

# The Chemical Mechanism of MECCA

KPP version: 2.2.1\_rs7

MECCA version: 3.8b

Date: December 18, 2017.

Selected reactions:

“Tr && G && !Cl && !Br && !I && !Hg”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 2664

Aqueous phase: 0

All species: 2664

Number of reactions in selected mechanism:

Gas phase (Gnnn): 1670

Aqueous phase (Annn): 0

Henry (Hnnn): 0

Photolysis (Jnnn): 324

Aqueous phase photolysis (PHnnn): 0

Heterogeneous (HETnnn): 0

Equilibria (EQnn): 0

Isotope exchange (IEXnnn): 0

Tagging equations (TAGnnn): 0

Dummy (Dnn): 0

All equations: 1994

This document is part of the electronic supplement to our article  
“Oxidation processes in the Eastern Mediterranean atmosphere:  
Evidence from the Modelling of HOx Measurements over Cyprus”

in Atmos. Chem. Phys. (2018), available at:

<https://www.atmospheric-chemistry-and-physics.net>

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$\text{O}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	$3.3\text{E}-11*\text{EXP}(55./\text{temp})$	Sander et al. (2011)
G1001	UpStTrG	$\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{O}_3$	$6.\text{E}-34*((\text{temp}/300.)**(-2.4))*\text{cair}$	Sander et al. (2011)
G2100	UpStTrG	$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	$\text{k\_3rd}(\text{temp}, \text{cair}, 4.4\text{E}-32, 1.3, 7.5\text{E}-11, -0.2, 0.6)$	Sander et al. (2011)
G2104	UpStTrG	$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$1.7\text{E}-12*\text{EXP}(-940./\text{temp})$	Sander et al. (2011)
G2105	UpStTrG	$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$2.8\text{E}-12*\text{EXP}(-1800./\text{temp})$	Sander et al. (2011)
G2107	UpStTrG	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2 \text{O}_2$	$1.\text{E}-14*\text{EXP}(-490./\text{temp})$	Sander et al. (2011)
G2109	UpStTrG	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	$4.8\text{E}-11*\text{EXP}(250./\text{temp})$	Sander et al. (2011)
G2110	UpStTrG	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$\text{k\_H02\_H02}$	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	UpStTrG	$\text{H}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 2 \text{OH}$	$1.63\text{E}-10*\text{EXP}(60./\text{temp})$	Sander et al. (2011)
G2112	UpStTrG	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	$1.8\text{E}-12$	Sander et al. (2011)
G2117	UpStTrG	$\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow (\text{H}_2\text{O})_2$	$6.521\text{E}-26*\text{temp}*\text{EXP}(1851.09/\text{temp})$ $*\text{EXP}(-5.10485\text{E}-3*\text{temp})$	Scribano et al. (2006)*
G2118	UpStTrG	$(\text{H}_2\text{O})_2 \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	$1.\text{E}0$	see note*
G3101	UpStTrGN	$\text{N}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{N}_2$	$2.15\text{E}-11*\text{EXP}(110./\text{temp})$	Sander et al. (2011)
G3103	UpStTrGN	$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$	$3.\text{E}-12*\text{EXP}(-1500./\text{temp})$	Sander et al. (2011)
G3106	StTrGN	$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$	$1.2\text{E}-13*\text{EXP}(-2450./\text{temp})$	Sander et al. (2011)
G3108	StTrGN	$\text{NO}_3 + \text{NO} \rightarrow 2 \text{NO}_2$	$1.5\text{E}-11*\text{EXP}(170./\text{temp})$	Sander et al. (2011)
G3109	UpStTrGN	$\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	$\text{k\_N03\_N02}$	Sander et al. (2011)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$\text{k\_N03\_N02}/(2.7\text{E}-27*\text{EXP}(11000./\text{temp}))$	Sander et al. (2011)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$\text{k\_3rd}(\text{temp}, \text{cair}, 7.0\text{E}-31, 2.6, 3.6\text{E}-11, 0.1, 0.6)$	Sander et al. (2011)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.3\text{E}-12*\text{EXP}(270./\text{temp})$	Sander et al. (2011)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$\text{k\_3rd}(\text{temp}, \text{cair}, 1.8\text{E}-30, 3.0, 2.8\text{E}-11, 0., 0.6)$	Sander et al. (2011)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	$\text{k\_N02\_H02}$	Sander et al. (2011)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E}-12$	Sander et al. (2011)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E}-11*\text{EXP}(-390./\text{temp})$	Sander et al. (2011)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	$\text{k\_HNO3\_OH}$	Sander et al. (2011)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$\text{k\_N02\_H02}/(2.1\text{E}-27*\text{EXP}(10900./\text{temp}))$	Sander et al. (2011)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E}-12*\text{EXP}(380./\text{temp})$	Sander et al. (2011)

