH)	see general notes*
H46027b_a01	TrAa01ScCN	DNPHENOOH(aq) → DNPHENOOH	k_exb(01,ind_DNPHENOOH)	see general notes*
H46028f_a01	TrAa01ScCN	NBZQOOH → NBZQOOH(aq)	k_exf(01,ind_NBZQOOH)	see general notes*
H46028b_a01	TrAa01ScCN	NBZQOOH(aq) → NBZQOOH	k_exb(01,ind_NBZQOOH)	see general notes*
H46029f_a01	TrAa01ScCN	NCATECHOL → NCATECHOL(aq)	k_exf(01,ind_NCATECHOL)	see general notes*
H46029b_a01	TrAa01ScCN	NCATECHOL(aq) → NCATECHOL	k_exb(01,ind_NCATECHOL)	see general notes*
H46030f_a01	TrAa01ScCN	NCATECOOH → NCATECOOH(aq)	k_exf(01,ind_NCATECOOH)	see general notes*
H46030b_a01	TrAa01ScCN	NCATECOOH(aq) → NCATECOOH	k_exb(01,ind_NCATECOOH)	see general notes*
H46031f_a01	TrAa01ScCN	NDNPHENOOH → NDNPHENOOH(aq)	k_exf(01,ind_NDNPHENOOH)	see general notes*
H46031b_a01	TrAa01ScCN	NDNPHENOOH(aq) → NDNPHENOOH	k_exb(01,ind_NDNPHENOOH)	see general notes*
H46032f_a01	TrAa01ScCN	NNCATECOOH → NNCATECOOH(aq)	k_exf(01,ind_NNCATECOOH)	see general notes*
H46032b_a01	TrAa01ScCN	NNCATECOOH(aq) → NNCATECOOH	k_exb(01,ind_NNCATECOOH)	see general notes*
H46033f_a01	TrAa01ScCN	NPHENOOH → NPHENOOH(aq)	k_exf(01,ind_NPHENOOH)	see general notes*
H46033b_a01	TrAa01ScCN	NPHENOOH(aq) → NPHENOOH	k_exb(01,ind_NPHENOOH)	see general notes*
H46034f_a01	TrAa01ScC	PBZQCO → PBZQCO(aq)	k_exf(01,ind_PBZQCO)	see general notes*
H46034b_a01	TrAa01ScC	PBZQCO(aq) → PBZQCO	k_exb(01,ind_PBZQCO)	see general notes*
H46035f_a01	TrAa01ScC	PBZQOOH → PBZQOOH(aq)	k_exf(01,ind_PBZQOOH)	see general notes*
H46035b_a01	TrAa01ScC	PBZQOOH(aq) → PBZQOOH	k_exb(01,ind_PBZQOOH)	see general notes*
H46036f_a01	TrAa01ScC	PHENOL → PHENOL(aq)	k_exf(01,ind_PHENOL)	see general notes*
H46036b_a01	TrAa01ScC	PHENOL(aq) → PHENOL	k_exb(01,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 → PHENOOH(aq)	k_exf(01,ind_PHENOOH)	see general notes*
H46037b_a01	TrAa01ScC	PHENOOH(aq) → PHENOOH	k_exb(01,ind_PHENOOH)	see general notes*
H47000f_a01	TrAa01ScC	C235C6CO3H → C235C6CO3H(aq)	k_exf(01,ind_C235C6CO3H)	see general notes*
H47000b_a01	TrAa01ScC	C235C6CO3H(aq) → C235C6CO3H	k_exb(01,ind_C235C6CO3H)	see general notes*
H47001f_a01	TrAa01ScCN	C6CO2OHPAN → C6CO2OHPAN(aq)	k_exf(01,ind_C6CO2OHPAN)	see general notes*
H47001b_a01	TrAa01ScCN	C6CO2OHPAN(aq) → C6CO2OHPAN	k_exb(01,ind_C6CO2OHPAN)	see general notes*
H47002f_a01	TrAa01ScC	C6COOHCO3H → C6COOHCO3H(aq)	k_exf(01,ind_C6COOHCO3H)	see general notes*
H47002b_a01	TrAa01ScC	C6COOHCO3H(aq) → C6COOHCO3H	k_exb(01,ind_C6COOHCO3H)	see general notes*
H47003f_a01	TrAa01ScC	C6H5CH2OOH → C6H5CH2OOH(aq)	k_exf(01,ind_C6H5CH2OOH)	see general notes*
H47003b_a01	TrAa01ScC	C6H5CH2OOH(aq) → C6H5CH2OOH	k_exb(01,ind_C6H5CH2OOH)	see general notes*
H47004f_a01	TrAa01ScC	C6H5CO3H → C6H5CO3H(aq)	k_exf(01,ind_C6H5CO3H)	see general notes*
H47004b_a01	TrAa01ScC	C6H5CO3H(aq) → C6H5CO3H	k_exb(01,ind_C6H5CO3H)	see general notes*
H47005f_a01	TrAa01ScC	C716OOH → C716OOH(aq)	k_exf(01,ind_C716OOH)	see general notes*
H47005b_a01	TrAa01ScC	C716OOH(aq) → C716OOH	k_exb(01,ind_C716OOH)	see general notes*
H47006f_a01	TrAa01ScC	C721OOH → C721OOH(aq)	k_exf(01,ind_C721OOH)	see general notes*
H47006b_a01	TrAa01ScC	C721OOH(aq) → C721OOH	k_exb(01,ind_C721OOH)	see general notes*
H47007f_a01	TrAa01ScC	C722OOH → C722OOH(aq)	k_exf(01,ind_C722OOH)	see general notes*
H47007b_a01	TrAa01ScC	C722OOH(aq) → C722OOH	k_exb(01,ind_C722OOH)	see general notes*
H47008f_a01	TrAa01ScC	C7CO4DB → C7CO4DB(aq)	k_exf(01,ind_C7CO4DB)	see general notes*
H47008b_a01	TrAa01ScC	C7CO4DB(aq) → C7CO4DB	k_exb(01,ind_C7CO4DB)	see general notes*
H47009f_a01	TrAa01ScCN	C7PAN3 → C7PAN3(aq)	k_exf(01,ind_C7PAN3)	see general notes*
H47009b_a01	TrAa01ScCN	C7PAN3(aq) → C7PAN3	k_exb(01,ind_C7PAN3)	see general notes*
H47010f_a01	TrAa01ScC	CO235C6CHO → CO235C6CHO(aq)	k_exf(01,ind_CO235C6CHO)	see general notes*
H47010b_a01	TrAa01ScC	CO235C6CHO(aq) → CO235C6CHO	k_exb(01,ind_CO235C6CHO)	see general notes*
H47011f_a01	TrAa01ScC	CRESOL → CRESOL(aq)	k_exf(01,ind_CRESOL)	see general notes*
H47011b_a01	TrAa01ScC	CRESOL(aq) → CRESOL	k_exb(01,ind_CRESOL)	see general notes*
H47012f_a01	TrAa01ScC	CRESOOH → CRESOOH(aq)	k_exf(01,ind_CRESOOH)	see general notes*
H47012b_a01	TrAa01ScC	CRESOOH(aq) → CRESOOH	k_exb(01,ind_CRESOOH)	see general notes*
H47013f_a01	TrAa01ScCN	DNCRES → DNCRES(aq)	k_exf(01,ind_DNCRES)	see general notes*
H47013b_a01	TrAa01ScCN	DNCRES(aq) → DNCRES	k_exb(01,ind_DNCRES)	see general notes*
H47014f_a01	TrAa01ScCN	DNCRESOOH → DNCRESOOH(aq)	k_exf(01,ind_DNCRESOOH)	see general notes*
H47014b_a01	TrAa01ScCN	DNCRESOOH(aq) → DNCRESOOH	k_exb(01,ind_DNCRESOOH)	see general notes*
H47015f_a01	TrAa01ScC	MCATEC1O → MCATEC1O(aq)	k_exf(01,ind_MCATEC1O)	see general notes*
H47015b_a01	TrAa01ScC	MCATEC1O(aq) → MCATEC1O	k_exb(01,ind_MCATEC1O)	see general notes*
H47016f_a01	TrAa01ScC	MCATEC1OOH → MCATEC1OOH(aq)	k_exf(01,ind_MCATEC1OOH)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H47016b_a01	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*
H48000f_a01	TrAa01ScC	C721CHO $\rightarrow$ C721CHO(aq)	k_exf(01,ind_C721CHO)	see general notes*
H48000b_a01	TrAa01ScC	C721CHO(aq) $\rightarrow$ C721CHO	k_exb(01,ind_C721CHO)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H48001f_a01	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*
H49000b_a01	TrAa01ScC	C811CO3H(aq) → C811CO3H	k_exb(01,ind_C811CO3H)	see general notes*
H49001f_a01	TrAa01ScCN	C811PAN → C811PAN(aq)	k_exf(01,ind_C811PAN)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H49001b_a01	TrAa01ScCN	C811PAN(aq) → C811PAN	k_exb(01,ind_C811PAN)	see general notes*
H49002f_a01	TrAa01ScC	C85CO3H → C85CO3H(aq)	k_exf(01,ind_C85CO3H)	see general notes*
H49002b_a01	TrAa01ScC	C85CO3H(aq) → C85CO3H	k_exb(01,ind_C85CO3H)	see general notes*
H49003f_a01	TrAa01ScC	C89CO2H → C89CO2H(aq)	k_exf(01,ind_C89CO2H)	see general notes*
H49003b_a01	TrAa01ScC	C89CO2H(aq) → C89CO2H	k_exb(01,ind_C89CO2H)	see general notes*
H49004f_a01	TrAa01ScC	C89CO3H → C89CO3H(aq)	k_exf(01,ind_C89CO3H)	see general notes*
H49004b_a01	TrAa01ScC	C89CO3H(aq) → C89CO3H	k_exb(01,ind_C89CO3H)	see general notes*
H49005f_a01	TrAa01ScCN	C89PAN → C89PAN(aq)	k_exf(01,ind_C89PAN)	see general notes*
H49005b_a01	TrAa01ScCN	C89PAN(aq) → C89PAN	k_exb(01,ind_C89PAN)	see general notes*
H49006f_a01	TrAa01ScCN	C96NO3 → C96NO3(aq)	k_exf(01,ind_C96NO3)	see general notes*
H49006b_a01	TrAa01ScCN	C96NO3(aq) → C96NO3	k_exb(01,ind_C96NO3)	see general notes*
H49007f_a01	TrAa01ScC	C96OOH → C96OOH(aq)	k_exf(01,ind_C96OOH)	see general notes*
H49007b_a01	TrAa01ScC	C96OOH(aq) → C96OOH	k_exb(01,ind_C96OOH)	see general notes*
H49008f_a01	TrAa01ScC	C97OOH → C97OOH(aq)	k_exf(01,ind_C97OOH)	see general notes*
H49008b_a01	TrAa01ScC	C97OOH(aq) → C97OOH	k_exb(01,ind_C97OOH)	see general notes*
