S1 Initial values in the CAABA/MECCA box model

Compound	Initial value in ppbv
nC_4H_{10}	0.2
NH_3	8
C_2H_6	0.9
C_3H_8	0.5
iC_4H_{10}	0.09
C_2H_2	0.3
Toluene	0.1
CH_3CO_3H	0.04
Benzene	0.05
CH_4	1800
Xylenes	0.09
Ethylbenzene	0.01
Trimethylbenzenes	0.009
$C_{11}H_{14}$ (LHAROM)	0.008
CH_3CO_2H	0.3
CH_3CN	0.01
PAN	0.2
CH_3OOH	0.25
HCN	0.07
MBO	0.002
Methylpropene	0.006
β-Pinene	0.03
Sabinene	0.006
Camphene	0.005

Compound	Initial value in ppbv
α-Pinene	0.025
Carene	0.004
HONO	0.009
cBut-2-ene	0.004
tBut-2-ene	0.003
CH_3OH	3
Styrene	0.003
H_2O_2	1.8
CH_3COCH_3	1
C_5H_8	0.5
HNO_3	0.8
Hydroxyacetone (Acetol)	0.35
Glyoxal	0.06
Methylglyoxal	0.1
CH_3CHO	0.4
$HOCH_2CHO$	0.25
HCOOH	0.25
CO	100
O_3	50
NO_2	2
NO	0.4
HCHO	2
O_2	2.1×10^8
N_2	7.8×10^8
CO_2	4×10^5

S2 Mechanism of MECCA

The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs7`

MECCA version: `3.8`

Date: February 9, 2016.

Selected reactions:
"`!Ara`"

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase:	699
Aqueous phase:	89
All species:	788

Number of reactions in selected mechanism:

Gas phase (Gnnn):	1789
Aqueous phase (Annn):	145
Henry (Hnnn):	93
Photolysis (Jnnn):	384
Aqueous phase photolysis (PHnnn):	2
Heterogeneous (HETnnn):	21
Equilibria (EQnn):	68
Isotope exchange (IEXnnn):	0
Tagging equations (TAGnnn):	0
Dummy (Dnn):	1
All equations:	2503

This document is part of the electronic supplement to our article "The atmospheric chemistry box model CAABA/MECCA-3.0" in Geosci. Model Dev. (2011), available at:
`http://www.geosci-model-dev.net`

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)	Sander et al. (2011)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4))*cair	Sander et al. (2011)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2\ O_2$	1.2E-10	Sander et al. (2011)*
G1002b	UpG	$O_3 + O(^1D) \rightarrow O_2 + 2\ O(^3P)$	1.2E-10	Sander et al. (2011)
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2\ O_2$	8.E-12*EXP(-2060./temp)	Sander et al. (2011)
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)	Sander et al. (2011)
G2101	UpStG	$H + O_3 \rightarrow OH + O_2$	1.4E-10*EXP(-470./temp)	Sander et al. (2011)
G2102	UpStG	$H_2 + O(^1D) \rightarrow H + OH$	1.2E-10	Sander et al. (2011)
G2103	UpStG	$OH + O(^3P) \rightarrow H + O_2$	1.8E-11*EXP(180./temp)	Sander et al. (2011)
G2104	UpStTrG	$OH + O_3 \rightarrow HO_2 + O_2$	1.7E-12*EXP(-940./temp)	Sander et al. (2011)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	2.8E-12*EXP(-1800./temp)	Sander et al. (2011)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow OH + O_2$	3.E-11*EXP(200./temp)	Sander et al. (2011)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	1.E-14*EXP(-490./temp)	Sander et al. (2011)
G2108a	UpStG	$HO_2 + H \rightarrow 2\ OH$	7.2E-11	Sander et al. (2011)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Sander et al. (2011)
G2108c	UpStG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	Sander et al. (2011)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	4.8E-11*EXP(250./temp)	Sander et al. (2011)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	1.63E-10*EXP(60./temp)	Sander et al. (2011)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Sander et al. (2011)
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)	Sander et al. (2011)
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)	Sander et al. (2011)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	2.15E-11*EXP(110./temp)	Sander et al. (2011)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow 2\ NO$	7.25E-11*EXP(20./temp)	Sander et al. (2011)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.63E-11*EXP(20./temp)	Sander et al. (2011)
G3103	UpStTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2011)
G3104	UpStGN	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Sander et al. (2011)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.1E-12*EXP(210./temp)	Sander et al. (2011)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2011)
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./temp)	Sander et al. (2011)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2011)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2011)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(2.7E-27*EXP(11000./ temp))	Sander et al. (2011)*
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)	Sander et al. (2011)
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)	Sander et al. (2011)
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)	Sander et al. (2011)

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)	Sander et al. (2011)
G3202	UpStTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,1.8E-30,3.0, 2.8E-11,0.,0.6)	Sander et al. (2011)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2011)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2011)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2011)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2011)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./ temp))	Sander et al. (2011)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2011)
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)
G4100	UpStG	$CH_4 + O(^1D) \rightarrow .75\ CH_3 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	1.75E-10	Sander et al. (2011)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3 + H_2O$	1.85E-20*EXP(2.82*LOG(temp) -987./temp)	Atkinson (2003)

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

#	labels	reaction	rate coefficient	reference
G4102	TrG	CH_3OH + OH → .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 → 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 → 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 → 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 → CH_3ONO2	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 → CH_3O + NO_2 + O_2	1.2E-12	Atkinson et al. (2006)
G4106a	StTrG	CH_3O_2 → CH_3O + .5 O_2	7.4E-13*EXP(-520./temp)*RO2*2.	Atkinson et al. (2006)
G4106b	StTrG	CH_3O_2 → .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 → .6 CH_3O_2 + .4 HCHO + .4 OH + H_2O	k_CH3OOH_OH	Wallington et al.
G4108	StTrG	HCHO + OH → CO + H_2O + HO_2	9.52E-18*EXP(2.03*LOG(temp)+636./temp)	Sivakumaran et al. (2003)
G4109	TrGN	HCHO + NO_3 → HNO_3 + CO + HO_2	3.4E-13*EXP(-1900./temp)	Sander et al. (2011)
G4110	UpStTrG	CO + OH → H + CO_2	(1.57E-13+cair*3.54E-33)	McCabe et al. (2001)
G4111	TrG	HCOOH + OH → 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 + $O(^3P)$ → CO_2	6.60E-33*EXP(-1103./temp)	Roble (1995)
G4113	UpStG	CH_4 + $O(^3P)$ → .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 → $CH_3O_2NO_2$	k_NO2_CH3O2	Sander et al. (2011)
G4115	StTrGN	$CH_3O_2NO_2$ → CH_3O_2 + NO_2	k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))	Sander et al. (2011)
G4116	StTrGN	$CH_3O_2NO_2$ + OH → HCHO + NO_3 + H_2O	3.00E-14	see note*
G4117	StTrGN	CH_3ONO2 + OH → H_2O + HCHO + NO_2	4.0E-13*EXP(-845./temp)	Atkinson et al. (2006)
G4118	StTrG	CH_3O → HO_2 + HCHO	1.3E-14*exp(-663./temp)*c(ind_O2)	Chai et al. (2014)
G4119a	StTrGN	CH_3O + NO_2 → CH_3ONO2	k_3rd_iupac(temp,cair,8.1E-29,4.5,2.1E-11,0.,0.44)	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
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)	Sander et al. (2011)
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	$HOCH_2OOH + OH \rightarrow HOCH_2O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2010)*
G4130b	StTrG	$HOCH_2OOH + OH \rightarrow HCOOH + H_2O + OH$	k_rohro + k_s*f_sooh*f_soh	Taraborrelli (2010)*
G4132	StTrG	$HOCH_2OH + OH \rightarrow HO_2 + HCOOH + H_2O$	k_rohro + 2.*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)
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)

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

#	labels	reaction	rate coefficient	reference
G4148	StTrGN	$HOCH_2O_2 + NO_2 \rightarrow HOCH_2O_2NO_2$	k_NO2_CH3O2	Sander et al. (2011)
G4149	StTrGN	$HOCH_2O_2NO_2 \rightarrow HOCH_2O_2 + NO_2$	k_NO2_CH3O2/(9.5E-29*EXP(11234./temp))	Sander et al. (2011), 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.E-11*EXP(-1600./temp)	Sander et al. (2011)
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)	Sander et al. (2011)*
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)*
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)

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

#	labels	reaction	rate coefficient	reference
G42003	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*EXP(700./temp)	Sander et al. (2011)
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.
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	Taraborrelli (2016), Atkinson et al. (2006)
G42007a	TrGC	$C_2H_5OOH + OH \rightarrow C_2H_5O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G42007b	TrGC	$C_2H_5OOH + OH \rightarrow CH_3CHO + OH$	k_s*f_sooh	Taraborrelli (2016)
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	$CH_3CHO + OH \rightarrow HCOCH2O2 + H_2O$	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	$CH_3COOH + OH \rightarrow CH_3 + CO_2 + H_2O$	4.0E-14*EXP(850./temp)	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	Sander et al. (2011)*
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	Taraborrelli (2016)
G42017b	TrGC	$CH_3C(O)OO \rightarrow CH_3COOH$	k1_RO2RCO3*0.1	Taraborrelli (2016)
G42018	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	0.6*k_CH3OOH_OH	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	Sander et al. (2011)*
G42022a	TrGC	$C_2H_2 + OH \rightarrow GLYOX + OH$	k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,2.,0.6)*.71	Sander et al. (2011), Glowacki et al. (2012)
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)*(1.-.71)	Sander et al. (2011), Glowacki et al. (2012)
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)*
G42024b	TrGC	$HOCH2CO + O_2 \rightarrow OH + HCHO + CO_2$	5.1E-12*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
G42025	TrGC	HOCHCHO → GLYOX + HO_2	KDEC	Taraborrelli (2016)
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	Taraborrelli (2016)
G42027b	TrGC	$HOCH_2CO_3$ → $HOCH_2CO_2H$	k1_RO2RCO3*0.1	Taraborrelli (2016)
G42028a	TrGC	$HOCH_2CO_3$ + HO_2 → HCHO + HO_2 + OH + CO_2	KAPHO2*rco3_oh	Taraborrelli (2016), Groß et al. (2014)
G42028b	TrGC	$HOCH_2CO_3$ + HO_2 → $HOCH_2CO_3H$	KAPHO2*rco3_ooh	Taraborrelli (2016), Groß et al. (2014)
G42028c	TrGC	$HOCH_2CO_3$ + HO_2 → $HOCH_2CO_2H$ + O_3	KAPHO2*rco3_o3	Taraborrelli (2016), 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*1.60	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	Taraborrelli (2016)
G42033a	TrGC	$HOCH_2CO_3H$ + OH → $HOCH_2CO_3$ + H_2O	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G42033b	TrGC	$HOCH_2CO_3H$ + OH → $HCOCO_3H$ + HO_2	k_s*f_soh*f_co2h	Taraborrelli (2016)
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	Taraborrelli (2016)
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	Taraborrelli (2016)
G42039b	TrGC	$HCOCO_3$ → $HCOCO_2H$	k1_RO2RCO3*0.1	Taraborrelli (2016)
G42040	TrGC	$HCOCO_3$ + HO_2 → HO_2 + CO + CO_2 + OH	KAPHO2	Feierabend et al. (2008), Taraborrelli (2016)
G42041	TrGCN	$HCOCO_3$ + NO → HO_2 + CO + NO_2 + CO_2	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G42042	TrGCN	$HCOCO_3 + NO_3 \rightarrow HO_2 + CO + NO_2 + CO_2$	KRO2NO3*1.60	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), Taraborrelli (2016)
G42044	TrGC	$HCOCO_2H + OH \rightarrow CO + HO_2 + CO_2 + H_2O$	k_co2h+k_t*f_o*f_co2h	Taraborrelli (2016)
G42045a	TrGC	$HCOCO_3H + OH \rightarrow HCOCO_3 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G42045b	TrGC	$HCOCO_3H + OH \rightarrow CO + CO_2 + H_2O + OH$	k_t*f_o*f_co2h	Taraborrelli (2016)
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)	Taraborrelli (2016)
G42049a	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow$ HYETHO2H	1.53E-13*EXP(1300./temp) *(1.-rchohch2o2_oh)	Rickard and Pascoe (2009)
G42049b	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow HOCH_2CH_2O + OH$	1.53E-13*EXP(1300./temp) *rchohch2o2_oh	Rickard and Pascoe (2009)
G42050	TrGCN	ETHOHNO3 + OH $\rightarrow$ .93 NO_3CH2CHO + .93 HO_2 + .07 $HOCH_2CHO$ + .07 NO_2 + H_2O	k_s*(f_soh*f_ch2ono2+f_ono2*f_ pch2oh)+k_rohro	Taraborrelli (2016)
G42051a	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CH_2O_2 + H_2O$	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G42051b	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CHO + OH + H_2O$	k_s*f_sooh*f_pch2oh	Taraborrelli (2016)
G42051c	TrGC	HYETHO2H + OH $\rightarrow$ HOOCH2CHO + $HO_2 + H_2O$	k_s*f_soh*f_pch2oh+k_rohro	Taraborrelli (2016)
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	Taraborrelli (2016)
G42054	TrGC	HCOCH2O2 $\rightarrow$ .6 HCHO + .6 CO + .6 HO_2 + .2 GLYOX + .2 $HOCH_2CHO$	k1_RO2pORO2	Taraborrelli (2016)
G42055a	TrGC	HCOCH2O2 + $HO_2 \rightarrow$ HOOCH2CHO	KRO2HO2(2)*rcoch2o2_ooh	Taraborrelli (2016)
G42055b	TrGC	HCOCH2O2 + $HO_2 \rightarrow$ HCHO + CO + HO_2 + OH	KRO2HO2(2)*rcoch2o2_oh	Taraborrelli (2016)
G42056a	TrGCN	HCOCH2O2 + NO $\rightarrow NO_2$ + HCHO + CO + HO_2	KRO2NO*(1.-alpha_AN(3,1,1,0,0, temp,cair))	Taraborrelli (2016)
G42056b	TrGCN	HCOCH2O2 + NO $\rightarrow NO_3$CH2CHO	KRO2NO*alpha_AN(3,1,1,0,0,temp, cair)	Taraborrelli (2016)
G42057	TrGCN	HCOCH2O2 + $NO_3 \rightarrow$ HCHO + CO + $HO_2 + NO_2$	KRO2NO3	Taraborrelli (2016)
G42058a	TrGC	HOOCH2CHO + OH $\rightarrow$ HCOCH2O2	0.6*k_CH3OOH_OH	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G42058b	TrGC	HOOCH2CHO + OH → HCHO + CO + OH	.8*8.E-12	Taraborrelli (2016)*
G42058c	TrGC	HOOCH2CHO + OH → GLYOX + OH	k_s*f_sooh*f_cho	Taraborrelli (2016)
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	Taraborrelli (2016)
G42061	TrGCN	$HOOCH_2CO_3$ + NO_3 → NO_2 + OH + HCHO + CO_2	KRO2NO3*1.60	Taraborrelli (2016)
G42062a	TrGC	$HOOCH_2CO_3$ + HO_2 → 2 OH + HCHO + CO_2	KAPHO2*rco3_oh	Taraborrelli (2016)
G42062b	TrGC	$HOOCH_2CO_3$ + HO_2 → HOOCH2CO3H	KAPHO2*rco3_ooh	Taraborrelli (2016)
G42062c	TrGC	$HOOCH_2CO_3$ + HO_2 → HOOCH2CO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2016)
G42063a	TrGC	$HOOCH_2CO_3$ → OH + HCHO + CO_2	k1_RO2RCO3*0.9	Taraborrelli (2016)
G42063b	TrGC	$HOOCH_2CO_3$ → HOOCH2CO2H	k1_RO2RCO3*0.1	Taraborrelli (2016)
G42064a	TrGC	HOOCH2CO3H + OH → $HOOCH_2CO_3$ + H_2O	2.*0.6*k_CH3OOH_OH	Taraborrelli (2016)
G42064b	TrGC	HOOCH2CO3H + OH → $HCOCO_3H$ + OH + H_2O	k_s*f_sooh*f_co2h	Taraborrelli (2016)
G42065	TrGC	HOOCH2CO2H + OH → $HCOCO_2H$ + OH + H_2O	k_s*f_sooh*f_co2h+k_co2h	Taraborrelli (2016)
G42066	TrGC	CH2CO + OH → .6 HCHO + .6 HO_2 + .6 CO + .4 HOOCH2CO2H	2.8E-12*exp(510./temp)	Baulch et al. (2005), Taraborrelli (2016)
G42067a	TrGC	CH3CHOHOOH + OH → CH_3COOH + OH	(k_t*f_tooh*f_toh + k_rohro)	Taraborrelli (2016)
G42067b	TrGC	CH3CHOHOOH + OH → CH3CHOHO2	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G42068	TrGC	CH3CHOHO2 → CH_3CHO + HO_2	3.46E12*EXP(-12500./(1.98*temp))	Hermans et al. (2005), Taraborrelli (2016)
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), Taraborrelli (2016)
G42070	TrGC	CH3CHOHO2 + HO_2 → .5 CH3CHOHOOH + .3 CH_3COOH + .2 CH_3 + .2 HCOOH + .2 OH	5.6E-15*EXP(2300./temp)	Taraborrelli (2016)
G42071	TrGC	CH3CHOHO2 → CH_3 + HCOOH + OH	k1_RO2sOR02	Taraborrelli (2016)
G42072	TrGCN	CH3CHOHO2 + NO → CH_3 + HCOOH + OH + NO_2	KRO2NO	Taraborrelli (2016)
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), Taraborrelli (2016)*
G42074b	TrGCN	NO_3CH2CHO + OH → NO_3CH2CO_3 + H_2O	k_t*f_o*f_ch2ono2*3.	Paulot et al. (2009a), Taraborrelli (2016)*
G42075	TrGCN	NO_3CH2CO_3 + HO_2 → HCHO + NO_2 + CO_2 + OH	KAPHO2	Rickard and Pascoe (2009)*
G42076	TrGCN	NO_3CH2CO_3 + NO → HCHO + NO_2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G42077	TrGCN	NO_3CH2CO_3 + NO_2 → NO_3CH2CHO	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G42078	TrGCN	NO_3CH2CO_3 → HCHO + NO_2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
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)	Taraborrelli (2016)*
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)	Taraborrelli (2016), 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	$NCCH_2O_2 + HO_2 \rightarrow HCN + CO_2 + HO_2$	KRO2HO2(2)	see note*
G42089a	TrGC	$CH_2CHOH + OH \rightarrow HCOOH + OH + HCHO$	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G42089b	TrGC	$CH_2CHOH + OH \rightarrow HOCH_2CHO + HO_2$	k_CH2CHOH_OH_ALD	Taraborrelli (2016), So et al. (2014)
G42090	TrGC	$CH_2CHOH + HCOOH \rightarrow CH_3CHO + HCOOH$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G42091	TrGC	$CH_3CHO + HCOOH \rightarrow CH_2CHOH + HCOOH$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G43000a	TrGC	$C_3H_8 + OH \rightarrow iC_3H_7O_2 + H_2O$	k_s	Taraborrelli (2016)
G43000b	TrGC	$C_3H_8 + OH \rightarrow C_3H_7O_2 + H_2O$	2.*k_p	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43001a	TrGC	C_3H_6 + O_3 → HCHO + .16 CH3CHOHOOH + .50 OH + .50 HCOCH2O2 + .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 → CH_3CHO + CH_2OO^*	5.5E-15*EXP(-1880./temp)*.43	Atkinson et al. (2006)*
G43002	TrGC	C_3H_6 + OH → 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 → PRONO3BO2	4.6E-13*EXP(-1155./temp)	Wallington et al.
G43004	TrGC	$iC_3H_7O_2$ + HO_2 → iC_3H_7OOH	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G43005a	TrGCN	$iC_3H_7O_2$ + NO → 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.
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.
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	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G43007b	TrGC	iC_3H_7OOH + OH → CH_3COCH_3 + H_2O + OH	k_t*f_tooh	Taraborrelli (2016)
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.
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.
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)*rcoch2o2_ ooh	Tyndall et al. (2001a), Taraborrelli (2016)
G43012b	TrGC	$CH_3COCH_2O_2$ + HO_2 → OH + $CH_3C(O)$ + HCHO	8.6E-13*EXP(700./temp)*rcoch2o2_ oh	Tyndall et al. (2001a), Taraborrelli (2016)
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))	Sander et al. (2011)
G43013b	TrGCN	$CH_3COCH_2O_2$ + NO → NOA	2.9E-12*EXP(300./temp)*alpha_ AN(4,1,1,0,0,temp,cair)	Sander et al. (2011)
G43014	TrGC	$CH_3COCH_2O_2$ → .3 $CH_3C(O)$ + .3 HCHO + .5 MGLYOX + .2 CH_3COCH_2OH	k1_RO2pORO2	Orlando and Tyndall (2012)