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

#	labels	reaction	rate coefficient	reference
G3209	TrGN	$\text{NH}_3 + \text{OH} \rightarrow \text{NH}_2 + \text{H}_2\text{O}$	$1.7\text{E-}12 \cdot \text{EXP}(-710./\text{temp})$	Kohlmann and Poppe (1999)
G3210	TrGN	$\text{NH}_2 + \text{O}_3 \rightarrow \text{NH}_2\text{O} + \text{O}_2$	$4.3\text{E-}12 \cdot \text{EXP}(-930./\text{temp})$	Kohlmann and Poppe (1999)
G3211	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{NH}_2\text{O} + \text{OH}$	$4.8\text{E-}07 \cdot \text{EXP}(-628./\text{temp})$ $\cdot \text{temp}^{**}(-1.32)$	Kohlmann and Poppe (1999)
G3212	TrGN	$\text{NH}_2 + \text{HO}_2 \rightarrow \text{HNO} + \text{H}_2\text{O}$	$9.4\text{E-}09 \cdot \text{EXP}(-356./\text{temp})$ $\cdot \text{temp}^{**}(-1.12)$	Kohlmann and Poppe (1999)
G3213	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{HO}_2 + \text{OH} + \text{N}_2$	$1.92\text{E-}12 \cdot ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3214	TrGN	$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$	$1.41\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-1.5))$	Kohlmann and Poppe (1999)
G3215	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$	$1.2\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-2.0))$	Kohlmann and Poppe (1999)
G3216	TrGN	$\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH}_2\text{O} + \text{NO}$	$0.8\text{E-}11 \cdot ((\text{temp}/298.)^{**}(-2.0))$	Kohlmann and Poppe (1999)
G3217	TrGN	$\text{NH}_2\text{O} + \text{O}_3 \rightarrow \text{NH}_2 + \text{O}_2$	$1.2\text{E-}14$	Kohlmann and Poppe (1999)
G3218	TrGN	$\text{NH}_2\text{O} \rightarrow \text{NHOH}$	$1.3\text{E}3$	Kohlmann and Poppe (1999)
G3219	TrGN	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	$8.0\text{E-}11 \cdot \text{EXP}(-500./\text{temp})$	Kohlmann and Poppe (1999)
G3220	TrGN	$\text{HNO} + \text{NHOH} \rightarrow \text{NH}_2\text{OH} + \text{NO}$	$1.66\text{E-}12 \cdot \text{EXP}(-1500./\text{temp})$	Kohlmann and Poppe (1999)
G3221	TrGN	$\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$	$1.0\text{E-}12 \cdot \text{EXP}(-1000./\text{temp})$	Kohlmann and Poppe (1999)
G3222	TrGN	$\text{NHOH} + \text{OH} \rightarrow \text{HNO} + \text{H}_2\text{O}$	$1.66\text{E-}12$	Kohlmann and Poppe (1999)
G3223	TrGN	$\text{NH}_2\text{OH} + \text{OH} \rightarrow \text{NHOH} + \text{H}_2\text{O}$	$4.13\text{E-}11 \cdot \text{EXP}(-2138./\text{temp})$	Kohlmann and Poppe (1999)
G3224	TrGN	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	$3.65\text{E-}14 \cdot \text{EXP}(-4600./\text{temp})$	Kohlmann and Poppe (1999)
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	$1.85\text{E-}20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp})$ $-987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow .85 \text{ HCHO} + .85 \text{ HO}_2 + .15 \text{ CH}_3\text{O} + \text{H}_2\text{O}$	$6.38\text{E-}18 \cdot \text{temp}^{**}2 \cdot \text{EXP}(144./\text{temp})$	Atkinson et al. (2006)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$3.8\text{E-}13 \cdot \text{EXP}(780./\text{temp}) / (1.+1./$ $498. \cdot \text{EXP}(1160./\text{temp}))$	Atkinson et al. (2006)
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$3.8\text{E-}13 \cdot \text{EXP}(780./\text{temp}) / (1.+$ $498. \cdot \text{EXP}(-1160./\text{temp}))$	Atkinson et al. (2006)
G4104a	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	$2.3\text{E-}12 \cdot \text{EXP}(360./\text{temp}) \cdot (1.-\text{beta}_$ $\text{CH3NO3})$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)
G4104b	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{ONO}_2$	$2.3\text{E-}12 \cdot \text{EXP}(360./\text{temp}) \cdot \text{beta}_$ $\text{CH3NO3}$	Atkinson et al. (2006), Butkovskaya et al. (2012), Flocke et al. (1998)*
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{O} + \text{NO}_2 + \text{O}_2$	$1.2\text{E-}12$	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + .5 \text{ O}_2$	$7.4\text{E-}13 \cdot \text{EXP}(-520./\text{temp}) \cdot \text{R02} \cdot 2.$	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{HCHO} + .5 \text{CH}_3\text{OH} + .5 \text{O}_2$	$(\text{k\_CH302}-7.4\text{E}-13*\text{EXP}(-520./\text{temp}))$ $*\text{R02}*2.$	Atkinson et al. (2006)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{CH}_3\text{O}_2 + .4 \text{HCHO} + .4 \text{OH} + \text{H}_2\text{O}$	$\text{k\_CH300H\_OH}$	Wallington et al.
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18*\text{EXP}(2.03*\text{LOG}(\text{temp})$ $+636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13*\text{EXP}(-1900./\text{temp})$	Sander et al. (2011)
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E}-13+\text{cair}*3.54\text{E}-33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$2.94\text{E}-14*\text{exp}(786./\text{temp})$ $+9.85\text{E}-13*\text{EXP}(-1036./\text{temp})$	Paulot et al. (2011)
G4114	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O}_2\text{NO}_2$	$\text{k\_NO2\_CH302}$	Sander et al. (2011)
G4115	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$\text{k\_NO2\_CH302}/(9.5\text{E}-29*\text{EXP}(11234./$ $\text{temp}))$	Sander et al. (2011)
G4116	StTrGN	$\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCHO} + \text{NO}_3 + \text{H}_2\text{O}$	$3.00\text{E}-14$	see note*
G4117	StTrGN	$\text{CH}_3\text{ONO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}_2$	$4.0\text{E}-13*\text{EXP}(-845./\text{temp})$	Atkinson et al. (2006)
G4118	StTrG	$\text{CH}_3\text{O} \rightarrow \text{HO}_2 + \text{HCHO}$	$1.3\text{E}-14*\text{exp}(-663./\text{temp})*\text{c}(\text{ind\_02})$	Chai et al. (2014)
G4119a	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{ONO}_2$	$\text{k\_3rd\_iupac}(\text{temp}, \text{cair}, 8.1\text{E}-29,$ $4.5, 2.1\text{E}-11, 0., 0.44)$	Atkinson et al. (2006)
G4119b	StTrGN	$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{HCHO} + \text{HONO}$	$9.6\text{E}-12*\text{EXP}(-1150./\text{temp})$	Atkinson et al. (2006)
G4120a	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_3\text{ONO}$	$\text{k\_3rd\_iupac}(\text{temp}, \text{cair}, 2.6\text{E}-29,$ $2.8, 3.3\text{E}-11, 0.6, \text{REAL}(\text{EXP}(-\text{temp}/$ $900.), \text{SP}))$	Atkinson et al. (2006)
G4120b	StTrGN	$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{HCHO} + \text{HNO}$	$2.3\text{E}-12*(\text{temp}/300.)*0.7$	Atkinson et al. (2006)
G4121	StTrG	$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{O} + 2 \text{O}_2$	$2.9\text{E}-16*\text{exp}(-1000./\text{temp})$	Sander et al. (2011)
G4122	StTrGN	$\text{CH}_3\text{ONO} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCHO} + \text{NO}$	$1.\text{E}-10*\text{exp}(-1764./\text{temp})$	Nielsen et al. (1991)
G4123	StTrG	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$9.7\text{E}-15*\text{EXP}(625./\text{temp})$	Atkinson et al. (2006)
G4124	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.4\text{E}12*\text{EXP}(-7000./\text{temp})$	Atkinson et al. (2006)
G4125	StTrG	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{HOCH}_2\text{OOH} + .5 \text{HCOOH} + .2$ $\text{OH} + .2 \text{HO}_2 + .3 \text{H}_2\text{O} + .8 \text{O}_2$	$5.6\text{E}-15*\text{EXP}(2300./\text{temp})$	Atkinson et al. (2006)
G4126	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$0.7275*2.3\text{E}-12*\text{EXP}(360./\text{temp})$	Atkinson et al. (2006)*
G4127	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$1.2\text{E}-12$	see note*
G4129a	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$	$(\text{k\_CH302}*5.5\text{E}-12)**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4129b	StTrG	$\text{HOCH}_2\text{O}_2 \rightarrow .5 \text{HCOOH} + .5 \text{HOCH}_2\text{OH} + .5 \text{O}_2$	$(\text{k\_CH302}*5.7\text{E}-14*\text{EXP}(750./\text{temp}))$ $**0.5*\text{R02}*2.$	Atkinson et al. (2006)
G4130a	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*\text{k\_CH300H\_OH}$	Taraborrelli (2010)*
G4130b	StTrG	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOOH} + \text{H}_2\text{O} + \text{OH}$	$\text{k\_rohro} + \text{k\_s*f\_sooh}*f\_soh$	Taraborrelli (2010)*