H49009f_a01	TrAa01ScC	C98OOH → C98OOH(aq)	k_exf(01,ind_C98OOH)	see general notes*
H49009b_a01	TrAa01ScC	C98OOH(aq) → C98OOH	k_exb(01,ind_C98OOH)	see general notes*
H49010f_a01	TrAa01ScCN	C9PAN2 → C9PAN2(aq)	k_exf(01,ind_C9PAN2)	see general notes*
H49010b_a01	TrAa01ScCN	C9PAN2(aq) → C9PAN2	k_exb(01,ind_C9PAN2)	see general notes*
H49011f_a01	TrAa01ScC	NOPINDCO → NOPINDCO(aq)	k_exf(01,ind_NOPINDCO)	see general notes*
H49011b_a01	TrAa01ScC	NOPINDCO(aq) → NOPINDCO	k_exb(01,ind_NOPINDCO)	see general notes*
H49012f_a01	TrAa01ScC	NOPINDOOH → NOPINDOOH(aq)	k_exf(01,ind_NOPINDOOH)	see general notes*
H49012b_a01	TrAa01ScC	NOPINDOOH(aq) → NOPINDOOH	k_exb(01,ind_NOPINDOOH)	see general notes*
H49013f_a01	TrAa01ScC	NOPINONE → NOPINONE(aq)	k_exf(01,ind_NOPINONE)	see general notes*
H49013b_a01	TrAa01ScC	NOPINONE(aq) → NOPINONE	k_exb(01,ind_NOPINONE)	see general notes*
H49014f_a01	TrAa01ScC	NOPINOO → NOPINOO(aq)	k_exf(01,ind_NOPINOO)	see general notes*
H49014b_a01	TrAa01ScC	NOPINOO(aq) → NOPINOO	k_exb(01,ind_NOPINOO)	see general notes*
H49015f_a01	TrAa01ScC	NORPINAL → NORPINAL(aq)	k_exf(01,ind_NORPINAL)	see general notes*
H49015b_a01	TrAa01ScC	NORPINAL(aq) → NORPINAL	k_exb(01,ind_NORPINAL)	see general notes*
H49016f_a01	TrAa01ScC	NORPINENOL → NORPINENOL(aq)	k_exf(01,ind_NORPINENOL)	see general notes*
H49016b_a01	TrAa01ScC	NORPINENOL(aq) → NORPINENOL	k_exb(01,ind_NORPINENOL)	see general notes*
H49017f_a01	TrAa01ScC	PINIC → PINIC(aq)	k_exf(01,ind_PINIC)	see general notes*
H49017b_a01	TrAa01ScC	PINIC(aq) → PINIC	k_exb(01,ind_PINIC)	see general notes*
H410000f_a01	TrAa01ScCN	BPINANO3 → BPINANO3(aq)	k_exf(01,ind_BPINANO3)	see general notes*
H410000b_a01	TrAa01ScCN	BPINANO3(aq) → BPINANO3	k_exb(01,ind_BPINANO3)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410001f_a01	TrAa01ScC	BPINAOOH → BPINAOOH(aq)	k_exf(01,ind_BPINAOOH)	see general notes*
H410001b_a01	TrAa01ScC	BPINAOOH(aq) → BPINAOOH	k_exb(01,ind_BPINAOOH)	see general notes*
H410002f_a01	TrAa01ScCN	C106NO3 → C106NO3(aq)	k_exf(01,ind_C106NO3)	see general notes*
H410002b_a01	TrAa01ScCN	C106NO3(aq) → C106NO3	k_exb(01,ind_C106NO3)	see general notes*
H410003f_a01	TrAa01ScC	C106OOH → C106OOH(aq)	k_exf(01,ind_C106OOH)	see general notes*
H410003b_a01	TrAa01ScC	C106OOH(aq) → C106OOH	k_exb(01,ind_C106OOH)	see general notes*
H410004f_a01	TrAa01ScC	C109CO → C109CO(aq)	k_exf(01,ind_C109CO)	see general notes*
H410004b_a01	TrAa01ScC	C109CO(aq) → C109CO	k_exb(01,ind_C109CO)	see general notes*
H410005f_a01	TrAa01ScC	C109OOH → C109OOH(aq)	k_exf(01,ind_C109OOH)	see general notes*
H410005b_a01	TrAa01ScC	C109OOH(aq) → C109OOH	k_exb(01,ind_C109OOH)	see general notes*
H410006f_a01	TrAa01ScCN	C10PAN2 → C10PAN2(aq)	k_exf(01,ind_C10PAN2)	see general notes*
H410006b_a01	TrAa01ScCN	C10PAN2(aq) → C10PAN2	k_exb(01,ind_C10PAN2)	see general notes*
H410007f_a01	TrAa01ScCN	LAPINABNO3 → LAPINABNO3(aq)	k_exf(01,ind_LAPINABNO3)	see general notes*
H410007b_a01	TrAa01ScCN	LAPINABNO3(aq) → LAPINABNO3	k_exb(01,ind_LAPINABNO3)	see general notes*
H410008f_a01	TrAa01ScC	LAPINABOOH → LAPINABOOH(aq)	k_exf(01,ind_LAPINABOOH)	see general notes*
H410008b_a01	TrAa01ScC	LAPINABOOH(aq) → LAPINABOOH	k_exb(01,ind_LAPINABOOH)	see general notes*
H410009f_a01	TrAa01ScCN	LNAPINABOOH → LNAPINABOOH(aq)	k_exf(01,ind_LNAPINABOOH)	see general notes*
H410009b_a01	TrAa01ScCN	LNAPINABOOH(aq) → LNAPINABOOH	k_exb(01,ind_LNAPINABOOH)	see general notes*
H410010f_a01	TrAa01ScCN	LNBPINABOOH → LNBPINABOOH(aq)	k_exf(01,ind_LNBPINABOOH)	see general notes*
H410010b_a01	TrAa01ScCN	LNBPINABOOH(aq) → LNBPINABOOH	k_exb(01,ind_LNBPINABOOH)	see general notes*
H410011f_a01	TrAa01ScC	MENTHEN6ONE → MENTHEN6ONE(aq)	k_exf(01,ind_MENTHEN6ONE)	see general notes*
H410011b_a01	TrAa01ScC	MENTHEN6ONE(aq) → MENTHEN6ONE	k_exb(01,ind_MENTHEN6ONE)	see general notes*
H410012f_a01	TrAa01ScC	2OHMENTHEN6ONE → 2OHMENTHEN6ONE(aq)	k_exf(01,ind_OH2MENTHEN6ONE)	see general notes*
H410012b_a01	TrAa01ScC	2OHMENTHEN6ONE(aq) → 2OHMENTHEN6ONE	k_exb(01,ind_OH2MENTHEN6ONE)	see general notes*
H410013f_a01	TrAa01ScC	PERPINONIC → PERPINONIC(aq)	k_exf(01,ind_PERPINONIC)	see general notes*
H410013b_a01	TrAa01ScC	PERPINONIC(aq) → PERPINONIC	k_exb(01,ind_PERPINONIC)	see general notes*
H410014f_a01	TrAa01ScC	PINAL → PINAL(aq)	k_exf(01,ind_PINAL)	see general notes*
H410014b_a01	TrAa01ScC	PINAL(aq) → PINAL	k_exb(01,ind_PINAL)	see general notes*
H410015f_a01	TrAa01ScCN	PINALNO3 → PINALNO3(aq)	k_exf(01,ind_PINALNO3)	see general notes*
H410015b_a01	TrAa01ScCN	PINALNO3(aq) → PINALNO3	k_exb(01,ind_PINALNO3)	see general notes*
H410016f_a01	TrAa01ScC	PINALOOH → PINALOOH(aq)	k_exf(01,ind_PINALOOH)	see general notes*
H410016b_a01	TrAa01ScC	PINALOOH(aq) → PINALOOH	k_exb(01,ind_PINALOOH)	see general notes*
H410017f_a01	TrAa01ScC	PINEOL → PINEOL(aq)	k_exf(01,ind_PINENOL)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H410017b_a01	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*
H63000_a01	TrAa01MblClN	$N_2O_5 + Cl^-$(aq) $\rightarrow ClNO_2 + NO_3^-$(aq)	k_exf_N2O5(01) * 5.E2	Behnke et al. (1994), Behnke et al. (1997)
H63001_a01	TrAa01MblClN	$ClNO_3 \rightarrow$ HOCl(aq) + HNO_3(aq)	k_exf_ClNO3(01) * C(ind_H2O_a01)	see general notes*
H63002_a01	TrAa01MblClN	$ClNO_3 + Cl^-$(aq) $\rightarrow Cl_2$(aq) + NO_3^-(aq)	k_exf_ClNO3(01) * 5.E2	see general notes*
H70000f_a01	TrAa01MblScBr	$Br_2 \rightarrow Br_2$(aq)	k_exf(01,ind_Br2)	see general notes*
H70000b_a01	TrAa01MblScBr	Br_2(aq) $\rightarrow Br_2$	k_exb(01,ind_Br2)	see general notes*
H72000f_a01	TrAa01MblScScmBr	HBr $\rightarrow$ HBr(aq)	k_exf(01,ind_HBr)	see general notes*
H72000b_a01	TrAa01MblScScmBr	HBr(aq) $\rightarrow$ HBr	k_exb(01,ind_HBr)	see general notes*
H72001f_a01	TrAa01MblScBr	HOBr $\rightarrow$ HOBr(aq)	k_exf(01,ind_HOBr)	see general notes*
H72001b_a01	TrAa01MblScBr	HOBr(aq) $\rightarrow$ HOBr	k_exb(01,ind_HOBr)	see general notes*
H73000_a01	TrAa01MblBrN	$N_2O_5 + Br^-$(aq) $\rightarrow BrNO_2 + NO_3^-$(aq)	k_exf_N2O5(01) * 3.E5	Behnke et al. (1994), Behnke et al. (1997)
H73001_a01	TrAa01MblBrN	$BrNO_3 \rightarrow$ HOBr(aq) + HNO_3(aq)	k_exf_BrNO3(01) * C(ind_H2O_a01)	see general notes*
H73002_a01	TrAa01MblBrN	$BrNO_3 + Br^-$(aq) $\rightarrow Br_2$(aq) + NO_3^-(aq)	k_exf_BrNO3(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_ClNO3(01) * 3.E5	see general notes*
H76002_a01	TrAa01MblBrClN	$BrNO_3 + Cl^-$(aq) $\rightarrow$ BrCl(aq) + NO_3^-(aq)	k_exf_BrNO3(01) * 5.E2	see general notes*
H80000f_a01	TrAa01ScI	$I_2 \rightarrow I_2$(aq)	k_exf(01,ind_I2)	see general notes*
H80000b_a01	TrAa01ScI	I_2(aq) $\rightarrow I_2$	k_exb(01,ind_I2)	see general notes*
H81000f_a01	TrAa01MblScI	IO $\rightarrow$ IO(aq)	k_exf(01,ind_IO)	see general notes*