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

#	labels	reaction	rate coefficient	reference
G43015a	TrGC	$CH_3COCH_2O_2H + OH \rightarrow CH_3COCH_2O_2 + H_2O$	0.6*k_CH3OOH_OH	see note*
G43015b	TrGC	$CH_3COCH_2O_2H + OH \rightarrow$ MGLYOX + OH + H_2O	k_s*f_sooh*f_co	Taraborrelli (2016)
G43016	TrGC	$CH_3COCH_2OH + OH \rightarrow$ MGLYOX + $HO_2 + H_2O$	1.6E-12*EXP(305./temp)	Atkinson et al. (2006)
G43017	TrGC	MGLYOX + OH $\rightarrow$ .4 CH_3 + .6 $CH_3C(O)$ + 1.4 CO + H_2O	1.9E-12*EXP(575./temp)	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$iC_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	6.2E-13*EXP(-230./temp)	Wallington et al.
G43021	TrGCN	$CH_3COCH_2O_2 + NO_3 \rightarrow CH_3C(O) + HCHO + NO_2$	KRO2NO3	Rickard and Pascoe (2009)
G43022	TrGC	HYPROPO2 $\rightarrow CH_3CHO + HCHO + HO_2$	k1_RO2sORO2	Rickard and Pascoe (2009)
G43023a	TrGC	HYPROPO2 + $HO_2 \rightarrow$ HYPROPO2H	KRO2HO2(3)*(1.-rchohch2o2_oh)	Rickard and Pascoe (2009)
G43023b	TrGC	HYPROPO2 + $HO_2 \rightarrow CH_3CHO + HCHO + HO_2 + OH$	KRO2HO2(3)*rchohch2o2_oh	Rickard and Pascoe (2009)
G43024a	TrGCN	HYPROPO2 + NO $\rightarrow CH_3CHO + HCHO + HO_2 + NO_2$	KRO2NO*(1.-alpha_AN(4,1,0,0,0, temp,cair))	Rickard and Pascoe (2009)
G43024b	TrGCN	HYPROPO2 + NO $\rightarrow$ PROPOLNO3	KRO2NO*alpha_AN(4,1,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G43025	TrGCN	HYPROPO2 + $NO_3 \rightarrow CH_3CHO + HCHO + HO_2 + NO_2$	KRO2NO3	Rickard and Pascoe (2009)
G43026a	TrGC	HYPROPO2H + OH $\rightarrow$ HYPROPO2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G43026b	TrGC	HYPROPO2H + OH $\rightarrow CH_3COCH_2OH$ + OH	(k_s*f_soh*f_pch2oh+k_t*f_ tooh*f_pch2oh)	Taraborrelli (2016)
G43027	TrGCN	PRONO3BO2 + $HO_2 \rightarrow$ PR2O2HNO3	KRO2HO2(3)	Rickard and Pascoe (2009)
G43028	TrGCN	PRONO3BO2 + NO $\rightarrow$ NOA + $HO_2 + NO_2$	KRO2NO	Rickard and Pascoe (2009)*
G43029	TrGCN	PRONO3BO2 + $NO_3 \rightarrow$ NOA + $HO_2 + NO_2$	KRO2NO3	Rickard and Pascoe (2009)
G43030a	TrGCN	PR2O2HNO3 + OH $\rightarrow$ PRONO3BO2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G43030b	TrGCN	PR2O2HNO3 + OH $\rightarrow$ NOA + OH	k_t*f_tooh*f_ch2ono2	Taraborrelli (2016)
G43031	TrGCN	MGLYOX + $NO_3 \rightarrow CH_3C(O) + CO + HNO_3$	KNO3AL*2.4	Rickard and Pascoe (2009)
G43032	TrGCN	NOA + OH $\rightarrow$ MGLYOX + NO_2	(k_s*f_co*f_ono2+k_p*f_co)	Taraborrelli (2016)
G43033	TrGC	HOCH2COCHO + OH $\rightarrow$ .8609 HOCH2CO + .8609 CO + .1391 HCOCOCHO + .1391 HO_2	(1.9E-12*EXP(575./temp)+k_s*f_ soh*f_co)	Taraborrelli (2016)
G43034	TrGCN	HOCH2COCHO + $NO_3 \rightarrow$ HOCH2CO + CO + HNO_3	KNO3AL*2.4	Taraborrelli (2016)
G43035	TrGC	$CH_3COCO_2H + OH \rightarrow CH_3C(O) + H_2O + CO_2$	4.9E-14*EXP(276./temp)	Mellouki and Mu (2003), Taraborrelli (2016)
G43036	TrGC	$HCOCOCH_2O_2 \rightarrow$ .6 HCOCO + .6 HCHO + .2 HCOCOCHO + .2 HOCH2COCHO	k1_RO2pORO2	Taraborrelli (2016)
G43037	TrGCN	$HCOCOCH_2O_2$ + NO $\rightarrow$ HCOCO + HCHO + NO_2	KRO2NO	Taraborrelli (2016)*
G43038a	TrGC	$HCOCOCH_2O_2 + HO_2 \rightarrow HCOCOCH_2OOH$	KRO2HO2(3)*rcoch2o2_ooh	Taraborrelli (2016)
G43038b	TrGC	$HCOCOCH_2O_2 + HO_2 \rightarrow$ HCOCO + HCHO + OH	KRO2HO2(3)*rcoch2o2_oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43039	TrGCN	$HCOCOCH_2O_2 + NO_3 \rightarrow HCOCO + HCHO + NO_2$	KRO2NO3	Taraborrelli (2016)
G43040a	TrGC	$HCOCOCH_2OOH + OH \rightarrow HOOCH_2CO_3 + CO + H_2O$	k_t*f_co*f_o	Taraborrelli (2016)*
G43040b	TrGC	$HCOCOCH_2OOH + OH \rightarrow HCOCOCHO + H_2O + OH$	k_s*f_sooh*f_co	Taraborrelli (2016)*
G43040c	TrGC	$HCOCOCH_2OOH + OH \rightarrow HCOCOCH_2O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G43041	TrGCN	$HCOCOCH_2OOH + NO_3 \rightarrow HOOCH_2CO_3 + CO + HNO_3$	KNO3AL*2.4	Taraborrelli (2016)
G43042	TrGC	HOCH2COCH2O2 $\rightarrow$ HCHO + HOCH2CO	k1_RO2pORO2	Taraborrelli (2016)
G43043a	TrGC	HOCH2COCH2O2 + HO_2 $\rightarrow$ HOCH2COCH2OOH	KRO2HO2(3)*rcoch2o2_ooh	Taraborrelli (2016)
G43043b	TrGC	HOCH2COCH2O2 + HO_2 $\rightarrow$ HCHO + HOCH2CO + OH	KRO2HO2(3)*rcoch2o2_oh	Taraborrelli (2016)
G43044	TrGCN	HOCH2COCH2O2 + NO $\rightarrow$ HCHO + HOCH2CO + NO_2	KRO2NO	Taraborrelli (2016)*
G43045a	TrGC	HOCH2COCH2OOH + OH $\rightarrow$ HOCH2COCHO + OH	k_s*f_sooh*f_co	Taraborrelli (2016)
G43045b	TrGC	HOCH2COCH2OOH + OH $\rightarrow$ HOCH2COCH2O2	.6*k_CH3OOH_OH	Taraborrelli (2016)
G43045c	TrGC	HOCH2COCH2OOH + OH $\rightarrow$ $HCOCOCH_2OOH + HO_2$	1.60E-12*EXP(305./temp)	Taraborrelli (2016)*
G43046	TrGC	CH3CHCO + OH $\rightarrow$ .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), Taraborrelli (2016)
G43047	TrGCN	PROPOLNO3 + OH $\rightarrow$ $CH_3COCH_2OH + NO_2$	k_t*f_ono2*f_pch2oh+k_s*f_soh*f_ch2ono2	Taraborrelli (2016)
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 $\rightarrow$ MGLYOX + $NO_3 + H_2O$	9.50E-13*EXP(-650./temp)*f_co	Taraborrelli (2016)*
G43051a	TrGC	$C_3H_7OOH + OH \rightarrow C_3H_7O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G43051b	TrGC	$C_3H_7OOH + OH \rightarrow C_2H_5CHO + H_2O + OH$	k_s*f_sooh	Taraborrelli (2016)
G43051c	TrGC	$C_3H_7OOH + OH \rightarrow C_2H_5CHO + HO_2 + H_2O$	k_s*f_pch2oh	Taraborrelli (2016)*
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	Taraborrelli (2016)
G43054b	TrGC	$C_2H_5CO_3 \rightarrow C_2H_5CO_2H$	k1_RO2RCO3*0.1	Taraborrelli (2016)
G43055a	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5O_2 + CO_2 + OH$	KAPHO2*rco3_oh	Taraborrelli (2016), Groß et al. (2014)
G43055b	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_3H$	KAPHO2*rco3_ooh	Taraborrelli (2016), Groß et al. (2014)
G43055c	TrGC	$C_2H_5CO_3 + HO_2 \rightarrow C_2H_5CO_2H + O_3$	KAPHO2*rco3_o3	Taraborrelli (2016), 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	$C_2H_5CO_3 + NO_2 \rightarrow$ PPN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43058	TrGCN	PPN $\rightarrow C_2H_5CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43059	TrGC	$C_2H_5CO_2H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	k_co2h+k_p+k_s*f_co2h	Taraborrelli (2016)*
G43060a	TrGC	$C_2H_5CO_3H + OH \rightarrow C_2H_5CO_3 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G43060b	TrGC	$C_2H_5CO_3H + OH \rightarrow CH_3CHO + CO_2 + H_2O$	k_s*f_co2h+k_p	Taraborrelli (2016)*
G43061	TrGCN	$PPN + OH \rightarrow CH_3CHO + CO_2 + NO_2 + H_2O$	k_s*f_cpan+k_p	Taraborrelli (2016)*
G43062	TrGC	$CH_3COCO_3H + OH \rightarrow CH_3COCO_3 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G43063a	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3C(O) + CO_2 + OH$	KAPHO2*rco3_oh	Taraborrelli (2016)
G43063b	TrGC	$CH_3COCO_3 + HO_2 \rightarrow CH_3COCO_3H$	KAPHO2*(rco3_ooh+rco3_o3)	Taraborrelli (2016)
G43064	TrGCN	$CH_3COCO_3 + NO \rightarrow CH_3C(O) + CO_2 + NO_2$	KAPNO	Taraborrelli (2016)
G43065	TrGCN	$CH_3COCO_3 + NO_2 \rightarrow CH_3C(O) + CO_2 + NO_3$	k_CH3CO3_NO2	Taraborrelli (2016)*
G43066	TrGCN	$CH_3COCO_3 + NO_3 \rightarrow CH_3C(O)OO + CO_2 + NO_2$	KRO2NO3*1.74	Taraborrelli (2016)
G43067	TrGC	$CH_3COCO_3 \rightarrow CH_3C(O)OO + CO_2$	k1_RO2RCO3	Taraborrelli (2016)
G43068	TrGC	$HCOCOCHO + OH \rightarrow 3\ CO + HO_2$	2.*k_t*f_co*f_o	Taraborrelli (2016)
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), Taraborrelli (2016)*
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), Taraborrelli (2016)*
G43071a	TrGC	$CH_2CHCH_2OH + OH \rightarrow HCOOH + OH + CH_3CHO$	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G43072	TrGC	$CH_2CHCH_2OH + HCOOH \rightarrow C_2H_5CHO + HCOOH$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G43073	TrGC	$C_2H_5CHO + HCOOH \rightarrow CH_2CHCH_2OH + HCOOH$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G43074	TrGC	$HCOCOCH_2OOH + OH \rightarrow HCOCO + CO + HO_2 + OH$	k_s*f_sooh*f_co+.6*k_CH3OOH_OH	Taraborrelli (2016)*
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	$HCOCH2CO3 \rightarrow HCOCH2O2 + CO_2$	k1_RO2RCO3*0.9	Taraborrelli (2016)
G43204b	TrGTerC	$HCOCH2CO3 \rightarrow HCOCH2CO2H$	k1_RO2RCO3*0.1	Taraborrelli (2016)
G43205	TrGTerCN	$HCOCH2CO3 + NO \rightarrow HCOCH2O2 + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G43206	TrGTerCN	$HCOCH2CO3 + NO_2 \rightarrow C3PAN2$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43207a	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH2CO3H$	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G43207b	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH2CO2H + O_3$	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G43207c	TrGTerC	$HCOCH2CO3 + HO_2 \rightarrow HCOCH2O2 + CO_2 + OH$	KAPHO2*rco3_oh	Rickard and Pascoe (2009)
G43210	TrGTerCN	$C3PAN2 \rightarrow HCOCH2CO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43211	TrGTerCN	C3PAN2 + OH → GLYOX + CO + NO_2	2.10E-11	Rickard and Pascoe (2009)
G43212	TrGTerC	HCOCH2CO2H + OH → HCOCH2O2 + CO_2	2.14E-11	Rickard and Pascoe (2009)
G43213a	TrGTerC	HOC2H4CO3 → $HOCH_2CH_2O_2$ + CO_2	k1_RO2RCO3*0.9	Taraborrelli (2016)
G43213b	TrGTerC	HOC2H4CO3 → HOC2H4CO2H	k1_RO2RCO3*0.1	Taraborrelli (2016)
G43214	TrGTerCN	HOC2H4CO3 + NO → $HOCH_2CH_2O_2$ + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	HOC2H4CO3 + HO_2 → HOC2H4CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G43215b	TrGTerC	HOC2H4CO3 + HO_2 → $HOCH_2CH_2O_2$ + CO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)
G43215c	TrGTerC	HOC2H4CO3 + HO_2 → HOC2H4CO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G43218	TrGTerCN	HOC2H4CO3 + NO_2 → C3PAN1	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43219	TrGTerC	HOC2H4CO2H + OH → $HOCH_2CH_2O_2$ + CO_2	1.39E-11	Rickard and Pascoe (2009)
G43220	TrGTerC	HOC2H4CO3H + OH → HOC2H4CO3	1.73E-11	Rickard and Pascoe (2009)
G43221	TrGTerCN	C3PAN1 → HOC2H4CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G43222	TrGTerCN	C3PAN1 + OH → $HOCH_2CHO$ + CO + NO_2	4.51E-12	Rickard and Pascoe (2009)
G43223	TrGTerC	HCOCH2CO3H + OH → HCOCH2O2 + CO_2 + H_2O	2.49E-11	Rickard and Pascoe (2009)*
G43415	TrGAroC	C3DIALOOH + OH → HCOCOCHO + OH	1.44E-10	Rickard and Pascoe (2009)
G43418a	TrGAroC	C3DIALO2 + HO_2 → C3DIALOOH	KRO2HO2(3)*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G43418b	TrGAroC	C3DIALO2 + HO_2 → GLYOX + CO + HO_2 + OH	KRO2HO2(3)*rco3_oh	Rickard and Pascoe (2009)
G43419	TrGAroCN	C3DIALO2 + NO → GLYOX + CO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G43420	TrGAroCN	C3DIALO2 + NO_3 → GLYOX + CO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G43421	TrGAroC	C3DIALO2 → GLYOX + CO + HO_2	k1_RO2sORO2	Rickard and Pascoe (2009)*
G43422a	TrGAroC	HCOCOHCO3 + HO_2 → GLYOX + CO_2 + HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)
G43422b	TrGAroC	HCOCOHCO3 + HO_2 → HCOCOHCO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G43424	TrGAroCN	HCOCOHCO3 + NO → GLYOX + CO_2 + HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G43425	TrGAroCN	HCOCOHCO3 + NO_2 → HCOCOHPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G43426	TrGAroCN	HCOCOHCO3 + NO_3 → GLYOX + CO_2 + HO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	HCOCOHCO3 → GLYOX + CO_2 + HO_2	k1_RO2RCO3	Rickard and Pascoe (2009)
G43428	TrGAroC	METACETHO + OH → $CH_3C(O)$ + CO_2	9.82E-11	Rickard and Pascoe (2009)
G43442	TrGAroCN	HCOCOHPAN + OH → GLYOX + CO + NO_2	6.97E-11	Rickard and Pascoe (2009)
G43443	TrGAroCN	HCOCOHPAN → HCOCOHCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	C32OH13CO + OH → HCOCOHCO3	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	HCOCOHCO3H + OH → HCOCOHCO3	7.33E-11	Rickard and Pascoe (2009)
G44000	TrGC	C_4H_{10} + OH → $LC_4H_9O_2$ + H_2O	2.03E-17*temp*temp*EXP(78./temp)	Atkinson et al. (2006)*
G44001a	TrGC	$LC_4H_9O_2$ → C_3H_7CHO + HO_2	(k1_RO2pRO2*0.1273+k1_ RO2sRO2*0.8727)*0.1273	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
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), Taraborrelli (2016)*
G44002	TrGC	$LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$	KRO2HO2(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), Taraborrelli (2016)
G44003b	TrGCN	$LC_4H_9O_2 + NO \rightarrow NO_2 + .636\ MEK + .636\ HO_2 + .364\ CH_3CHO + .364\ C_2H_5O_2$	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), Taraborrelli (2016)
G44003c	TrGCN	$LC_4H_9O_2 + NO \rightarrow$ 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	$LC_4H_9O_2 + NO_3 \rightarrow NO_2 + C_3H_7CHO + HO_2$	KRO2NO3*0.1273	Rickard and Pascoe (2009), Taraborrelli (2016)
G44004b	TrGCN	$LC_4H_9O_2 + NO_3 \rightarrow NO_2 + .636\ MEK + .636\ HO_2 + .364\ CH_3CHO + .364\ C_2H_5O_2$	KRO2NO3*0.8727	Rickard and Pascoe (2009), Taraborrelli (2016)
G44005a	TrGC	$LC_4H_9OOH + OH \rightarrow LC_4H_9O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G44005b	TrGC	$LC_4H_9OOH + OH \rightarrow C_3H_7CHO + H_2O + OH$	k_s*f_tooh*f_alk*(k_p/(k_p+k_s))	Taraborrelli (2016)
G44005c	TrGC	$LC_4H_9OOH + OH \rightarrow MEK + H_2O + OH$	k_t*f_tooh*f_alk*(k_s/(k_p+k_s))	Taraborrelli (2016)
G44006a	TrGC	$iC_4H_{10} + OH \rightarrow TC_4H_9O_2 + H_2O$	1.17E-17*temp*temp*EXP(213./temp)*k_t/(3.*k_p+k_t)	Atkinson (2003)
G44006b	TrGC	$iC_4H_{10} + OH \rightarrow IC_4H_9O_2 + H_2O$	1.17E-17*temp*temp*EXP(213./temp)*3.*k_p/(3.*k_p+k_t)	Atkinson (2003)
G44007	TrGC	$TC_4H_9O_2 \rightarrow CH_3COCH_3 + CH_3$	k1_RO2tRO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G44008	TrGC	$TC_4H_9O_2 + HO_2 \rightarrow TC_4H_9OOH$	KRO2HO2(4)	Rickard and Pascoe (2009)
G44009a	TrGCN	$TC_4H_9O_2 + NO \rightarrow NO_2 + CH_3COCH_3 + CH_3$	KRO2NO*(1.-alpha_AN(4,3,0,0,0,temp,cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G44009b	TrGCN	$TC_4H_9O_2 + NO \rightarrow$ TC4H9NO3	KRO2NO*alpha_AN(4,3,0,0,0,temp,cair)	Rickard and Pascoe (2009)
G44010a	TrGC	$TC_4H_9OOH + OH \rightarrow TC_4H_9O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G44010b	TrGC	$TC_4H_9OOH + OH \rightarrow CH_3COCH_3 + HCHO + OH + H_2O$	3.*k_p*f_tch2oh	Taraborrelli (2016)*
G44011	TrGCN	TC4H9NO3 $+ OH \rightarrow CH_3COCH_3 + HCHO + NO_2 + H_2O$	3.*k_p*f_ch2ono2	Taraborrelli (2016)*
G44012	TrGC	$IC_4H_9O_2 \rightarrow$ IPRCHO	k1_RO2sRO2	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44013	TrGC	$IC_4H_9O_2 + HO_2 \rightarrow IC_4H_9OOH$	KRO2HO2(4)	Rickard and Pascoe (2009)
G44014a	TrGCN	$IC_4H_9O_2 + NO \rightarrow NO_2 + IPRCHO$	KRO2NO*(1.-alpha_AN(4,2,0,0,0, temp,cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G44014b	TrGCN	$IC_4H_9O_2 + NO \rightarrow IC4H9NO3$	KRO2NO*alpha_AN(4,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G44015a	TrGC	$IC_4H_9OOH + OH \rightarrow IC_4H_9O_2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G44015b	TrGC	$IC_4H_9OOH + OH \rightarrow IPRCHO + OH + H_2O$	k_s*f_sooh+2.*k_s+k_t*f_pch2oh	Taraborrelli (2016)*
G44016	TrGCN	$IC4H9NO3 + OH \rightarrow IPRCHO + NO_2 + H_2O$	k_s*f_ono2+2.*k_p+k_t*f_ch2ono2	Taraborrelli (2016)*
G44017	TrGC	$MVK + O_3 \rightarrow .87\ MGLYOX + .5481\ CO + .1392\ HO_2 + .1392\ OH + .3219\ CH_2OO + .13\ HCHO + .04680\ OH + .04680\ CO + .07280\ CH_3C(O) + .026\ CH_3CHO + .026\ CO_2 + .026\ HCHO + .026\ HO_2 + .02402\ MGLYOX + .02402\ H_2O_2 + .00718\ CH_3COCO_2H$	8.5E-16*EXP(-1520./temp)	Taraborrelli (2016)
G44018	TrGC	$MVK + OH \rightarrow LHMVKABO2$	2.6E-12*EXP(610./temp)	Taraborrelli (2016), Atkinson et al. (2006)*
G44019	TrGC	$MEK + OH \rightarrow LMEKO2 + H_2O$	1.5E-12*EXP(-90./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44020	TrGC	$LMEKO2 + HO_2 \rightarrow LMEKOOH$	KRO2HO2(4)	Taraborrelli (2016)
G44021a	TrGCN	$LMEKO2 + NO \rightarrow .62\ CH_3CHO + .62\ CH_3C(O) + .38\ HCHO + .38\ CO_2 + .38\ HOCH_2CH_2O_2 + NO_2$	KRO2NO*(1.-(.62*alpha_AN(4,2,1, 0,0,temp,cair)+.38*alpha_AN(4,1, 0,1,0,temp,cair)))	Taraborrelli (2016)*
G44021b	TrGCN	$LMEKO2 + NO \rightarrow LMEKNO3$	KRO2NO*(.62*alpha_AN(4,2,1,0,0, temp,cair)+.38*alpha_AN(4,1,0,1, 0,temp,cair))	Taraborrelli (2016)
G44022a	TrGC	$LMEKOOH + OH \rightarrow LMEKO2 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G44022b	TrGC	$LMEKOOH + OH \rightarrow .62\ BIACET + .38\ HCHO + .38\ CO_2 + .38\ HOCH_2CH_2O_2 + H_2O + OH$	(.62*k_t*f_tooh*f_co+.38*k_s*f_ sooh)	Taraborrelli (2016)
G44023a	TrGCN	$LC4H9NO3 + OH \rightarrow MEK + NO_2 + H_2O$	(k_t*f_ono2*f_alk+k_p*f_alk+k_ s*f_ch2ono2+k_p)*(k_s/(k_p+k_s))	Taraborrelli (2016)*
G44023b	TrGCN	$LC4H9NO3 + OH \rightarrow C_3H_7CHO + NO_2 + H_2O$	(k_p+k_s*(1+f_ch2ono2+f_ono2) *f_alk)*(k_p/(k_p+k_s))	Taraborrelli (2016)*
G44024	TrGCN	$MPAN + OH \rightarrow CH_3COCH_2OH + CO + NO_2$	3.2E-11	Orlando et al. (2002)
G44025	TrGCN	$MPAN \rightarrow MACO3 + NO_2$	k_PAN_M	see note*