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

#	labels	reaction	rate coefficient	reference
G4132	StTrG	$\text{HOCH}_2\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{HCOOH} + \text{H}_2\text{O}$	$k_{\text{rohro}} + 2 \cdot k_{\text{s}} \cdot f_{\text{soh}} \cdot f_{\text{soh}}$	Taraborrelli (2010)*
G4133	StTrG	$\text{CH}_3\text{O}_2 + \text{OH} \rightarrow \text{CH}_3\text{O} + \text{HO}_2$	1.4E-10	Bossolasco et al. (2014)*
G4134	StTrG	$\text{CH}_2\text{OO} \rightarrow \text{CO} + \text{HO}_2 + \text{OH}$	$1.124\text{E}+14 \cdot \text{EXP}(-10000/\text{temp})$	see note*
G4135	StTrG	$\text{CH}_2\text{OO} + \text{H}_2\text{O} \rightarrow \text{HOCH}_2\text{OOH}$	$k_{\text{CH200\_N02}} \cdot 3.6\text{E}-6$	Ouyang et al. (2013)*
G4136	StTrG	$\text{CH}_2\text{OO} + (\text{H}_2\text{O})_2 \rightarrow \text{HOCH}_2\text{OOH} + \text{H}_2\text{O}$	5.2E-12	Chao et al. (2015), Lewis et al. (2015)*
G4137	StTrGN	$\text{CH}_2\text{OO} + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2$	6.E-14	Welz et al. (2012)*
G4138	StTrGN	$\text{CH}_2\text{OO} + \text{NO}_2 \rightarrow \text{HCHO} + \text{NO}_3$	$k_{\text{CH200\_N02}}$	Welz et al. (2012), Stone et al. (2014)*
G4140	StTrG	$\text{CH}_2\text{OO} + \text{CO} \rightarrow \text{HCHO} + \text{CO}_2$	3.6E-14	Vereecken et al. (2012)
G4141	StTrG	$\text{CH}_2\text{OO} + \text{HCOOH} \rightarrow 2 \text{HCOOH}$	1.E-10	Welz et al. (2014)*
G4142	StTrG	$\text{CH}_2\text{OO} + \text{HCHO} \rightarrow 2 \text{LCARBON}$	1.7E-12	Stone et al. (2014)*
G4143	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{OH} \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4144	StTrG	$\text{CH}_2\text{OO} + \text{CH}_3\text{O}_2 \rightarrow 2 \text{LCARBON}$	5.E-12	Vereecken et al. (2012)*
G4145	StTrG	$\text{CH}_2\text{OO} + \text{HO}_2 \rightarrow \text{LCARBON}$	5.E-12	Vereecken et al. (2012)
G4146	StTrG	$\text{CH}_2\text{OO} + \text{O}_3 \rightarrow \text{HCHO} + 2 \text{O}_2$	1.E-12	Vereecken et al. (2014)
G4147	StTrG	$\text{CH}_2\text{OO} + \text{CH}_2\text{OO} \rightarrow 2 \text{HCHO} + \text{O}_2$	6.E-11	Buras et al. (2014)
G4148	StTrGN	$\text{HOCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2\text{NO}_2$	$k_{\text{N02\_CH302}}$	Sander et al. (2011)
G4149	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 \rightarrow \text{HOCH}_2\text{O}_2 + \text{NO}_2$	$k_{\text{N02\_CH302}} / (9.5\text{E}-29 \cdot \text{EXP}(11234./\text{temp}))$	Sander et al. (2011), Barnes et al. (1985)*
G4150	StTrGN	$\text{HOCH}_2\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp}) \cdot f_{\text{soh}}$	see note*
G4151	StTrG	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2$	$k_{\text{3rd\_iupac}}(\text{temp}, \text{cair}, 7.0\text{E}-31, 3., 1.8\text{E}-12, -1.1, 0.33)$	Atkinson et al. (2006)
G4152	StTrG	$\text{CH}_3 + \text{O}_3 \rightarrow .956 \text{HCHO} + .956 \text{H} + .044 \text{CH}_3\text{O} + \text{O}_2$	$5.1\text{E}-12 \cdot \exp(-210./\text{temp})$	Albaladejo et al. (2002), Ogryzlo et al. (1981)
G4153	StTrG	$\text{CH}_3 + \text{O}(^3\text{P}) \rightarrow .83 \text{HCHO} + .83 \text{H} + .17 \text{CO} + .17 \text{H}_2 + .17 \text{H}$	1.3E-10	Atkinson et al. (2006)
G4154	StTrG	$\text{CH}_3\text{O} + \text{O}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{O}_2$	2.53E-14	Albaladejo et al. (2002)*
G4155	StTrG	$\text{CH}_3\text{O} + \text{O}(^3\text{P}) \rightarrow .75 \text{CH}_3 + .75 \text{O}_2 + .25 \text{HCHO} + .25 \text{OH}$	2.5E-11	Baulch et al. (2005)
G4156	StTrG	$\text{CH}_3\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{CH}_3\text{O} + \text{O}_2$	4.3E-11	Zellner et al. (1988)
G4157	StTrG	$\text{HCHO} + \text{O}(^3\text{P}) \rightarrow .7 \text{OH} + .7 \text{CO} + .3 \text{H} + .3 \text{CO}_2 + \text{HO}_2$	$3.\text{E}-11 \cdot \text{EXP}(-1600./\text{temp})$	Sander et al. (2011)
G4158	TrG	$\text{CH}_2\text{OO}^* \rightarrow .37 \text{CH}_2\text{OO} + .47 \text{CO} + .47 \text{H}_2\text{O} + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH}$	KDEC	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4159	TrGN	$\text{HCN} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CN}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 4.28\text{E-}33, 1.0, \text{REAL}(4.25\text{E-}13 * \text{EXP}(-1150./\text{temp}), \text{SP}), 1.0, 0.8)$	Kleinböhle et al. (2006)
G4160a	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{HCN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.15 * \text{EXP}(200/\text{temp})$	Strekowski et al. (2010)
G4160b	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{H} + \text{NCO}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * 0.68/2.$	Strekowski et al. (2010)*
G4160c	TrGN	$\text{HCN} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{CN}$	$1.08\text{E-}10 * \text{EXP}(105./\text{temp}) * (1. - (0.68/2. + 0.15 * \text{EXP}(200/\text{temp})))$	Strekowski et al. (2010)*
G4161	TrGN	$\text{HCN} + \text{O}(^3\text{P}) \rightarrow \text{H} + \text{NCO}$	$1.0\text{E-}11 * \text{EXP}(-4000./\text{temp})$	Sander et al. (2011)*
G4162	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}(^3\text{P})$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.75$	Baulch et al. (2005)
G4163	TrGN	$\text{CN} + \text{O}_2 \rightarrow \text{CO} + \text{NO}$	$1.2\text{E-}11 * \text{EXP}(210./\text{temp}) * 0.25$	Baulch et al. (2005)
G4164	TrGN	$\text{NCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{NO}$	$7.\text{E-}15$	Becker et al. (2000)*
G42000	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(-499./\text{temp})$	Atkinson et al. (2006)
G42001	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + \text{CH}_2\text{OO}^*$	$9.1\text{E-}15 * \text{EXP}(-2580./\text{temp})$	Atkinson et al. (2006)*
G42002	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2$	$k_{\text{3rd\_iupac}}(\text{temp}, \text{cair}, 8.6\text{E-}29, 3.1, 9.\text{E-}12, 0.85, 0.48)$	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42003	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E-}13 * \text{EXP}(700./\text{temp})$	Sander et al. (2011)
G42004a	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * (1. - \text{beta\_C2H5N03})$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42004b	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{ONO}_2$	$2.55\text{E-}12 * \text{EXP}(380./\text{temp}) * \text{beta\_C2H5N03}$	Atkinson et al. (2006), Butkovskaya et al. (2010)
G42005	TrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E-}12$	Wallington et al.
G42006	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .8 \text{CH}_3\text{CHO} + .6 \text{HO}_2 + .2 \text{C}_2\text{H}_5\text{OH}$	$2. * (7.6\text{E-}14 * k_{\text{CH302}}) * (.5) * \text{R02}$	Taraborrelli (2016), Atkinson et al. (2006)
G42007a	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$0.6 * k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G42007b	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{OH}$	$k_{\text{s*f\_sooh}}$	Taraborrelli (2016)
G42008a	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.95$	Atkinson et al. (2006)
G42008b	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$4.4\text{E-}12 * \text{EXP}(365./\text{temp}) * 0.05$	Atkinson et al. (2006)
G42009	TrGCN	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42010	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{H}_2\text{O}$	$4.0\text{E-}14 * \text{EXP}(850./\text{temp})$	Atkinson et al. (2006)*
G42011a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3 + \text{CO}_2$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.61$	Groß et al. (2014)
G42011b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.23$	Groß et al. (2014)
G42011c	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$5.20\text{E-}13 * \text{EXP}(980./\text{temp}) * 1.507 * 0.16$	Groß et al. (2014)
G42012	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$	$8.1\text{E-}12 * \text{EXP}(270./\text{temp})$	Tyndall et al. (2001a)