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

#	labels	reaction	rate coefficient	reference
H81000b_a01	TrAa01MblScI	$IO(aq) \rightarrow IO$	k_exb(01,ind_IO)	see general notes*
H81001_a01	TrAa01I	$OIO \rightarrow HOI(aq) + HO_2(aq)$	k_exf(01,ind_OIO)	see general notes*
H81002_a01	TrAa01I	$I_2O_2 \rightarrow HOI(aq) + H^+(aq) + IO_2^-(aq)$	k_exf(01,ind_I2O2)	see general notes*
H82000f_a01	TrAa01MblScI	$HOI \rightarrow HOI(aq)$	k_exf(01,ind_HOI)	see general notes*
H82000b_a01	TrAa01MblScI	$HOI(aq) \rightarrow HOI$	k_exb(01,ind_HOI)	see general notes*
H82001_a01	TrAa01MblScI	$HI \rightarrow H^+(aq) + I^-(aq)$	$k_{\mathrm{mt}}(\mathrm{HI}) \cdot lwc$	see general notes*
H82002_a01	TrAa01ScI	$HIO_3 \rightarrow IO_3^-(aq) + H^+(aq)$	$k_{\mathrm{mt}}(\mathrm{HIO_3}) \cdot lwc$	see general notes*
H83000_a01	TrAa01IN	$INO_2 \rightarrow HOI(aq) + HONO(aq)$	k_exf(01,ind_INO2)	see general notes*
H83001_a01	TrAa01MblIN	$INO_3 \rightarrow HOI(aq) + HNO_3(aq)$	k_exf(01,ind_INO3)	see general notes*
H86000f_a01	TrAa01MblScClI	$ICl \rightarrow ICl(aq)$	k_exf(01,ind_ICl)	see general notes*
H86000b_a01	TrAa01MblScClI	$ICl(aq) \rightarrow ICl$	k_exb(01,ind_ICl)	see general notes*
H87000f_a01	TrAa01MblScBrI	$IBr \rightarrow IBr(aq)$	k_exf(01,ind_IBr)	see general notes*
H87000b_a01	TrAa01MblScBrI	$IBr(aq) \rightarrow IBr$	k_exb(01,ind_IBr)	see general notes*
H91000f_a01	TrAa01MblScScmS	$SO_2 \rightarrow SO_2(aq)$	k_exf(01,ind_SO2)	see general notes*
H91000b_a01	TrAa01MblScScmS	$SO_2(aq) \rightarrow SO_2$	k_exb(01,ind_SO2)	see general notes*
H92000_a01	TrAa01MblScScmS	$H_2SO_4 \rightarrow H_2SO_4(aq)$	xnom7sulf*k_exf(01,ind_H2SO4)	see general notes*
H94000f_a01	TrAa01CS	$DMSO \rightarrow DMSO(aq)$	k_exf(01,ind_DMSO)	see general notes*
H94000b_a01	TrAa01CS	$DMSO(aq) \rightarrow DMSO$	k_exb(01,ind_DMSO)	see general notes*
H94001_a01	TrAa01MblS	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	k_exf(01,ind_CH3SO3H)	see general notes*
H94002f_a01	TrAa01CS	$DMS \rightarrow DMS(aq)$	k_exf(01,ind_DMS)	see general notes*
H94002b_a01	TrAa01CS	$DMS(aq) \rightarrow DMS$	k_exb(01,ind_DMS)	see general notes*
H100000f_a01	TrAa01Hg	$Hg \rightarrow Hg(aq)$	k_exf(01,ind_Hg)	see general notes*
H100000b_a01	TrAa01Hg	$Hg(aq) \rightarrow Hg$	k_exb(01,ind_Hg)	see general notes*
H100100f_a01	TrAa01Hg	$HgO \rightarrow HgO(aq)$	k_exf(01,ind_HgO)	see general notes*
H100100b_a01	TrAa01Hg	$HgO(aq) \rightarrow HgO$	k_exb(01,ind_HgO)	see general notes*
H100600f_a01	TrAa01ClHg	$HgCl_2 \rightarrow HgCl_2(aq)$	k_exf(01,ind_HgCl2)	see general notes*
H100600b_a01	TrAa01ClHg	$HgCl_2(aq) \rightarrow HgCl_2$	k_exb(01,ind_HgCl2)	see general notes*
H100700f_a01	TrAa01BrHg	$HgBr_2 \rightarrow HgBr_2(aq)$	k_exf(01,ind_HgBr2)	see general notes*
H100700b_a01	TrAa01BrHg	$HgBr_2(aq) \rightarrow HgBr_2$	k_exb(01,ind_HgBr2)	see general notes*
H100701f_a01	TrAa01BrClHg	$ClHgBr \rightarrow ClHgBr(aq)$	k_exf(01,ind_ClHgBr)	see general notes*
H100701b_a01	TrAa01BrClHg	$ClHgBr(aq) \rightarrow ClHgBr$	k_exb(01,ind_ClHgBr)	see general notes*
H100702f_a01	TrAa01BrHg	$BrHgOBr \rightarrow BrHgOBr(aq)$	k_exf(01,ind_BrHgOBr)	see general notes*
H100702b_a01	TrAa01BrHg	$BrHgOBr(aq) \rightarrow BrHgOBr$	k_exb(01,ind_BrHgOBr)	see general notes*
H100703f_a01	TrAa01BrClHg	$ClHgOBr \rightarrow ClHgOBr(aq)$	k_exf(01,ind_ClHgOBr)	see general notes*
H100703b_a01	TrAa01BrClHg	$ClHgOBr(aq) \rightarrow ClHgOBr$	k_exb(01,ind_ClHgOBr)	see general notes*

General notes

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

For uptake of X (X = N_2O_5, $ClNO_3$, or $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\rm exf}(\mathrm{X}) = \frac{k_{\rm mt}(\mathrm{X}) \times \mathrm{LWC}}{[\mathrm{H_2O}] + 5 \times 10^2 [\mathrm{Cl^-}] + 3 \times 10^5 [\mathrm{Br^-}]}$$

Here, $k_{\rm mt}$ = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by $k_{\rm mt}$. 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 $[\mathrm{Cl^-}] > 0.1$ M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\mathrm{H_2O}]/[\mathrm{Cl^-}]$ is less than 5×10^2. The ratio $5\times10^2/3\times10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N_2O_5. Here, they are also used for $ClNO_3$ and $BrNO_3$.

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET300	StHetN	$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	`khet_St(ihs_N2O5_H2O)`	see general notes*
HET301	TrHetN	$N_2O_5 \rightarrow 2\ NO_3^-(cs) + 2\ H^+(cs)$	`khet_Tr(iht_N2O5)`	see general notes*
HET610	StHetCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_St(ihs_HOCl_HCl)`	see general notes*
HET620	StHetClN	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_St(ihs_ClNO3_HCl)`	see general notes*
HET621	StHetClN	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_St(ihs_ClNO3_H2O)`	see general notes*
HET622	StHetClN	$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	`khet_St(ihs_N2O5_HCl)`	see general notes*
HET710	StHetBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_St(ihs_HOBr_HBr)`	see general notes*
HET720	StHetBrN	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_St(ihs_BrNO3_H2O)`	see general notes*
HET740	StHetBrClN	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_St(ihs_ClNO3_HBr)`	see general notes*
HET741	StHetBrClN	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_St(ihs_BrNO3_HCl)`	see general notes*
HET742	StHetBrCl	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_St(ihs_HOCl_HBr)`	see general notes*
HET743	StHetBrCl	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_St(ihs_HOBr_HCl)`	see general notes*
HET1001	StTrHetHg	$Hg \rightarrow Hg(cs)$	`khet_Tr(iht_Hg) + khet_St(ihs_Hg)`	see general notes*
HET1002	StTrHetHg	$HgO \rightarrow Hg(cs)$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1003	StTrHetClHg	$HgCl \rightarrow Hg(cs) + LCHLORINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1004	StTrHetClHg	$HgCl_2 \rightarrow Hg(cs) + 2\ LCHLORINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1005	StTrHetBrHg	$HgBr \rightarrow Hg(cs) + LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1006	StTrHetBrHg	$HgBr_2 \rightarrow Hg(cs) + 2\ LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1007	StTrHetBrClHg	$ClHgBr \rightarrow Hg(cs) + LCHLORINE + LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1008	StTrHetBrHg	$BrHgOBr \rightarrow Hg(cs) + 2\ LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1009	StTrHetBrClHg	$ClHgOBr \rightarrow Hg(cs) + LCHLORINE + LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*