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

#	labels	reaction	rate coefficient	reference
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), Taraborrelli (2016)
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)`	Taraborrelli (2016)
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`	Taraborrelli (2016)
G44030b	TrGC	MACO3 → MACO2H	`k1_RO2RCO3*0.1`	Taraborrelli (2016)
G44031a	TrGC	MACO3 + HO_2 → MACO2 + OH	`KAPHO2*rco3_oh`	Taraborrelli (2016)
G44031b	TrGC	MACO3 + HO_2 → MACO3H	`KAPHO2*rco3_ooh`	Taraborrelli (2016)
G44031c	TrGC	MACO3 + HO_2 → MACO2H + O_3	`KAPHO2*rco3_o3`	Taraborrelli (2016)
G44032	TrGCN	MACO3 + NO → MACO2 + NO_2	`8.70E-12*EXP(290./temp)`	Taraborrelli (2016)
G44033	TrGCN	MACO3 + NO_2 → MPAN	`k_CH3CO3_NO2`	Rickard and Pascoe (2009)
G44034	TrGCN	MACO3 + NO_3 → MACO2 + NO_2	`KRO2NO3*1.60`	Taraborrelli (2016)
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	`KRO2HO2(4)*rcoch2o2_oh`	Taraborrelli (2016)
G44036b	TrGC	MACRO2 + HO_2 → MACROOH	`KRO2HO2(4)*rcoch2o2_ooh`	Taraborrelli (2016)
G44037a	TrGCN	MACRO2 + NO → MACRO + NO_2	`KRO2NO*(1.-alpha_AN(6,3,1,0,0, temp,cair))`	Taraborrelli (2016)
G44037b	TrGCN	MACRO2 + NO → MACRN	`KRO2NO*alpha_AN(6,3,1,0,0,temp, cair)`	Taraborrelli (2016)
G44038	TrGCN	MACRO2 + NO_3 → MACRO + NO_2	`KRO2NO3`	Taraborrelli (2016)
G44039a	TrGC	MACROOH + OH → MACRO2	`0.6*k_CH3OOH_OH`	Taraborrelli (2016)
G44039b	TrGC	MACROOH + OH → CO + CH_3COCH_2OH + OH	`k_t*f_o*f_tch2oh*f_alk`	Taraborrelli (2016)
G44039c	TrGC	MACROOH + OH → CO + MGLYOX + HO_2	`(k_s*f_soh*f_pch2oh + k_rohro)`	Taraborrelli (2016)
G44040	TrGC	MACROH + OH → CH_3COCH_2OH + CO + HO_2	`k_t*f_o*f_tch2oh*f_alk`	Taraborrelli (2016)
G44041	TrGC	MACRO → .885 CH_3COCH_2OH + .885 CO + .115 MGLYOX + .115 HCHO + HO_2	`KDEC`	Taraborrelli (2016)
G44042	TrGC	MACO2H + OH → CH_3COCH_2OH + HO_2 + CO_2	`((k_adt+k_adp)*a_co2h+k_co2h)`	Taraborrelli (2016)
G44043a	TrGC	MACO3H + OH → CH_3COCH_2OH + CO_2 + OH	`(k_adt+k_adp)*a_co2h`	Taraborrelli (2016)
G44043b	TrGC	MACO3H + OH → MACO3	`0.6*k_CH3OOH_OH`	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
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)`	Taraborrelli (2016)
G44045a	TrGC	LHMVKABO2 + HO_2 → OH + $HOCH_2CHO$ + $CH_3C(O)$	`KRO2HO2(4)*.88*rcoch2o2_oh`	Taraborrelli (2016)
G44045b	TrGC	LHMVKABO2 + HO_2 → LHMVKABOOH	`KRO2HO2(4)*(.12+.88*rcoch2o2_ooh)`	Taraborrelli (2016)
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)))`	Taraborrelli (2016)
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))`	Taraborrelli (2016)*
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`	Taraborrelli (2016)
G44048a	TrGC	LHMVKABOOH + OH → LHMVKABO2	`0.6*k_CH3OOH_OH`	Taraborrelli (2016)
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)`	Taraborrelli (2016)
G44049a	TrGC	CO2H3CHO + OH → CO2H3CO3	`k_t*f_o*f_alk`	Taraborrelli (2016)
G44049b	TrGC	CO2H3CHO + OH → $CH_3COCOCHO$ + HO_2 + H_2O	`k_t*f_co*f_toh*f_cho`	Taraborrelli (2016)
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`	Taraborrelli (2016)
G44052a	TrGC	CO2H3CO3 + HO_2 → OH + MGLYOX + HO_2 + CO_2	`KAPHO2*rco3_oh`	Taraborrelli (2016)
G44052b	TrGC	CO2H3CO3 + HO_2 → CO2H3CO2H + O_3	`KAPHO2*rco3_o3`	Taraborrelli (2016)
G44052c	TrGC	CO2H3CO3 + HO_2 → CO2H3CO3H	`KAPHO2*rco3_ooh`	Taraborrelli (2016)
G44053	TrGCN	CO2H3CO3 + NO → MGLYOX + HO_2 + NO_2 + CO_2	`KAPNO`	Taraborrelli (2016)
G44054	TrGCN	CO2H3CO3 + NO_3 → MGLYOX + HO_2 + NO_2 + CO_2	`KRO2NO3*1.60`	Taraborrelli (2016)
G44055a	TrGC	CO2H3CO3H + OH → CO2H3CO3	`0.6*k_CH3OOH_OH`	Taraborrelli (2016)
G44055b	TrGC	CO2H3CO3H + OH → $CH_3C(O)$ + CO + CO_2 + OH	`(k_t*f_co2h*f_co*f_toh)`	Taraborrelli (2016)
G44056	TrGC	CO2H3CO2H + OH → CH3COCOCO2H + HO_2	`k_t*f_co2h*f_co*f_toh+k_co2h`	Taraborrelli (2016)
G44057a	TrGC	HO12CO3C4 + OH → BIACETOH + HO_2	`k_t*f_toh*f_alk*f_co`	Taraborrelli (2016)
G44057b	TrGC	HO12CO3C4 + OH → CO2H3CHO + HO_2	`k_s*f_soh*f_alk`	Taraborrelli (2016)
G44058	TrGC	MACO2 → .65 CH_3 + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + CO_2	`KDEC`	Taraborrelli (2016)
G44059	TrGC	LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 $CH_3C(O)$ + OH	`KHSD`	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44060	TrGC	MACRO2 → MGLYOX + HCHO + OH	KHSB	Taraborrelli (2016)
G44061a	TrGCN	MVKNO3 + OH → MGLYOX + CO_2 + HO_2 + NO_2 + H_2O	k_s*f_sooh*f_ch2ono2+k_rohro	Taraborrelli (2016)*
G44061b	TrGCN	MVKNO3 + OH → BIACETOH + NO_2 + H_2O	k_t*f_ono2*f_co*f_pch2oh	Taraborrelli (2016)*
G44062a	TrGCN	MACRN + OH → CH_3COCH_2OH + CO_2 + NO_2 + H_2O	k_t*f_o*f_ch2ono2	Taraborrelli (2016)*
G44062b	TrGCN	MACRN + OH → MGLYOX + CO + NO_2 + H_2O	k_rohro+k_s*f_sooh*f_ch2ono2	Taraborrelli (2016)*
G44063	TrGC	MACRO2 → CH_3COCH_2OH + OH + CO	K14HSAL	Taraborrelli (2016)
G44064	TrGC	EZCH3CO2CHCHO → .9 $CH_3COCHCO$ + .1 $CH_3C(O)$ + .01 GLYOX + .18 CO + .09 HO_2 + OH	K15HS24VYNAL	Taraborrelli (2016)
G44065	TrGC	EZCH3CO2CHCHO + HO_2→ $CH_3COOHCHCHO$	KRO2HO2(4)	Taraborrelli (2016)
G44066	TrGCN	EZCH3CO2CHCHO + NO → CH_3COCHO_2CHO + NO_2	KRO2NO	Taraborrelli (2016)*
G44067	TrGCN	EZCH3CO2CHCHO + NO_3→ CH_3COCHO_2CHO + NO_2	kRO2NO3	Taraborrelli (2016)
G44068	TrGC	EZCH3CO2CHCHO → CH_3COCHO_2CHO	k1_RO2sORO2	Taraborrelli (2016)
G44069	TrGC	EZCHOCCH3CHO2 → $HCOCCH_3CO$ + OH	K15HS24VYNAL	Taraborrelli (2016)
G44070	TrGCN	EZCHOCCH3CHO2 + NO → $HCOCO_2CH_3CHO$ + NO_2	KRO2NO	Taraborrelli (2016)*
G44071	TrGC	EZCHOCCH3CHO2 + HO_2→ $HCOCCH_3CHOOH$	KRO2HO2(4)	Taraborrelli (2016)
G44072	TrGCN	EZCHOCCH3CHO2 + NO_3→ $HCOCO_2CH_3CHO$ + NO_2	KRO2NO3	Taraborrelli (2016)
G44073	TrGC	EZCHOCCH3CHO2 → $HCOCO_2CH_3CHO$	k1_RO2pORO2	Taraborrelli (2016)
G44074	TrGC	$CH_3COOHCHCHO$ → CH_3COCHO_2CHO + OH	KHYDEC	Taraborrelli (2016)
G44075	TrGC	$HCOCCH_3CHOOH$ → $HCOCO_2CH_3CHO$ + OH	KHYDEC	Taraborrelli (2016)
G44076	TrGCN	CH_3COCHO_2CHO + NO → $CH_3C(O)$ + GLYOX + NO_2	KRO2NO	Taraborrelli (2016)*
G44077	TrGCN	CH_3COCHO_2CHO + NO_3 → $CH_3C(O)$ + GLYOX + NO_2	KRO2NO3	Taraborrelli (2016)
G44078	TrGC	CH_3COCHO_2CHO + HO_2 → $CH_3C(O)$ + GLYOX + OH	KRO2HO2(4)	Taraborrelli (2016)*
G44079	TrGC	CH_3COCHO_2CHO → $CH_3C(O)$ + GLYOX	k1_RO2sORO2	Taraborrelli (2016)
G44080	TrGC	$HCOCO_2CH_3CHO$ → MGLYOX + CO + HO_2	k1_RO2tORO2	Taraborrelli (2016)
G44081	TrGCN	$HCOCO_2CH_3CHO$ + NO → MGLYOX + CO + HO_2 + NO_2	KRO2NO	Taraborrelli (2016)*
G44082	TrGC	$HCOCO_2CH_3CHO$ + HO_2 → MGLYOX + CO + HO_2 + OH	KRO2HO2(4)	Taraborrelli (2016)*
G44083	TrGCN	$HCOCO_2CH_3CHO$ + NO_3 → MGLYOX + CO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2016)
G44084	TrGC	$HCOCCH_3CO$ + OH → CO + MGLYOX + HO_2	1E-10*a_cho	Hatakeyama et al. (1985), Taraborrelli (2016)
G44085	TrGC	$CH_3COCHCO$ + OH → CO + MGLYOX + HO_2	7.6E-11*a_coch3	Hatakeyama et al. (1985), Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
G44086	TrGCN	LMEKNO3 + OH → .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)	Taraborrelli (2016)*
G44087	TrGC	MEPROPENE + OH → IBUTOLBO2	9.4E-12*EXP(505./temp)	Atkinson et al. (2006)
G44088a	TrGC	MEPROPENE + O_3 → CH_3COCH_3 + CH_2OO^*	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Taraborrelli (2016)
G44088b	TrGC	MEPROPENE + O_3 → $CH_3COCH_2O_2$ + OH + HCHO	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Taraborrelli (2016)
G44089	TrGCN	MEPROPENE + NO_3 → CH_3COCH_3 + HCHO + NO_2	3.4E-13	Atkinson et al. (2006), Taraborrelli (2016)*
G44090	TrGC	IBUTOLBO2 → CH_3COCH_3 + HCHO + HO_2	k1_RO2tORO2	Taraborrelli (2016)
G44091a	TrGC	IBUTOLBO2 + HO_2 → IBUTOLBOOH	KRO2HO2(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44091b	TrGC	IBUTOLBO2 + HO_2 → CH_3COCH_3 + HCHO + HO_2 + OH	KRO2HO2(4)*rcoch2o2_oh	Taraborrelli (2016)
G44092a	TrGCN	IBUTOLBO2 + NO → CH_3COCH_3 + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,3,0,0,0, temp,cair))	Taraborrelli (2016)
G44092b	TrGCN	IBUTOLBO2 + NO → IBUTOLBNO3	KRO2NO*alpha_AN(5,3,0,0,0,temp, cair)	Taraborrelli (2016)
G44093	TrGCN	IBUTOLBO2 + NO_3 → CH_3COCH_3 + HCHO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2016)
G44094a	TrGC	IBUTOLBOOH + OH → IBUTOLBO2	.6*k_CH3OOH_OH	Taraborrelli (2016)
G44094b	TrGC	IBUTOLBOOH + OH → CH_3COCH_3 + HCHO + HO_2	k_s*f_sooh*f_pch2oh	Taraborrelli (2016)
G44095	TrGCN	IBUTOLBNO3 + OH → CH_3COCH_3 + HCHO + HO_2 + NO_2	3.*k_p	Taraborrelli (2016)
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), Taraborrelli (2016)*
G44097b	TrGC	BUT1ENE + O_3 → C_2H_5CHO + CH_2OO^*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Taraborrelli (2016)*
G44098	TrGCN	BUT1ENE + NO_3 → C_2H_5CHO + HCHO + NO_2	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44099	TrGC	LBUT1ENO2 → C_2H_5CHO + HCHO + HO_2	k1_RO2sORO2	Taraborrelli (2016)
G44100a	TrGC	LBUT1ENO2 + HO_2 → LBUT1ENOOH	KRO2HO2(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44100b	TrGC	LBUT1ENO2 + HO_2 → C_2H_5CHO + HCHO + HO_2 + OH	KRO2HO2(4)*rcoch2o2_oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44101a	TrGCN	LBUT1ENO2 + NO → C_2H_5CHO + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair))	Taraborrelli (2016)
G44101b	TrGCN	LBUT1ENO2 + NO → LBUT1ENNO3	KRO2NO*alpha_AN(5,2,0,0,0,temp, cair)	Taraborrelli (2016)
G44102	TrGCN	LBUT1ENO2 + NO_3 → C_2H_5CHO + HCHO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2016)
G44103a	TrGC	LBUT1ENOOH + OH → LBUT1ENO2	.6*k_CH3OOH_OH	Taraborrelli (2016)
G44103b	TrGC	LBUT1ENOOH + OH → $C_2H_5CO_3$ + HCHO + HO_2	k_t*f_tooh*f_pch2oh	Taraborrelli (2016)*
G44104	TrGCN	LBUT1ENNO3 + OH → C_2H_5CHO + CO + HO_2 + NO_2	k_s*f_soh*f_ch2ono2	Taraborrelli (2016)*
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 HCOCH2O2 + .05 CH2CO + .09 CH_3OH + .09 CO + .2 CH_4 + .2 CO_2	3.2E-15*EXP(-965./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44107	TrGCN	CBUT2ENE + NO_3 → 2 CH_3CHO + NO_2	3.5E-13	Atkinson et al. (2006), Taraborrelli (2016)*
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 HCOCH2O2 + .05 CH2CO + .09 CH_3OH + .09 CO + .2 CH_4 + .2 CO_2	6.6E-15*EXP(-1060./temp)	Atkinson et al. (2006), Taraborrelli (2016)
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), Taraborrelli (2016)*
G44111	TrGC	BUT2OLO2 → C_2H_5CHO + HCHO + HO_2	k1_RO2sOR02	Taraborrelli (2016)
G44112a	TrGC	BUT2OLO2 + HO_2 → BUT2OLOOH	KRO2HO2(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44112b	TrGC	BUT2OLO2 + HO_2 → 2 CH_3CHO + HO_2 + OH	KRO2HO2(4)*rcoch2o2_oh	Taraborrelli (2016)
G44113a	TrGCN	BUT2OLO2 + NO → 2 CH_3CHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(5,2,0,0,0, temp,cair))	Taraborrelli (2016)
G44113b	TrGCN	BUT2OLO2 + NO → BUT2OLNO3	KRO2NO*alpha_AN(5,2,0,0,0,temp, cair)	Taraborrelli (2016)
G44114	TrGCN	BUT2OLO2 + NO_3 → 2 CH_3CHO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2016)
G44115a	TrGC	BUT2OLOOH + OH → BUT2OLO2	.6*k_CH3OOH_OH	Taraborrelli (2016)
G44115b	TrGC	BUT2OLOOH + OH → LMEKOOH + HO_2	k_t*f_toh*f_pch2oh	Taraborrelli (2016)
G44115c	TrGC	BUT2OLOOH + OH → BUT2OLO + OH	k_t*f_tooh*f_pch2oh	Taraborrelli (2016)
G44116	TrGCN	BUT2OLNO3 + OH → LMEKNO3 + HO_2	k_t*f_toh*f_ch2ono2	Taraborrelli (2016)
G44117	TrGC	BUT2OLO + OH → BIACET + HO_2	k_t*f_toh*f_co	Taraborrelli (2016)
G44118	TrGC	IPRCHO + OH → IPRCO3 + H_2O	6.8E-12*EXP(410./temp)	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
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*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44121b	TrGC	IPRCO3 + HO_2 → $iC_3H_7O_2$ + CO_2 + OH	KAPHO2*(1-rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
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	.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G44124b	TrGC	PERIBUACID + OH → CH_3COCH_3 + H_2O + CO_2	k_s*f_co2h	Taraborrelli (2016)*
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	Taraborrelli (2016)*
G44127	TrGC	MPROPENOL + OH → HCOOH + OH + CH_3COCH_3	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44128	TrGC	MPROPENOL + HCOOH → IPRCHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44129	TrGC	IPRCHO + HCOOH → MPROPENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44130	TrGC	BUTENOL + OH → HCOOH + OH + C_2H_5CHO	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44131	TrGC	BUTENOL + HCOOH → C_3H_7CHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44132	TrGC	C_3H_7CHO + HCOOH → BUTENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44133	TrGC	HVMK + OH → HCOOH + OH + MGLYOX	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	HVMK + HCOOH → CO2C3CHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44135	TrGC	CO2C3CHO + HCOOH → HVMK + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44136	TrGC	HMAC + OH → HCOOH + OH + MGLYOX	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	HMAC + HCOOH → IBUTDIAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*

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

#	labels	reaction	rate coefficient	reference
G44138	TrGC	IBUTDIAL + HCOOH → HMAC + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (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	Taraborrelli (2016)*
G44140	TrGCN	CO2C3CHO + NO_3 → $CH_3COCH_2O_2$ + CO_2 + HNO_3	KNO3AL*4.0	Taraborrelli (2016)*
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	Taraborrelli (2016)*
G44142	TrGCN	IBUTDIAL + NO_3 → CH_3CHO + CO + HO_2 + CO_2 + HNO_3	2.*KNO3AL*4.0	Taraborrelli (2016)*
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 → $CH_3COCOCH_2OOH$	KRO2HO2(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 → $CH_3COCOCH_2O_2$	.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G44204	TrGTerC	C44O2 + HO_2 → C44OOH	KRO2HO2(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	KRO2HO2(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*rco3_ooh	Rickard and Pascoe (2009)
G44215b	TrGTerC	C312COCO3 + HO_2 → $HCOCOCH_2O_2$ + CO_2 + OH	KAPHO2*(1-rco3_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)	Taraborrelli (2016)*
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)

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

#	labels	reaction	rate coefficient	reference
G44224a	TrGTerC	IPRHOCO3 + HO_2 → CH_3COCH_3 + CO_2 + HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44224b	TrGTerC	IPRHOCO3 + HO_2 → IPRHOCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2016)
G44224c	TrGTerC	IPRHOCO3 + HO_2 → IPRHOCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
G44233b	TrGTerC	MBOOO → IBUTALOH + H_2O_2	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2016)
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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G44402	TrGAroCN	NC4DCO2H + OH → MALANHY + NO_2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G44403	TrGAroC	CO14O3CO2H + OH → HCOCH2O2 + 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*rco3_o3	Rickard and Pascoe (2009)
G44406b	TrGAroC	MALDIALCO3 + HO_2 → MALDALCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G44406c	TrGAroC	MALDIALCO3 + HO_2 → .6 MALANHY + HO_2 + .4 GLYOX + .4 CO + .4 CO_2 + OH	KAPHO2*rco3_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)*