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

#	labels	reaction	rate coefficient	reference
G42013	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3C03_NO2	Sander et al. (2011)*
G42014	TrGCN	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G42017a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3 + \text{CO}_2$	k1_R02RC03*0.9	Taraborrelli (2016)
G42017b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{COOH}$	k1_R02RC03*0.1	Taraborrelli (2016)
G42018	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G42020	TrGCN	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	3.00E-14	Rickard and Pascoe (2009)
G42021	TrGCN	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2011)*
G42022a	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,2.,0.6)*.71	Sander et al. (2011), Glowacki et al. (2012)
G42022b	TrGC	$\text{C}_2\text{H}_2 + \text{OH} \rightarrow \text{HCOOH} + \text{CO} + \text{HO}_2$	k_3rd(temp,cair,5.5e-30,0.0, 8.3e-13,2.,0.6)*(1.-.71)	Sander et al. (2011), Glowacki et al. (2012)
G42023a	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCH}_2\text{CO} + \text{H}_2\text{O}$	8.00E-12*0.80	Atkinson et al. (2006)
G42023b	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HOCHCHO} + \text{H}_2\text{O}$	8.00E-12*0.20	Atkinson et al. (2006)
G42024a	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CO}_3$	5.1E-12*(1.-1./(1+1.85E-18*cair))	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42024b	TrGC	$\text{HOCH}_2\text{CO} + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	5.1E-12*1./(1+1.85E-18*cair)	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42025	TrGC	$\text{HOCHCHO} \rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Taraborrelli (2016)
G42026	TrGCN	$\text{HOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO} + \text{HNO}_3$	KN03AL	Rickard and Pascoe (2009)
G42027a	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.9	Taraborrelli (2016)
G42027b	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow \text{HOCH}_2\text{CO}_2\text{H}$	k1_R02RC03*0.1	Taraborrelli (2016)
G42028a	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2$	KAPH02*rco3_oh	Taraborrelli (2016), Groß et al. (2014)
G42028b	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Taraborrelli (2016), Groß et al. (2014)
G42028c	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_2\text{H} + \text{O}_3$	KAPH02*rco3_o3	Taraborrelli (2016), Groß et al. (2014)
G42029	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G42030	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$	k_CH3C03_NO2	Rickard and Pascoe (2009)
G42031	TrGCN	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KR02N03*1.60	Rickard and Pascoe (2009)
G42032	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{ HCHO} + .09 \text{ CO}_2 + .91 \text{ HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O}$	k_co2h+k_sf_soh*f_co2h	Taraborrelli (2016)
G42033a	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	0.6*k_CH300H_OH	Taraborrelli (2016)
G42033b	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2$	k_sf_soh*f_co2h	Taraborrelli (2016)
G42034	TrGCN	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G42035	TrGCN	PHAN + OH $\rightarrow$ HCHO + CO + NO <sub>2</sub> + H <sub>2</sub> O	k_s*f_soh*f_cpan+k_rohro	Taraborrelli (2016)
G42036	TrGC	GLYOX + OH $\rightarrow$ HCOCO + H <sub>2</sub> O	3.1E-12*EXP(340./temp)	Atkinson et al. (2006), Orlando and Tyndall (2001), Lockhart et al. (2013)
G42037	TrGCN	GLYOX + NO <sub>3</sub> $\rightarrow$ HCOCO + HNO <sub>3</sub>	KN03AL	Rickard and Pascoe (2009)
G42038a	TrGC	HCOCO $\rightarrow$ CO + CO + HO <sub>2</sub>	7.E11*EXP(-3160./temp) +5.E-12*c(ind_02)	Orlando and Tyndall (2001), Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037b	TrGC	HCOCO $\rightarrow$ HCOCO <sub>3</sub>	5.E-12*c(ind_02)*3.2*exp(-550./temp)	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42037c	TrGC	HCOCO $\rightarrow$ OH + CO + CO <sub>2</sub>	5.E-12*c(ind_02) *(1.-3.2*exp(-550./temp))	Lockhart et al. (2013), Rickard and Pascoe (2009)
G42039a	TrGC	HCOCO <sub>3</sub> $\rightarrow$ CO + HO <sub>2</sub> + CO <sub>2</sub>	k1_R02RC03*0.9	Taraborrelli (2016)
G42039b	TrGC	HCOCO <sub>3</sub> $\rightarrow$ HCOCO <sub>2</sub> H	k1_R02RC03*0.1	Taraborrelli (2016)
G42040	TrGC	HCOCO <sub>3</sub> + HO <sub>2</sub> $\rightarrow$ HO <sub>2</sub> + CO + CO <sub>2</sub> + OH	KAPH02	Feierabend et al. (2008), Taraborrelli (2016)
G42041	TrGCN	HCOCO <sub>3</sub> + NO $\rightarrow$ HO <sub>2</sub> + CO + NO <sub>2</sub> + CO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G42042	TrGCN	HCOCO <sub>3</sub> + NO <sub>3</sub> $\rightarrow$ HO <sub>2</sub> + CO + NO <sub>2</sub> + CO <sub>2</sub>	KR02N03*1.60	Rickard and Pascoe (2009)
G42043	TrGCN	HCOCO <sub>3</sub> + NO <sub>2</sub> $\rightarrow$ HO <sub>2</sub> + CO + NO <sub>3</sub> + CO <sub>2</sub>	k_CH3C03_N02	Orlando and Tyndall (2001), Taraborrelli (2016)
G42044	TrGC	HCOCO <sub>2</sub> H + OH $\rightarrow$ CO + HO <sub>2</sub> + CO <sub>2</sub> + H <sub>2</sub> O	k_co2h+k_t*f_o*f_co2h	Taraborrelli (2016)
G42045a	TrGC	HCOCO <sub>3</sub> H + OH $\rightarrow$ HCOCO <sub>3</sub> + H <sub>2</sub> O	0.6*k_CH300H_OH	Taraborrelli (2016)
G42045b	TrGC	HCOCO <sub>3</sub> H + OH $\rightarrow$ CO + CO <sub>2</sub> + H <sub>2</sub> O + OH	k_t*f_o*f_co2h	Taraborrelli (2016)
G42046	TrGC	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> $\rightarrow$ .6 HOCH <sub>2</sub> CH <sub>2</sub> O + .2 HOCH <sub>2</sub> CHO + .2 ETHGLY	2.*(7.8E-14*EXP(1000./temp) *k_CH302)**(.5)*R02	Atkinson et al. (2006), Rickard and Pascoe (2009)
G42047	TrGCN	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + NO $\rightarrow$ .25 HO <sub>2</sub> + .5 HCHO + .75 HOCH <sub>2</sub> CH <sub>2</sub> O + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(3,1,0,0,0, temp, cair))	Rickard and Pascoe (2009)*
G42048	TrGCN	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + NO $\rightarrow$ ETHOHNO3	KR02N0*alpha_AN(3,1,0,0,0,temp, cair)	Taraborrelli (2016)
G42049a	TrGC	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ HYETHO2H	1.53E-13*EXP(1300./temp) *(1.-rchohch2o2_oh)	Rickard and Pascoe (2009)
G42049b	TrGC	HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ HOCH <sub>2</sub> CH <sub>2</sub> O + OH	1.53E-13*EXP(1300./temp) *rchohch2o2_oh	Rickard and Pascoe (2009)
G42050	TrGCN	ETHOHNO3 + OH $\rightarrow$ .93 NO <sub>3</sub> CH <sub>2</sub> CHO + .93 HO <sub>2</sub> + .07 HOCH <sub>2</sub> CHO + .07 NO <sub>2</sub> + H <sub>2</sub> O	k_s*(f_soh*f_ch2ono2+f_ono2*f_pch2oh)+k_rohro	Taraborrelli (2016)