General notes

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

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ2100_a01	TrAa01Sc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ2101_a01	TrAa01MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ2102_a01	TrAa01Sc	$HO_3 \rightleftharpoons O_3^- + H^+$	4.4E-9		Staehelin et al. (1984)
EQ3200_a01	TrAa01MblScScmN	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ3201_a01	TrAa01ScN	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ3202_a01	TrAa01MblScScmN	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ3203_a01	TrAa01ScN	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5		Warneck (1999)
EQ4100_a01	TrAa01MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ4101_a01	TrAa01ScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4		Weast (1980)
EQ4150_a01	TrAa01Sc	$HCHO \rightleftharpoons HOCH_2OH$	4.11E-3	-3769	see note*
EQ4151_a01	TrAa01Sc	$HCO_3 \rightleftharpoons HCOHOHO_2$	1.08E1	-2936	see note*
EQ4200_a01	TrAraScScmC	$CH_3COOH \rightleftharpoons H^+ + CH_3COO^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4201_a01	TrAa01ScC	$CH_3C(O)OOH \rightleftharpoons CH_3COOO^- + H^+$	6.3E-9		Schuchmann and von Sonntag (1988)
EQ4202_a01	TrAa01ScC	$HOCH_2CO_3H \rightleftharpoons CH_2OHCO_2O^- + H^+$	6.3E-9		Schuchmann and von Sonntag (1988)*
EQ4203_a01	TrAa01ScC	$HOOCCOOH \rightleftharpoons H^+ + HOOCCOO^-$	5.6E-2		Martell (1977)
EQ4204_a01	TrAa01ScC	$HOOCCOO^- \rightleftharpoons H^+ + C_2O_4^{2-}$	5.4E-5		Martell (1977)
EQ4205_a01	TrAa01ScC	$HOOCH2CO2H \rightleftharpoons H^+ + CH_2OOHCO_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4206_a01	TrAa01ScC	$CH_2OOCOOH \rightleftharpoons H^+ + CH_2OOCO_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4207_a01	TrAa01ScC	$CHOOHOOCOOH \rightleftharpoons H^+ + CHOOHOOCO_2^-$	1.754E-5		Fisher and Barnes (1972)*
EQ4208_a01	TrAa01ScC	$HOCH_2CO_2H \rightleftharpoons H^+ + CH_2OHCO_2^-$	1.5E-4		Rumble (2020)
EQ4209_a01	TrAa01ScC	$CHOHOOCOOH \rightleftharpoons H^+ + CHOHOOCOO_2^-$	1.5E-4		Rumble (2020)*
EQ4210_a01	TrAa01ScC	$CHOCOOH \rightleftharpoons H^+ + CHOCOO^-$	1.754E-5		Fisher and Barnes (1972)
EQ4211_a01	TrAa01ScC	$COOHCO_3 \rightleftharpoons H^+ + CO_2^-CO_3$	1.754E-5		Fisher and Barnes (1972)
EQ4250_a01	TrAa01ScC	$CH_3CHO \rightleftharpoons CH_3CHOHOH$	1.22		Tur'yan (2000)
EQ4251_a01	TrAa01ScC	$CHOHOOCHO \rightleftharpoons CHOHOOCHOHOH$	1.57E1		see note*
EQ4252_a01	TrAa01ScC	$CH_2OHCHO \rightleftharpoons CH_2OHCHOHOH$	1.56E1		Doussin and Monod (2013)
EQ4253_a01	TrAa01ScC	$GLYOX \rightleftharpoons CHOCHOHOH$	3.5E2		Ervens and Volkamer (2010)
EQ4254_a01	TrAa01ScC	$CHOCHOHOH \rightleftharpoons CHOHOHCHOHOH$	2.0E2		Ervens and Volkamer (2010)
EQ4255_a01	TrAa01ScC	$CHOCOOH \rightleftharpoons CHOOHOHCOOH$	1.1E3		Doussin and Monod (2013)
EQ4256_a01	TrAa01ScC	$CHOCOO^- \rightleftharpoons CHOHOHCO_2^-$	6.6E1		Doussin and Monod (2013)
EQ4257_a01	TrAa01ScC	$CO_2^-CO_3 \rightleftharpoons CO2^-COHOHO_2$	6.6E1		see note*
EQ4258_a01	TrAa01ScC	$CH_2OOHCHO \rightleftharpoons HOOCH_2CHOHOH$	1.56E1		see note*
EQ4300_a01	TrAa01ScScmC	$CH_3COCOOH \rightleftharpoons H^+ + CH_3COCO2^-$	4.1E-3		Rumble (2020)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ4350_a01	TrAa01ScC	$CH_3C(O)CHO \rightleftharpoons CH_3COCHOHOH$	1.98E3		Doussin and Monod (2013)
EQ6000_a01	TrAa01Cl	$Cl_2^- \rightleftharpoons Cl + Cl^-$	7.3E-6		Yu (2004)
EQ6200_a01	TrAa01MblScScmCl	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ6201_a01	TrAa01ScCl	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8		Lax (1969)
EQ7000_a01	TrAa01Br	$Br_2^- \rightleftharpoons Br + Br^-$	2.54E-6	-2256	Liu et al. (2002)
EQ7200_a01	TrAa01MblScScmBr	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ7201_a01	TrAa01ScBr	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ7600_a01	TrAa01MblBrCl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ7601_a01	TrAa01MblBrCl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ7602_a01	TrAa01MblBrCl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ7603_a01	TrAa01MblBrCl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ8600_a01	TrAa01MblScClI	$ICl + Cl^- \rightleftharpoons ICl_2^-$	7.7E1		Wang et al. (1989)
EQ8700_a01	TrAa01MblScBrI	$IBr + Br^- \rightleftharpoons IBr_2^-$	2.9E2		Troy and Margerum (1991)
EQ8701_a01	TrAa01MblScBrClI	$ICl + Br^- \rightleftharpoons IBr + Cl^-$	3.3E2		see note*
EQ9200_a01	TrAa01MblScScmS	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ9201_a01	TrAa01MblScScmS	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ9202_a01	TrAa01MblScScmS	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ9203_a01	TrAa01MblScScmS	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ10200_a01	TrAa01Hg	$Hg^{2+} + OH^- \rightleftharpoons HgOH^+$	4.0E10		Ammann and Pöschl (2007)
EQ10201_a01	TrAa01Hg	$HgOH^+ + OH^- \rightleftharpoons Hg(OH)_2$	1.58E11		Ammann and Pöschl (2007)
EQ10600_a01	TrAa01ClHg	$Hg^{2+} + Cl^- \rightleftharpoons HgCl^+$	5.8E6		Ammann and Pöschl (2007)
EQ10601_a01	TrAa01ClHg	$HgCl^+ + Cl^- \rightleftharpoons HgCl_2$	2.5E6		Ammann and Pöschl (2007)
EQ10602_a01	TrAa01ClHg	$HgOH^+ + Cl^- \rightleftharpoons Hg(OH)Cl$	2.69E7		Ammann and Pöschl (2007)
EQ10700_a01	TrAa01BrHg	$Hg^{2+} + Br^- \rightleftharpoons HgBr^+$	1.1E9		Raofie and Ariya (2004)
EQ10701_a01	TrAa01BrHg	$HgBr^+ + Br^- \rightleftharpoons HgBr_2$	2.5E8		Raofie and Ariya (2004)
EQ10800_a01	TrAa01HgS	$Hg^{2+} + SO_3^{2-} \rightleftharpoons HgSO_3$	2.E13		van Loon et al. (2001)
EQ10801_a01	TrAa01HgS	$HgSO_3 + SO_3^{2-} \rightleftharpoons Hg(SO_3)_2^{2-}$	1.E10		van Loon et al. (2001)
EQ11200_a01	TrAa01Fe	$Fe^{3+} \rightleftharpoons FeOH^{2+} + H^+$	2.34E-3		de Laat and Le (2006)*
EQ11201_a01	TrAa01Fe	$FeOH^{2+} \rightleftharpoons Fe(OH)_2^+ + H^+$	2E-4		de Laat and Le (2006)*
EQ11202_a01	TrAa01Fe	$Fe^{3+} + H_2O_2 \rightleftharpoons FeHO_2^{2+} + H^+$	3.1E-3		de Laat and Le (2006)
EQ11203_a01	TrAa01Fe	$FeOH^{2+} + H_2O_2 \rightleftharpoons Fe(OH)(HO_2)^+ + H^+$	2E-4		de Laat and Le (2006)
EQ11600_a01	TrAa01ClFe	$Fe^{3+} + Cl^- \rightleftharpoons FeCl^{2+}$	6.61		de Laat and Le (2006)*
EQ11601_a01	TrAa01ClFe	$FeCl^{2+} + Cl^- \rightleftharpoons FeCl_2^+$	1.6		de Laat and Le (2006)*
EQ11800_a01	TrAa01FeS	$Fe^{3+} + SO_4^{2-} \rightleftharpoons FeSO_4^+$	120		Brand and van Eldik (1995)*

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ11801_a01	TrAa01FeS	$FeOH^{2+} + HSO_3^- \rightleftharpoons FeSO_3^+$	8.25E2		Warneck (2018)*
EQ11802_a01	TrAa01FeS	$Fe^{2+} + SO_3^- \rightleftharpoons FeSO_3^+$	1.6E7		Warneck (2018)

Specific notes

EQ4100_a01: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

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

EQ4151_a01: Assumed to be the same as for HCHO.

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

EQ4202_a01: Same as for CH3CO3H.

EQ4205_a01: Same as for CH3CO2H.

EQ4206_a01: Same as for CH3CO2H.

EQ4207_a01: Same as for CH3CO2H.

EQ4209_a01: Same as HOCH2CO2H.

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

EQ4257_a01: Assumed to be equal to CHOCO2m.

EQ4258_a01: Same as for $HOCH_2CHO$.

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

EQ8701_a01: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):

ICl	+	Br^-	$\rightleftharpoons$	IBr	+	Cl^-
-17.1		-103.96	=	-4.2		-131.228

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

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

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

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

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

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

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

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

EQ11801_a01: Rate of equilibration assumed.