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

#	labels	reaction	rate coefficient	reference
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)*
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 HCOCH2O2 + .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*rco3_oh	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO_2 → EPXDLCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO_2 → EPXDLCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO → C3DIALO2 + CO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G44419	TrGAroCN	EPXDLCO3 + NO_2 → EPXDLPAN	k_CH3CO3_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	KRO2HO2(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44429b	TrGAroC	MALANHYO2 + HO_2 → HCOCOHCO3 + CO_2 + OH	KRO2HO2(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCOHCO3 + CO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G44431	TrGAroCN	MALANHYO2 + NO_3 → HCOCOHCO3 + CO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 → HCOCOHCO3 + CO_2	k1_RO2sOR02	Rickard and Pascoe (2009)*
G44433	TrGAroC	EPXDLCO3H + OH → EPXDLCO3	2.62E-11	Rickard and Pascoe (2009)
G44434	TrGAroC	CO2C4DIAL + OH → CO + CO + CO + CO + HO_2	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	NBZFUO2 + HO_2 → NBZFUOOH	KRO2HO2(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44435b	TrGAroCN	NBZFUO2 + HO_2 → .5 CO14O3CHO + .5 NO_2 + .5 NBZFUONE + .5 HO_2 + OH	KRO2HO2(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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_RO2sOR02	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	KRO2HO2(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44442b	TrGAroC	MECOACETO2 + HO_2 → $CH_3C(O)OO$ + HCHO + CO_2 + OH	KRO2HO2(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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_RO2pOR02	Rickard and Pascoe (2009)*
G44446	TrGAroCN	CO14O3CHO + NO_3 → CO + HCOCH2O2 + CO_2 + HNO_3	KNO3AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	CO14O3CHO + OH → CO + HCOCH2O2 + 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	KRO2HO2(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44449b	TrGAroC	BZFUO2 + HO_2 → CO14O3CHO + HO_2 + OH	KRO2HO2(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44450	TrGAroCN	BZFUO2 + NO → CO14O3CHO + HO_2 + NO_2	`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)*
G44453	TrGAroC	BZFUCO + OH → CO14O3CHO + HO_2	`1.78E-11`	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO_2 → MALDIALOOH	`KRO2HO2(4)*(1-rcoch2o2_oh-rchohch2o2_oh)`	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO_2 → GLYOX + GLYOX + HO_2 + OH	`KRO2HO2(4)*(rcoch2o2_oh+rchohch2o2_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 HCOCH2O2 + .01782 CO + 0.05408 LCARBON	`1.03E-14*EXP(-1995./temp)`	Atkinson et al. (2006), Taraborrelli (2016)
G45001	TrGC	C_5H_8 + OH → .63 ISOPAB + .30 ISOPCD + .07 LISOPEFO2	`2.7E-11*EXP(390./temp)`	Atkinson et al. (2006), Taraborrelli (2016)
G45002	TrGCN	C_5H_8 + NO_3 → NISOPO2	`3.0E-12*EXP(-450./temp)`	Atkinson et al. (2006)
G45003a	TrGC	ISOPAB + O_2 → LISOPACO2	`5.530E-13`	Taraborrelli (2016)
G45003b	TrGC	ISOPAB + O_2 → ISOPBO2	`3.E-12`	Taraborrelli (2016)
G45004a	TrGC	ISOPCD + O_2 → LDISOPACO2	`6.780E-13`	Taraborrelli (2016)
G45004b	TrGC	ISOPCD + O_2 → ISOPDO2	`3.E-12`	Taraborrelli (2016)
G45005	TrGC	LISOPACO2 → ISOPAB + O_2	`3.1E12*exp(-7900./temp)*.6+7.8E13*exp(-8600./temp)*.4`	Taraborrelli (2016)
G45006	TrGC	ISOPBO2 → ISOPAB + O_2	`3.7E14*exp(-9570./temp)+4.2E14*exp(-9970./temp)`	Taraborrelli (2016)
G45007	TrGC	LDISOPACO2 → ISOPCD + O_2	`5.65E12*exp(-8410./temp)*.42+1.4E14*exp(-9110./temp)*.58`	Taraborrelli (2016)
G45008	TrGC	ISOPDO2 → ISOPCD + O_2	`5.0E14*exp(-10120./temp)+8.25E14*exp(-10220/temp)`	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45009a	TrGC	LISOPACO2 → C1ODC2O2C4OOH	K16HSZ14 * 2./3.*(1-fhpal)	Taraborrelli (2016)
G45009b	TrGC	LISOPACO2 → ZCODC23DBCOOH + HO_2	K16HSZ14 * (2./3.*fhpal + 1./3.)	Taraborrelli (2016)
G45010a	TrGC	LDISOPACO2 → C1OOHC3O2C4OD	k16HSZ41 * 2./3.*(1-fhpal)	Taraborrelli (2016)
G45010b	TrGC	LDISOPACO2 → ZCODC23DBCOOH + HO_2	k16HSZ41 * (2./3.*fhpal + 1./3.)	Taraborrelli (2016)
G45011	TrGC	LISOPACO2 → .9 LISOPACO + .1 ISOPAOH	k1_RO2LISOPACO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G45012	TrGC	LISOPACO2 + HO_2 → LISOPACOOH	KRO2HO2(5)	Rickard and Pascoe (2009)
G45013a	TrGCN	LISOPACO2 + NO → LISOPACO + NO_2	KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45013b	TrGCN	LISOPACO2 + NO → LISOPACNO3	KRO2NO*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45014	TrGCN	LISOPACO2 + NO_3 → LISOPACO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45015	TrGC	LDISOPACO2 → .9 LISOPACO + .1 ISOPAOH	k1_RO2LISOPACO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G45016	TrGC	LDISOPACO2 + HO_2 → LISOPACOOH	KRO2HO2(5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO → LISOPACO + NO_2	KRO2NO*(1.-alpha_AN(6,1,0,0,0, temp,cair))	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45017b	TrGCN	LDISOPACO2 + NO → LISOPACNO3	KRO2NO*alpha_AN(6,1,0,0,0,temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45018	TrGCN	LDISOPACO2 + NO_3 → LISOPACO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH → LISOPACO2	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G45019b	TrGC	LISOPACOOH + OH → ZCODC23DBCOOH + HO_2	k_s*f_allyl*f_soh	Taraborrelli (2016)
G45019c	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH	(k_s*f_sooh*f_allyl+ k_rohro)	Taraborrelli (2016)
G45019d	TrGC	LISOPACOOH + OH → LIEPOX + OH	(k_adt+k_ads)*a_ch2oh*a_ch2ooh	Taraborrelli (2016)*
G45020	TrGC	ISOPAOH + OH → LHC4ACCHO + HO_2	(k_adt+k_ads)*a_ch2oh*a_ch2oh+k_ s*f_soh*f_allyl+k_rohro	Taraborrelli (2016)
G45021	TrGCN	LISOPACNO3 + OH → LISOPACNO3O2	(k_adt+k_ads)*a_ch2ono2*a_ch2oh	Taraborrelli (2016)*
G45022	TrGC	ISOPBO2 → .8 MVK + .8 HCHO + .8 HO_2 + .2 ISOPBOH	k1_RO2ISOPBO2	Rickard and Pascoe (2009)
G45023a	TrGC	ISOPBO2 + HO_2 → ISOPBOOH	KRO2HO2(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45023b	TrGC	ISOPBO2 + HO_2 → MVK + HCHO + HO_2 + OH	KRO2HO2(5)*rchohch2o2_oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45024a	TrGCN	ISOPBO2 + NO → MVK + HCHO + HO_2 + NO_2	KRO2NO*(1.-alpha_AN(6,3,0,0,0, temp,cair))	Lockwood et al. (2010), Taraborrelli (2016)
G45024b	TrGCN	ISOPBO2 + NO → ISOPBNO3	KRO2NO*alpha_AN(6,3,0,0,0,temp, cair)	Lockwood et al. (2010), Taraborrelli (2016)
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), Taraborrelli (2016)
G45026b	TrGC	ISOPBOOH + OH → ISOPBO2	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G45026c	TrGC	ISOPBOOH + OH → MGLYOX + $HOCH_2CHO$	k_rohro+k_s*f_alk*f_soh	Taraborrelli (2016)
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	Taraborrelli (2016)
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	Taraborrelli (2016)
G45029	TrGCN	ISOPBNO3 + OH → ISOPBDNO3O2	(k_adt+k_adp)*f_ch2ono2	Taraborrelli (2016)
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	KRO2HO2(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45031b	TrGC	ISOPDO2 + HO_2 → MACR + HCHO + HO_2 + OH	KRO2HO2(5)*rchohch2o2_oh	Taraborrelli (2016)
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), Taraborrelli (2016)
G45032b	TrGCN	ISOPDO2 + NO → ISOPDNO3	KRO2NO*alpha_AN(6,2,0,0,0,temp, cair)	Lockwood et al. (2010), Taraborrelli (2016)
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), Taraborrelli (2016)
G45034b	TrGC	ISOPDOOH + OH → ISOPDO2	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G45034c	TrGC	ISOPDOOH + OH → HCOC5 + OH	k_t*f_tooh*f_allyl*f_pch2oh	Taraborrelli (2016)
G45034d	TrGC	ISOPDOOH + OH → CH_3COCH_2OH + GLYOX + OH	k_s*f_pch2oh*f_soh	Taraborrelli (2016)
G45035	TrGC	ISOPDOOH + O_3 → 1.393 OH + BIACETOH + .67 HCHO + .05280 HO_2 + .2079 CO + .1221 CH_2OO	1.E-17	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
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	Taraborrelli (2016)
G45037	TrGCN	ISOPDNO3 + OH → ISOPBDNO3O2	(k_adp+k_ads)*a_ch2ono2	Taraborrelli (2016)*
G45038	TrGCN	NISOPO2 → .8 NC4CHO + .6 HO_2 + .2 LISOPACNO3	k1_RO2LISOPACO2	Rickard and Pascoe (2009)
G45039	TrGCN	NISOPO2 + HO_2 → NISOPOOH	KRO2HO2(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	Taraborrelli (2016)*
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	Taraborrelli (2016)
G45045	TrGCN	NC4CHO + NO_3 → LNISO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO3 + HO_2 → LNISOOH	.5*KRO2HO2(5) + .5*KAPHO2	Rickard and Pascoe (2009)
G45047	TrGCN	LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	.5*KAPNO +.5*KRO2NO	Rickard and Pascoe (2009)*
G45048	TrGCN	LNISO3 + NO_3 → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	1.3*KRO2NO3	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	Taraborrelli (2016)
G45050b	TrGC	LHC4ACCHO + OH → LHC4ACCO3	k_t*f_o	Taraborrelli (2016)
G45050c	TrGC	LHC4ACCHO + OH → ZCODC23DBCOD + HO_2	k_s*f_soh*f_allyl	Taraborrelli (2016)
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	KRO2HO2(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45054b	TrGC	LC578O2 + HO_2 → LC578OOH	KRO2HO2(5)*rcoch2o2_ooh	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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)*
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	KHSB	Taraborrelli (2016)
G45058a	TrGC	LC578OOH + OH → LC578O2	0.6*k_CH3OOH_OH	Taraborrelli (2016)
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	Taraborrelli (2016)
G45059a	TrGC	LHC4ACCO3 → OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	k1_RO2RCO3*0.9	Taraborrelli (2016)
G45059b	TrGC	LHC4ACCO3 → LHC4ACCO2H	k1_RO2RCO3*0.1	Taraborrelli (2016)
G45060a	TrGC	LHC4ACCO3 + HO_2 → 2 OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	KAPHO2*rco3_oh	Taraborrelli (2016)
G45060b	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO3H	KAPHO2*rco3_ooh	Taraborrelli (2016)
G45060c	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2016)
G45061	TrGCN	LHC4ACCO3 + NO → .5 MACRO2 + .5 LHMVKABO2 + NO_2 + CO_2	KAPNO	Taraborrelli (2016)
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	1.6*KRO2NO3	Taraborrelli (2016)
G45064a	TrGC	LHC4ACCO2H + OH → OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	2.52E-11	Taraborrelli (2016)
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)	Taraborrelli (2016)
G45069	TrGC	C59O2 → CH_3COCH_2OH + HOCH2CO	k1_RO2tORO2	Taraborrelli (2016)
G45070a	TrGC	C59O2 + HO_2 → OH + CH_3COCH_2OH + HOCH2CO	KRO2HO2(5)*rcoch2o2_oh	Taraborrelli (2016)
G45070b	TrGC	C59O2 + HO_2 → C59OOH	KRO2HO2(5)*rcoch2o2_ooh	Taraborrelli (2016)
G45071	TrGCN	C59O2 + NO → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO	Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
G45072	TrGCN	C59O2 + NO_3 → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO3	Taraborrelli (2016)
G45073	TrGC	C59OOH + OH → C59O2	9.7E-12	Rickard and Pascoe (2009)
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), Taraborrelli (2016)*
G45075	TrGC	ISOPBO2 → MVK + HCHO + OH	KHSB	Taraborrelli (2016)
G45076	TrGC	ISOPDO2 → MACR + HCHO + OH	KHSD	Taraborrelli (2016)
G45077a	TrGC	ZCODC23DBCOOH + OH → .6 C1ODC2O2C4OOH + .4 C1OOHC2O2C4OD	k_adt*a_cho*a_ch2ooh	Taraborrelli (2016)
G45077b	TrGC	ZCODC23DBCOOH + OH → .6 C1ODC3O2C4OOH + .4 C1OOHC3O2C4OD	k_ads*a_cho*a_ch2ooh	Taraborrelli (2016)
G45077c	TrGC	ZCODC23DBCOOH + OH → ZCO3HC23DBCOD	k_t*f_o*f_alk+0.6*k_CH3OOH_OH	Taraborrelli (2016)
G45077d	TrGC	ZCODC23DBCOOH + OH → ZCODC23DBCOD + OH	k_s*f_sooh*f_allyl	Taraborrelli (2016)
G45078	TrGC	ZCODC23DBCOOH + 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	Taraborrelli (2016)
G45079	TrGC	C1OOHC2O2C4OD → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH	k1_RO2tORO2	Taraborrelli (2016)
G45080	TrGCN	C1OOHC2O2C4OD + NO → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH + NO_2	KRO2NO	Taraborrelli (2016)*
G45081a	TrGC	C1OOHC2O2C4OD + HO_2 → C1OOHC2OOHC4OD	KRO2HO2(5)*rcoch2o2_ooh	Taraborrelli (2016)
G45081b	TrGC	C1OOHC2O2C4OD + HO_2 → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + 1.22 OH	KRO2HO2(5)*rcoch2o2_oh	Taraborrelli (2016)
G45082	TrGC	C1OOHC2O2C4OD → $CH_3COCH_2O_2H$ + GLYOX + OH	KHSB	Taraborrelli (2016)
G45083	TrGC	C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD	K15HSDHB	Taraborrelli (2016)
G45084a	TrGC	C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH	2.*k_s*f_sooh*f_tch2oh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45084b	TrGC	C1OOHC2OOHC4OD + OH → $CH_3COCH_2O_2H$ + 2 CO + 2 HO_2 + OH	k_t*f_toh*f_pch2oh*f_pch2oh	Taraborrelli (2016)
G45084c	TrGC	C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD	0.6*k_CH3OOH_OH	Taraborrelli (2016)
G45085	TrGC	C1ODC2OOHC4OD + OH → CO2H3CHO + CO + H_2O + OH	k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho	Taraborrelli (2016)
G45086	TrGC	C1ODC3O2C4OOH → MGLYOX + HOOCH2CHO + HO_2	k1_RO2sORO2	Taraborrelli (2016)
G45087	TrGCN	C1ODC3O2C4OOH + NO → MGLYOX + HOOCH2CHO + HO_2 + NO_2	KRO2NO	Taraborrelli (2016)
G45088	TrGC	C1ODC3O2C4OOH + HO_2 → .5 $CH_3C(O)$ + .5 CO + .5 MGLYOX + .5 HO_2 + $HOOCH_2CO_3$	KRO2HO2(5)	Taraborrelli (2016)
G45089	TrGC	C1ODC3O2C4OOH → MGLYOX + OH + HOOCH2CHO	KHSD	Taraborrelli (2016)
G45090	TrGC	C1OOHC3O2C4OD → .625 MGLYOX + 2 CO + 1.625 HO_2 + .375 $CH_3C(O)$ + .375 CO_2 + OH	K15HSDHB	Taraborrelli (2016)
G45091	TrGC	LHC4ACCO3 → ZCO3HC23DBCOD + HO_2	K16HS	Taraborrelli (2016)
G45092a	TrGC	ZCODC23DBCOD + OH → C1ODC2O2C4OD	(k_adt+k_ads)*a_cho*a_cho	Taraborrelli (2016)*
G45092b	TrGC	ZCODC23DBCOD + OH → ZCO3C23DBCOD	2*k_t*f_o*f_alk	Taraborrelli (2016)*
G45093	TrGCN	ZCODC23DBCOD + NO_3 → ZCO3C23DBCOD + HNO_3	KNO3AL*4.25*2.	Taraborrelli (2016)*
G45094a	TrGC	C1ODC2O2C4OD + HO_2 → OH + MGLYOX + HOCHCHO	KRO2HO2(5)*rcoch2o2_oh	Taraborrelli (2016)
G45094b	TrGC	C1ODC2O2C4OD + HO_2 → C1ODC2OOHC4OD	KRO2HO2(5)*rcoch2o2_ooh	Taraborrelli (2016)
G45095	TrGCN	C1ODC2O2C4OD + NO → NO_2 + MGLYOX + HOCHCHO	KRO2NO	Taraborrelli (2016)*
G45096	TrGC	C1ODC2O2C4OD → MGLYOX + HOCHCHO	k1_RO2tORO2	Taraborrelli (2016)
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	Taraborrelli (2016)
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	Taraborrelli (2016)
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	Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
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+KRO2HO2(5)*c(ind_HO2)`	Taraborrelli (2016)
G45100	TrGCN	ISOPBDNO3O2 + NO → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO_2 + 1.6 NO_2	`KRO2NO`	Taraborrelli (2016)*
G45101	TrGCN	ISOPBDNO3O2 → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRN + .14 MVKNO3 + .4 HCHO + .4 HO_2 + .6 NO_2	`k1_RO2sORO2+KRO2HO2(5)*c(ind_HO2)`	Taraborrelli (2016)
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), Taraborrelli (2016)
G45103	TrGC	DB1O2 → DB1O2	`k1_RO2sORO2`	Taraborrelli (2016)
G45104a	TrGC	DB1O2 + HO_2 → DB1OOH	`KRO2HO2(5)*(1.-rchohch2o2_oh)`	Taraborrelli (2016)*
G45104b	TrGC	DB1O2 + HO_2 → DB1O2 + OH	`KRO2HO2(5)*rchohch2o2_oh`	Taraborrelli (2016)
G45105a	TrGCN	DB1O2 + NO → DB1O2 + NO_2	`KRO2NO*(1.-alpha_AN(7,2,0,0,0,temp,cair))`	Taraborrelli (2016)
G45105b	TrGCN	DB1O2 + NO → DB1NO3	`KRO2NO*alpha_AN(7,2,0,0,0,temp,cair)`	Taraborrelli (2016)
G45106	TrGCN	DB1O2 + NO_3 → DB1O2 + NO_2	`KRO2NO3`	Taraborrelli (2016)
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`	Taraborrelli (2016)
G45110a	TrGC	DB1O2 + HO_2 → DB2OOH	`KRO2HO2(5)*(1.-rchohch2o2_oh)`	Taraborrelli (2016)
G45110b	TrGC	DB1O2 + HO_2 → .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + OH	`KRO2HO2(5)*rchohch2o2_oh`	Taraborrelli (2016)
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`	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45113	TrGC	DB1O2 → .48 MACROOH + .52 LHMVKABOOH + CO + OH	K14HSAL	Taraborrelli (2016)
G45114a	TrGC	DB1OOH + OH → DB1O2	.6*k_CH3OOH_OH	Taraborrelli (2016)
G45114b	TrGC	DB1OOH + OH → HCOOH + HO_2 + CH_3COCHO_2CHO	k_adt	Taraborrelli (2016)*
G45115	TrGC	DB1OOH + HCOOH → C1ODC2OOHC4OD + HCOOH	4.67E-26*temp**3.286*EXP(4509./(1.987*temp))	Taraborrelli (2016), daSilva (2010)*
G45116	TrGCN	DB1NO3 + OH → HCOOH + NO_2 + CH_3COCHO_2CHO	k_adt	Taraborrelli (2016)*
G45117	TrGC	DB2OOH + OH → DB1O2	.6*k_CH3OOH_OH	Taraborrelli (2016)*
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	Taraborrelli (2016)
G45119a	TrGC	ZCO3HC23DBCOD + OH → .62 CO2H3CHO + .62 OH + .62 CO_2 + .38 MGLYOX + .38 $HCOCO_3H$ + .38 HO_2	k_adt*a_cho*a_co2h	Taraborrelli (2016)
G45119b	TrGC	ZCO3HC23DBCOD + 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	Taraborrelli (2016)
G45120	TrGC	LISOPEFO2 → LISOPEFO	k1_RO2pORO2	Taraborrelli (2016)
G45121a	TrGCN	LISOPEFO2 + NO → LISOPEFO + NO_2	KRO2NO*(1.-alpha_AN(6,1,0,0,0,temp,cair))	Taraborrelli (2016)
G45121b	TrGCN	LISOPEFO2 + NO → ISOPDNO3	KRO2NO*alpha_AN(6,1,0,0,0,temp,cair)	Taraborrelli (2016)*
G45122a	TrGC	LISOPEFO2 + HO_2 → .7143 ISOPDOOH + .2857 ISOPBOOH	KRO2HO2(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45122b	TrGC	LISOPEFO2 + HO_2 → LISOPEFO + OH	KRO2HO2(5)*rchohch2o2_oh	Taraborrelli (2016)
G45123	TrGCN	LISOPEFO2 + NO_3 → LISOPEFO + NO_2	KRO2NO3	Taraborrelli (2016)
G45124	TrGC	LISOPEFO2 → .7143 MACR + .2857 MVK + HCHO + OH	.7143*KHSD+.2857*KHSB	Taraborrelli (2016)
G45125	TrGC	LISOPEFO → .7143 MACR + .2857 MVK + HCHO + HO_2	KDEC	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45126a	TrGC	LISOPACO → 3METHYLFURAN + HO_2	KDEC*0.37	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO_2 + .35 DB1O2	KDEC*(1.-0.37)	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	LISOPACO → 3METHYLFURAN + HO_2	KDEC*0.37	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	LISOPACO → .65 LHC4ACCHO + .65 HO_2 + .35 DB1O2	KDEC*(1.-0.37)	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	3METHYLFURAN + OH → L3METHYLFURANO2	3.2E-11*EXP(310./temp)	Taraborrelli (2016)*
G45129	TrGCN	3METHYLFURAN + NO_3 → L3METHYLFURANO2 + NO_2	1.9E-11	Taraborrelli (2016), Atkinson et al. (2006)*
G45130	TrGC	L3METHYLFURANO2 → ZCODC23DBCOD + HO_2	k1_RO2sOR02	Taraborrelli (2016)
G45131	TrGCN	L3METHYLFURANO2 + NO → ZCODC23DBCOD + HO_2 + NO_2	KRO2NO	Taraborrelli (2016)*
G45132	TrGC	L3METHYLFURANO2 + HO_2 → ZCODC23DBCOD + HO_2	KRO2HO2(5)	Taraborrelli (2016)*
G45133	TrGC	ZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2	k1_RO2RCO3	Taraborrelli (2016)
G45134a	TrGC	ZCO3C23DBCOD + HO_2 → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + OH	KAPHO2*rco3_oh	Taraborrelli (2016)
G45134b	TrGC	ZCO3C23DBCOD + HO_2 → ZCO3HC23DBCOD	KAPHO2*(rco3_ooh+rco3_o3)	Taraborrelli (2016)*
G45135	TrGCN	ZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	KAPNO	Taraborrelli (2016)
G45136	TrGCN	ZCO3C23DBCOD + NO_2 → ZCPANC23DBCOD	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45137	TrGCN	ZCO3C23DBCOD + NO_3 → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	1.6*KRO2NO3	Taraborrelli (2016)
G45138	TrGCN	ZCPANC23DBCOD → ZCO3C23DBCOD + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	ZCPANC23DBCOD + OH → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO_2 + NO_2	2.52E-11	Taraborrelli (2016)*
G45200	TrGTerC	C511O2 → $CH_3C(O)$ + HCOCH2CHO	k1_RO2sOR02	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO → $CH_3C(O)$ + HCOCH2CHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45202a	TrGTerC	C511O2 + HO_2 → C511OOH	KRO2HO2(5)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45202b	TrGTerC	C511O2 + HO_2 → $CH_3C(O)$ + HCOCH2CHO + OH	KRO2HO2(5)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45209b	TrGTerC	CO23C4CO3 + HO_2 → $CH_3COCOCH_2O_2$ + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(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 + HOC2H4CO3	k1_RO2sORO2	Rickard and Pascoe (2009)
G45217	TrGTerCN	C513O2 + NO → GLYOX + HOC2H4CO3 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G45218a	TrGTerC	C513O2 + HO_2 → C513OOH	KRO2HO2(5)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45218b	TrGTerC	C513O2 + HO_2 → GLYOX + HOC2H4CO3 + OH	KRO2HO2(5)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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 → HOC2H4CO3 + CO + CO	2.64E-11	Rickard and Pascoe (2009)
G45227	TrGTerC	C514O2 + HO_2 → C514OOH	KRO2HO2(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), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45228b	TrGTerCN	C514O2 + NO → C514NO3	KRO2NO*alpha_AN(7,2,0,1,0,temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
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)
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), Taraborrelli (2016)*
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G45238	TrGTerCN	MBO + NO_3 → LNMBOABO2	4.6E-14*EXP(-400./TEMP)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45239	TrGTerC	LMBOABO2 + HO_2 → LMBOABOOH	KRO2HO2(5)	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G45241a	TrGTerC	LMBOABO2 → $HOCH_2CHO$ + CH_3COCH_3 + HO_2	k1_RO2sORO2*.67	Rickard and Pascoe (2009), Taraborrelli (2016)
G45241b	TrGTerC	LMBOABO2 → IBUTALOH + HCHO + HO_2	k1_RO2pORO2*.33	Rickard and Pascoe (2009), Taraborrelli (2016)
G45242a	TrGTerC	LMBOABOOH + OH → MBOACO	.67*2.93E-11+.33*2.05E-12	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45242b	TrGTerC	LMBOABOOH + OH → LMBOABO2	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2016)
G45243	TrGTerCN	LMBOABNO3 + OH → MBOACO + NO_2	.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45244	TrGTerC	MBOACO + OH → MBOCOCO + HO_2	3.79E-12	Rickard and Pascoe (2009)
G45245	TrGTerC	MBOCOCO + OH → CO + IPRHOCO3	1.38E-11	Rickard and Pascoe (2009)
G45246	TrGTerCN	LNMBOABO2 + HO_2 → LNMBOABOOH	KRO2HO2(5)	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)*
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), Taraborrelli (2016)
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), Taraborrelli (2016)
G45250a	TrGTerCN	LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBCO	.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45250b	TrGTerCN	LNMBOABOOH + OH → LNMBOABO2	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2016)
G45251	TrGTerCN	NMBOBCO + OH → NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45252a	TrGTerCN	NC4OHCO3 + HO_2 → IBUTALOH + CO_2 + NO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45252b	TrGTerCN	NC4OHCO3 + HO_2 → NC4OHCO3H	KAPHO2*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
G45400	TrGAroCN	NC4MDCO2HN + OH → MMALANHY + NO_2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G45401	TrGAroCN	$C54CO + NO_3 \rightarrow 3\ CO + CH_3C(O)OO + HNO_3$	KNO3AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	$C54CO + OH \rightarrow 3\ CO + CH_3C(O)OO$	1.72E-11	Rickard and Pascoe (2009)
G45403a	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow NTLFUOOH$	KRO2HO2(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	$NTLFUO2 + HO_2 \rightarrow ACCOMECHO + NO_2 + OH$	KRO2HO2(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45404	TrGAroCN	$NTLFUO2 + NO \rightarrow ACCOMECHO + NO_2 + NO_2$	KRO2NO	Rickard and Pascoe (2009)*
G45405	TrGAroCN	$NTLFUO2 + NO_3 \rightarrow ACCOMECHO + NO_2 + NO_2$	KRO2NO3	Rickard and Pascoe (2009)*
G45406	TrGAroCN	$NTLFUO2 \rightarrow ACCOMECHO + NO_2$	k1_RO2tORO2	Rickard and Pascoe (2009)*
G45407	TrGAroC	$C5134CO2OH + OH \rightarrow C54CO + HO_2$	7.48E-11	Rickard and Pascoe (2009)
G45408	TrGAroCN	$C5COO2NO2 + OH \rightarrow MGLYOX + CO + CO + NO_2$	5.43E-11	Rickard and Pascoe (2009)
G45409	TrGAroCN	$C5COO2NO2 \rightarrow C5CO14O2 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45410	TrGAroC	$C5DIALOOH + OH \rightarrow C5DIALCO + OH$	7.52E-11	Rickard and Pascoe (2009)
G45411a	TrGAroC	$C4CO2DBCO3 + HO_2 \rightarrow C4CO2DCO3H$	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45411b	TrGAroC	$C4CO2DBCO3 + HO_2 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + OH$	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45412	TrGAroCN	$C4CO2DBCO3 + NO \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	KAPNO	Rickard and Pascoe (2009)
G45413	TrGAroCN	$C4CO2DBCO3 + NO_2 \rightarrow C4CO2DBPAN$	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$C4CO2DBCO3 + NO_3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2 + NO_2$	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45415	TrGAroC	$C4CO2DBCO3 \rightarrow HO_2 + CO + HCOCOCHO + CO_2$	k1_RO2RCO3	Rickard and Pascoe (2009)
G45416	TrGAroC	$MMALANHY + OH \rightarrow MMALANHYO2$	1.50E-12	Rickard and Pascoe (2009)
G45421a	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow MMALNHYOOH$	KRO2HO2(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45421b	TrGAroC	$MMALANHYO2 + HO_2 \rightarrow CO2H3CO3 + CO_2 + OH$	KRO2HO2(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45422	TrGAroCN	$MMALANHYO2 + NO \rightarrow CO2H3CO3 + CO_2 + NO_2$	KRO2NO	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$MMALANHYO2 + NO_3 \rightarrow CO2H3CO3 + CO_2 + NO_2$	KRO2NO3	Rickard and Pascoe (2009)*
G45424	TrGAroC	$MMALANHYO2 \rightarrow CO2H3CO3 + CO_2$	k1_RO2tORO2	Rickard and Pascoe (2009)*
G45428	TrGAroCN	$C4CO2DBPAN + OH \rightarrow HCOCOCHO + CO_2 + CO + NO_2$	2.74E-11	Rickard and Pascoe (2009)
G45429	TrGAroCN	$C4CO2DBPAN \rightarrow C4CO2DBCO3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	$C5CO14O2 + HO_2 \rightarrow .83\ MALANHY + .83\ CH_3 + .17\ MGLYOX + .17\ HO_2 + .17\ CO + .17\ CO_2 + OH$	KAPHO2*rco3_oh	Rickard and Pascoe (2009)*
G45430b	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OH + O_3$	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G45430c	TrGAroC	$C5CO14O2 + HO_2 \rightarrow C5CO14OOH$	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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)*
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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	ACCOMECO3 + HO_2 → MECOACETO2 + CO_2 + OH	KAPHO2*rco3_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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G45468	TrGAroC	C24O3CCO2H + OH → MECOACETO2 + CO_2	8.76E-13	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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)
G45471	TrGAroCN	ACCOMEPAN → ACCOMECO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G45476a	TrGAroC	TLFUO2 + HO_2 → TLFUOOH	KRO2HO2(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
G45476b	TrGAroC	TLFUO2 + HO_2 → ACCOMECHO + HO_2 + OH	KRO2HO2(5)*(rcoch2o2_oh+rchohch2o2_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	KRO2HO2(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45486b	TrGAroC	C5DIALO2 + HO_2 → MALDIAL + CO + HO_2 + OH	KRO2HO2(5)*rcoch2o2_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	KRO2HO2(5)*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45491b	TrGAroC	C5DICARBO2 + HO_2 → MGLYOX + GLYOX + HO_2 + OH	KRO2HO2(5)*rco3_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	KRO2HO2(6)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G46200b	TrGTerC	CO235C6O2 + HO_2 → CO23C4CO3 + HCHO + OH	KRO2HO2(6)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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	KRO2HO2(6)*(1.-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G46206b	TrGTerC	C614O2 + HO_2 → CO23C4CHO + HCHO + HO_2 + OH	KRO2HO2(6)*rchohch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G46404a	TrGAroC	C615CO2O2 + HO_2 → C615CO2OOH	KRO2HO2(6)*(1.-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46404b	TrGAroC	C615CO2O2 + HO_2 → C5DICARB + CO + HO_2 + OH	KRO2HO2(6)*rcoch2o2_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	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46413b	TrGAroCN	NDNPHENO2 + HO_2 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + OH	KRO2HO2(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46414	TrGAroCN	NDNPHENO2 + NO → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G46415	TrGAroCN	NDNPHENO2 + NO_3 → NC4DCO2H + HNO_3 + CO + CO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46424b	TrGAroC	C5CO2OHCO3 + HO_2 → HOCOC4DIAL + HO_2 + CO + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	NCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	KRO2HO2(6)*rchohch2o2_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)*
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	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46437b	TrGAroCN	NPHENO2 + HO_2 → MALDALCO2H + GLYOX + NO_2 + OH	KRO2HO2(6)*rchohch2o2_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	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46447b	TrGAroCN	NNCATECO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	KRO2HO2(6)*rchohch2o2_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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G46453	TrGAroCN	NPHEN1O + NO_2 → DNPHEN	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)
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)*

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

#	labels	reaction	rate coefficient	reference
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	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46461b	TrGAroC	PHENO2 + HO_2 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO_2 + OH	KRO2HO2(6)*rchohch2o2_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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBCO3 + HO_2 → $CH_3C(O)$ + HCOCOCHO + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(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)
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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH → PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46480a	TrGAroC	PBZQO2 + HO_2 → PBZQOOH	KRO2HO2(6)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46480b	TrGAroC	PBZQO2 + HO_2 → C5CO2OHCO3 + OH	KRO2HO2(6)*(rchohch2o2_oh+rcoch2o2_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_RO2sOR02	Rickard and Pascoe (2009)*
G46484	TrGAroC	BZOBIPEROH + OH → MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	DNPHENO2 + HO_2 → DNPHENOOH	KRO2HO2(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46485b	TrGAroCN	DNPHENO2 + HO_2 → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	KRO2HO2(6)*rchohch2o2_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	KRO2HO2(6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	BZEMUCO2 + HO_2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO + OH	KRO2HO2(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)*
G46493	TrGAroC	BZEMUCO2 → .5 EPXC4DIAL + .5 GLYOX + .5 HO_2 + .5 C3DIALO2 + .5 C32OH13CO	k1_RO2sOR02	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	.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G46498	TrGAroC	C6125CO + OH → C5CO14O2 + CO	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	NBZQO2 + HO_2 → NBZQOOH	KRO2HO2(6)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46499b	TrGAroCN	NBZQO2 + HO_2 → C6CO4DB + NO_2 + OH	KRO2HO2(6)*rcoch2o2_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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G46504	TrGAroC	CATEC1O2 + HO_2 → CATEC1OOH	KRO2HO2(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*rco3_o3	Rickard and Pascoe (2009)
G46511b	TrGAroC	BZEMUCCO3 + HO_2 → BZEMUCCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G46511c	TrGAroC	BZEMUCCO3 + HO_2 → C5DIALO2 + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(6)	Rickard and Pascoe (2009)
G46517a	TrGAroCN	C6H5O2 + NO → C6H5O + NO_2	KRO2NO	Rickard and Pascoe (2009)
G46517b	TrGAroCN	C6H5O2 + NO_2 → C6H5O + NO_3	K_C6H5O2_NO2	Jagiella and Zabel (2007)*
G46518	TrGAroCN	C6H5O2 + NO_3 → C6H5O + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G46519	TrGAroC	C6H5O2 → C6H5O	k1_RO2sRO2	Rickard and Pascoe (2009)
G46521	TrGAroCN	BZEMUCNO3 + OH → BZEMUCCO + NO_2	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	BZBIPERO2 + HO_2 → BZBIPEROOH	KRO2HO2(6)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G46522b	TrGAroC	BZBIPERO2 + HO_2 → OH + GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE	KRO2HO2(6)*rbipero2_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)*