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

#	labels	reaction	rate coefficient	reference
G42051a	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)*
G42051b	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f\_sooh*f\_pch2oh}}$	Taraborrelli (2016)
G42051c	TrGC	$\text{HYETHO}_2\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f\_soh*f\_pch2oh}+k_{\text{rohro}}}$	Taraborrelli (2016)
G42052a	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HOCH}_2\text{CHO}$	$6.00\text{E-}14 \cdot \text{EXP}(-550./\text{temp})$ $\cdot C(\text{ind\_02})$	Rickard and Pascoe (2009)
G42052b	TrGC	$\text{HOCH}_2\text{CH}_2\text{O} \rightarrow \text{HO}_2 + \text{HCHO} + \text{HCHO}$	$9.50\text{E}13 \cdot \text{EXP}(-5988./\text{temp})$	Rickard and Pascoe (2009)
G42053	TrGC	$\text{ETHGLY} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$2 \cdot k_{\text{s*f\_soh*f\_pch2oh}} + 2 \cdot k_{\text{rohro}}$	Taraborrelli (2016)
G42054	TrGC	$\text{HCOCH}_2\text{O}_2 \rightarrow .6 \text{ HCHO} + .6 \text{ CO} + .6 \text{ HO}_2 + .2 \text{ GLYOX}$ $+ .2 \text{ HOCH}_2\text{CHO}$	$k1_{\text{R02p0R02}}$	Taraborrelli (2016)
G42055a	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CHO}$	$\text{KR02H02}(2) \cdot r_{\text{coch2o2\_ooh}}$	Taraborrelli (2016)
G42055b	TrGC	$\text{HCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(2) \cdot r_{\text{coch2o2\_oh}}$	Taraborrelli (2016)
G42056a	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO} + \text{HO}_2$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair}))$	Taraborrelli (2016)
G42056b	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(3, 1, 1, 0, 0, \text{temp}, \text{cair})$	Taraborrelli (2016)
G42057	TrGCN	$\text{HCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03}$	Taraborrelli (2016)
G42058a	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G42058b	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{OH}$	$.8 \cdot 8.\text{E-}12$	Taraborrelli (2016)*
G42058c	TrGC	$\text{HOOCH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{OH}$	$k_{\text{s*f\_sooh*f\_cho}}$	Taraborrelli (2016)
G42059	TrGCN	$\text{HOOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL}$	Rickard and Pascoe (2009)
G42060	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	$\text{KAPNO}$	Taraborrelli (2016)
G42061	TrGCN	$\text{HOOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{OH} + \text{HCHO} + \text{CO}_2$	$\text{KR02N03} \cdot 1.60$	Taraborrelli (2016)
G42062a	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow 2 \text{ OH} + \text{HCHO} + \text{CO}_2$	$\text{KAPH02} \cdot r_{\text{co3\_oh}}$	Taraborrelli (2016)
G42062b	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02} \cdot r_{\text{co3\_ooh}}$	Taraborrelli (2016)
G42062c	TrGC	$\text{HOOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot r_{\text{co3\_o3}}$	Taraborrelli (2016)
G42063a	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Taraborrelli (2016)
G42063b	TrGC	$\text{HOOCH}_2\text{CO}_3 \rightarrow \text{HOOCH}_2\text{CO}_2\text{H}$	$k1_{\text{R02RC03}} \cdot 0.1$	Taraborrelli (2016)
G42064a	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{H}_2\text{O}$	$2 \cdot 0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G42064b	TrGC	$\text{HOOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f\_sooh*f\_co2h}}$	Taraborrelli (2016)
G42065	TrGC	$\text{HOOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCO}_2\text{H} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s*f\_sooh*f\_co2h}} + k_{\text{co2h}}$	Taraborrelli (2016)
G42066	TrGC	$\text{CH}_2\text{CO} + \text{OH} \rightarrow .6 \text{ HCHO} + .6 \text{ HO}_2 + .6 \text{ CO} + .4$ $\text{HOOCH}_2\text{CO}_2\text{H}$	$2.8\text{E-}12 \cdot \exp(510./\text{temp})$	Baulch et al. (2005), Taraborrelli (2016)
G42067a	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{COOH} + \text{OH}$	$(k_{\text{t*f\_tooh*f\_toh}} + k_{\text{rohro}})$	Taraborrelli (2016)
G42067b	TrGC	$\text{CH}_3\text{CHOHOOH} + \text{OH} \rightarrow \text{CH}_3\text{CHOHO}_2$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G42068	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$3.46\text{E}12 \cdot \text{EXP}(-12500./(1.98 \cdot \text{temp}))$	Hermans et al. (2005), Taraborrelli (2016)
G42069	TrGC	$\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHOHO}_2$	$3.46\text{E}12 \cdot \text{EXP}(-12500./(1.98 \cdot \text{temp})) / (6.34\text{E}26 \cdot \text{EXP}(-14700./(1.98 \cdot \text{temp})))$	Hermans et al. (2005), Taraborrelli (2016)
G42070	TrGC	$\text{CH}_3\text{CHOHO}_2 + \text{HO}_2 \rightarrow .5 \text{ CH}_3\text{CHOHOOH} + .3 \text{ CH}_3\text{COOH} + .2 \text{ CH}_3 + .2 \text{ HCOOH} + .2 \text{ OH}$	$5.6\text{E}-15 \cdot \text{EXP}(2300./\text{temp})$	Taraborrelli (2016)
G42071	TrGC	$\text{CH}_3\text{CHOHO}_2 \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	k1_R02s0R02	Taraborrelli (2016)
G42072	TrGCN	$\text{CH}_3\text{CHOHO}_2 + \text{NO} \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH} + \text{NO}_2$	KR02N0	Taraborrelli (2016)
G42073	TrGCN	$\text{C}_2\text{H}_5\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{H}_2\text{O} + \text{NO}_2$	$6.7\text{E}-13 \cdot \text{EXP}(-395./\text{temp})$	Atkinson et al. (2006)
G42074a	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{GLYOX} + \text{NO}_2 + \text{H}_2\text{O}$	k_s*f_ch2ono2*f_cho	Paulot et al. (2009a), Taraborrelli (2016)*
G42074b	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} + \text{OH} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{H}_2\text{O}$	k_t*f_o*f_ch2ono2*3.	Paulot et al. (2009a), Taraborrelli (2016)*
G42075	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{OH}$	KAPH02	Rickard and Pascoe (2009)*
G42076	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G42077	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{NO}_3\text{CH}_2\text{CHO}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G42078	TrGCN	$\text{NO}_3\text{CH}_2\text{CO}_3 \rightarrow \text{HCHO} + \text{NO}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G42079	TrGCN	$\text{NO}_3\text{CH}_2\text{CHO} \rightarrow \text{NO}_3\text{CH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G42080	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2\text{NO}_2$	k_3rd_iupac(temp, cair, 1.3E-29, 6.2, 8.8E-12, 0.0, 0.31)	Atkinson et al. (2006)
G42081	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$	k_3rd_iupac(temp, cair, REAL(4.8E-4*EXP(-9285./temp), SP), 0.0, REAL(8.8E15*EXP(-10440./temp), SP), 0.0, 0.31)	Atkinson et al. (2006)
G42082	StTrGCN	$\text{C}_2\text{H}_5\text{O}_2\text{NO}_2 + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp})$	Taraborrelli (2016)*
G42083a	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	$5.1\text{E}-12 \cdot (1. - 1./(1. + 9.4\text{E}-18 \cdot \text{cair}))$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42083b	TrGC	$\text{CH}_3\text{C}(\text{O}) + \text{O}_2 \rightarrow \text{OH} + \text{HCHO} + \text{CO}$	$5.1\text{E}-12 \cdot 1./(1. + 9.4\text{E}-18 \cdot \text{cair})$	Atkinson et al. (2006), Beyersdorf et al. (2010)*
G42084	TrGC	$\text{C}_2\text{H}_5\text{OH} + \text{OH} \rightarrow .95 \text{ C}_2\text{H}_5\text{O}_2 + .95 \text{ HO}_2 + .05 \text{ HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	$3.0\text{E}-12 \cdot \text{EXP}(20./\text{temp})$	Taraborrelli (2016), Atkinson et al. (2006)
G42085a	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{NCCH}_2\text{O}_2 + \text{H}_2\text{O}$	$8.1\text{E}-13 \cdot \text{EXP}(-1080./\text{temp}) \cdot 0.40$	Atkinson et al. (2006), Tyndall et al. (2001b)*