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A10000_a01	TrAa01Sc	$O_3 + O_2^- \rightarrow O_3^- + O_2$	1.50E9		Staehelin et al. (1984)
A21000_a01	TrAa01Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10		Sehested et al. (1968)
A21001_a01	TrAa01Sc	$OH + OH \rightarrow H_2O_2$	5.5E9		Buxton et al. (1988)
A21002_a01	TrAa01Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900	Christensen and Sehested (1988)
A21003_a01	TrAa01Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9		Sehested et al. (1968)
A21004_a01	TrAa01Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500	Christensen and Sehested (1988)
A21005_a01	TrAa01Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684	Christensen et al. (1982)
A21006_a01	TrAa01Sc	$O_3 + OH \rightarrow HO_4$	1.10E8		Staehelin et al. (1984)
A21007_a01	TrAa01Sc	$O_3 + OH^- \rightarrow HO_2 + O_2^-$	7.00E1		Staehelin et al. (1984)
A21008_a01	TrAa01Sc	$HO_3 \rightarrow OH + O_2$	1.10E5		Staehelin et al. (1984)
A21009_a01	TrAa01Sc	$HO_4 \rightarrow HO_2 + O_2$	2.80E4		Staehelin et al. (1984)
A21010_a01	TrAa01Sc	$HO_4 + HO_4 \rightarrow H_2O_2 + 2\ O_3$	5.00E9		Staehelin et al. (1984)
A21011_a01	TrAa01Sc	$HO_4 + HO_3 \rightarrow H_2O_2 + O_3 + O_2$	5.00E9		Staehelin et al. (1984)
A31000_a01	TrAa01ScN	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950	Damschen and Martin (1983)
A31001_a01	TrAa01ScN	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8		Lee and Schwartz (1981)
A31002_a01	TrAa01ScN	$NO_4^- \rightarrow NO_2^-$	8.0E1		Warneck (1999)
A32000_a01	TrAa01ScN	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9		Warneck (1999)
A32001_a01	TrAa01ScN	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10		Wingenter et al. (1999)
A32002_a01	TrAa01ScN	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700	Exner et al. (1992)
A32003_a01	TrAa01ScN	$HONO + OH \rightarrow NO_2$	1.0E10		Barker et al. (1970)
A32004_a01	TrAa01ScN	$HONO + H_2O_2 + H^+ \rightarrow HNO_3 + H^+$	4.6E3	-6800	Damschen and Martin (1983)
A41000_a01	TrAa01Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8		Ross et al. (1992)
A41001_a01	TrAa01Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5		Ross et al. (1992)
A41002_a01	TrAa01Sc	$HCOO^- + CO_3^- \rightarrow 2\ HCO_3^- + HO_2$	1.5E5		Ross et al. (1992)
A41003_a01	TrAa01Sc	$HCOO^- + OH \rightarrow O_2^- + H_2O + CO_2$	3.1E9	-1240	Chin and Wine (1994)
A41004_a01	TrAa01ScN	$HCOO^- + NO_3 \rightarrow NO_3^- + H^+ + O_2^- + CO_2$	5.119E+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)
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)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A41012b_a01	TrAa01Sc	$CH_3OO + CH_3OO \rightarrow 2\ HOCH_2O_2$	0.80 × 2.145E+08	-2139	Herrmann et al. (1999b)
A41013a_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HOCH_2O_2 + H_2O$	0.93 × 9.70E8	-600	Elliot and McCracken (1989)*
A41013b_a01	TrAa01Sc	$CH_3OH + OH \rightarrow HCHO + HO_2 + H_2O$	0.07 × 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 × 6.30E8		Monod et al. (2007)*
A41016b_a01	TrAa01Sc	$CH_3OOH + OH \rightarrow HCHO + OH + H_2O$	0.75 × 6.30E8		Monod et al. (2007)*
A41017a_a01	TrAa01ScN	$CH_3OOH + NO_3 \rightarrow CH_3OO + NO_3^- + H^+$	0.25 × 4.90E6	-2000	see note*
A41017b_a01	TrAa01ScN	$CH_3OOH + NO_3 \rightarrow HCHO + HO_2 + NO_3^- + H^+$	0.75 × 4.90E6	-2000	see note*
A41018a_a01	TrAa01Sc	$CH_3OOH + CO_3^- \rightarrow CH_3OO + HCO_3^-$	0.25 × 4.30E5		see note*
A41018b_a01	TrAa01Sc	$CH_3OOH + CO_3^- \rightarrow HCHO + HO_2 + HCO_3^-$	0.75 × 4.30E5		see note*
A41019a_a01	TrAa01Sc	$HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$	0.25 × 6.30E8		see note*
A41019b_a01	TrAa01Sc	$HOCH_2OOH + OH \rightarrow CHOOOH + HO_2 + H_2O$	0.75 × 6.30E8		see note*
A41020a_a01	TrAa01ScN	$HOCH_2OOH + NO_3 \rightarrow HOCH_2O_2 + NO_3^- + H^+$	0.25 × 4.90E6	-2000	see note*
A41020b_a01	TrAa01ScN	$HOCH_2OOH + NO_3 \rightarrow CHOOOH + HO_2 + NO_3^- + H^+$	0.75 × 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*
A42000a_a01	TrAa01ScC	$CH_3CH_2OH + OH \rightarrow CH_3CHO + HO_2 + H_2O$	0.90 × 2.002E+09	-830	Monod et al. (2005)*
A42000b_a01	TrAa01ScC	$CH_3CH_2OH + OH \rightarrow CH_2OHCH_2OO + H_2O$	0.10 × 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 × 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 × 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 × 1.00E8		Piesiak et al. (1984)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42002b_a01	TrAa01ScC	CH_2OHCH_2OO + CH_2OHCH_2OO → CH_2OHCHO + ETHGLY	0.33 × 1.00E8		Piesiak et al. (1984)
A42002c_a01	TrAa01ScC	CH_2OHCH_2OO + CH_2OHCH_2OO → 2 $HOCH_2O_2$ + 2 HCHO	0.17 × 1.00E8		Piesiak et al. (1984)
A42003_a01	TrAa01ScC	CH_2OHCH_2OO + O_2^- → HYETHO2H + OH^-	1.0E8	-900	see note*
A42004_a01	TrAa01ScC	CH_2OHCH_2OO + HO_2 → HYETHO2H	9.7E5	-2500	see note*
A42005_a01	TrAa01ScC	HYETHO2H + OH → CH_2OHCHO	1.10E9		see note*
A42006_a01	TrAa01ScC	ETHGLY + OH → CH_2OHCHO + HO_2 + H_2O	1.657E+09	-1191	Hoffmann et al. (2009)*
A42007_a01	TrAa01ScCN	ETHGLY + NO_3 → CH_2OHCHO + HO_2 + NO_3^- + H^+	5.856E+06	-2117	Hoffmann et al. (2009)*
A42008_a01	TrAa01ScC	CH_3CHO + OH → CH_3COOO + H_2O	3.60E9		Schuchmann and von Sonntag (1988)
A42009_a01	TrAa01ScCN	CH_3CHO + NO_3 → CH_3COOO + NO_3^- + H^+	3.10E6		Rousse and George (2004)
A42010_a01	TrAa01ScC	CH_3COOO + CH_3COOO → CH_3OO + CH_3OO + CO_2 + CO_2	1.891E+08	1563	see note*
A42011_a01	TrAa01ScC	CH_3COOO + O_2^- → CH_3COOO^- + O_2	1.00E9		Schuchmann and von Sonntag (1988)
A42012_a01	TrAa01ScC	$CH_3CHOHOH$ + OH → $CH_3COHOHOO$ + H_2O	1.20E9		Schuchmann and von Sonntag (1988)
A42013_a01	TrAa01ScCN	$CH_3CHOHOH$ + NO_3 → $CH_3COHOHOO$ + NO_3^- + H^+	1.10E6		Rousse and George (2004)
A42014_a01	TrAa01ScC	$CH_3COHOHOO$ → CH_3COOH + HO_2	1.00E6		see note*
A42015a_a01	TrAa01ScC	CH_2OHCHO + OH → CH_2OHCO3 + H_2O	0.77 × 1.40E9		Doussin and Monod (2013)
A42015b_a01	TrAa01ScC	CH_2OHCHO + OH → CHOHOOCHO + H_2O	0.23 × 1.40E9		Doussin and Monod (2013)
A42016a_a01	TrAa01ScCN	CH_2OHCHO + NO_3 → CH_2OHCO3 + NO_3^- + H^+	0.77 × 3.10E6		see note*
A42016b_a01	TrAa01ScCN	CH_2OHCHO + NO_3 → CHOHOOCHO + NO_3^- + H^+	0.23 × 3.10E6		see note*
A42017_a01	TrAa01ScC	CH_2OHCO3 + O_2^- → $CH_2OHCO_2O^-$	1.00E9		see note*
A42018_a01	TrAa01ScC	$CH_2OHCOHOHO_2$ → $HOCH_2CO_2H$ + HO_2	1.00E6		see note*
A42019_a01	TrAa01ScC	CHOHOOCHO → GLYOX + HO_2	1.90E2		see note*
A42020_a01	TrAa01ScC	CHOHOOCHOHOH → CHOCHOHOH + HO_2	1.90E2		see note*
A42021a_a01	TrAa01ScC	$CH_2OHCHOHOH$ + OH → $CH_2OHCOHOHO_2$ + H_2O	0.33 × 1.10E9		Doussin and Monod (2013)
A42021b_a01	TrAa01ScC	$CH_2OHCHOHOH$ + OH → CHOHOOCHOHOH + H_2O	0.28 × 1.10E9		Doussin and Monod (2013)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42021c_a01	TrAa01ScC	$CH_2OHCHOHOH + OH \rightarrow HCOOH + HOCH_2O_2 + H_2O$	0.39 × 1.10E9		Doussin and Monod (2013)
A42022a_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow CH_2OHCOHOHO_2 + NO_3^- + H^+$	0.33 × 1.10E6		see note*
A42022b_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow CHOHOOCHOHOH + NO_3^- + H^+$	0.28 × 1.10E6		see note*
A42022c_a01	TrAa01ScCN	$CH_2OHCHOHOH + NO_3 \rightarrow HCOOH + HOCH_2O_2 + NO_3^- + H^+$	0.39 × 1.10E6		see note*
A42023a_a01	TrAa01ScC	$CHOHOHCHOHOH + OH \rightarrow CHOHOHCOHOHO_2 + H_2O$	0.27 × 1.114E+09	-1516	Buxton et al. (1997)
A42023b_a01	TrAa01ScC	$CHOHOHCHOHOH + OH \rightarrow HCOOH + HCOHOHO_2 + HO_2 + H_2O$	0.73 × 1.114E+09	-1516	Buxton et al. (1997)*
A42024a_a01	TrAa01ScCN	$CHOHOHCHOHOH + NO_3 \rightarrow CHOHOHCOHOHO_2 + NO_3^- + H^+$	0.27 × 1.00E6		see note*
A42024b_a01	TrAa01ScCN	$CHOHOHCHOHOH + NO_3 \rightarrow HCOOH + HCOHOHO_2 + HO_2 + NO_3^- + H^+$	0.73 × 1.00E6		see note*
A42025_a01	TrAa01ScC	$CHOHOHCOHOHO_2 \rightarrow CHOOHOHCOOH + HO_2$	0.77 × 1.00E6		see note*
A42026_a01	TrAa01ScC	$CH_3COOH + OH \rightarrow CH_2OOCOOH + H_2O$	1.50E7	-1330	Chin and Wine (1994)
A42027_a01	TrAa01ScCN	$CH_3COOH + NO_3 \rightarrow CH_2OOCOOH + NO_3^- + H^+$	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)
A42030a_a01	TrAa01ScC	C2H5OOH + OH → C2H5OO + H_2O	0.80 × 5.80E8		Monod et al. (2007)
A42030b_a01	TrAa01ScC	C2H5OOH + OH → $CH_3COOH + HO_2 + H_2O$	0.20 × 5.80E8		Monod et al. (2007)*
A42031a_a01	TrAa01ScC	C2H5OO + C2H5OO → $CH_3CHO + CH_3CHO + H_2O_2$	0.20 × 1.891E+08	1563	Herrmann et al. (1999b)
A42031b_a01	TrAa01ScC	C2H5OO + C2H5OO → 2 CH_3CHO + 2 HO_2	0.80 × 1.891E+08	1563	Herrmann et al. (1999b)*
A42032_a01	TrAa01ScC	C2H5OO + O_2^- → C2H5OOH + OH^-	1.0E8	-900	see note*
A42033_a01	TrAa01ScC	C2H5OO + HO_2 → C2H5OOH	9.7E5	-2500	see note*
A42034_a01	TrAa01ScC	$CH_2OOCOOH + HO_2$ → HOOCH2CO2H	9.7E5	-2500	see note*
A42035_a01	TrAa01ScC	$CH_2OOCOOH + O_2^- + H^+$ → HOOCH2CO2H	1.0E8	-900	see note*
A42036a_a01	TrAa01ScC	$CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOCOOH + CHOCOOH + H_2O_2$	0.30 × 7.50E7		Schuchmann et al. (1985)
A42036b_a01	TrAa01ScC	$CH_2OOCOOH + CH_2OOCOOH \rightarrow 2\ HCHO + 2\ CO_2 + H_2O_2$	0.30 × 7.50E7		Schuchmann et al. (1985)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42036c_a01	TrAa01ScC	$CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOCOOH + HOCH_2CO_2H$	0.30 × 7.50E7		Schuchmann et al. (1985)
A42036d_a01	TrAa01ScC	$CH_2OOCOOH + CH_2OOCOOH \rightarrow CHOHOOCOOH + CHOHOOCOOH$	0.10 × 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	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CHOCOO^- + H_2O_2$	0.30 × 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 × 7.50E7		Schuchmann et al. (1985)
A42039c_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow CHOCOO^- + CH_2OHCO_2^-$	0.30 × 7.50E7		Schuchmann et al. (1985)
A42039d_a01	TrAa01ScC	$CH_2OOCO_2^- + CH_2OOCO_2^- \rightarrow 2\ CHOHOOCOO_2^-$	0.10 × 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	$HOOCCOO^- + OH \rightarrow C_2O_4^- + H_2O$	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	$HOOCH2CO2H + OH \rightarrow CH_2OOCOOH + H_2O$	0.80 × 5.80E8		see note*
A42144b_a01	TrAa01ScC	$HOOCH2CO2H + OH \rightarrow CHOOHOOCOOH + H_2O$	0.20 × 5.80E8		see note*
A42145a_a01	TrAa01ScCN	$HOOCH2CO2H + NO_3 \rightarrow CH_2OOCOOH + NO_3^- + H^+$	0.80 × 1.70E6		Herrmann and Zellner (1998)
A42145b_a01	TrAa01ScCN	$HOOCH2CO2H + NO_3 \rightarrow CHOOHOOCOOH + NO_3^- + H^+$	0.20 × 1.70E6		Herrmann and Zellner (1998)
A42146a_a01	TrAa01ScC	$CH_2OOHCO_2^- + OH \rightarrow CH_2OOCO_2^- + H_2O$	0.80 × 5.80E8		see note*
A42146b_a01	TrAa01ScC	$CH_2OOHCO_2^- + OH \rightarrow CHOOHOOCO_2^- + H_2O$	0.20 × 5.80E8		see note*
A42147a_a01	TrAa01ScCN	$CH_2OOHCO_2^- + NO_3 \rightarrow CH_2OOCO_2^- + NO_3^- + H^+$	0.80 × 7.10E6		Herrmann and Zellner (1998)
A42147b_a01	TrAa01ScCN	$CH_2OOHCO_2^- + NO_3 \rightarrow CHOOHOOCO_2^- + NO_3^- + H^+$	0.20 × 7.10E6		Herrmann and Zellner (1998)
A42148_a01	TrAa01ScC	$CHOOHOOCOOH \rightarrow HOOCCOOH + HO_2$	1.90E2		see note*
A42149_a01	TrAa01ScC	$CHOOHOOCO_2^- \rightarrow HOOCCOO^- + HO_2$	1.90E2		see note*
A42150a_a01	TrAa01ScC	$HOCH_2CO_2H + OH \rightarrow CHOHOOCOOH + H_2O$	0.62 × 6.00E8		see note*
A42150b_a01	TrAa01ScC	$HOCH_2CO_2H + OH \rightarrow HCHO + CO_2 + HO_2 + H_2O$	0.38 × 6.00E8		see note*