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

#	labels	reaction	rate coefficient	reference
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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	CO235C6CO3 + HO_2 → CO235C6O2 + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(7)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G47209b	TrGTerC	C716O2 + HO_2 → CO13C4CHO + $CH_3C(O)$ + OH	KRO2HO2(7)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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	KRO2HO2(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	KRO2HO2(7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	C722O2 + NO → CH_3COCH_3 + C44O2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
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	KRO2HO2(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)*

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

#	labels	reaction	rate coefficient	reference
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	KRO2HO2(7)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G47407b	TrGAroC	TLBIPERO2 + HO_2 → OH + .6 GLYOX + .4 MGLYOX + HO_2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KRO2HO2(7)*rbipero2_oh	Rickard and Pascoe (2009), Birdsall et al. (2010)*
G47408a	TrGAroCN	TLBIPERO2 + NO → NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 ZCODC23DBCOD + .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)*
G47409	TrGAroCN	TLBIPERO2 + NO_3 → NO_2 + .6 GLYOX + .4 MGLYOX + HO_2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KRO2NO3	Rickard and Pascoe (2009)*
G47410	TrGAroC	TLBIPERO2 → .6 GLYOX + .4 MGLYOX + HO_2 + .2 ZCODC23DBCOD + .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)

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

#	labels	reaction	rate coefficient	reference
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	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO2 + HO_2 → .68 C5CO14OH + .68 GLYOX + HO_2 + .32 PTLQONE + OH	KRO2HO2(7)*rchohch2o2_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	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO2 + HO_2 → C5CO14OH + GLYOX + NO_2 + OH	KRO2HO2(7)*rchohch2o2_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)*
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*rco3_oh	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO3 + HO_2 → TLEMUCCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO3 + HO_2 → TLEMUCCO3H	KAPHO2*rco3_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)

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

#	labels	reaction	rate coefficient	reference
G47438	TrGAroC	TLEMUCCO3 → C615CO2O2 + CO_2	k1_RO2RCO3	Rickard and Pascoe (2009)*
G47439a	TrGAroC	TLEMUCO2 + HO_2 → TLEMUCOOH	KRO2HO2(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47439b	TrGAroC	TLEMUCO2 + HO_2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO_2 + OH	KRO2HO2(7)*(rchohch2o2_oh+rcoch2o2_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)*
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	KRO2HO2(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)

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

#	labels	reaction	rate coefficient	reference
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)
G47477	TrGAroC	MCATEC1O2 + HO_2 → MCATEC1OOH	KRO2HO2(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	KRO2HO2(7)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO_2 → C7CO4DB + NO_2 + OH	KRO2HO2(7)*rcoch2o2_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	KRO2HO2(7)*(1-rchohch2o2_ oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO_2 → C6CO2OHCO3 + OH	KRO2HO2(7)*(rchohch2o2_oh+ rcoch2o2_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)*

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

#	labels	reaction	rate coefficient	reference
G47490	TrGAroCN	DNCRES + NO_3 → NDNCRESO2	7.83E-15	Rickard and Pascoe (2009)
G47491	TrGAroCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard and Pascoe (2009)
G47492	TrGAroCN	NCRES1O2 + HO_2 → NCRES1OOH	KRO2HO2(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	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47497b	TrGAroCN	MNNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	KRO2HO2(7)*rchohch2o2_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)
G47501a	TrGAroCN	MNCATECO2 + HO_2 → MNCATECOOH	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47501b	TrGAroCN	MNCATECO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	KRO2HO2(7)*rchohch2o2_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	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47509b	TrGAroCN	NDNCRESO2 + HO_2 → NC4MDCO2HN + HNO_3 + 2 CO + NO_2 + OH	KRO2HO2(7)*rchohch2o2_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)*

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

#	labels	reaction	rate coefficient	reference
G47513a	TrGAroCN	DNCRESO2 + HO_2 → DNCRESOOH	KRO2HO2(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47513b	TrGAroCN	DNCRESO2 + HO_2 → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	KRO2HO2(7)*rchohch2o2_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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G47519	TrGAroCN	MNCATECOOH + OH → MNCATECO2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
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*rco3_oh	Rickard and Pascoe (2009)
G47521b	TrGAroC	C6CO2OHCO3 + HO_2 → C6COOHCO3H	KAPHO2*(rco3_ooh+rco3_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	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G47527	TrGAroCN	DNCRESOOH + OH → DNCRESO2	0.6*k_CH3OOH_OH	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	KRO2HO2(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	KRO2HO2(8)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
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	KRO2HO2(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	KRO2HO2(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	KRO2HO2(8)	Rickard and Pascoe (2009)
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*rco3_ooh	Rickard and Pascoe (2009)
G48221b	TrGTerC	C721CO3 + HO_2 → C721O2 + CO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009)
G48221c	TrGTerC	C721CO3 + HO_2 → NORPINIC + O_3	KAPHO2*rco3_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	Taraborrelli (2016)
G48226	TrGTerC	C721CO3 → NORPINIC	k1_RO2RCO3*0.1	Taraborrelli (2016)
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	KRO2HO2(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)

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

#	labels	reaction	rate coefficient	reference
G48237	TrGTerC	C8BCCO + OH → C89O2	3.94E-12	Rickard and Pascoe (2009)
G48238	TrGTerC	C89O2 + HO_2 → C89OOH	KRO2HO2(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	KRO2HO2(8)	Rickard and Pascoe (2009)
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	KRO2HO2(8)	Rickard and Pascoe (2009)
G48408	TrGAroCN	NSTYRENO2 + NO → NO_2 + NO_2 + HCHO + BENZAL	KRO2NO	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G48409	TrGAroCN	NSTYRENO2 + NO_3 → NO_2 + NO_2 + HCHO + BENZAL	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	KRO2HO2(8)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G48412b	TrGAroC	STYRENO2 + HO_2 → HO_2 + OH + HCHO + BENZAL	KRO2HO2(8)*rchohch2o2_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)
G49201	TrGTerC	C96O2 + HO_2 → C96OOH	KRO2HO2(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	0.6*k_CH3OOH_OH	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	KRO2HO2(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49208b	TrGTerC	C97O2 + HO_2 → C98O2 + OH	KRO2HO2(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49209	TrGTerC	C97OOH + OH → C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 → C614O2 + CH_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	KRO2HO2(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)

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

#	labels	reaction	rate coefficient	reference
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*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G49219b	TrGTerC	C85CO3 + HO_2 → C85O2 + CO_2 + OH	KAPHO2*rco3_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	Taraborrelli (2016)
G49223b	TrGTerC	C89CO3 → C89CO2H	k1_RO2RCO3*0.1	Taraborrelli (2016)
G49224a	TrGTerC	C89CO3 + HO_2 → C89CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G49224b	TrGTerC	C89CO3 + HO_2 → C89CO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G49224c	TrGTerC	C89CO3 + HO_2 → .80 C811CO3 + .20 C89O2 + .2 CO_2 + OH	KAPHO2*rco3_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	Taraborrelli (2016)
G49231b	TrGTerC	C811CO3 → PINIC	k1_RO2RCO3*0.1	Taraborrelli (2016)
G49232a	TrGTerC	C811CO3 + HO_2 → C811CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009)
G49232b	TrGTerC	C811CO3 + HO_2 → PINIC + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G49232c	TrGTerC	C811CO3 + HO_2 → C811O2 + CO_2 + OH	KAPHO2*rco3_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	KRO2HO2(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G49237b	TrGTerC	NOPINDO2 + HO_2 → C89CO3 + OH	KRO2HO2(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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	Taraborrelli (2016), So et al. (2014)*
G49247	TrGTerC	NORPINENOL + HCOOH → NORPINAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G49248	TrGTerC	NORPINAL + HCOOH → NORPINENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (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), Taraborrelli (2016)
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), Taraborrelli (2016)
G40202a	TrGTerC	LAPINABO2 + HO_2 → LAPINABOOH	KRO2HO2(10)*(1.-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G40202b	TrGTerC	LAPINABO2 + HO_2 → PINAL + HO_2 + OH	KRO2HO2(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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	KRO2HO2(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)	T. J. Wallington et al. (2014)*
G40212	TrGTerCN	PINAL + NO_3 → C96CO3 + HNO_3	2.0E-14	T. J. Wallington et al. (2014)*
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*rco3_ooh	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO_2 → PINONIC + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO_2 → C96O2 + OH + CO_2	KAPHO2*rco3_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*1.60	Rickard and Pascoe (2009)
G40218	TrGTerCN	C10PAN2 → C96CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G40219	TrGTerCN	C10PAN2 + OH → NORPINAL + CO + NO_2	3.66E-12	Rickard and Pascoe (2009)
G40220	TrGTerC	PINONIC + OH → C96O2 + CO_2	6.65E-12	Rickard and Pascoe (2009)
G40221	TrGTerC	PERPINONIC + OH → C96CO3	9.73E-12	Rickard and Pascoe (2009)
G40222	TrGTerC	PINALO2 + HO_2 → PINALOOH	KRO2HO2(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), Taraborrelli (2016)
G40223b	TrGTerCN	PINALO2 + NO → PINALNO3	KRO2NO*alpha_AN(12,3,0,1,0,temp,cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
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)

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

#	labels	reaction	rate coefficient	reference
G40227	TrGTerC	C106O2 + HO_2 → C106OOH	KRO2HO2(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), Taraborrelli (2016)
G40228b	TrGTerCN	C106O2 + NO → C106NO3	KRO2NO*0.875*alpha_AN(13,3,0,0,0,temp,cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
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)	T. J. Wallington et al. (2014)*
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)
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	KRO2HO2(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40243b	TrGTerC	C109O2 + HO_2 → C89CO3 + HCHO + OH	KRO2HO2(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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)	T. J. Wallington et al. (2014)*
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	KRO2HO2(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)

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

#	labels	reaction	rate coefficient	reference
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	KRO2HO2(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40253b	TrGTerC	BPINAO2 + HO_2 → NOPINONE + HCHO + HO_2 + OH	KRO2HO2(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KRO2NO*alpha_AN(11,3,0,0,0, temp,cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO_2	k1_RO2tORO2	Rickard and Pascoe (2009)
G40256	TrGTerC	BPINAOOH + OH → BPINAO2	1.33E-11	Rickard and Pascoe (2009)
G40257	TrGTerCN	BPINANO3 + OH → NOPINONE + HCHO + NO_2	4.70E-12	Rickard and Pascoe (2009)
G40258a	TrGTerCN	ROO6R1O2 + NO → ROO6R3O2 + CH_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	KRO2HO2(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	KRO2HO2(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	KRO2HO2(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)	T. J. Wallington et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
G40267b	TrGTerC	BPINENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40267c	TrGTerC	BPINENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40267d	TrGTerC	BPINENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40268	TrGTerCN	BPINENE + NO_3 → LNBPINABO2	2.51E-12	T. J. Wallington et al. (2014)*
G40269	TrGTerCN	LNBPINABO2 + HO_2 → LNBPINABOOH	KRO2HO2(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)
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	Taraborrelli (2016), So et al. (2014)*
G40277	TrGTerC	PINEOL + HCOOH → PINAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G40278	TrGTerC	PINAL + HCOOH → PINEOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G40279a	TrGC	CARENE + OH → LAPINABO2	8.7E-11*(.50+.25)	Wolfe et al. (2011), Taraborrelli (2016)
G40279b	TrGC	CARENE + OH → MENTHEN6ONE + HO_2	8.7E-11*.25*.60	Wolfe et al. (2011), Taraborrelli (2016)
G40279c	TrGC	CARENE + OH → ROO6R1O2	8.7E-11*.25*.40	Wolfe et al. (2011), Taraborrelli (2016)
G40280a	TrGC	CARENE + O_3 → APINBOO	2.E-16*.50*.18	Wolfe et al. (2011), Taraborrelli (2016)
G40280b	TrGC	CARENE + O_3 → PINONIC	2.E-16*.50*.16	Wolfe et al. (2011), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G40280c	TrGC	CARENE + O_3 → OH + NORPINAL + CO + HO_2	2.E-16*.50*.66	Wolfe et al. (2011), Taraborrelli (2016)
G40280d	TrGC	CARENE + O_3 → APINAOO	2.E-16*.50*.12	Wolfe et al. (2011), Taraborrelli (2016)
G40280e	TrGC	CARENE + O_3 → OH + C109O2	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Taraborrelli (2016)
G40281	TrGCN	CARENE + NO_3 → LNAPINABO2	9.5E-12	Wolfe et al. (2011), Taraborrelli (2016)
G40282a	TrGTerC	SABINENE + OH → BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40282b	TrGTerC	SABINENE + OH → ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40283a	TrGTerC	SABINENE + O_3 → NOPINONE + .63 CO + .37 $HOCH_2OOH$ + .16 OH + .16 HO_2	1.35E-15*EXP(-1270./TEMP) *.051/(1-.027)	T. J. Wallington et al. (2014)*
G40283b	TrGTerC	SABINENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40283c	TrGTerC	SABINENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40283d	TrGTerC	SABINENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40284	TrGTerCN	SABINENE + NO_3 → LNBPINABO2	2.51E-12	T. J. Wallington et al. (2014)*
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)	T. J. Wallington et al. (2014)*
G40286b	TrGTerC	CAMPHENE + O_3 → NOPINOO + CO_2	1.35E-15*EXP(-1270./TEMP) *.368/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40286c	TrGTerC	CAMPHENE + O_3 → NOPINDO2 + CO_2 + OH	1.35E-15*EXP(-1270./TEMP) *.283/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40286d	TrGTerC	CAMPHENE + O_3 → C8BC + 2 CO_2	1.35E-15*EXP(-1270./TEMP) *(.104+.167)/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40287	TrGTerCN	CAMPHENE + NO_3 → LNBPINABO2	2.51E-12	T. J. Wallington et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
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	Atkinson et al. (2007)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(1.72E-27*EXP(8649./temp))	Atkinson et al. (2007), Sander et al. (2011)*
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)	Sander et al. (2011)
G6300	UpStTrGClN	ClO + NO → NO_2 + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGClN	ClO + NO_2 → $ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31,3.4,7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGClN	$ClNO_3$ → ClO + NO_2	6.918E-7*EXP(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGClN	$ClNO_3$ + $O(^3P)$ → ClO + NO_3	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGClN	$ClNO_3$ + Cl → Cl_2 + NO_3	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH_4 → HCl + CH_3	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO_2	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH_3OOH → HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH_3O_2 → HO_2 + Cl + HCHO	3.3E-12*EXP(-115./temp)	Sander et al. (2011)
G6404	StGCl	CCl_4 + $O(^1D)$ → LCARBON + ClO + 3 Cl	3.3E-10	Sander et al. (2011)
G6405	StGCl	CH_3Cl + $O(^1D)$ → LCARBON + OH + Cl	1.65E-10	see note*
G6406	StGCl	CH_3Cl + OH → LCARBON + H_2O + Cl	2.4E-12*EXP(-1250./temp)	Sander et al. (2011)
G6407	StGCCl	CH_3CCl_3 + $O(^1D)$ → 2 LCARBON + OH + 3 Cl	3.E-10	see note*

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

#	labels	reaction	rate coefficient	reference
G6408	StTrGCCl	CH_3CCl_3 + OH → 2 LCARBON + H_2O + 3 Cl	1.64E-12*EXP(-1520./temp)	Sander et al. (2011)
G6409	TrGCCl	Cl + C_2H_4 → $HOCH_2CH_2O_2$ + 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 → HCl + $CH_3C(O)$	8.0e-11	Atkinson et al. (2006)
G6411	TrGCCl	C_2H_2 + Cl → 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 → $C_2H_5O_2$ + HCl	8.3E-11*EXP(-100./temp)	Atkinson et al. (2006)
G6413	StTrGClN	Cl + CH_3ONO2 → HCl + HCHO + NO_2	1.3E-11*EXP(-1200./temp)	Sander et al. (2011)
G6414	StTrGClN	Cl + CH_3ONO → HCl + HCHO + NO	2.1E-12	Sokolov et al. (1999)
G6415	StTrGCCl	Cl + CH_3O_2 → .5 ClO + .5 CH_3O + .5 HCl + .5 CH_2OO	1.6E-10	Sander et al. (2011)
G6416	TrGCClN	Cl + CH_3CN → $NCCH_2O_2$ + HCl	1.6E-11*EXP(-2104./temp)	Tyndall et al. (1996), Tyndall et al. (2001b), Taraborrelli (2016)
G6500	StGClF	CF_2Cl_2 + $O(^1D)$ → LCARBON + 2 LFLUORINE + ClO + Cl	1.4E-10	Sander et al. (2011)
G6501	StGClF	$CFCl_3$ + $O(^1D)$ → LCARBON + LFLUORINE + ClO + 2 Cl	2.3E-10	Sander et al. (2011)
G7100	StTrGBr	Br + O_3 → BrO + O_2	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	BrO + $O(^3P)$ → Br + O_2	1.9E-11*EXP(230./temp)	Atkinson et al. (2007)
G7102a	StTrGBr	BrO + BrO → 2 Br + O_2	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	BrO + BrO → Br_2 + O_2	2.9E-14*EXP(840./temp)	Atkinson et al. (2007)
G7200	StTrGBr	Br + HO_2 → HBr + O_2	7.7E-12*EXP(-450./temp)	Atkinson et al. (2007)
G7201	StTrGBr	BrO + HO_2 → HOBr + O_2	4.5E-12*EXP(500./temp)	Atkinson et al. (2007)
G7202	StTrGBr	HBr + OH → Br + H_2O	6.7E-12*EXP(155./temp)	Atkinson et al. (2007)
G7203	StGBr	HOBr + $O(^3P)$ → OH + BrO	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	Br_2 + OH → HOBr + Br	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGBrN	Br + $BrNO_3$ → Br_2 + NO_3	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGBrN	BrO + NO → Br + NO_2	8.7E-12*EXP(260./temp)	Atkinson et al. (2007)
G7302	StTrGBrN	BrO + NO_2 → $BrNO_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7303	TrGBrN	$BrNO_3$ → 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 → HBr + CO + HO_2	7.7E-12*EXP(-580./temp)	Atkinson et al. (2006)
G7401	TrGBr	Br + CH_3OOH → CH_3O_2 + HBr	2.6E-12*EXP(-1600./temp)	Kondo and Benson (1984)
G7402	TrGBr	BrO + CH_3O_2 → HOBr + CH_2OO	2.42E-14*EXP(1617./temp)	Shallcross et al. (2015)

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

#	labels	reaction	rate coefficient	reference
G7403	StTrGBr	$CH_3Br + OH \rightarrow LCARBON + H_2O + Br$	2.35E-12*EXP(-1300./temp)	Sander et al. (2011)
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	$CHBr_3 + OH \rightarrow LCARBON + H_2O + 3\ Br$	1.35E-12*EXP(-600./temp)	Sander et al. (2011)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow LCARBON + H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	Sander et al. (2011)*
G7600	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	3.32E-15	Manion et al. (2010)
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	$CHCl_2Br + OH \rightarrow LCARBON + 2\ LCHLORINE + H_2O + Br$	2.0E-12*EXP(-840./temp)	see note*
G7606	TrGBrCl	$CHClBr_2 + OH \rightarrow LCARBON + LCHLORINE + H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	see note*
G7607	TrGBrCl	$CH_2ClBr + OH \rightarrow LCARBON + LCHLORINE + H_2O + Br$	2.4E-12*EXP(-920./temp)	Sander et al. (2011)*
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)*
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)
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)

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

#	labels	reaction	rate coefficient	reference
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	$INO_3 \rightarrow IO + NO_2$	0.	see note*
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)
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	Sander et al. (2011)
G8701	TrGBrI	$IO + BrO \rightarrow Br + .8\ OIO + .2\ I + .2\ O_2$	1.5E-11*EXP(510./temp)	Atkinson et al. (2007)*
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)	Sander et al. (2011)
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)
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)*

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

#	labels	reaction	rate coefficient	reference
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:

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by T. J. Wallington et al. (2014) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

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 $k^{\mathrm{1st}} = 2 \times \sqrt{k_{\mathrm{self}} \times \texttt{k\_CH3O2}} \times [\mathrm{RO_2}]$ 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 $[\mathrm{RO_2}]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

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

`G2110`: The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp) *cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_ H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

`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.E-30,4.4,1.4E-12,0.7,0.6)`.

`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,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

`G3206`: The rate coefficient is: `k_HNO3_ OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./ (6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)) )`

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

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

`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.

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.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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).

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 (Sander et al., 2011).

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.

G43223: Products simplified

G43419: KDEC C3DIALO → GLYOX + CO + HO2

G43420: KDEC C3DIALO → 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 → .6 MALANHY + HO2 + .4 GLYOX + .4 CO + .4 CO2

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

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

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

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

G44421: Only major channel.

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

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCOHCO3

G44431: KDEC MALANHYO → HCOCOHCO3

G44432: Only major channel. KDEC MALANHYO → HCOCOHCO3

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

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

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

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

G44443: KDEC MECOACETO → CH3CO3 + HCHO

G44444: KDEC MECOACETO → CH3CO3 + HCHO

G44445: KDEC MECOACETO → CH3CO3 + HCHO

G44450: KDEC BZFUO → CO14O3CHO + HO2

G44451: KDEC BZFUO → CO14O3CHO + HO2

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

G44457: KDEC MALDIALO → 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: ZCODC23DBCOD = 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 (ZCODC23DBCOD) 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: ZCPANC23DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO2 = .67 MBOAO2 + .33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2 → 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 →.83 MALANHY + .83 CH3 + .17 MGLYOX + .17 HO2 + .17 CO + .17 CO2

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

G45432: KFPAN →k_CH3CO3_NO2 (renaming)

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

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

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

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

G45452: KDEC TLFUONOOA →.5 CO + .5 OH + .5 MECOACETO2 + .5 TLFUONOO and H2O subs TLFUONOO →.625 C24O3CCO2H + .375 ACCOMECHO + .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 → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

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

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

G46464: KDEC PHENO → .71 MALDALCO2H + .71 GLYOX + .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 → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO.

G46491b: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO.

G46492: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .5 C32OH13CO

G46493: KDEC BZEMUCO → .5 EPXC4DIAL + .5 GLYOX + .5 HO2 + .5 C3DIALO2 + .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.

G46517b: New channel.

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

G46523b: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

G46524: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE

G46525: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .5 BZFUONE and Only major channel.

G47210: Alkyl nitrate formation neglected.

G47214: Alkyl nitrate formation neglected.

G47218: Alkyl nitrate formation neglected.

G47222: Alkyl nitrate formation neglected.

G47223: ROO6R3OOH produced but no sink for it.

G47225: ROO6R4P produced but no sink for it.

G47226: ROO6R5P produced but no sink for it

G47400: Merged.

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

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

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

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

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero2_oh is set to 0.40 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

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

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

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

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

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

G47413: Merged.

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

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

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

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

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

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

G47442: KDEC TLEMUCO→ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .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 → .24 CH2OO + .40 CO + .36 HO2 + .36 CO + .36 OH and H2Osubs PHCHOO → .625 PHCOOH + .375 BENZAL + .375 H2O2 + .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 = .65 APINAO2 + .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.

G6405: Average of reactions with CH_3Br and CH_3F from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F from Sander et al. (2006).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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))`.