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

#	labels	reaction	rate coefficient	reference
G42085b	TrGCN	$\text{CH}_3\text{CN} + \text{OH} \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{NO}$	$8.1\text{E-}13*\text{EXP}(-1080./\text{temp})*(1.-0.40)$	Atkinson et al. (2006), Tyndall et al. (2001b)*
G42086a	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{CH}_3\text{CN}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})$ $*0.0269*\text{EXP}(137./\text{temp})$	Strekowski et al. (2010)
G42086b	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow 2 \text{H} + \text{CO} + \text{HCN}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})*0.16$	Strekowski et al. (2010)*
G42086c	TrGCN	$\text{CH}_3\text{CN} + \text{O}(^1\text{D}) \rightarrow .5 \text{CH}_3 + .5 \text{NCO} + .5 \text{NCCH}_2\text{O}_2 + .5 \text{OH}$	$2.54\text{E-}10*\text{EXP}(-24./\text{temp})*(1.-(0.16+0.0269*\text{EXP}(137./\text{temp})))$	Strekowski et al. (2010)*
G42087	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N0	see note*
G42088	TrGCN	$\text{NCCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCN} + \text{CO}_2 + \text{HO}_2$	KR02H02(2)	see note*
G42089a	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{HCHO}$	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G42089b	TrGC	$\text{CH}_2\text{CHOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2$	k_CH2CHOH_OH_ALD	Taraborrelli (2016), So et al. (2014)
G42090	TrGC	$\text{CH}_2\text{CHOH} + \text{HCOOH} \rightarrow \text{CH}_3\text{CHO} + \text{HCOOH}$	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G42091	TrGC	$\text{CH}_3\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHOH} + \text{HCOOH}$	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G43000a	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	k_s	Taraborrelli (2016)
G43000b	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	2.*k_p	Taraborrelli (2016)
G43001a	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{CHOHOOH} + .50 \text{OH} + .50 \text{HCOCH}_2\text{O}_2 + .05 \text{CH}_2\text{CO} + .09 \text{CH}_3\text{OH} + .09 \text{CO} + .2 \text{CH}_4 + .2 \text{CO}_2$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.57$	Atkinson et al. (2006)*
G43001b	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{OO}^*$	$5.5\text{E-}15*\text{EXP}(-1880./\text{temp})*.43$	Atkinson et al. (2006)*
G43002	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO}_2$	k_3rd_iupac(temp, cair, 8.6E-27, 3.5, 3.E-11, 1., 0.5)	Atkinson et al. (2006), Rickard and Pascoe (2009)
G43003	TrGCN	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO}_3\text{BO}_2$	$4.6\text{E-}13*\text{EXP}(-1155./\text{temp})$	Wallington et al.
G43004	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{iC}_3\text{H}_7\text{OOH}$	$1.9\text{E-}13*\text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43005a	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*(1.-\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Wallington et al.
G43005b	TrGCN	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{iC}_3\text{H}_7\text{ONO}_2$	$2.7\text{E-}12*\text{EXP}(360./\text{temp})*\alpha_{\text{AN}}(3, 2, 0, 0, 0, \text{temp}, \text{cair})$	Wallington et al.
G43006	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{CH}_3\text{COCH}_3 + .2 \text{IPROPOL} + .6 \text{HO}_2$	$2.*(1.6\text{E-}12*\text{EXP}(-2200./\text{temp})*\text{k\_CH302})*(.5)*\text{R02}$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43007a	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	0.6*k_CH300H_OH	Taraborrelli (2016)
G43007b	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{H}_2\text{O} + \text{OH}$	k_t*f_tooh	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43008	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	$1.9\text{E}-13 \cdot \text{EXP}(1300./\text{temp})$	Atkinson (1997)*
G43009a	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.7\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot (1.-\text{alpha\_AN}(3,1,0,0,0,\text{temp},\text{cair}))$	Wallington et al.
G43009b	TrGCN	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow \text{C}_3\text{H}_7\text{ONO}_2$	$2.7\text{E}-12 \cdot \text{EXP}(360./\text{temp}) \cdot \text{alpha\_AN}(3,1,0,0,0,\text{temp},\text{cair})$	Wallington et al.
G43010	TrGC	$\text{C}_3\text{H}_7\text{O}_2 \rightarrow .8 \text{ CH}_3\text{COCH}_3 + .2 \text{ NPROPOL} + .6 \text{ HO}_2$	$2. \cdot (\text{k\_CH302} \cdot 3.\text{E}-13) \cdot (.5) \cdot \text{R02}$	Rickard and Pascoe (2009), Atkinson et al. (2006)
G43011	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$(8.8\text{E}-12 \cdot \text{EXP}(-1320./\text{temp}) + 1.7\text{E}-14 \cdot \text{EXP}(423./\text{temp}))$	Atkinson et al. (2006)*
G43012a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E}-13 \cdot \text{EXP}(700./\text{temp}) \cdot \text{rcoch2o2\_ooh}$	Tyndall et al. (2001a), Taraborrelli (2016)
G43012b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{C}(\text{O}) + \text{HCHO}$	$8.6\text{E}-13 \cdot \text{EXP}(700./\text{temp}) \cdot \text{rcoch2o2\_oh}$	Tyndall et al. (2001a), Taraborrelli (2016)
G43013a	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12 \cdot \text{EXP}(300./\text{temp}) \cdot (1.-\text{alpha\_AN}(4,1,1,0,0,\text{temp},\text{cair}))$	Sander et al. (2011)
G43013b	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NOA}$	$2.9\text{E}-12 \cdot \text{EXP}(300./\text{temp}) \cdot \text{alpha\_AN}(4,1,1,0,0,\text{temp},\text{cair})$	Sander et al. (2011)
G43014	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .3 \text{ CH}_3\text{C}(\text{O}) + .3 \text{ HCHO} + .5 \text{ MGLYOX} + .2 \text{ CH}_3\text{COCH}_2\text{OH}$	$\text{k1\_R02p0R02}$	Orlando and Tyndall (2012)
G43015a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	see note*
G43015b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O}$	$\text{k\_s} \cdot \text{f\_sooh} \cdot \text{f\_co}$	Taraborrelli (2016)
G43016	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{H}_2\text{O}$	$1.6\text{E}-12 \cdot \text{EXP}(305./\text{temp})$	Atkinson et al. (2006)
G43017	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{ CH}_3 + .6 \text{ CH}_3\text{C}(\text{O}) + 1.4 \text{ CO} + \text{H}_2\text{O}$	$1.9\text{E}-12 \cdot \text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007), Atkinson et al. (2006)
G43020	TrGCN	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E}-13 \cdot \text{EXP}(-230./\text{temp})$	Wallington et al.
G43021	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)
G43022	TrGC	$\text{HYPROPO2} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	$\text{k1\_R02s0R02}$	Rickard and Pascoe (2009)
G43023a	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{HYPROPO2H}$	$\text{KR02H02}(3) \cdot (1.-\text{rchohch2o2\_oh})$	Rickard and Pascoe (2009)
G43023b	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02}(3) \cdot \text{rchohch2o2\_oh}$	Rickard and Pascoe (2009)
G43024a	TrGCN	$\text{HYPROPO2} + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} \cdot (1.-\text{alpha\_AN}(4,1,0,0,0,\text{temp},\text{cair}))$	Rickard and Pascoe (2009)
G43024b	TrGCN	$\text{HYPROPO2} + \text{NO} \rightarrow \text{PROPOLNO3}$	$\text{KR02N0} \cdot \text{alpha\_AN}(4,1,0,0,0,\text{temp},\text{cair})$	Rickard and Pascoe (2009)
G43025	TrGCN	$\text{HYPROPO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)
G43026a	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{HYPROPO2}$	$0.6 \cdot \text{k\_CH300H\_OH}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43026b	TrGC	$\text{HYPROPO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH}$	$(k_{s*f\_soh*f\_pch2oh} + k_{t*f\_tooh*f\_pch2oh})$	Taraborrelli (2016)
G43027	TrGCN	$\text{PRONO3BO2} + \text{HO}_2 \rightarrow \text{PR2O2HNO3}$	$\text{KR02H02(3)}$	Rickard and Pascoe (2009)
G43028	TrGCN	$\text{PRONO3BO2} + \text{NO} \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0}$	Rickard and Pascoe (2009)*
G43029	TrGCN	$\text{PRONO3BO2} + \text{NO}_3 \rightarrow \text{NOA} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)
G43030a	TrGCN	$\text{PR2O2HNO3} + \text{OH} \rightarrow \text{PRONO3BO2}$	$0.6*k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)
G43030b	TrGCN	$\text{PR2O2HNO3} + \text{OH} \rightarrow \text{NOA} + \text{OH}$	$k_{t*f\_tooh*f\_ch2ono2}$	Taraborrelli (2016)
G43031	TrGCN	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{HNO}_3$	$\text{KN03AL*2.4}$	Rickard and Pascoe (2009)
G43032	TrGCN	$\text{NOA} + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_2$	$(k_{s*f\_co*f\_ono2} + k_{p*f\_co})$	Taraborrelli (2016)
G43033	TrGC	$\text{HOCH2COCHO} + \text{OH} \rightarrow .8609 \text{ HOCH2CO} + .8609 \text{ CO} + .1391 \text{ HCOCOCHO} + .1391 \text{ HO}_2$	$(1.9\text{E-}12*\text{EXP}(575./\text{temp}) + k_{s*f\_soh*f\_co})$	Taraborrelli (2016)
G43034	TrGCN	$\text{HOCH2COCHO} + \text{NO}_3 \rightarrow \text{HOCH2CO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL*2.4}$	Taraborrelli (2016)
G43035	TrGC	$\text{CH}_3\text{COCO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{H}_2\text{O} + \text{CO}_2$	$4.9\text{E-}14*\text{EXP}(276./\text{temp})$	Mellouki and Mu (2003), Taraborrelli (2016)
G43036	TrGC	$\text{HCOCOCH}_2\text{O}_2 \rightarrow .6 \text{ HCOCO} + .6 \text{ HCHO} + .2 \text{ HCOCOCHO} + .2 \text{ HOCH2COCHO}$	$k1\_R02p0R02$	Taraborrelli (2016)
G43037	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	$\text{KR02N0}$	Taraborrelli (2016)*
G43038a	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{OOH}$	$\text{KR02H02(3)*rcoch2o2\_ooh}$	Taraborrelli (2016)
G43038b	TrGC	$\text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{KR02H02(3)*rcoch2o2\_oh}$	Taraborrelli (2016)
G43039	TrGCN	$\text{HCOCOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{HCOCO} + \text{HCHO} + \text{NO}_2$	$\text{KR02N03}$	Taraborrelli (2016)
G43040a	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{H}_2\text{O}$	$k_{t*f\_co*f\_o}$	Taraborrelli (2016)*
G43040b	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{H}_2\text{O} + \text{OH}$	$k_{s*f\_sooh*f\_co}$	Taraborrelli (2016)*
G43040c	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{H}_2\text{O}$	$0.6*k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G43041	TrGCN	$\text{HCOCOCH}_2\text{OOH} + \text{NO}_3 \rightarrow \text{HOCH}_2\text{CO}_3 + \text{CO} + \text{HNO}_3$	$\text{KN03AL*2.4}$	Taraborrelli (2016)
G43042	TrGC	$\text{HOCH2COCH2O2} \rightarrow \text{HCHO} + \text{HOCH2CO}$	$k1\_R02p0R02$	Taraborrelli (2016)
G43043a	TrGC	$\text{HOCH2COCH2O2} + \text{HO}_2 \rightarrow \text{HOCH2COCH2OOH}$	$\text{KR02H02(3)*rcoch2o2\_ooh}$	Taraborrelli (2016)
G43043b	TrGC	$\text{HOCH2COCH2O2} + \text{HO}_2 \rightarrow \text{HCHO} + \text{HOCH2CO} + \text{OH}$	$\text{KR02H02(3)*rcoch2o2\_oh}$	Taraborrelli (2016)
G43044	TrGCN	$\text{HOCH2COCH2O2} + \text{NO} \rightarrow \text{HCHO} + \text{HOCH2CO} + \text{NO}_2$	$\text{KR02N0}$	Taraborrelli (2016)*
G43045a	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HOCH2COCHO} + \text{OH}$	$k_{s*f\_sooh*f\_co}$	Taraborrelli (2016)
G43045b	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HOCH2COCH2O2}$	$.6*k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G43045c	TrGC	$\text{HOCH2COCH2OOH} + \text{OH} \rightarrow \text{HCOCOCH}_2\text{OOH} + \text{HO}_2$	$1.60\text{E-}12*\text{EXP}(305./\text{temp})$	Taraborrelli (2016)*
G43046	TrGC	$\text{CH3CHCO} + \text{OH} \rightarrow .72 \text{ CO} + .72 \text{ CH}_3\text{CHO} + .72 \text{ HO}_2 + .21 \text{ CH}_3\text{COCO}_2\text{H} + .07 \text{ CH}_3\text{CHO} + .07 \text{ HO}_2 + .07 \text{ CO}_2$	$7.6\text{E-}11$	Hatakeyama et al. (1985), Taraborrelli (2016)
G43047	TrGCN	$\text{PROPOLNO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	$k_{t*f\_ono2*f\_pch2oh} + k_{s*f\_soh*f\_ch2ono2}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G43048	TrGCN	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OONO}_2$	$2.3\text{E}-12 \cdot \text{EXP}(300./\text{temp})$	Tyndall et al. (2001a)*
G43049	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_2$	$1.9\text{E}16 \cdot \text{EXP}(-10830./\text{temp})$	Sehested et al. (1998)*
G43050	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + \text{OH} \rightarrow \text{MGLYOX} + \text{NO}_3 + \text{H}_2\text{O}$	$9.50\text{E}-13 \cdot \text{EXP}(-650./\text{temp}) \cdot \text{f\_co}$	Taraborrelli (2016)*
G43051a	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	Taraborrelli (2016)
G43051b	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$\text{k\_s*f\_sooh}$	Taraborrelli (2016)
G43051c	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$\text{k\_s*f\_pch2oh}$	Taraborrelli (2016)*
G43052	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$4.9\text{E}-12 \cdot \text{EXP}(405./\text{temp})$	Atkinson et al. (2006)*
G43053	TrGCN	$\text{C}_2\text{H}_5\text{CHO} + \text{NO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{HNO}_3$	$6.3\text{E}-15$	Atkinson et al. (2006)
G43054a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	$\text{k1\_R02RC03} \cdot 0.9$	Taraborrelli (2016)
G43054b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H}$	$\text{k1\_R02RC03} \cdot 0.1$	Taraborrelli (2016)
G43055a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3\_oh}$	Taraborrelli (2016), Groß et al. (2014)
G43055b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{rco3\_ooh}$	Taraborrelli (2016), Groß et al. (2014)
G43055c	TrGC	$\text{C}_2\text{H}_5\text{CO}_3 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{rco3\_o3}$	Taraborrelli (2016), Groß et al. (2014)
G43056	TrGCN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G43057	TrGCN	$\text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2 \rightarrow \text{PPN}$	$\text{k\_CH3C03\_N02}$	Rickard and Pascoe (2009)
G43058	TrGCN	$\text{PPN} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{NO}_2$	$\text{k\_PAN\_M}$	Rickard and Pascoe (2009)
G43059	TrGC	$\text{C}_2\text{H}_5\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$\text{k\_co2h} + \text{k\_p} + \text{k\_s*f\_co2h}$	Taraborrelli (2016)*
G43060a	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CO}_3 + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	Taraborrelli (2016)
G43060b	TrGC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{H}_2\text{O}$	$\text{k\_s*f\_co2h} + \text{k\_p}$	Taraborrelli (2016)*
G43061	TrGCN	$\text{PPN} + \text{OH} \rightarrow \text{CH}_3\text{CHO} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$\text{k\_s*f\_cpan} + \text{k\_p}$	Taraborrelli (2016)*
G43062	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_3 + \text{H}_2\text{O}$	$0.6 \cdot \text{k\_CH300H\_OH}$	Taraborrelli (2016)
G43063a	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3\_oh}$	Taraborrelli (2016)
G43063b	TrGC	$\text{CH}_3\text{COCO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCO}_3\text{H}$	$\text{KAPH02} \cdot (\text{rco3\_ooh} + \text{rco3\_o3})$	Taraborrelli (2016)
G43064	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO} \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_2$	KAPNO	Taraborrelli (2016)
G43065	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2 + \text{NO}_3$	$\text{k\_CH3C03\_N02}$	Taraborrelli (2016)*
G43066	TrGCN	$\text{CH}_3\text{COCO}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2 + \text{NO}_2$	$\text{KR02N03} \cdot 1.74$	Taraborrelli (2016)
G43067	TrGC	$\text{CH}_3\text{COCO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2$	$\text{k1\_R02RC03}$	Taraborrelli (2016)
G43068	TrGC	$\text{HCOCOCHO} + \text{OH} \rightarrow 3 \text{ CO} + \text{HO}_2$	$2 \cdot \text{k\_t*f\_co*f\_o}$	Taraborrelli (2016)
G43069	TrGC	$\text{IPROPOL} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{H}_2\text{O}$	$2.6\text{E}-12 \cdot \text{EXP}(200./\text{temp})$	Atkinson et al. (2006)
G43070a	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{H}_2\text{O}$	$4.6\text{E}-12 \cdot \text{EXP}(70./\text{temp}) \cdot (\text{k\_s*f\_soh} / (\text{k\_p} + \text{k\_s*f\_pch2oh} + \text{k\_s*f\_soh}))$	Atkinson et al. (2006), Taraborrelli (2016)*