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42151a_a01	TrAa01ScCN	$HOCH_2CO_2H + NO_3 \rightarrow CHOHOOCOOH + NO_3^- + H^+$	0.62 × 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 × 7.445E+05	-3969	see note*
A42152_a01	TrAa01ScC	$CHOHOOCOOH \rightarrow CHOCOOH + HO_2$	1.90E2		von Sonntag (1987)
A42153a_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow CHOHOOCOO_2^- + H_2O$	0.60 × 8.60E8		Buxton et al. (1988)
A42153b_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow HCHO + CO_2 + O_2^- + H_2O$	0.19 × 8.60E8		Buxton et al. (1988)
A42153c_a01	TrAa01ScC	$CH_2OHCO_2^- + OH \rightarrow HOCH_2O_2 + CO_2 + OH^-$	0.21 × 8.60E8		Buxton et al. (1988)
A42154a_a01	TrAa01ScCN	$CH_2OHCO_2^- + NO_3 \rightarrow CHOHOOCOO_2^- + NO_3^- + H^+$	0.76 × 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 × 7.502E+06	-3007	Gaillard de Sémainville et al. (2007)
A42155_a01	TrAa01ScC	$CHOHOOCOO_2^- \rightarrow CHOCOO^- + HO_2$	1.90E2		von Sonntag (1987)
A42156a_a01	TrAa01ScC	$CHOOHOHCOOH + OH \rightarrow COOHCOHOHO_2 + H_2O$	0.15 × 2.830E+08	-1000	Ervens et al. (2003)
A42156b_a01	TrAa01ScC	$CHOOHOHCOOH + OH \rightarrow HCOOH + CO_2 + HO_2 + H_2O$	0.85 × 2.830E+08	-1000	Ervens et al. (2003)*
A42157a_a01	TrAa01ScCN	$CHOOHOHCOOH + NO_3 \rightarrow COOHCOHOHO_2 + NO_3^- + H^+$	0.15 × 1.00E6		see note*
A42157b_a01	TrAa01ScCN	$CHOOHOHCOOH + NO_3 \rightarrow HCOOH + CO_2 + HO_2 + NO_3^- + H^+$	0.85 × 1.00E6		see note*
A42158a_a01	TrAa01ScC	$CHOHOHCO_2^- + OH \rightarrow CO2^-COHOHO_2 + H_2O$	0.26 × 3.271E+09	-4300	Ervens et al. (2003)
A42158b_a01	TrAa01ScC	$CHOHOHCO_2^- + OH \rightarrow HCOOH + CO_2 + O_2^- + H_2O$	0.74 × 3.271E+09	-4300	Ervens et al. (2003)
A42159a_a01	TrAa01ScCN	$CHOHOHCO_2^- + NO_3 \rightarrow CO2^-COHOHO_2 + NO_3^- + H^+$	0.26 × 1.80E5		Herrmann and Zellner (1998)
A42159b_a01	TrAa01ScCN	$CHOHOHCO_2^- + NO_3 \rightarrow HCOOH + CO_2 + O_2^- + NO_3^- + H^+$	0.74 × 1.80E5		Herrmann and Zellner (1998)
A42160_a01	TrAa01ScC	$CHOHOHCO_2^- + H_2O_2 \rightarrow HCOO^- + CO_2 + H_2O + H_2O$	1.10E-1		Schöne and Herrmann (2014)
A42161_a01	TrAa01ScC	$COOHCOHOHO_2 \rightarrow HOOCCOOH + HO_2$	1.00E6		see note*
A42162_a01	TrAa01ScC	$CO2^-COHOHO_2 \rightarrow HOOCCOO^- + HO_2$	1.00E6		see note*
A42163a_a01	TrAa01ScC	$CH_2OOHCHO + OH \rightarrow HCHO + CO + OH + H_2O$	0.77 × 1.40E9		see note*
A42163b_a01	TrAa01ScC	$CH_2OOHCHO + OH \rightarrow GLYOX + HO_2 + H_2O$	0.23 × 1.40E9		see note*