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

G10201: Upper limit.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J0001	UpGJ	$O(^3P) \rightarrow O^+ + e^-$	`jx(ip_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)
J41001b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	`jx(ip_CHOH)`	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J41002	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	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	$CH_3ONO2 + h\nu \rightarrow CH_3O + NO_2$	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), Sander et al. (2011)
J42005a	TrGJC	$HOCH_2CHO + h\nu \rightarrow HCHO + 2\ HO_2 + CO$	jx(ip_HOCH2CHO)*0.83	Sander et al. (2011)
J42005b	TrGJC	$HOCH_2CHO + h\nu \rightarrow OH + HCOCH2O2$	jx(ip_HOCH2CHO)*0.07	Sander et al. (2011)
J42005c	TrGJC	$HOCH_2CHO + h\nu \rightarrow CH_3OH + CO$	jx(ip_HOCH2CHO)*0.10	Sander et al. (2011)
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)	Taraborrelli (2016)
J42014	TrGC	$HOOCH2CO2H + h\nu \rightarrow OH + HCHO + HO_2 + CO_2$	jx(ip_CH3OOH)	Taraborrelli (2016)
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	Taraborrelli (2016)
J42016	TrGC	$CH3CHOHOOH + h\nu \rightarrow CH_3 + HCOOH + OH$	jx(ip_CH3OOH)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42017	TrGJCN	$NO_3CH2CHO + h\nu \rightarrow HO_2 + CO + HCHO + NO_2$	`(jx(ip_C2H5NO3)+jx(ip_CH3CHO))*(jx(ip_NOA)+1E-10)/(0.59*J_IC3H7NO3+jx(ip_CH3COCH3)+1E-10)`	Taraborrelli (2016)*
J42018	TrGJC	$HOOCH2CHO + h\nu \rightarrow OH + HCHO + CO + HO_2$	`jx(ip_CH3OOH)+jx(ip_HOCH2CHO)`	Taraborrelli (2016)
J42019	TrGJCN	$C_2H_5ONO_2 + h\nu \rightarrow CH_3CHO + HO_2 + NO_2$	`jx(ip_C2H5NO3)`	Taraborrelli (2016)
J42020	TrGJCN	$NO_3CH2CHO + h\nu \rightarrow .7\ NO_3CH2CO_3 + .7\ NO_2 + .3\ HCHO + .3\ NO_2 + .3\ CO_2 + .3\ NO_3$	`jx(ip_PAN)`	Taraborrelli (2016)*
J42021	StTrGJCN	$C_2H_5O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ C_2H_5O_2 + .333\ NO_3 + .333\ CH_3CHO + .333\ HO_2$	`jx(ip_CH3O2NO2)`	Taraborrelli (2016)*
J43000	TrGJC	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	`jx(ip_CH3OOH)`	von Kuhlmann (2001)
J43001	TrGJC	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O) + CH_3$	`jx(ip_CH3COCH3)`	Sander et al. (2014)
J43002	TrGJC	$CH_3COCH_2OH + h\nu \rightarrow .5\ CH_3C(O) + .5\ HCHO + .5\ HO_2 + .5\ HOCH2CO + .5\ CH_3$	`J_ACETOL`	Sander et al. (2011)*
J43003	TrGJC	$MGLYOX + h\nu \rightarrow CH_3C(O) + CO + HO_2$	`jx(ip_MGLYOX)`	Sander et al. (2014)
J43004	TrGJC	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O) + HCHO + OH$	`jx(ip_CH3OOH)+J_ACETOL`	Rickard and Pascoe (2009)
J43005	TrGJC	$HOCH2COCH2OOH + h\nu \rightarrow HOCH2CO + HCHO + OH$	`jx(ip_CH3OOH)+J_ACETOL`	Taraborrelli (2016)
J43006	TrGJCN	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	`J_IC3H7NO3`	von Kuhlmann et al. (2003)*
J43007	TrGJCN	$NOA + h\nu \rightarrow CH_3C(O) + HCHO + NO_2$	`jx(ip_NOA)`	Barnes et al. (1993)
J43009	TrGJC	$HYPROPO2H + h\nu \rightarrow CH_3CHO + HCHO + HO_2 + OH$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J43010	TrGJCN	$PR2O2HNO3 + h\nu \rightarrow NOA + HO_2 + OH$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J43011	TrGJC	$HOCH2COCHO + h\nu \rightarrow HOCH2CO + CO + HO_2$	`jx(ip_MGLYOX)`	Rickard and Pascoe (2009)
J43012	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HCOCO + HCHO + OH$	`jx(ip_CH3OOH)+J_ACETOL`	Taraborrelli (2016)
J43013	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HOOCH_2CO_3 + CO + HO_2$	`jx(ip_MGLYOX)`	Taraborrelli (2016)
J43014	TrGJTerC	$HCOCH2CHO + h\nu \rightarrow HCOCH2O2 + HO_2 + CO$	`jx(ip_HOCH2CHO)*2.`	Rickard and Pascoe (2009)
J43015	TrGJTerC	$HCOCH2CO2H + h\nu \rightarrow HCOCH2O2 + CO_2 + HO_2$	`jx(ip_HOCH2CHO)`	Rickard and Pascoe (2009)
J43016	TrGJTerC	$HOC2H4CO3H + h\nu \rightarrow HOCH_2CH_2O_2 + CO_2 + OH$	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)
J43017	TrGJC	$HCOCOCHO + h\nu \rightarrow HCOCO + HO_2 + CO$	`2.*jx(ip_MGLYOX)`	Taraborrelli (2016)
J43018	TrGJC	$CH_3COCO_2H + h\nu \rightarrow .32\ CH_3CHO + .16\ CH_2CHOH + .54\ CO_2 + .38\ CH_3C(O) + .38\ HO_2 + .38\ CO_2 + .07\ CH_3COOH + .07\ CO + .05\ CH_3C(O) + .05\ CO + .05\ OH$	`JX(IP_CH3COCO2H)`	Sander et al. (2011), Taraborrelli (2016)*
J43019	TrGC	$CH_3COCO_3H + h\nu \rightarrow CH_3C(O) + OH + CO_2$	`JX(IP_MGLYOX)+jx(ip_CH3OOH)`	Taraborrelli (2016)
J43020	TrGC	$CH3CHCO + h\nu \rightarrow C_2H_4 + CO$	`J_ketene*0.36*2.`	Taraborrelli (2016)
J43021	TrGCN	$PROPOLNO3 + h\nu \rightarrow HOCH_2CHO + HCHO + HO_2 + NO_2$	`J_IC3H7NO3`	Taraborrelli (2016)
J43022	TrGCN	$CH_3COCH_2OONO_2 + h\nu \rightarrow CH_3C(O) + HCHO + NO_3$	`jx(ip_CH3O2NO2)+jx(ip_CH3COCH3)`	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43023	TrGJC	$C_3H_7OOH + h\nu \rightarrow C_2H_5CHO + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)
J43024	TrGJCN	$C_3H_7ONO_2 + h\nu \rightarrow C_2H_5CHO + NO_2 + HO_2$	0.59*J_IC3H7NO3	see note*
J43025a	TrGJC	$C_2H_5CHO + h\nu \rightarrow C_2H_5O_2 + HO_2 + CO$	jx(ip_C2H5CHO2HCO)	see note*
J43025b	TrGJC	$C_2H_5CHO + h\nu \rightarrow CH_2CHCH_2OH$	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Taraborrelli (2016)*
J43026	TrGJCN	PPN + $h\nu \rightarrow .7\ C_2H_5CO_3 + .7\ NO_2 + .3\ C_2H_5O_2 + .3\ CO_2 + .3\ NO_3$	jx(ip_PAN)	Sander et al. (2014), Sander et al. (2011)
J43027	TrGJC	$C_2H_5CO_3H + h\nu \rightarrow C_2H_5O_2 + CO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)
J43028a	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HOOCH_2CO_3 + CO + HO_2$	jx(ip_MGLYOX)	Taraborrelli (2016)
J43028b	TrGJC	$HCOCOCH_2OOH + h\nu \rightarrow HCOCO + HCHO + OH$	jx(ip_HOCH2CHO)+jx(ip_CH3OOH)	Taraborrelli (2016)
J43200	TrGJTerC	HCOCH2CO3H + $h\nu \rightarrow$ HCOCH2O2 + CO_2 + OH	jx(ip_HOCH2CHO)+jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J43400	TrGJAroC	C3DIALOOH + $h\nu \rightarrow$ GLYOX + CO + HO_2 + OH	jx(ip_HOCH2CHO)*2+jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J43401	TrGJAroC	C32OH13CO + $h\nu \rightarrow$ GLYOX + HO_2 + HO_2 + CO	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J43402	TrGJAroC	HCOCOHCO3H + $h\nu \rightarrow$ GLYOX + HO_2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44000a	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + C_3H_7CHO + HO_2$	jx(ip_CH3OOH)*(k_p/(k_p+k_s))	Rickard and Pascoe (2009), Taraborrelli (2016)
J44000b	TrGJC	$LC_4H_9OOH + h\nu \rightarrow OH + .636$ MEK $+ .636\ HO_2 + .364\ CH_3CHO + .364\ C_2H_5O_2$	jx(ip_CH3OOH)*(k_s/(k_p+k_s))	Rickard and Pascoe (2009), Taraborrelli (2016)
J44001	TrGJC	MVK + $h\nu \rightarrow .5\ C_3H_6 + .5\ CH_3C(O) + .5$ HCHO + CO + .5 HO_2	jx(ip_MVK)	Sander et al. (2014)
J44002	TrGJC	MEK + $h\nu \rightarrow CH_3C(O) + C_2H_5O_2$	0.42*jx(ip_CHOH)	von Kuhlmann et al. (2003)
J44003	TrGJC	LMEKOOH + $h\nu \rightarrow .62\ CH_3C(O) + .62\ CH_3CHO + .38$ HCHO $+ .38\ CO_2 + .38\ HOCH_2CH_2O_2$ + OH	jx(ip_CH3OOH)+0.42*jx(ip_CHOH)	Taraborrelli (2016)
J44004	TrGJC	BIACET + $h\nu \rightarrow 2\ CH_3C(O)$	2.15*jx(ip_MGLYOX)	see note*
J44005a	TrGJCN	LC4H9NO3 + $h\nu \rightarrow NO_2 + C_3H_7CHO + HO_2$	J_IC3H7NO3*(k_p/(k_p+k_s))	see note*
J44005b	TrGJCN	LC4H9NO3 + $h\nu \rightarrow NO_2$ + MEK + HO_2	J_IC3H7NO3*(k_s/(k_p+k_s))	see note*
J44006	TrGJCN	MPAN + $h\nu \rightarrow$ .7 MACO3 + .7 NO_2 + .3 MACO2 + .3 NO_3	jx(ip_PAN)	see note*
J44007a	TrGJC	CO2H3CO3H + $h\nu \rightarrow$ MGLYOX + HO_2 + OH + CO_2	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44007b	TrGJC	CO2H3CO3H + $h\nu \rightarrow CH_3C(O) + HO_2 + HCOCO_3H$	J_ACETOL	Rickard and Pascoe (2009)
J44008	TrGJC	MACR + $h\nu \rightarrow$ .5 MACO3 + .5 $CH_3C(O)$ + .5 HCHO + .5 CO + HO_2	jx(ip_MACR)	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44009	TrGJC	MACROOH + hν → MACRO + OH	jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)	Taraborrelli (2016)*
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)	Taraborrelli (2016)
J44012	TrGJC	LHMVKABOOH + hν → .12 MGLYOX + .12 HO_2 + .88 $CH_3C(O)$ + .88 $HOCH_2CHO$ + .12 HCHO + OH	jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2016)
J44013	TrGJC	CO2H3CHO + hν → MGLYOX + CO + HO_2 + HO_2	jx(ip_HOCH2CHO)+J_ACETOL	Taraborrelli (2016)
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	Taraborrelli (2016)
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	Taraborrelli (2016),Rickard and Pascoe (2009)*
J44017b	TrGC	$CH_3COCHCO$ + hν → CH3CHCO + CO	J_KETENE*0.5	Taraborrelli (2016)
J44018a	TrGJC	$CH_3COCOCHO$ + hν → $CH_3C(O)$ + 2 CO + HO_2	jx(ip_MGLYOX)	Taraborrelli (2016)
J44018b	TrGJC	$CH_3COCOCHO$ + hν → HCOCO + $CH_3C(O)$	2.15*jx(ip_MGLYOX)	Taraborrelli (2016)
J44019	TrGJC	CH3COCOCO2H + hν → $CH_3C(O)$ + CO + CO_2 + HO_2	3.15*jx(ip_MGLYOX)	Taraborrelli (2016)
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), Taraborrelli (2016)*
J44026	TrGJCN	MVKNO3 + hν → $CH_3C(O)$ + $HOCH_2CHO$ + NO_2	jx(ip_MEKNO3)	Barnes et al. (1993), Taraborrelli (2016)*
J44027	TrGJCN	MACRN + hν → 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), Taraborrelli (2016)*
J44028	TrGJCN	TC4H9NO3 + hν → CH_3COCH_3 + CH_3 + NO_2	2.84*J_IC3H7NO3	Taraborrelli (2016)
J44029	TrGJC	TC_4H_9OOH + hν → CH_3COCH_3 + CH_3 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44030	TrGJCN	IBUTOLBNO3 + hν → CH_3COCH_3 + HCHO + HO_2 + NO_2	2.84*J_IC3H7NO3	Taraborrelli (2016)
J44031	TrGJC	IBUTOLBOOH + hν → CH_3COCH_3 + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)
J44032	TrGJC	LBUT1ENOOH + hν → C_2H_5CHO + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)
J44033	TrGJCN	LBUT1ENNO3 + hν → C_2H_5CHO + HCHO + HO_2 + NO_2	J_IC3H7NO3	Taraborrelli (2016)
J44034	TrGJC	BUT2OLOOH + hν → 2 CH_3CHO + HO_2 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)
J44035	TrGJCN	BUT2OLNO3 + hν → 2 CH_3CHO + HO_2 + NO_2	J_IC3H7NO3	Taraborrelli (2016)
J44036	TrGJC	BUT2OLO + hν → $CH_3C(O)$ + HOCH2CO	J_ACETOL	Taraborrelli (2016)
J44037a	TrGJC	C_3H_7CHO + hν → $C_3H_7O_2$ + CO + HO_2	jx(ip_C3H7CHO2HCO)	Taraborrelli (2016)
J44037b	TrGJC	C_3H_7CHO + hν → C_2H_4 + CH_2CHOH	jx(ip_C3H7CHO2VINY)	Taraborrelli (2016)*
J44038	TrGJC	IPRCHO + hν → $iC_3H_7O_2$ + CO + HO_2	jx(ip_IPRCHO2HCO)	Taraborrelli (2016)
J44039	TrGJCN	IC4H9NO3 + hν → IPRCHO + NO_2	J_IC3H7NO3	Taraborrelli (2016)
J44040	TrGJC	IC_4H_9OOH + hν → IPRCHO + HO_2 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)
J44041	TrGJC	PERIBUACID + hν → $iC_3H_7O_2$ + CO_2 + OH	jx(ip_CH3OOH)	Taraborrelli (2016)
J44042	TrGJCN	PIPN + hν → .7 IPRCO3 + .7 NO_2 + .3 $iC_3H_7O_2$ + .3 CO_2 + .3 NO_3	jx(ip_PAN)	Taraborrelli (2016), Sander et al. (2014), Sander et al. (2011)
J44043	TrGJC	HVMK + hν → MGLYOX + CO + 2 OH	jx(ip_PeDIONE24)	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44044	TrGJC	HMAC + hν → $HCOCCH_3CO$ + 2 OH	jx(ip_PeDIONE24)	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	CO2C3CHO + hν → $CH_3COCH_2O_2$ + HO_2 + CO	jx(ip_C2H5CHO2HCO)	Rickard and Pascoe (2009)
J44045b	TrGJC	CO2C3CHO + hν → HVMK	jx(ip_C2H5CHO2ENOL)	Andrews et al. (2012), Taraborrelli (2016)
J44046a	TrGJC	IBUTDIAL + hν → CH_3CHO + CO + HO_2 + CO_2 + H_2O	jx(ip_C2H5CHO2HCO)*2.	see note*
J44046b	TrGJC	IBUTDIAL + hν → HMAC	jx(ip_C2H5CHO2ENOL)*2.	Andrews et al. (2012), Taraborrelli (2016)
J44200	TrGJTerC	IBUTALOH + hν → CH_3COCH_3 + HO_2 + HO_2 + CO	J_ACETOL	Rickard and Pascoe (2009)
J44201	TrGJTerC	IPRHOCO3H + hν → CH_3COCH_3 + HO_2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J44400a	TrGJAroC	MALDIALOOH + hν → C32OH13CO + CO + OH + HO_2	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)
J44400b	TrGJAroC	MALDIALOOH + hν → GLYOX + GLYOX + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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 + HCOCH2O2 + 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), Taraborrelli (2016)*
J45010	TrGJCN	LNISOOH + hν $\rightarrow$ NOA + OH + .5 HOCHCHO + .5 CO + .5 HO_2 + .5 CO_2	jx(ip_CH3OOH)	Taraborrelli et al. (2009), Taraborrelli (2016)
J45011	TrGJC	LHC4ACCHO + hν $\rightarrow$ .5 LHC4ACCO3 + .5 HO_2 + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2	jx(ip_MACR)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45012	TrGJC	LC578OOH + hν → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + OH	jx(ip_CH3OOH)+ 2.77*jx(ip_ HOCH2CHO)	Taraborrelli (2016)
J45013	TrGJC	LHC4ACCO3H + hν → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO_2	J_HPALD	Taraborrelli (2016)
J45014	TrGJCN	LC5PAN1719 + hν → .7 LHC4ACCO3 + .7 NO_2 + .15 MACRO2 + .15 LHMVKABO2 + .3 CO_2 + .3 NO_3	jx(ip_PAN)	Taraborrelli (2016)
J45015	TrGJC	HCOC5 + hν → .65 CH_3 + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + HOCH2CO	0.5*jx(ip_MVK)	Taraborrelli (2016)*
J45016	TrGJC	C59OOH + hν → CH_3COCH_2OH + HOCH2CO + OH	J_ACETOL+jx(ip_CH3OOH)	Taraborrelli (2016)
J45017	TrGJTerC	C511OOH + hν → $CH_3C(O)$ + HCOCH2CHO + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018a	TrGJTerC	CO23C4CHO + hν → $CH_3COCOCH_2O_2$ + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018b	TrGJTerC	CO23C4CHO + hν → $CH_3C(O)$ + HCOCH2CO3	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45019	TrGJTerC	CO23C4CO3H + hν → $CH_3COCOCH_2O_2$ + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45020	TrGJTerC	C512OOH + hν → C513O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45021	TrGJTerC	CO13C4CHO + hν → CHOC3COO2 + CO + HO_2	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45022	TrGJTerC	C513OOH + hν → GLYOX + HOC2H4CO3 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45023	TrGJTerC	C513CO + hν → HOC2H4CO3 + HO_2 + CO + CO	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45024	TrGJTerC	C514OOH + hν → CO13C4CHO + HO_2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45025	TrGJTerCN	C514NO3 + hν → CO13C4CHO + HO_2 + NO_2	J_IC3H7NO3+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45026a	TrGJC	ZCODC23DBCOOH + hν → OH + CO + HVMK + OH	J_HPALD*0.6*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	ZCODC23DBCOOH + hν → OH + CO + $CH_3C(O)$ + $HOCH_2CHO$	J_HPALD*0.6*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	ZCODC23DBCOOH + hν → OH + CO + HMAC + OH	J_HPALD*0.4*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	ZCODC23DBCOOH + hν → OH + CO + CO + CH_3COCH_2OH + HO_2	J_HPALD*0.4*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	ZCO3HC23DBCOD + hν → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO_2	J_HPALD	Taraborrelli (2016)
J45028a	TrGJC	C1OOHC2OOHC4OD + hν → $CH_3COCH_2O_2H$ + OH + 2 CO + HO_2	2.77*JX(IP_HOCH2CHO)	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45028b	TrGJC	C1OOHC2OOHC4OD + hν $\rightarrow$ .5 $CH_3COCH_2O_2H$ + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH	`2.*JX(IP_CH3OOH)`	Taraborrelli (2016)
J45029	TrGC	DB1OOH + hν $\rightarrow$ DB1O2 + OH	`JX(IP_CH3OOH)`	Taraborrelli (2016)
J45030	TrGC	DB2OOH + hν $\rightarrow$ .48 CH_3COCH_2OH + .52 $HOCH_2CHO$ + .52 MGLYOX + .48 GLYOX + HO_2 + OH	`JX(ip_CH3OOH)`	Taraborrelli (2016)
J45031a	TrGJC	C1ODC2OOHC4OD + hν $\rightarrow$ MGLYOX + HOCHCHO + OH	`JX(ip_CH3OOH)`	Taraborrelli (2016)
J45031b	TrGJC	C1ODC2OOHC4OD + hν $\rightarrow$ CO2H3CHO + CO + HO_2 + OH	`2.*2.77*JX(IP_HOCH2CHO)`	Taraborrelli (2016)
J45032	TrGJC	ZCODC23DBCOD + hν $\rightarrow$ .5 $CH_3COCHCO$ + .5 $HCOCCH_3CO$ + CO + HO_2 + OH	`jx(ip_NO2)*0.1*0.5`	Taraborrelli (2016)*
J45033	TrGCN	DB1NO3 + hν $\rightarrow$ DB1O2 + NO_2	`J_IC3H7NO3`	Taraborrelli (2016)
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), Taraborrelli (2016)
J45200b	TrGJTerC	LMBOABOOH + hν $\rightarrow$ IBUTALOH + HCHO + HO_2 + OH	`jx(ip_CH3OOH)*.33`	Rickard and Pascoe (2009), Taraborrelli (2016)
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), Taraborrelli (2016)
J45203b	TrGJTerCN	LNMBOABOOH + hν $\rightarrow$ IBUTALOH + HCHO + NO_2 + OH	`jx(ip_CH3OOH)*.35`	Rickard and Pascoe (2009), Taraborrelli (2016)
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)
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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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*
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)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46409	TrGJAroCN	NPHEN1OOH + hν → NPHEN1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46410	TrGJAroC	BZEMUCCO + hν → HCOCOHCO3 + C3DIALO2	jx(ip_HOCH2CHO)*2+J_ACETOL	Rickard and Pascoe (2009)
J46411	TrGJAroC	BZEMUCCO2H + hν → C5DIALO2 + CO_2 + HO_2	jx(ip_MACR)	Rickard and Pascoe (2009)
J46412	TrGJAroCN	NNCATECOOH + hν → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46413	TrGJAroC	C615CO2OOH + hν → C5DICARB + CO + HO_2 + OH	jx(ip_MVK)+jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46414	TrGJAroCN	NPHENOOH + hν → MALDALCO2H + GLYOX + OH + NO_2	J_IC3H7NO3 + jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46415	TrGJAroCN	NCATECOOH + hν → NC4DCO2H + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46416	TrGJAroC	PBZQOOH + hν → C5CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46417	TrGJAroC	BZOBIPEROH + hν → MALDIALCO3 + GLYOX + HO_2	J_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	BZBIPEROOH + hν → GLYOX + HO_2 + .5 BZFUONE + .5 BZFUONE + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	NBZQOOH + hν → C6CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46420	TrGJAroC	CATEC1OOH + hν → CATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46421	TrGJAroC	C6125CO + hν → C5CO14O2 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_MVK)	Rickard and Pascoe (2009)
J46422	TrGJAroCN	DNPHENOOH + hν → NC4DCO2H + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J46423	TrGJAroC	BZEMUCCO3H + hν → C5DIALO2 + CO_2 + OH	jx(ip_CH3OOH)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46424	TrGJAroC	C6H5OOH + hν → C6H5O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J46425	TrGJAroC	BZEMUCOOH + hν → .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 → EPXC4DIAL + NO_2 + GLYOX + HO_2	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J46428	TrGJAroCN	DNPHEN + hν → HONO + NCPDKETENE	jx(ip_HOC6H4NO2)	Taraborrelli (2016)
J46429	TrGJAroCN	NCPDKETENE + hν → CO_2 + CO + 2 HO_2 + NC4DCO2H	J_KETENE	see note*
J47200	TrGJTerC	CO235C6CHO + hν → CHOC3COCO3 + $CH_3C(O)$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47201	TrGJTerC	C235C6CO3H + hν → CO235C6O2 + CO_2 + OH	jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47202	TrGJTerC	C716OOH + hν → CO13C4CHO + $CH_3C(O)$ + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J47203	TrGJTerC	C721OOH + hν → C722O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47204	TrGJTerC	C722OOH + hν → CH_3COCH_3 + C44O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47400	TrGJAroC	TLEPOXMUC + hν → .5 C615CO2O2 + HO_2 + CO + .5 EPXC4DIAL + .5 $CH_3C(O)$	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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)	T. J. Wallington et al. (2014)
J47404	TrGJAroC	TLBIPEROOH + hν $\rightarrow$ .6 GLYOX + .4 MGLYOX + HO_2 + .2 ZCODC23DBCOD + .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 ZCODC23DBCOD + .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 + ZCODC23DBCOD	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 → CO_2 + CO + 2 HO_2 + NC4MDCO2HN	J_KETENE	see note*
J47421	TrGJAroC	MCATEC1OOH + hν → MCATEC1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47422	TrGJAroCN	NPTLQOOH + hν → C7CO4DB + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47423	TrGJAroC	PTLQOOH + hν → C6CO2OHCO3 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47424	TrGJAroCN	NCRES1OOH + hν → NCRES1O + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J47425	TrGJAroCN	MNNCATCOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47426	TrGJAroCN	MNCATECOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47427	TrGJAroC	C7CO4DB + hν → C5CO2DBCO3 + HO_2 + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
J47428	TrGJAroCN	NDNCRESOOH + hν → NC4MDCO2HN + HNO_3 + CO + CO + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47429	TrGJAroCN	DNCRESOOH + hν → NC4MDCO2HN + $HCOCO_2H$ + NO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J47430	TrGJAroC	C6COOHCO3H + hν → C5134CO2OH + HO_2 + CO + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48200	TrGJTerC	C86OOH + hν → C511O2 + CH_3COCH_3 + OH	jx(ip_CH3OOH)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48201	TrGJTerC	C812OOH + hν → C813O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48202	TrGJTerC	C813OOH + hν → CH_3COCH_3 + C512O2 + OH	jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J48203	TrGJTerC	C721CHO + hν → C721O2 + CO + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48204	TrGJTerC	C721CO3H + hν → C721O2 + CO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48205	TrGJTerC	C8BCOOH + hν → C89O2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J48206	TrGJTerC	C89OOH + hν → C810O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48207	TrGJTerCN	C89NO3 + hν → C810O2 + NO_2	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48208	TrGJTerC	C810OOH + hν → CH_3COCH_3 + C514O2 + OH	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48209	TrGJTerCN	C810NO3 + hν → CH_3COCH_3 + C514O2 + NO_2	2.84*J_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48210	TrGJTerCN	C8BCNO3 + hν → C89O2 + NO_2	J_IC3H7NO3	Rickard and Pascoe (2009)
J48211	TrGJTerC	C85OOH + hν → C86O2 + OH	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)
J48400	TrGJAroC	STYRENOOH + hν → HO_2 + HCHO + BENZAL + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J49200	TrGJTerC	C96OOH + hν → C97O2 + OH	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)
J49201	TrGJTerC	C97OOH + hν → C98O2 + OH	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J49202	TrGJTerC	$C98OOH + h\nu \rightarrow C614O2 + CH_3COCH_3 + OH$	(jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX))	Rickard and Pascoe (2009)
J49203a	TrGJTerC	$NORPINAL + h\nu \rightarrow C85O2 + CO + HO_2$	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009), Taraborrelli (2016)
J49203b	TrGJTerC	$NORPINAL + h\nu \rightarrow NORPINENOL$	jx(ip_PINAL2ENOL)	Taraborrelli (2016), Andrews et al. (2012)
J49204	TrGJTerC	$C85CO3H + h\nu \rightarrow C85O2 + CO_2 + OH$	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)
J49205	TrGJTerC	$C89CO2H + h\nu \rightarrow .8\ C811CO3 + .2\ C89O2 + .2\ CO_2 + HO_2$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49206	TrGJTerC	$C89CO3H + h\nu \rightarrow .8\ C811CO3 + .2\ C89O2 + .2\ CO_2 + OH$	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J49207	TrGJTerC	$C811CO3H + h\nu \rightarrow C811O2 + CO_2 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J49208	TrGJTerC	$NOPINDOOH + h\nu \rightarrow C89CO3 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40200	TrGJTerC	$LAPINABOOH + h\nu \rightarrow PINAL + HO_2 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40201	TrGJTerC	$MENTHEN6ONE + h\nu \rightarrow RO6R1O2 + OH$	jx(ip_CH3OOH)	Vereecken et al. (2007)
J40202	TrGJTerC	$2OHMENTHEN6ONE + h\nu \rightarrow 10\ LCARBON + OH$	jx(ip_CH3OOH)	Vereecken et al. (2007)
J40203a	TrGJTerC	$PINAL + h\nu \rightarrow C96O2 + CO + HO_2$	jx(ip_PINAL2HCO)	Rickard and Pascoe (2009)
J40203b	TrGJTerC	$PINAL + h\nu \rightarrow PINEOL$	jx(ip_PINAL2ENOL)	Taraborrelli (2016), Andrews et al. (2012)*
J40204	TrGJTerC	$PERPINONIC + h\nu \rightarrow C96O2 + CO_2 + OH$	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)
J40205	TrGJTerC	$PINALOOH + h\nu \rightarrow C106O2 + OH$	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40206	TrGJTerCN	$PINALNO3 + h\nu \rightarrow C106O2 + NO_2$	J_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40207	TrGJTerC	$C106OOH + h\nu \rightarrow C716O2 + CH_3COCH_3 + OH$	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40208	TrGJTerCN	$C106NO3 + h\nu \rightarrow C716O2 + CH_3COCH_3 + NO_2$	J_IC3H7NO3+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40209	TrGJTerC	$C109OOH + h\nu \rightarrow C89CO3 + HCHO + OH$	jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40210	TrGJTerC	$C109CO + h\nu \rightarrow C89CO3 + CO + HO_2$	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J40211	TrGJTerCN	$LNAPINABOOH + h\nu \rightarrow PINAL + NO_2 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40212	TrGJTerC	$BPINAOOH + h\nu \rightarrow NOPINONE + HCHO + HO_2 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40213	TrGJTerCN	$LNBPINABOOH + h\nu \rightarrow NOPINONE + HCHO + NO_2 + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)
J40214	TrGJTerCN	$ROO6R1NO3 + h\nu \rightarrow ROO6R3O2 + CH_3COCH_3 + NO_2$	2.84*J_IC3H7NO3+jx(ip_CH3OOH)	Taraborrelli (2016)
J40215	TrGJTerCN	$RO6R1NO3 + h\nu \rightarrow 9\ LCARBON + HCHO + HO_2 + NO_2$	2.84*J_IC3H7NO3	Taraborrelli (2016)
J6000	StTrGJCl	$Cl_2 + h\nu \rightarrow Cl + Cl$	jx(ip_Cl2)	Sander et al. (2014)
J6100	StTrGJCl	$Cl_2O_2 + h\nu \rightarrow 2\ Cl$	jx(ip_Cl2O2)	Sander et al. (2014)
J6101	StTrGJCl	$OClO + h\nu \rightarrow ClO + O(^3P)$	jx(ip_OClO)	Sander et al. (2014)
J6200	StGJCl	$HCl + h\nu \rightarrow Cl + H$	jx(ip_HCl)	Sander et al. (2014)
J6201	StTrGJCl	$HOCl + h\nu \rightarrow OH + Cl$	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)
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*
PH10200_a01	TrAa01JHg	$Hg(OH)_2(aq) + h\nu \rightarrow Hg(aq)$	xaer(01)*6E-5*jx(ip_NO2)	see note*