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

#	labels	reaction	rate coefficient	reference
G43070b	TrGC	$\text{NPROPOL} + \text{OH} \rightarrow \text{HYPROPO2} + \text{H}_2\text{O}$	$4.6\text{E-}12 \cdot \text{EXP}(70./\text{temp}) \cdot ((k_p + k_{\text{s*f\_pch2oh}})/(k_p + k_{\text{s*f\_pch2oh}} + k_{\text{s*f\_soh}}))$	Atkinson et al. (2006), Taraborrelli (2016)*
G43071a	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{OH} \rightarrow \text{HCOOH} + \text{OH} + \text{CH}_3\text{CHO}$	$k_{\text{CH2CHOH\_OH\_HCOOH}}$	Taraborrelli (2016), So et al. (2014)*
G43072	TrGC	$\text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH} \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCOOH}$	$k_{\text{CH2CHOH\_HCOOH}}$	Taraborrelli (2016), daSilva (2010)*
G43073	TrGC	$\text{C}_2\text{H}_5\text{CHO} + \text{HCOOH} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{HCOOH}$	$k_{\text{ALD\_HCOOH}}$	Taraborrelli (2016), daSilva (2010)*
G43074	TrGC	$\text{HCOCOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HCOCO} + \text{CO} + \text{HO}_2 + \text{OH}$	$k_{\text{s*f\_sooh*f\_co}} + 0.6 \cdot k_{\text{CH3OOH\_OH}}$	Taraborrelli (2016)*
G43202	TrGTerC	$\text{HCOCH}_2\text{CHO} + \text{OH} \rightarrow \text{HCOCH}_2\text{CO}_3$	$4.29\text{E-}11$	Rickard and Pascoe (2009)
G43203	TrGTerCN	$\text{HCOCH}_2\text{CHO} + \text{NO}_3 \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HNO}_3$	$2 \cdot \text{KN03AL} \cdot 2.4$	Rickard and Pascoe (2009)
G43204a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Taraborrelli (2016)
G43204b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H}$	$k1_{\text{R02RC03}} \cdot 0.1$	Taraborrelli (2016)
G43205	TrGTerCN	$\text{HCOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43206	TrGTerCN	$\text{HCOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN2}$	$k_{\text{CH3CO3\_NO2}}$	Rickard and Pascoe (2009)
G43207a	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{rco3\_ooh}$	Rickard and Pascoe (2009)
G43207b	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{rco3\_o3}$	Rickard and Pascoe (2009)
G43207c	TrGTerC	$\text{HCOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3\_oh}$	Rickard and Pascoe (2009)
G43210	TrGTerCN	$\text{C}_3\text{PAN2} \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN\_M}}$	Rickard and Pascoe (2009)
G43211	TrGTerCN	$\text{C}_3\text{PAN2} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	$2.10\text{E-}11$	Rickard and Pascoe (2009)
G43212	TrGTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$2.14\text{E-}11$	Rickard and Pascoe (2009)
G43213a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$k1_{\text{R02RC03}} \cdot 0.9$	Taraborrelli (2016)
G43213b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H}$	$k1_{\text{R02RC03}} \cdot 0.1$	Taraborrelli (2016)
G43214	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G43215a	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3\text{H}$	$\text{KAPH02} \cdot \text{rco3\_ooh}$	Rickard and Pascoe (2009)
G43215b	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3\_oh}$	Rickard and Pascoe (2009)
G43215c	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02} \cdot \text{rco3\_o3}$	Rickard and Pascoe (2009)
G43218	TrGTerCN	$\text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2 \rightarrow \text{C}_3\text{PAN1}$	$k_{\text{CH3CO3\_NO2}}$	Rickard and Pascoe (2009)
G43219	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_2\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2$	$1.39\text{E-}11$	Rickard and Pascoe (2009)
G43220	TrGTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3$	$1.73\text{E-}11$	Rickard and Pascoe (2009)
G43221	TrGTerCN	$\text{C}_3\text{PAN1} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	$k_{\text{PAN\_M}}$	Rickard and Pascoe (2009)
G43222	TrGTerCN	$\text{C}_3\text{PAN1} + \text{OH} \rightarrow \text{HOCH}_2\text{CHO} + \text{CO} + \text{NO}_2$	$4.51\text{E-}12$	Rickard and Pascoe (2009)
G43223	TrGTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$2.49\text{E-}11$	Rickard and Pascoe (2009)*
G43415	TrGAroC	$\text{C3DIALOOH} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{OH}$	$1.44\text{E-}10$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G43418a	TrGAroC	$\text{C3DIALO2} + \text{HO}_2 \rightarrow \text{C3DIALOOH}$	$\text{KR02H02(3)} * (\text{rco3\_ooh} + \text{rco3\_o3})$	Rickard and Pascoe (2009)
G43418b	TrGAroC	$\text{C3DIALO2} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(3)} * \text{rco3\_oh}$	Rickard and Pascoe (2009)
G43419	TrGAroCN	$\text{C3DIALO2} + \text{NO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G43420	TrGAroCN	$\text{C3DIALO2} + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G43421	TrGAroC	$\text{C3DIALO2} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G43422a	TrGAroC	$\text{HCOCOHCO3} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G43422b	TrGAroC	$\text{HCOCOHCO3} + \text{HO}_2 \rightarrow \text{HCOCOHCO3H}$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G43424	TrGAroCN	$\text{HCOCOHCO3} + \text{NO} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G43425	TrGAroCN	$\text{HCOCOHCO3} + \text{NO}_2 \rightarrow \text{HCOCOHHPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G43426	TrGAroCN	$\text{HCOCOHCO3} + \text{NO}_3 \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G43427	TrGAroC	$\text{HCOCOHCO3} \rightarrow \text{GLYOX} + \text{CO}_2 + \text{HO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G43428	TrGAroC	$\text{METACETHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + \text{CO}_2$	9.82E-11	Rickard and Pascoe (2009)
G43442	TrGAroCN	$\text{HCOCOHHPAN} + \text{OH} \rightarrow \text{GLYOX} + \text{CO} + \text{NO}_2$	6.97E-11	Rickard and Pascoe (2009)
G43443	TrGAroCN	$\text{HCOCOHHPAN} \rightarrow \text{HCOCOHCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G43444	TrGAroC	$\text{C32OH13CO} + \text{OH} \rightarrow \text{HCOCOHCO3}$	1.36E-10	Rickard and Pascoe (2009)
G43446	TrGAroC	$\text{HCOCOHCO3H} + \text{OH} \rightarrow \text{HCOCOHCO3}$	7.33E-11	Rickard and Pascoe (2009)
G44000	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$2.03\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(78./\text{temp})$	Atkinson et al. (2006)*
G44001a	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$(\text{k1\_R02pR02} * 0.1273 + \text{k1\_R02sR02} * 0.8727) * 0.1273$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44001b	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 \rightarrow .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$(\text{k1\_R02pR02} * 0.1273 + \text{k1\_R02sR02} * 0.8727) * 0.8727$	Rickard and Pascoe (2009), Taraborrelli (2016)*
G44002	TrGC	$\text{LC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{LC}_4\text{H}_9\text{OOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44003a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{KR02N0} * (1 - (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) * 0.1273$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44003b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	$\text{KR02N0} * (1 - (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))) * 0.8727$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44003c	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{LC}_4\text{H}_9\text{NO3}$	$\text{KR02N0} * (0.1273 * \alpha_{\text{AN}}(4, 1, 0, 0, 0, \text{temp}, \text{cair}) + 0.8727 * \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009)*
G44004a	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	KR02N03*0.1273	Rickard and Pascoe (2009), Taraborrelli (2016)
G44004b	TrGCN	$\text{LC}_4\text{H}_9\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + .636 \text{ MEK} + .636 \text{ HO}_2 + .364 \text{ CH}_3\text{CHO} + .364 \text{ C}_2\text{H}_5\text{O}_2$	KR02N03*0.8727	Rickard and Pascoe (2009), Taraborrelli (2016)