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A42164a_a01	TrAa01ScCN	$CH_2OOHCHO + NO_3 \rightarrow HCHO + CO + NO_3 + H_2O$	0.77 × 3.10E6		see note*
A42164b_a01	TrAa01ScCN	$CH_2OOHCHO + NO_3 \rightarrow GLYOX + NO_3^- + H_2O + H^+$	0.23 × 3.10E6		see note*
A42165a_a01	TrAa01ScC	$HOOCH_2CHOHOH + OH \rightarrow HOOCH2CO2H + HO_2 + H_2O$	0.33 × 1.10E9		see note*
A42165b_a01	TrAa01ScC	$HOOCH_2CHOHOH + OH \rightarrow CHOCHOHOH + OH + H_2O$	0.28 × 1.10E9		see note*
A42165c_a01	TrAa01ScC	$HOOCH_2CHOHOH + OH \rightarrow HCOOH + HCHO + OH + H_2O$	0.39 × 1.10E9		see note*
A42166a_a01	TrAa01ScCN	$HOOCH_2CHOHOH + NO_3 \rightarrow HOOCH2CO2H + NO_3^- + H_2O + H^+$	0.33 × 1.10E6		see note*
A42166b_a01	TrAa01ScCN	$HOOCH_2CHOHOH + NO_3 \rightarrow CHOCHOHOH + NO_3 + H_2O$	0.28 × 1.10E6		see note*
A42166c_a01	TrAa01ScCN	$HOOCH_2CHOHOH + NO_3 \rightarrow HCOOH + HCHO + NO_3 + H_2O$	0.39 × 1.10E6		see note*
A42167_a01	TrAa01ScC	$HOCH_2OH + HOCH_2OH \rightarrow MG2 + H_2O$	see note	see note	Hahnenstein et al. (1995)*
A42168_a01	TrAa01ScC	$MG2 + H_2O \rightarrow HOCH_2OH + HOCH_2OH$	see note	see note	Hahnenstein et al. (1995)
A42169_a01	TrAa01ScC	$MG2 + OH \rightarrow HMF + HO_2$	1.54E9	-1020	see note*
A42470_a01	TrAa01ScC	$CH_3COOO + H_2O \rightarrow CH_3COOH + HO_2$	7.0E5		Villalta et al. (1996)
A42471_a01	TrAa01ScC	$CH_2OHCO3 + H_2O \rightarrow HOCH_2CO_2H + HO_2$	7.0E5		see note*
A42472_a01	TrAa01ScC	$CHOCO_3 + H_2O \rightarrow CHOCOOH + HO_2$	7.0E5		see note*
A42473_a01	TrAa01ScC	$COOHCO_3 + H_2O \rightarrow HOOCCOOH + HO_2$	7.0E5		see note*
A43000a_a01	TrAa01ScC	$CH_3COCHOHOH + OH \rightarrow CH_3COCOOH + HO_2$	0.29 × 9.215E+08	-1235	Schaefer et al. (2015)*
A43000b_a01	TrAa01ScC	$CH_3COCHOHOH + OH \rightarrow HCOOH + CH_3COOO$	0.71 × 9.215E+08	-1235	Schaefer et al. (2015)
A43001_a01	TrAa01ScCN	$CH_3COCHOHOH + NO_3 \rightarrow CH_3COCOOH + NO_3^- + H^+$	4.539E+06	-4213	Schaefer et al. (2015)*
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)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A43008a_a01	TrAa01ScC	$CH_3COCH_2O_2 + CH_3COCH_2O_2 \rightarrow CH_3COCH_2OH + CH_3C(O)CHO$	0.20 × 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 × 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 × 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 × 4.00E8		Zegota et al. (1986)
A43010a_a01	TrAa01ScC	$CH_3COCH_2OH + OH \rightarrow CH_3COCHOHO_2$	0.85 × 5.10E8		Doussin and Monod (2013)*
A43010b_a01	TrAa01ScC	$CH_3COCH_2OH + OH \rightarrow HCHO + CH_3COOO$	0.15 × 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*
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)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A44002_a01	TrAa01ScC	MVK + OH → $CH_3COCHO_2CH_2OH$	7.117E+09	-1443	Schöne and Herrmann (2014)
A44003_a01	TrAa01ScC	$CH_3COCHO_2CH_2OH$ + $CH_3COCHO_2CH_2OH$ → 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 → GOLIG1 + H_2O	1.00E2		Ervens and Volkamer (2010)
A44005_a01	TrAa01ScC	GOLIG1 + H_2O → GLYOX + CHOCHOHOH	1.00E-1		Ervens and Volkamer (2010)
A44006_a01	TrAa01ScC	CHOCHOHOH + CHOCHOHOH → GOLIG2 + H_2O	1.00E2		Ervens and Volkamer (2010)
A44007_a01	TrAa01ScC	GOLIG2 + H_2O → CHOCHOHOH + CHOCHOHOH	1.00E-1		Ervens and Volkamer (2010)
A44008_a01	TrAa01ScC	CHOHOHCHOHOH + CHOCHOHOH → GOLIG3 + H_2O	1.00E2		Ervens and Volkamer (2010)
A44009_a01	TrAa01ScC	GOLIG3 + H_2O → CHOHOHCHOHOH + CHOCHOHOH	1.00E-1		Ervens and Volkamer (2010)
A44010_a01	TrAa01ScC	GOLIG1 + OH → GOLIGO1 + HO_2	1.610E+09	-1516	see note*
A44011_a01	TrAa01ScC	GOLIG2 + OH → GOLIGO2 + HO_2	1.610E+09	-1516	see note*
A44012_a01	TrAa01ScC	GOLIG3 + OH → GOLIGO3 + HO_2	1.610E+09	-1516	see note*
A46000_a01	TrAa01ScC	$CH_3C(O)CHO$ + $CH_3COCHOHOH$ → $CH_3COCHOHOCHOHCOCH_3$ + H_2O	1.00E2		Ervens and Volkamer (2010)*
A46001_a01	TrAa01ScC	$CH_3COCHOHOCHOHCOCH_3$ + H_2O → $CH_3COCHOHOH$ + $CH_3C(O)CHO$	1.00E-1		Ervens and Volkamer (2010)*
A46002_a01	TrAa01ScC	$CH_3COCHOHOCHOHCOCH_3$ + OH → $CH_3COCOHOCOHCOCH_3$ + HO_2	1.303E+09	-1235	see note*
A46003_a01	TrAa01ScC	$CH_3COCHOHOH$ + $CH_3COCHOHOH$ → $CH_3COCHOHOCOHC_3CHOHOH$ + H_2O	1.00E2		Ervens and Volkamer (2010)*
A46004_a01	TrAa01ScC	$CH_3COCHOHOCOHC_3CHOHOH$ + H_2O → 2 $CH_3COCHOHOH$	1.00E-1		Ervens and Volkamer (2010)*
A46005_a01	TrAa01ScC	$CH_3COCHOHOCOHC_3CHOHOH$ + OH → $CH_3COCOHOCOHC_3COHOH$ + HO_2	1.303E+09	-1235	see note*
A60000_a01	TrAa01Cl	Cl + Cl → Cl_2	8.8E7		Wu et al. (1980)
A60001_a01	TrAa01Cl	Cl_2^- + Cl_2^- → Cl_2 + 2 Cl^-	3.5E9		Yu (2004)
A61000_a01	TrAa01Cl	Cl^- + O_3 → ClO^-	3.0E-3		Hoigné et al. (1985)
A61001_a01	TrAa01Cl	Cl_2 + O_2^- → Cl_2^-	1.0E9		Bjergbakke et al. (1981)
A61002_a01	TrAa01Cl	Cl_2^- + O_2^- → 2 Cl^-	1.0E9		Jacobi (1996)*

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

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

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

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

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A92003_a01	TrAa01ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A92004_a01	TrAa01ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)
A92005_a01	TrAa01ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note*
A92006_a01	TrAa01MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A92007_a01	TrAa01ScS	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A92008_a01	TrAa01ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note*
A92009_a01	TrAa01MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A92010_a01	TrAa01ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A92011_a01	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75\ SO_4^- + .75\ SO_4^{2-} + .75\ H^+ + .25\ SO_3^- + .25\ HSO_5^-$	1.0E5		Huie and Neta (1987)
A92012_a01	TrAa01ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2\ HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988)
A93001_a01	TrAa01ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A93002_a01	TrAa01ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Løgager et al. (1993)
A93004_a01	TrAa01ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A93005_a01	TrAa01ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A94100_a01	TrAa01ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)*
A94101_a01	TrAa01ScS	$SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A94102_a01	TrAa01ScS	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	4.3E-1		Boyce and Hoffmann (1984)*
A94103_a01	TrAa01ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A94104_a01	TrAa01ScS	$HSO_3^- + CH_3OO \rightarrow SO_3^- + CH_3OOH$	5.00E5		Herrmann et al. (1999b)
A94105_a01	TrAa01ScS	$SO_4^- + HCOO^- \rightarrow SO_4^{2-} + CO_2 + HO_2$	1.7E8	-1500	Jacob (1986)
A94106_a01	TrAa01ScS	$SO_4^- + HCOOH \rightarrow SO_4^{2-} + CO_2 + H^+ + HO_2$	1.7E8	-1500	Jacob (1986)
A94107_a01	TrAa01ScS	$SO_4^- + CH_3OH \rightarrow SO_4^{2-} + HOCH_2O_2 + H^+$	9.039E+06	-2190	Clifton and Huie (1989)
A94108a_a01	TrAa01ScS	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + CH_3OO + H^+$	0.25 × 1.20E7		see note*
A94108b_a01	TrAa01ScS	$SO_4^- + CH_3OOH \rightarrow SO_4^{2-} + HCHO + HO_2 + H^+$	0.75 × 1.20E7		see note*
A94109_a01	TrAa01ScS	$SO_4^- + HOCH_2OH \rightarrow SO_4^{2-} + HCOHOHO_2 + H^+$	1.40E7	-1300	Buxton et al. (1990)
A94110_a01	TrAa01ScS	$SO_5^- + HCOO^- \rightarrow HSO_5^- + CO_2 + O_2^-$	1.4E4	-4000	Jacob (1986)
A94111_a01	TrAa01ScS	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A94200_a01	TrAa01ScCS	$HSO_3^- + CH_2OOCOOH \rightarrow SO_3^- + HOOCH2CO2H$	5.00E5		see note*
A94201_a01	TrAa01ScCS	$HSO_3^- + CH_2OOCO_2^- \rightarrow SO_3^- + CH_2OOHCO_2^-$	5.00E5		see note*
A94202a_a01	TrAa01ScCS	$SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_3CHO + HO_2 + H^+$	0.90 × 4.236E+07	-1750	Clifton and Huie (1989)*
A94202b_a01	TrAa01ScCS	$SO_4^- + CH_3CH_2OH \rightarrow SO_4^{2-} + CH_2OHCH_2OO + H^+$	0.10 × 4.236E+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	$SO_4^- + CHOHOHCHOHOH \rightarrow SO_4^{2-} + CHOHOHCOHOHO_2 + H^+$	0.27 × 2.40E7		George et al. (2001)
A94203b_a01	TrAa01ScCS	$SO_4^- + CHOHOHCHOHOH \rightarrow SO_4^{2-} + HCOHOHO_2 + HCOOH + HO_2 + H^+$	0.73 × 2.40E7		George et al. (2001)*
A94204_a01	TrAa01ScCS	$SO_4^- + CH_3COO^- \rightarrow SO_4^{2-} + CH_2OOCO_2^- + H^+$	5.10E6		Huie and Clifton (1990)
A94205_a01	TrAa01ScCS	$SO_4^- + HOOCCOO^- \rightarrow SO_4^{2-} + C_2O_4^- + H^+$	1.70E6		Grgić et al. (2007)
A94206_a01	TrAa01ScCS	$SO_4^- + C_2O_4^{2-} \rightarrow SO_4^{2-} + C_2O_4^-$	1.30E7		Grgić et al. (2007)
A96000_a01	TrAa01ClS	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2\ Cl^-$	6.2E7		Jacobi et al. (1996)
A96001_a01	TrAa01MblClS	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A96002_a01	TrAa01ClS	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A96003_a01	TrAa01ClS	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A96004_a01	TrAa01ClS	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2\ Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A96005_a01	TrAa01MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A96006_a01	TrAa01ClS	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A97000_a01	TrAa01BrS	$SO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + SO_3^-$	2.2E8	-649	Shoute et al. (1991)
A97001_a01	TrAa01BrS	$SO_3^{2-} + BrO^- \rightarrow Br^- + SO_4^{2-}$	1.0E8		Troy and Margerum (1991)
A97002_a01	TrAa01MblBrS	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A97003_a01	TrAa01BrS	$SO_4^- + Br^- \rightarrow Br + SO_4^{2-}$	2.1E9		Jacobi (1996)
A97004_a01	TrAa01BrS	$HSO_3^- + Br_2^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	6.3E7	-782	Shoute et al. (1991)
A97005_a01	TrAa01MblBrS	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note*
A97006_a01	TrAa01BrS	$HSO_5^- + Br^- \rightarrow HOBr + SO_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)
A98000_a01	TrAa01IS	$HSO_3^- + I_2 \rightarrow 2\ I^- + HSO_4^- + 2\ H^+$	1.7E9		Yiin and Margerum (1990)
A101000_a01	TrAa01Hg	$Hg + O_3 \rightarrow HgO + O_2$	4.7E7		Munthe (1992)
A102000_a01	TrAa01Hg	$HgO + H^+ \rightarrow Hg^{2+} + OH^-$	1.0E10		Pleijel and Munthe (1995)
A102001_a01	TrAa01Hg	$Hg + OH \rightarrow Hg^+ + OH^-$	2.0E9		Lin and Pehkonen (1997)
A102002_a01	TrAa01Hg	$Hg^+ + OH \rightarrow Hg^{2+} + OH^-$	1.0E10		Lin and Pehkonen (1997)
A102003_a01	TrAa01Hg	$Hg^{2+} + HO_2 \rightarrow Hg^+ + O_2 + H^+$	1.7E4		Enami et al. (2007)
A102004_a01	TrAa01Hg	$Hg^+ + HO_2 \rightarrow Hg + O_2 + H^+$	1.0E10		Lin and Pehkonen (1997)
A106000_a01	TrAa01ClHg	$Hg + HOCl \rightarrow Hg^{2+} + Cl^- + OH^-$	2.09E6		Lin and Pehkonen (1998)
A106001_a01	TrAa01ClHg	$Hg + ClO^- \rightarrow Hg^{2+} + Cl^- + 2\ OH^-$	1.99E6		Lin and Pehkonen (1998)
A107000_a01	TrAa01BrHg	$Hg + HOBr \rightarrow Hg^{2+} + Br^- + OH^-$	0.279		Wang and Pehkonen (2004)
A107001_a01	TrAa01BrHg	$Hg + BrO^- \rightarrow Hg^{2+} + Br^- + 2\ OH^-$	0.273		Wang and Pehkonen (2004)
A107002_a01	TrAa01BrHg	$Hg + Br_2 \rightarrow Hg^{2+} + 2\ Br^-$	0.196		Wang and Pehkonen (2004)
A109000_a01	TrAa01HgS	$HgSO_3 \rightarrow Hg + HSO_4^- + H^+$	0.0106		van Loon et al. (2000)