General notes

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

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:
J(11) → `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($iC_3H_7ONO_2$)
J(54) → J($iC_3H_7ONO_2$)
J(55) → J($iC_3H_7ONO_2$)
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 + .18 HCHO + .18 $O(^3P)$ + .33 OH + .33 HO_2 + .44 CO_2 + .38 CO + .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

`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 × 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 → .5 CO14O3CHO + .5 NO2 + .5 NBZFUONE + .5 HO2

J44404b: KDEC MALDIALCO2 → .6 MALANHY + HO2 + .4 GLYOX + .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 → .6 C5CO14O2 + .6 HO2 + .4 TLFUONE

J45410: KDEC MMALANHYO → CO2H3CO3

J45411: KDEC C5DICARBO → MGLYOX + GLYOX + HO2

J45412: KDEC NTLFUO → ACCOMECHO + NO2

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

J45415: KDEC TLFUO → ACCOMECHO + HO2

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

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

J46404: KDEC BZBIPERO → GLYOX + HO2 + .5 BZFUONE + .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 + .5 BZFUONE + .5 BZFUONE

J46419: KDEC NBZQO → C6CO4DB + NO2

J46422: KDEC DNPHENO → NC4DCO2H + HCOCO2H + NO2

J46425: KDEC BZEMUCO → .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 → .6 GLYOX + .4 MGLYOX + HO2 + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

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

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

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

J47408b: KDEC NCRESO → C5CO14OH + GLYOX + NO2

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

J47412: KDEC TLEMUCO → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

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

J47418: new channel

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

J47420: new channel

J47422: KDEC NPTLQO → 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.

J7301: The quantum yields are recommended by Sander et al. (2011) for $\lambda > 300$nm and used here for the entire spectrum.

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

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

Table 3: Henry's law coefficients

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{soln}H/R}{\text{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^{5}$	6338.	Lind and Kok (1994)
H_2O	BIG	0.	see note
NH_3	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
N_2O_5	BIG	0.	see note
HONO	4.9×10^{1}	4780.	Schwartz and White (1981)
HNO_3	$2.45\times10^{6}/1.5\times10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3OH	2.20×10^{2}	5200.	Snider and Dawson (1985)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CH_3COOH	4.1×10^{3}	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
$C_2H_5O_2$	6.	5600.	see note
CH_3CHO	1.29×10^{1}	5890.	Sander et al. (2006)
GLYOX	4.19×10^{5}	7481.	Sander et al. (2011)
$HOCH_2CO_2H$	2.83×10^{4}	4029.	Ip et al. (2009)
$HOCH_2CHO$	4.10×10^{4}	4600.	Betterton and Hoffmann (1988a)
CH_3COCH_3	28.1	5050.	Sander et al. (2006)
MGLYOX	3.70×10^{3}	7500.	Betterton and Hoffmann (1988a)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.6×10^{2}	5862.	Huthwelker et al. (1995)
$ClNO_3$	BIG	0.	see note

Table 3: Henry's law coefficients (... continued)

substance	$\frac{k_H^{\ominus}}{M/atm}$	$\frac{-\Delta_{soln}H/R}{K}$	reference
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	1.3×10^{3}	5862.	Blatchley et al. (1992)*
$BrNO_3$	BIG	0.	see note
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
I_2	3.	4431.	Palmer et al. (1985)
IO	4.5×10^{2}	5862.	see note
OIO	BIG	0.	see note
I_2O_2	BIG	0.	see note
HI	BIG	0.	see note
HOI	4.5×10^{2}	5862.	Chatfield and Crutzen (1990)*
HIO_3	BIG	0.	see note
INO_2	BIG	0.	see note
INO_3	BIG	0.	see note
ICl	1.1×10^{2}	5600.	see note
IBr	2.4×10^{1}	5600.	see note
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
CH_3SO_3H	BIG	0.	see note
DMS	5.4×10^{-1}	3500.	Staudinger and Roberts (2001)
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*
Hg	0.13	0.	Schroeder and Munthe (1998)
HgO	3.2×10^{6}	0.	Shon et al. (2005)
$HgCl_2$	2.4×10^{7}	0.	Shon et al. (2005)
$HgBr_2$	2.4×10^{7}	0.	see note
HgCl	2.4×10^{7}	0.	Shon et al. (2005)
HgBr	2.4×10^{7}	0.	see note
ClHgBr	2.4×10^{7}	0.	see note
BrHgOBr	2.4×10^{7}	0.	see note
ClHgOBr	2.4×10^{7}	0.	see note

General notes

The value "BIG" corresponds to virtually infinite solubility which is represented in the model using a very large but arbitrary number.

The temperature dependence of the Henry constants is:

$$K_{\mathrm{H}} = K_{\mathrm{H}}^{\ominus} \times \exp\left(\frac{-\Delta_{\mathrm{soln}} H}{R}\left(\frac{1}{T} - \frac{1}{T^{\ominus}}\right)\right)$$

where $\Delta_{\mathrm{soln}} H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314$ J/(mol K).

Specific notes

NO_2: The temperature dependence is from Chameides (1984).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

$C_2H_5O_2$: Assumed to be the same as $K_{\mathrm{H}}(CH_3O_2)$.

HBr: Calculated using the acidity constant from Lax (1969).

HOBr: Twice the value of HOCl, according to Blatchley et al. (1992). Same temperature dependence as for HOCl assumed.

IO: Assumed to be the same as K_{H}(HOI).

HOI: Lower limit.

ICl: Calculated using thermodynamic data from Wagman et al. (1982).

IBr: Calculated using thermodynamic data from Wagman et al. (1982).

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

$HgBr_2$: Assumed to be the same as for $HgCl_2$.

ClHgBr: Assumed to be the same as for $HgCl_2$.

BrHgOBr: Assumed to be the same as for $HgCl_2$.

ClHgOBr: Assumed to be the same as for $HgCl_2$.

Table 4: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\rm obs}H/R}{\rm K}$	reference
O_2	0.01	2000.	see note
O_3	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO_2	0.5	(default)	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
H_2O	0.0	(default)	see note
NH_3	0.06	(default)	DeMore et al. (1997)*
NO	5.0×10^{-5}	(default)	Saastad et al. (1993)*
NO_2	0.0015	(default)	Ponche et al. (1993)*
NO_3	0.04	(default)	Rudich et al. (1996)*
N_2O_5	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO_3	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO_4	(default)	(default)	DeMore et al. (1997)*
CH_3OH	(default)	(default)	see note
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
CO_2	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH_3COOH	2.0×10^{-2}	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
$C_2H_5O_2$	(default)	(default)	see note
CH_3CHO	3.0×10^{-2}	(default)	see note
GLYOX	(default)	(default)	see note
$HOCH_2CO_2H$	(default)	(default)	see note
$HOCH_2CHO$	(default)	(default)	see note
CH_3COCH_3	3.72×10^{-3}	6395.	Davidovits et al. (1995)
MGLYOX	(default)	(default)	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
$ClNO_3$	0.108	(default)	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^\ominus$	$\frac{-\Delta_{\rm obs}H/R}{\rm K}$	reference
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	(default)	Deiber et al. (2004)*
BrCl	0.038	6546.	see note
I_2	0.01	2000.	see note
IO	0.5	2000.	see note
OIO	0.01	(default)	see note
I_2O_2	(default)	2000.	see note
HI	0.036	4130.	Schweitzer et al. (2000)*
HOI	0.5	(default)	see note
HIO_3	0.01	(default)	see note
INO_2	(default)	2000.	see note
INO_3	(default)	2000.	see note
ICl	0.018	2000.	Braban et al. (2007)
IBr	0.018	2000.	see note
SO_2	0.11	(default)	DeMore et al. (1997)
H_2SO_4	0.65	(default)	Pöschl et al. (1998)*
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)
Hg	(default)	(default)	see note
HgO	(default)	(default)	see note
$HgCl_2$	(default)	(default)	see note
$HgBr_2$	(default)	(default)	see note
HgCl	(default)	(default)	see note
HgBr	(default)	(default)	see note
ClHgBr	(default)	(default)	see note
BrHgOBr	(default)	(default)	see note
ClHgOBr	(default)	(default)	see note

General notes

If no data are available, the following default values are used:

$\alpha^\ominus = 0.1$
$-\Delta_{\rm obs}H/R = 0$ K

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta_{\rm obs}G}{RT}\right) = \exp\left(\frac{-\Delta_{\rm obs}H}{RT}+\frac{\Delta_{\rm obs}S}{R}\right)$$

where $\Delta_{\rm obs}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\rm obs}H$ and $\Delta_{\rm obs}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\rm obs}H}{R}\times\frac{1}{T}+\frac{-\Delta_{\rm obs}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right)\Big/\mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\rm obs}H}{R}$$

Specific notes

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NH_3: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

N_2O_5: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

CO_2: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

$C_2H_5O_2$: Estimate.

CH_3CHO: Using the same estimate as in the CAPRAM 2.4 model (`http://projects.tropos.de/capram/capram_24.html`).

HCl: Temperature dependence derived from published data at 2 different temperatures

HOCl: Assumed to be the same as α(HOBr).

$ClNO_3$: Value measured at 274.5 K.

HBr: Temperature dependence derived from published data at 2 different temperatures

HOBr: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

$BrNO_3$: Value measured at 273 K.

BrCl: Assumed to be the same as $\alpha(Cl_2)$.

I_2: Estimate.

IO: Estimate.

OIO: Estimate.

I_2O_2: Estimate.

HI: Temperature dependence derived from published data at 2 different temperatures

HOI: Assumed to be the same as α(HOBr). See also Mössinger and Cox (2001) and Holmes et al. (2001).

HIO_3: Estimate.

INO_2: Estimate.

INO_3: Estimate.

IBr: Assumed to be the same as α(ICl).

H_2SO_4: Value measured at 303 K.

Hg: Estimate.

HgO: Estimate.

$HgCl_2$: Estimate.

$HgBr_2$: Estimate.

ClHgBr: Estimate.

BrHgOBr: Estimate.

ClHgOBr: Estimate.

Table 5: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H1000f_a01	TrAa01Sc	$O_2 \rightarrow O_2(aq)$	k_exf(01,ind_O2)	see general notes*
H1000b_a01	TrAa01Sc	$O_2(aq) \rightarrow O_2$	k_exb(01,ind_O2)	see general notes*
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	k_exf(01,ind_O3)	see general notes*
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	k_exb(01,ind_O3)	see general notes*
H2100f_a01	TrAa01Sc	$OH \rightarrow OH(aq)$	k_exf(01,ind_OH)	see general notes*
H2100b_a01	TrAa01Sc	$OH(aq) \rightarrow OH$	k_exb(01,ind_OH)	see general notes*
H2101f_a01	TrAa01Sc	$HO_2 \rightarrow HO_2(aq)$	k_exf(01,ind_HO2)	see general notes*
H2101b_a01	TrAa01Sc	$HO_2(aq) \rightarrow HO_2$	k_exb(01,ind_HO2)	see general notes*
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	k_exf(01,ind_H2O2)	see general notes*
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	k_exb(01,ind_H2O2)	see general notes*
H3101f_a01	TrAa01ScN	$NO_2 \rightarrow NO_2(aq)$	k_exf(01,ind_NO2)	see general notes*
H3101b_a01	TrAa01ScN	$NO_2(aq) \rightarrow NO_2$	k_exb(01,ind_NO2)	see general notes*
H3102f_a01	TrAa01ScN	$NO_3 \rightarrow NO_3(aq)$	k_exf(01,ind_NO3)	see general notes*
H3102b_a01	TrAa01ScN	$NO_3(aq) \rightarrow NO_3$	k_exb(01,ind_NO3)	see general notes*
H3200f_a01	TrAa01MblScScmN	$NH_3 \rightarrow NH_3(aq)$	k_exf(01,ind_NH3)	see general notes*
H3200b_a01	TrAa01MblScScmN	$NH_3(aq) \rightarrow NH_3$	k_exb(01,ind_NH3)	see general notes*
H3201_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)
H3202f_a01	TrAa01ScN	$HONO \rightarrow HONO(aq)$	k_exf(01,ind_HONO)	see general notes*
H3202b_a01	TrAa01ScN	$HONO(aq) \rightarrow HONO$	k_exb(01,ind_HONO)	see general notes*
H3203f_a01	TrAa01MblScScmN	$HNO_3 \rightarrow HNO_3(aq)$	k_exf(01,ind_HNO3)	see general notes*
H3203b_a01	TrAa01MblScScmN	$HNO_3(aq) \rightarrow HNO_3$	k_exb(01,ind_HNO3)	see general notes*
H3204f_a01	TrAa01ScN	$HNO_4 \rightarrow HNO_4(aq)$	k_exf(01,ind_HNO4)	see general notes*
H3204b_a01	TrAa01ScN	$HNO_4(aq) \rightarrow HNO_4$	k_exb(01,ind_HNO4)	see general notes*
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	k_exf(01,ind_CO2)	see general notes*
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	k_exb(01,ind_CO2)	see general notes*
H4101f_a01	TrAa01ScScm	$HCHO \rightarrow HCHO(aq)$	k_exf(01,ind_HCHO)	see general notes*
H4101b_a01	TrAa01ScScm	$HCHO(aq) \rightarrow HCHO$	k_exb(01,ind_HCHO)	see general notes*
H4102f_a01	TrAa01Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	k_exf(01,ind_CH3O2)	see general notes*
H4102b_a01	TrAa01Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	k_exb(01,ind_CH3O2)	see general notes*
H4103f_a01	TrAa01ScScm	$HCOOH \rightarrow HCOOH(aq)$	k_exf(01,ind_HCOOH)	see general notes*
H4103b_a01	TrAa01ScScm	$HCOOH(aq) \rightarrow HCOOH$	k_exb(01,ind_HCOOH)	see general notes*
H4104f_a01	TrAa01ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	k_exf(01,ind_CH3OOH)	see general notes*
H4104b_a01	TrAa01ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	k_exb(01,ind_CH3OOH)	see general notes*

Table 5: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H6000f_a01	TrAa01MblScCl	$Cl_2 \rightarrow Cl_2(aq)$	k_exf(01,ind_Cl2)	see general notes*
H6000b_a01	TrAa01MblScCl	$Cl_2(aq) \rightarrow Cl_2$	k_exb(01,ind_Cl2)	see general notes*
H6200f_a01	TrAa01MblScScmCl	$HCl \rightarrow HCl(aq)$	k_exf(01,ind_HCl)	see general notes*
H6200b_a01	TrAa01MblScScmCl	$HCl(aq) \rightarrow HCl$	k_exb(01,ind_HCl)	see general notes*
H6201f_a01	TrAa01MblScCl	$HOCl \rightarrow HOCl(aq)$	k_exf(01,ind_HOCl)	see general notes*
H6201b_a01	TrAa01MblScCl	$HOCl(aq) \rightarrow HOCl$	k_exb(01,ind_HOCl)	see general notes*
H6300_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)
H6301_a01	TrAa01MblClN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	k_exf_ClNO3(01) * C(ind_ H2O_a01)	see general notes*
H6302_a01	TrAa01MblClN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 5.E2	see general notes*
H7000f_a01	TrAa01MblScBr	$Br_2 \rightarrow Br_2(aq)$	k_exf(01,ind_Br2)	see general notes*
H7000b_a01	TrAa01MblScBr	$Br_2(aq) \rightarrow Br_2$	k_exb(01,ind_Br2)	see general notes*
H7200f_a01	TrAa01MblScScmBr	$HBr \rightarrow HBr(aq)$	k_exf(01,ind_HBr)	see general notes*
H7200b_a01	TrAa01MblScScmBr	$HBr(aq) \rightarrow HBr$	k_exb(01,ind_HBr)	see general notes*
H7201f_a01	TrAa01MblScBr	$HOBr \rightarrow HOBr(aq)$	k_exf(01,ind_HOBr)	see general notes*
H7201b_a01	TrAa01MblScBr	$HOBr(aq) \rightarrow HOBr$	k_exb(01,ind_HOBr)	see general notes*
H7300_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)
H7301_a01	TrAa01MblBrN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	k_exf_BrNO3(01) * C(ind_ H2O_a01)	see general notes*
H7302_a01	TrAa01MblBrN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 3.E5	see general notes*
H7600f_a01	TrAa01MblScBrCl	$BrCl \rightarrow BrCl(aq)$	k_exf(01,ind_BrCl)	see general notes*
H7600b_a01	TrAa01MblScBrCl	$BrCl(aq) \rightarrow BrCl$	k_exb(01,ind_BrCl)	see general notes*
H7601_a01	TrAa01MblBrClN	$ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 3.E5	see general notes*
H7602_a01	TrAa01MblBrClN	$BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 5.E2	see general notes*
H8000f_a01	TrAa01ScI	$I_2 \rightarrow I_2(aq)$	k_exf(01,ind_I2)	see general notes*
H8000b_a01	TrAa01ScI	$I_2(aq) \rightarrow I_2$	k_exb(01,ind_I2)	see general notes*
H8100f_a01	TrAa01MblScI	$IO \rightarrow IO(aq)$	k_exf(01,ind_IO)	see general notes*
H8100b_a01	TrAa01MblScI	$IO(aq) \rightarrow IO$	k_exb(01,ind_IO)	see general notes*
H8101_a01	TrAa01I	$OIO \rightarrow HOI(aq) + HO_2(aq)$	k_exf(01,ind_OIO)	see general notes*
H8102_a01	TrAa01I	$I_2O_2 \rightarrow HOI(aq) + H^+(aq) + IO_2^-(aq)$	k_exf(01,ind_I2O2)	see general notes*
H8200f_a01	TrAa01MblScI	$HOI \rightarrow HOI(aq)$	k_exf(01,ind_HOI)	see general notes*
H8200b_a01	TrAa01MblScI	$HOI(aq) \rightarrow HOI$	k_exb(01,ind_HOI)	see general notes*
H8201_a01	TrAa01MblScI	$HI \rightarrow H^+(aq) + I^-(aq)$	$k_{mt}(HI) \cdot lwc$	see general notes*

Table 5: Reversible (Henry's law) equilibria and irreversible ("heterogenous") uptake

#	labels	reaction	rate coefficient	reference
H8202_a01	TrAa01ScI	$HIO_3 \rightarrow IO_3^-(aq) + H^+(aq)$	$k_{mt}(HIO_3) \cdot lwc$	see general notes*
H8300_a01	TrAa01IN	$INO_2 \rightarrow HOI(aq) + HONO(aq)$	`k_exf(01,ind_INO2)`	see general notes*
H8301_a01	TrAa01MblIN	$INO_3 \rightarrow HOI(aq) + HNO_3(aq)$	`k_exf(01,ind_INO3)`	see general notes*
H8600f_a01	TrAa01MblScClI	$ICl \rightarrow ICl(aq)$	`k_exf(01,ind_ICl)`	see general notes*
H8600b_a01	TrAa01MblScClI	$ICl(aq) \rightarrow ICl$	`k_exb(01,ind_ICl)`	see general notes*
H8700f_a01	TrAa01MblScBrI	$IBr \rightarrow IBr(aq)$	`k_exf(01,ind_IBr)`	see general notes*
H8700b_a01	TrAa01MblScBrI	$IBr(aq) \rightarrow IBr$	`k_exb(01,ind_IBr)`	see general notes*
H9100f_a01	TrAa01MblScScmS	$SO_2 \rightarrow SO_2(aq)$	`k_exf(01,ind_SO2)`	see general notes*
H9100b_a01	TrAa01MblScScmS	$SO_2(aq) \rightarrow SO_2$	`k_exb(01,ind_SO2)`	see general notes*
H9200_a01	TrAa01MblScScmS	$H_2SO_4 \rightarrow H_2SO_4(aq)$	`xnom7sulf*k_exf(01,ind_H2SO4)`	see general notes*
H9400f_a01	TrAa01CS	$DMSO \rightarrow DMSO(aq)$	`k_exf(01,ind_DMSO)`	see general notes*
H9400b_a01	TrAa01CS	$DMSO(aq) \rightarrow DMSO$	`k_exb(01,ind_DMSO)`	see general notes*
H9401_a01	TrAa01MblS	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	`k_exf(01,ind_CH3SO3H)`	see general notes*
H9402f_a01	TrAa01CS	$DMS \rightarrow DMS(aq)$	`k_exf(01,ind_DMS)`	see general notes*
H9402b_a01	TrAa01CS	$DMS(aq) \rightarrow DMS$	`k_exb(01,ind_DMS)`	see general notes*
H10000f_a01	TrAa01Hg	$Hg \rightarrow Hg(aq)$	`k_exf(01,ind_Hg)`	see general notes*
H10000b_a01	TrAa01Hg	$Hg(aq) \rightarrow Hg$	`k_exb(01,ind_Hg)`	see general notes*
H10100f_a01	TrAa01Hg	$HgO \rightarrow HgO(aq)$	`k_exf(01,ind_HgO)`	see general notes*
H10100b_a01	TrAa01Hg	$HgO(aq) \rightarrow HgO$	`k_exb(01,ind_HgO)`	see general notes*
H10600f_a01	TrAa01ClHg	$HgCl_2 \rightarrow HgCl_2(aq)$	`k_exf(01,ind_HgCl2)`	see general notes*
H10600b_a01	TrAa01ClHg	$HgCl_2(aq) \rightarrow HgCl_2$	`k_exb(01,ind_HgCl2)`	see general notes*
H10700f_a01	TrAa01BrHg	$HgBr_2 \rightarrow HgBr_2(aq)$	`k_exf(01,ind_HgBr2)`	see general notes*
H10700b_a01	TrAa01BrHg	$HgBr_2(aq) \rightarrow HgBr_2$	`k_exb(01,ind_HgBr2)`	see general notes*
H10701f_a01	TrAa01BrClHg	$ClHgBr \rightarrow ClHgBr(aq)$	`k_exf(01,ind_ClHgBr)`	see general notes*
H10701b_a01	TrAa01BrClHg	$ClHgBr(aq) \rightarrow ClHgBr$	`k_exb(01,ind_ClHgBr)`	see general notes*
H10702f_a01	TrAa01BrHg	$BrHgOBr \rightarrow BrHgOBr(aq)$	`k_exf(01,ind_BrHgOBr)`	see general notes*
H10702b_a01	TrAa01BrHg	$BrHgOBr(aq) \rightarrow BrHgOBr$	`k_exb(01,ind_BrHgOBr)`	see general notes*
H10703f_a01	TrAa01BrClHg	$ClHgOBr \rightarrow ClHgOBr(aq)$	`k_exf(01,ind_ClHgOBr)`	see general notes*
H10703b_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 the file `messy_mecca_aero.f90` using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry's law constants in subroutine `mecca_aero_henry`.