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

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A111001_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + HO2^- + OH^-$	1E7		de Laat and Le (2006)
A111002_a01	TrAa01Fe	$Fe^{3+} + O_2^- \rightarrow O_2 + Fe^{2+}$	5E7		de Laat and Le (2006)
A111003_a01	TrAa01Fe	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	8.2E5		Løgager et al. (1992)
A112001a_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow Fe^{3+} + OH^-$	2.7E8		de Laat and Le (2006)
A112001b_a01	TrAa01Fe	$FeOH^+ + OH \rightarrow Fe^{3+} + 2\ OH^-$	2.7E8		de Laat and Le (2006)
A112002a_a01	TrAa01Fe	$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + OH + OH^-$	5.5E1		de Laat and Le (2006)
A112002b_a01	TrAa01Fe	$FeOH^+ + H_2O_2 \rightarrow Fe^{3+} + OH + 2\ OH^-$	5.9E6		de Laat and Le (2006)
A112003_a01	TrAa01Fe	$FeHO_2^{2+} \rightarrow Fe^{2+} + HO_2$	2.3E-3		de Laat and Le (2006)
A112004_a01	TrAa01Fe	$Fe(OH)(HO_2)^+ \rightarrow Fe^{2+} + HO_2 + OH^-$	2.3E-3		de Laat and Le (2006)
A112006_a01	TrAa01Fe	$Fe^{2+} + HO_2 \rightarrow Fe^{3+} + HO2^-$	1.2E6		de Laat and Le (2006)
A112008a_a01	TrAa01Fe	$FeOH^{2+} + O_2^- \rightarrow Fe^{2+} + O_2 + OH^-$	1.5E8		Rush and Bielski (1985)
A112008b_a01	TrAa01Fe	$Fe(OH)_2^+ + O_2^- \rightarrow Fe^{2+} + O_2 + 2\ OH^-$	1.5E8		Rush and Bielski (1985)
A112009_a01	TrAa01Fe	$Fe^{2+} + O_2^- \rightarrow Fe^{3+} + H_2O_2 + 2\ OH^-$	1.0E7		Rush and Bielski (1985)
A112010_a01	TrAa01Fe	$Fe^{2+} + OH \rightarrow FeOH^{2+}$	4.3E8		Christensen and Sehested (1981)
A112011_a01	TrAa01Fe	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^-$	9.5E3		Løgager et al. (1992)
A112012_a01	TrAa01Fe	$FeO^{2+} \rightarrow Fe^{3+} + OH + OH^-$	1.3E-2		Løgager et al. (1992)
A112013_a01	TrAa01Fe	$FeO^{2+} + HO_2 \rightarrow Fe^{3+} + O_2 + OH^-$	2.0E6		Løgager et al. (1992)
A112014_a01	TrAa01Fe	$FeO^{2+} + OH \rightarrow Fe^{3+} + HO2^-$	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	$FeCl^+ + HO_2 \rightarrow Fe^{3+} + Cl^- + HO2^-$	1.2E6		de Laat and Le (2006)
A116003b_a01	TrAa01ClFe	$FeCl^+ + O_2^- \rightarrow Fe^{3+} + Cl^- + HO2^- + OH^-$	1E7		de Laat and Le (2006)
A116004a_a01	TrAa01ClFe	$FeCl^{2+} + HO_2 \rightarrow Fe^{2+} + Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A116004b_a01	TrAa01ClFe	$FeCl_2^+ + HO_2 \rightarrow Fe^{2+} + 2\ Cl^- + O_2 + H^+$	2E4		de Laat and Le (2006)
A116004c_a01	TrAa01ClFe	$FeCl^{2+} + O_2^- \rightarrow Fe^{2+} + Cl^- + O_2$	5E7		de Laat and Le (2006)
A116004d_a01	TrAa01ClFe	$FeCl_2^+ + O_2^- \rightarrow Fe^{2+} + 2\ Cl^- + O_2$	5E7		de Laat and Le (2006)
A116005_a01	TrAa01ClFe	$FeO^{2+} + Cl^- \rightarrow Fe^{3+} + Cl + 2\ OH^-$	1E2		Jacobsen et al. (1998)*

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

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

Specific notes

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

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

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

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

A41017b_a01: See branch a.

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

A41018b_a01: See branch a.

A41019a_a01: Branching ratio as for CH_3OOH + OH

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

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

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

A41021_a01: HO_2 elimination

A41022_a01: $k(HO_2+HO_2)$

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

A41030_a01: HO_2 elimination

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

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

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

A42004_a01: $k(HO_2+HO_2)$

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

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

A42007_a01: $CH_2OHCHOHO_2$ is assumed to directly decompose into $HOCH_2CHO$ + HO_2

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

A42014_a01: HO_2 elimination

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

A42016b_a01: See branch a.

A42017_a01: $k(CH_3CHOHOH+O_2^-)$

A42018_a01: HO_2 elimination

A42019_a01: k based on von Sonntag (1987)

A42020_a01: k based on von Sonntag (1987)

A42022a_a01: $k(CH_3CHOHOH+NO_3)$

A42022b_a01: See branch a.

A42022c_a01: See branch a.

A42023b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + HO_2

A42024a_a01: k based on Neta and Huie (1986)

A42024b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + HO_2

A42025_a01: HO_2 elimination

A42030b_a01: $CH_3CHOOHO_2$ is assumed to directly decompose into CH_3CO_2H and HO_2

A42031b_a01: CH_3CHOHO_2 is assumed to directly decompose into CH_3CHO + HO_2

A42032_a01: $k(HO_2+O_2^-)$

A42033_a01: $k(HO_2+HO_2)$

A42034_a01: $k(HO_2+HO_2)$

A42035_a01: $k(HO_2+O_2^-)$

A42037_a01: $k(HO_2+HO_2)$

A42038_a01: $k(HO_2+O_2^-)$

A42144a_a01: k assumed to be the same as C_2H_5OOH + OH based on Monod et al. (2007)

A42144b_a01: See branch a.

A42146a_a01: k assumed to be the same as C_2H_5OOH + OH based on Monod et al. (2007)

A42146b_a01: See branch a.

A42148_a01: HO_2 elimination

A42149_a01: HO_2 elimination

A42150a_a01: COOHOO is not formed but directly dissociates into CO_2 + HO_2. Rate coefficient based on Buxton et al. (1988)

A42150b_a01: See branch a.

A42151a_a01: COOHOO is not formed but directly dissociates into CO_2 + HO_2. 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 CO_2 + HO_2.

A42157a_a01: $k(CHOHOHCHOHOH+NO_3)$

A42157b_a01: COOHOO is not formed but directly dissociates into CO_2 + HO_2

A42161_a01: HO_2 elimination

A42162_a01: HO_2 elimination

A42163a_a01: $k(HOCH_2CHO + OH)$

A42163b_a01: See branch a.

A42164a_a01: $k(HOCH_2CHO+NO_3)$

A42164b_a01: See branch a.

A42165a_a01: $k(HOCH_2CHOHOH+OH)$

A42165b_a01: See branch a.

A42165c_a01: See branch a.

A42166a_a01: $k(HOCH_2CHOHOH+NO_3)$

A42166b_a01: See branch a.

A42166c_a01: See branch a.

A42167_a01: pH-dependent

A42169_a01: $k = 2 \times k(HOCH_2OH+OH)$

A42471_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

A42472_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

A42473_a01: Assumed to be the same as CH3CO3 + H2O, following Villalta et al. (1996)

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

A43001_a01: $CH(OH)_2COCH_2O_2$ neglected

A43002_a01: CO_2 added for mass balance intermediate reactions neglected

A43004_a01: CO_2 added for mass balance intermediate reactions neglected

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

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

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

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

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

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

A43017_a01: k from $CH_3O_2 + HO_2$

A43018_a01: k from $CH_3O_2 + O_2^-$

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

A43019b_a01: k calculated comparing $CH3OH + OH$ / $CH3OOH + OH$ with $ACETOL + OH$ / $HYPERCET + OH$

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

A43021_a01: k from $CH_3O_2 + HO_2$

A43022_a01: k from $CH_3O_2 + O_2^-$

A43023_a01: pH-dependent

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

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

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

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

A46000_a01: Assumed to be the same as for glyoxal

A46001_a01: Assumed to be the same as for glyoxal

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

A46003_a01: Assumed to be the same as for glyoxal

A46004_a01: Assumed to be the same as for glyoxal

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

A61002_a01: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A63001_a01: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

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

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

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

A91005_a01: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A91006_a01: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, SO_4^{2-} is used as a proxy and the second sulfur atom is put into the lumped LSULFUR.

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

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

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

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

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

A94108b_a01: See branch a.

A94200_a01: $k(CH_3OO+HSO_3^-)$

A94201_a01: $k(CH_3OO+HSO_3^-)$

A94202a_a01: CH_3CHOHO_2 is assumed to directly decompose into CH_3CHO + HO_2

A94203b_a01: $CHOHOHO_2$ directly decomposes into HCOOH + HO_2

A96005_a01: Assumed to be the same as for SO_3^{2-} + HOCl.

A97005_a01: Assumed to be the same as for SO_3^{2-} + HOBr.

A116005_a01: products assumed

A119001_a01: products assumed

A119002_a01: products assumed

A119004_a01: Assumed. Note that CAPRAM 2.4 lists k=4.3E7 from Herrmann Air Pollution Research Report 57 and it also lists k= 2.65E7 from Williams PhD 1996 http://lib.leeds.ac.uk/record=b1835184~S5. Brand and van Eldik (1995) also list k=3.56E4 from Waygood EUROTRAC 1992 report.

A119006_a01: 3E8*6500/(48000+6500)

A119008_a01: Assuming that the intermediate $S_2O_6^{2-}$ dissociates quickly.

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