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

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

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt}. The factors only affect the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[\text{Cl}^-] > 0.1$ M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\text{H}_2\text{O}]/[\text{Cl}^-]$ is less than 5×10^2. The ratio $5\times10^2/3\times10^5$ 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 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	`khet_St(ihs_N2O5_H2O)`	see general notes*
HET201	TrHetN	$N_2O_5 \rightarrow 2\ NO_3^-(aq) + 2\ H^+(aq)$	`khet_Tr(iht_N2O5)`	see general notes*
HET410	StHetCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_St(ihs_HOCl_HCl)`	see general notes*
HET420	StHetClN	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_St(ihs_ClNO3_HCl)`	see general notes*
HET421	StHetClN	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_St(ihs_ClNO3_H2O)`	see general notes*
HET422	StHetClN	$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	`khet_St(ihs_N2O5_HCl)`	see general notes*
HET510	StHetBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_St(ihs_HOBr_HBr)`	see general notes*
HET520	StHetBrN	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_St(ihs_BrNO3_H2O)`	see general notes*
HET540	StHetBrClN	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_St(ihs_ClNO3_HBr)`	see general notes*
HET541	StHetBrClN	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_St(ihs_BrNO3_HCl)`	see general notes*
HET542	StHetBrCl	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_St(ihs_HOCl_HBr)`	see general notes*
HET543	StHetBrCl	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_St(ihs_HOBr_HCl)`	see general notes*
HET1001	StTrHetHg	$Hg \rightarrow Hg(aq)$	`khet_Tr(iht_Hg) + khet_St(ihs_Hg)`	see general notes*
HET1002	StTrHetHg	$HgO \rightarrow Hg(aq)$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1003	StTrHetClHg	$HgCl \rightarrow Hg(aq) + LCHLORINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1004	StTrHetClHg	$HgCl_2 \rightarrow Hg(aq) + 2\ LCHLORINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1005	StTrHetBrHg	$HgBr \rightarrow Hg(aq) + LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1006	StTrHetBrHg	$HgBr_2 \rightarrow Hg(aq) + 2\ LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1007	StTrHetBrClHg	$ClHgBr \rightarrow Hg(aq) + LCHLORINE + LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1008	StTrHetBrHg	$BrHgOBr \rightarrow Hg(aq) + 2\ LBROMINE$	`khet_Tr(iht_RGM) + khet_St(ihs_RGM)`	see general notes*
HET1009	StTrHetBrClHg	$ClHgOBr \rightarrow Hg(aq) + LCHLORINE + LBROMINE$	`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 7: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$	reference
EQ20_a01	TrAa01Sc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5		Weinstein-Lloyd and Schwartz (1991)
EQ21_a01	TrAa01MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a01	TrAa01MblScScmN	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ31_a01	TrAa01ScN	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260	Schwartz and White (1981)
EQ32_a01	TrAa01MblScScmN	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ33_a01	TrAa01ScN	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5		Warneck (1999)
EQ40_a01	TrAa01MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ41_a01	TrAa01ScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4		Weast (1980)
EQ60_a01	TrAa01Cl	$Cl_2^- \rightleftharpoons Cl + Cl^-$	7.3E-6		Yu (2004)
EQ61_a01	TrAa01MblScScmCl	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ62_a01	TrAa01ScCl	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8		Lax (1969)
EQ70_a01	TrAa01Br	$Br_2^- \rightleftharpoons Br + Br^-$	2.54E-6	-2256	Liu et al. (2002)
EQ71_a01	TrAa01MblScScmBr	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ72_a01	TrAa01ScBr	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091	Kelley and Tartar (1956)*
EQ73_a01	TrAa01MblBrCl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01MblBrCl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01MblBrCl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01MblBrCl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ80_a01	TrAa01MblScClI	$ICl + Cl^- \rightleftharpoons ICl_2^-$	7.7E1		Wang et al. (1989)
EQ81_a01	TrAa01MblScBrI	$IBr + Br^- \rightleftharpoons IBr_2^-$	2.9E2		Troy and Margerum (1991)
EQ82_a01	TrAa01MblScBrClI	$ICl + Br^- \rightleftharpoons IBr + Cl^-$	3.3E2		see note*
EQ90_a01	TrAa01MblScScmS	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01MblScScmS	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01MblScScmS	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01MblScScmS	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ100_a01	TrAa01Hg	$Hg^{2+} + OH^- \rightleftharpoons HgOH^+$	4.0E10		Ammann and Pöschl (2007)
EQ101_a01	TrAa01Hg	$HgOH^+ + OH^- \rightleftharpoons Hg(OH)_2$	1.58E11		Ammann and Pöschl (2007)
EQ102_a01	TrAa01ClHg	$Hg^{2+} + Cl^- \rightleftharpoons HgCl^+$	5.8E6		Ammann and Pöschl (2007)
EQ103_a01	TrAa01ClHg	$HgCl^+ + Cl^- \rightleftharpoons HgCl_2$	2.5E6		Ammann and Pöschl (2007)
EQ104_a01	TrAa01ClHg	$HgOH^+ + Cl^- \rightleftharpoons Hg(OH)Cl$	2.69E7		Ammann and Pöschl (2007)
EQ105_a01	TrAa01BrHg	$Hg^{2+} + Br^- \rightleftharpoons HgBr^+$	1.1E9		Raofie and Ariya (2004)
EQ106_a01	TrAa01BrHg	$HgBr^+ + Br^- \rightleftharpoons HgBr_2$	2.5E8		Raofie and Ariya (2004)
EQ107_a01	TrAa01HgS	$Hg^{2+} + SO_3^{2-} \rightleftharpoons HgSO_3$	2.E13		van Loon et al. (2001)
EQ108_a01	TrAa01HgS	$HgSO_3 + SO_3^{2-} \rightleftharpoons Hg(SO_3)_2^{2-}$	1.E10		van Loon et al. (2001)

Specific notes

EQ40_a01: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

EQ72_a01: For pK_a(HOBr), see also Keller-Rudek et al. (1992).

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

$$\begin{array}{ccccccccc} \mathrm{ICl} & + & \mathrm{Br^-} & \rightleftharpoons & \mathrm{IBr} & + & \mathrm{Cl^-} \\ \text{-17.1} & & \text{-103.96} & = & \text{-4.2} & & \text{-131.228} \end{array}$$

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

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

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

Table 8: Aqueous phase reactions

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

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A6202_a01	TrAa01Cl	$Cl^- + OH \rightarrow ClOH^-$	4.2E9		Yu (2004)
A6203_a01	TrAa01Cl	$Cl_2 + HO_2 \rightarrow Cl_2^- + H^+$	1.0E9		Bjergbakke et al. (1981)
A6204_a01	TrAa01MblCl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6205_a01	TrAa01Cl	$Cl_2^- + HO_2 \rightarrow 2\ Cl^- + H^+$	1.3E10		Jacobi (1996)
A6206_a01	TrAa01Cl	$HOCl + O_2^- \rightarrow Cl + OH^-$	7.5E6		Long and Bielski (1980)
A6207_a01	TrAa01Cl	$HOCl + HO_2 \rightarrow Cl$	7.5E6		Long and Bielski (1980)
A6208_a01	TrAa01MblCl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A6209_a01	TrAa01Cl	$ClOH^- \rightarrow Cl^- + OH$	6.0E9		Yu (2004)
A6210_a01	TrAa01Cl	$ClOH^- + H^+ \rightarrow Cl$	2.4E10		Yu (2004)
A6300_a01	TrAa01ClN	$Cl + NO_3^- \rightarrow NO_3 + Cl^-$	1.0E8		Buxton et al. (1999b)
A6301_a01	TrAa01ClN	$Cl^- + NO_3 \rightarrow NO_3^- + Cl$	3.4E8		Buxton et al. (1999b)*
A6302_a01	TrAa01ClN	$Cl_2^- + NO_2^- \rightarrow 2\ Cl^- + NO_2$	6.0E7		Jacobi et al. (1996)
A6400_a01	TrAa01Cl	$Cl_2^- + CH_3OOH \rightarrow 2\ Cl^- + H^+ + CH_3OO$	5.0E4		Jacobi et al. (1996)
A7000_a01	TrAa01Br	$Br_2^- + Br_2^- \rightarrow 2\ Br^- + Br_2$	1.9E9		Ross et al. (1992)
A7100_a01	TrAa01Br	$Br^- + O_3 \rightarrow BrO^-$	2.1E2	-4450	Haag and Hoigné (1983)
A7101_a01	TrAa01Br	$Br_2 + O_2^- \rightarrow Br_2^-$	5.6E9		Sutton and Downes (1972)
A7102_a01	TrAa01Br	$Br_2^- + O_2^- \rightarrow 2\ Br^-$	1.7E8		Wagner and Strehlow (1987)
A7200_a01	TrAa01Br	$Br^- + OH \rightarrow BrOH^-$	1.1E10		Zehavi and Rabani (1972)
A7201_a01	TrAa01Br	$Br_2 + HO_2 \rightarrow Br_2^- + H^+$	1.1E8		Sutton and Downes (1972)
A7202_a01	TrAa01MblBr	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7203_a01	TrAa01Br	$Br_2^- + HO_2 \rightarrow Br_2 + H_2O_2 + OH^-$	4.4E9		Matthew et al. (2003)
A7204_a01	TrAa01Br	$Br_2^- + H_2O_2 \rightarrow 2\ Br^- + H^+ + HO_2$	1.0E5		Jacobi (1996)
A7205_a01	TrAa01Br	$HOBr + O_2^- \rightarrow Br + OH^-$	3.5E9		Schwarz and Bielski (1986)
A7206_a01	TrAa01Br	$HOBr + HO_2 \rightarrow Br$	1.0E9		Herrmann et al. (1999)
A7207_a01	TrAa01Br	$HOBr + H_2O_2 \rightarrow Br^- + H^+$	1.2E6		Bichsel and von Gunten (1999)
A7208_a01	TrAa01MblBr	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7209a_a01	TrAa01Br	$BrOH^- \rightarrow Br^- + OH$	3.3E7		Zehavi and Rabani (1972)
A7209b_a01	TrAa01Br	$BrOH^- \rightarrow Br + OH^-$	4.2E6		Zehavi and Rabani (1972)
A7210_a01	TrAa01Br	$BrOH^- + H^+ \rightarrow Br$	4.4E10		Zehavi and Rabani (1972)
A7300_a01	TrAa01BrN	$Br^- + NO_3 \rightarrow Br + NO_3^-$	4.0E9		Neta and Huie (1986)
A7301_a01	TrAa01BrN	$Br_2^- + NO_2^- \rightarrow 2\ Br^- + NO_2$	1.7E7	-1720	Shoute et al. (1991)
A7400_a01	TrAa01Br	$Br_2^- + CH_3OOH \rightarrow 2\ Br^- + H^+ + CH_3OO$	1.0E5		Jacobi (1996)*
A7601_a01	TrAa01BrCl	$Br^- + ClO^- + H^+ \rightarrow BrCl + OH^-$	3.7E10		Kumar and Margerum (1987)
A7602_a01	TrAa01MblBrCl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A7603_a01	TrAa01MblBrCl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		Liu and Margerum (2001)*
A7604_a01	TrAa01MblBrCl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A8100_a01	TrAa01MblI	$I^- + O_3 \rightarrow HOI + OH^-$	4.2E9	-9311	Magi et al. (1997)
A8101_a01	TrAa01MblI	$IO + IO \rightarrow HOI + IO_2^- + H^+$	1.5E9		Buxton et al. (1986)
A8200_a01	TrAa01MblI	$IO_2^- + H_2O_2 \rightarrow IO_3^-$	6.0E1		Furrow (1987)
A8201_a01	TrAa01I	$HOI + IO_2^- \rightarrow IO_3^- + I^- + H^+$	6.0E2		Chinake and Simoyi (1996)
A8202_a01	TrAa01MblI	$HOI + I^- + H^+ \rightarrow I_2$	4.4E12		Eigen and Kustin (1962)
A8203_a01	TrAa01MblI	$IO_2^- + I^- + H^+ \rightarrow 2\ HOI + OH^-$	2.0E10		Edblom et al. (1987)
A8600_a01	TrAa01MblClI	$ICl \rightarrow HOI + Cl^- + H^+$	2.4E6		Wang et al. (1989)
A8601_a01	TrAa01MblClI	$I^- + HOCl + H^+ \rightarrow ICl$	3.5E11		Nagy et al. (1988)
A8602_a01	TrAa01ClI	$IO_2^- + HOCl \rightarrow IO_3^- + Cl^- + H^+$	1.5E3		Lengyel et al. (1996)
A8603_a01	TrAa01MblClI	$HOI + Cl^- + H^+ \rightarrow ICl$	2.9E10		Wang et al. (1989)
A8604_a01	TrAa01ClI	$HOI + Cl_2 \rightarrow IO_2^- + 2\ Cl^- + 3H^+$	1.0E6		Lengyel et al. (1996)
A8605_a01	TrAa01ClI	$HOI + HOCl \rightarrow IO_2^- + Cl^- + 2\ H^+$	5.0E5		Citri and Epstein (1988)
A8606_a01	TrAa01ClI	$ICl + I^- \rightarrow I_2 + Cl^-$	1.1E9		Margerum et al. (1986)
A8700_a01	TrAa01MblBrI	$IBr \rightarrow HOI + H^+ + Br^-$	8.0E5		Troy et al. (1991)
A8701_a01	TrAa01MblBrI	$I^- + HOBr \rightarrow IBr + OH^-$	5.0E9		Troy and Margerum (1991)
A8702_a01	TrAa01BrI	$IO_2^- + HOBr \rightarrow IO_3^- + Br^- + H^+$	1.0E6		Chinake and Simoyi (1996)
A8703_a01	TrAa01MblBrI	$HOI + Br^- + H^+ \rightarrow IBr$	3.3E12		Troy et al. (1991)
A8704_a01	TrAa01BrI	$HOI + HOBr \rightarrow IO_2^- + Br^- + 2\ H^+$	1.0E6		Chinake and Simoyi (1996)
A8705_a01	TrAa01BrI	$IBr + I^- \rightarrow I_2 + Br^-$	2.0E9		Faria et al. (1993)
A9100_a01	TrAa01ScS	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9		Huie and Neta (1987)
A9101_a01	TrAa01MblScScmS	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9102_a01	TrAa01ScS	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9		Jiang et al. (1992)
A9103_a01	TrAa01ScS	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8		Huie and Neta (1987)
A9104_a01	TrAa01ScS	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8		Buxton et al. (1996)
A9105_a01	TrAa01S	$SO_5^- + SO_3^{2-} \rightarrow .72\ SO_4^- + .72\ SO_4^{2-} + .28\ SO_3^- + .28\ HSO_5^- + .28\ OH^-$	1.3E7		Huie and Neta (1987), Deister and Warneck (1990)*
A9106_a01	TrAa01S	$SO_5^- + SO_5^- \rightarrow O_2 + SO_4^{2-} + LSULFUR$	1.0E8		Ross et al. (1992)*
A9200_a01	TrAa01ScS	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9		Buxton et al. (1988)
A9201_a01	TrAa01ScS	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9		Jiang et al. (1992)
A9202_a01	TrAa01ScS	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9		Jiang et al. (1992)
A9203_a01	TrAa01ScS	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110	Herrmann et al. (1995)
A9204_a01	TrAa01ScS	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7		Wine et al. (1989)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A9205_a01	TrAa01ScS	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3		see note*
A9206_a01	TrAa01MblScScmS	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9207_a01	TrAa01ScS	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9		Buxton et al. (1988)
A9208_a01	TrAa01ScS	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3		see note*
A9209_a01	TrAa01MblScScmS	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9210_a01	TrAa01ScS	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8		Huie and Neta (1987)
A9211_a01	TrAa01S	$HSO_3^- + SO_5^- \rightarrow .75\ SO_4^- + .75\ SO_4^{2-} + .75\ H^+ + .25\ SO_3^- + .25\ HSO_5^-$	1.0E5		Huie and Neta (1987)
A9212_a01	TrAa01ScS	$HSO_3^- + HSO_5^- + H^+ \rightarrow 2\ HSO_4^- + H^+$	7.1E6		Betterton and Hoffmann (1988b)
A9301_a01	TrAa01ScNS	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4		Exner et al. (1992)
A9302_a01	TrAa01ScNS	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5		Logager et al. (1993)
A9304_a01	TrAa01ScNS	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000	Exner et al. (1992)
A9305_a01	TrAa01ScNS	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5		Warneck (1999)
A9400_a01	TrAa01ScS	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	1.4E4		Boyce and Hoffmann (1984)
A9401_a01	TrAa01ScS	$SO_3^{2-} + CH_3OOH + H^+ \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9402_a01	TrAa01ScS	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	4.3E-1		Boyce and Hoffmann (1984)
A9403_a01	TrAa01ScS	$HSO_3^- + CH_3OOH + H^+ \rightarrow HSO_4^- + H^+ + CH_3OH$	1.6E7	-3800	Lind et al. (1987)
A9404_a01	TrAa01ScS	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3		Seinfeld and Pandis (1998)
A9600_a01	TrAa01ClS	$SO_3^{2-} + Cl_2^- \rightarrow SO_3^- + 2\ Cl^-$	6.2E7		Jacobi et al. (1996)
A9601_a01	TrAa01MblClS	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9602_a01	TrAa01ClS	$SO_4^- + Cl^- \rightarrow SO_4^{2-} + Cl$	2.5E8		Buxton et al. (1999a)
A9603_a01	TrAa01ClS	$SO_4^{2-} + Cl \rightarrow SO_4^- + Cl^-$	2.1E8		Buxton et al. (1999a)
A9604_a01	TrAa01ClS	$HSO_3^- + Cl_2^- \rightarrow SO_3^- + 2\ Cl^- + H^+$	4.7E8	-1082	Shoute et al. (1991)
A9605_a01	TrAa01MblClS	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note*
A9606_a01	TrAa01ClS	$HSO_5^- + Cl^- \rightarrow HOCl + SO_4^{2-}$	1.8E-3	-7352	Fortnum et al. (1960)
A9700_a01	TrAa01BrS	$SO_3^{2-} + Br_2^- \rightarrow 2\ Br^- + SO_3^-$	2.2E8	-649	Shoute et al. (1991)
A9701_a01	TrAa01BrS	$SO_3^{2-} + BrO^- \rightarrow Br^- + SO_4^{2-}$	1.0E8		Troy and Margerum (1991)
A9702_a01	TrAa01MblBrS	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9703_a01	TrAa01BrS	$SO_4^- + Br^- \rightarrow Br + SO_4^{2-}$	2.1E9		Jacobi (1996)
A9704_a01	TrAa01BrS	$HSO_3^- + Br_2^- \rightarrow 2\ Br^- + H^+ + SO_3^-$	6.3E7	-782	Shoute et al. (1991)
A9705_a01	TrAa01MblBrS	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note*
A9706_a01	TrAa01BrS	$HSO_5^- + Br^- \rightarrow HOBr + SO_4^{2-}$	1.0E0	-5338	Fogelman et al. (1989)
A9800_a01	TrAa01IS	$HSO_3^- + I_2 \rightarrow 2\ I^- + HSO_4^- + 2\ H^+$	1.7E9		Yiin and Margerum (1990)
A10100_a01	TrAa01Hg	$Hg + O_3 \rightarrow HgO + O_2$	4.7E7		Munthe (1992)

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A10200_a01	TrAa01Hg	$HgO + H^+ \rightarrow Hg^{2+} + OH^-$	1.0E10		Pleijel and Munthe (1995)
A10201_a01	TrAa01Hg	$Hg + OH \rightarrow Hg^+ + OH^-$	2.0E9		Lin and Pehkonen (1997)
A10202_a01	TrAa01Hg	$Hg^+ + OH \rightarrow Hg^{2+} + OH^-$	1.0E10		Lin and Pehkonen (1997)
A10203_a01	TrAa01Hg	$Hg^{2+} + HO_2 \rightarrow Hg^+ + O_2 + H^+$	1.7E4		Enami et al. (2007)
A10204_a01	TrAa01Hg	$Hg^+ + HO_2 \rightarrow Hg + O_2 + H^+$	1.0E10		Lin and Pehkonen (1997)
A10600_a01	TrAa01ClHg	$Hg + HOCl \rightarrow Hg^{2+} + Cl^- + OH^-$	2.09E6		Lin and Pehkonen (1998)
A10601_a01	TrAa01ClHg	$Hg + ClO^- \rightarrow Hg^{2+} + Cl^- + 2\ OH^-$	1.99E6		Lin and Pehkonen (1998)
A10700_a01	TrAa01BrHg	$Hg + HOBr \rightarrow Hg^{2+} + Br^- + OH^-$	0.279		Wang and Pehkonen (2004)
A10701_a01	TrAa01BrHg	$Hg + BrO^- \rightarrow Hg^{2+} + Br^- + 2\ OH^-$	0.273		Wang and Pehkonen (2004)
A10702_a01	TrAa01BrHg	$Hg + Br_2 \rightarrow Hg^{2+} + 2\ Br^-$	0.196		Wang and Pehkonen (2004)
A10900_a01	TrAa01HgS	$HgSO_3 \rightarrow Hg + HSO_4^- + H^+$	0.0106		van Loon et al. (2000)

Specific notes

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

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

A7400_a01: Assumed to be the same as for Br_2^- + H_2O_2.

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

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

A9106_a01: See also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ 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.

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

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

A9605_a01: Assumed to be the same as for SO_3^{2-} + HOCl.

A9705_a01: Assumed to be the same as for SO_3^{2-} + HOBr.

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