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

#	labels	reaction	rate coefficient	reference
G44005a	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{LC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G44005b	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{C}_3\text{H}_7\text{CHO} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{s}} \cdot f_{\text{tooh}} \cdot f_{\text{alk}} \cdot (k_{\text{p}} / (k_{\text{p}} + k_{\text{s}}))$	Taraborrelli (2016)
G44005c	TrGC	$\text{LC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{MEK} + \text{H}_2\text{O} + \text{OH}$	$k_{\text{t}} \cdot f_{\text{tooh}} \cdot f_{\text{alk}} \cdot (k_{\text{s}} / (k_{\text{p}} + k_{\text{s}}))$	Taraborrelli (2016)
G44006a	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.17\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp})$	Atkinson (2003)
G44006b	TrGC	$\text{iC}_4\text{H}_{10} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$k_{\text{t}} / (3 \cdot k_{\text{p}} + k_{\text{t}})$ $1.17\text{E-}17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(213./\text{temp})$ $\cdot 3 \cdot k_{\text{p}} / (3 \cdot k_{\text{p}} + k_{\text{t}})$	Atkinson (2003)
G44007	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$k1_{\text{R02tR02}}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44008	TrGC	$\text{TC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{TC}_4\text{H}_9\text{OOH}$	$\text{KR02H02}(4)$	Rickard and Pascoe (2009)
G44009a	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{COCH}_3 + \text{CH}_3$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 3, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44009b	TrGCN	$\text{TC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{TC4H9NO3}$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 3, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G44010a	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{TC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G44010b	TrGC	$\text{TC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{OH} + \text{H}_2\text{O}$	$3 \cdot k_{\text{p}} \cdot f_{\text{tch2oh}}$	Taraborrelli (2016)*
G44011	TrGCN	$\text{TC4H9NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$3 \cdot k_{\text{p}} \cdot f_{\text{ch2ono2}}$	Taraborrelli (2016)*
G44012	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 \rightarrow \text{IPRCHO}$	$k1_{\text{R02sR02}}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44013	TrGC	$\text{IC}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{IC}_4\text{H}_9\text{OOH}$	$\text{KR02H02}(4)$	Rickard and Pascoe (2009)
G44014a	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{IPRCHO}$	$\text{KR02N0} \cdot (1 - \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G44014b	TrGCN	$\text{IC}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow \text{IC4H9NO3}$	$\text{KR02N0} \cdot \alpha_{\text{AN}}(4, 2, 0, 0, 0, \text{temp}, \text{cair})$	Rickard and Pascoe (2009)
G44015a	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IC}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G44015b	TrGC	$\text{IC}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow \text{IPRCHO} + \text{OH} + \text{H}_2\text{O}$	$k_{\text{s}} \cdot f_{\text{sooh}} + 2 \cdot k_{\text{s}} + k_{\text{t}} \cdot f_{\text{pch2oh}}$	Taraborrelli (2016)*
G44016	TrGCN	$\text{IC4H9NO3} + \text{OH} \rightarrow \text{IPRCHO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s}} \cdot f_{\text{ono2}} + 2 \cdot k_{\text{p}} + k_{\text{t}} \cdot f_{\text{ch2ono2}}$	Taraborrelli (2016)*
G44017	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .87 \text{ MGLYOX} + .5481 \text{ CO} + .1392 \text{ HO}_2$ $+ .1392 \text{ OH} + .3219 \text{ CH}_2\text{OO} + .13 \text{ HCHO} + .04680 \text{ OH}$ $+ .04680 \text{ CO} + .07280 \text{ CH}_3\text{C(O)} + .026 \text{ CH}_3\text{CHO} + .026$ $\text{CO}_2 + .026 \text{ HCHO} + .026 \text{ HO}_2 + .02402 \text{ MGLYOX} +$ $.02402 \text{ H}_2\text{O}_2 + .00718 \text{ CH}_3\text{COCO}_2\text{H}$	$8.5\text{E-}16 \cdot \text{EXP}(-1520./\text{temp})$	Taraborrelli (2016)
G44018	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{LHMVKABO2}$	$2.6\text{E-}12 \cdot \text{EXP}(610./\text{temp})$	Taraborrelli (2016), Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G44019	TrGC	MEK + OH $\rightarrow$ LMEKO2 + H <sub>2</sub> O	1.5E-12*EXP(-90./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44020	TrGC	LMEKO2 + HO <sub>2</sub> $\rightarrow$ LMEKOOH	KR02H02(4)	Taraborrelli (2016)
G44021a	TrGCN	LMEKO2 + NO $\rightarrow$ .62 CH <sub>3</sub> CHO + .62 CH <sub>3</sub> C(O) + .38 HCHO + .38 CO <sub>2</sub> + .38 HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + NO <sub>2</sub>	KR02N0*(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	KR02N0*(.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 <sub>2</sub> O	0.6*k_CH300H_OH	Taraborrelli (2016)
G44022b	TrGC	LMEKOOH + OH $\rightarrow$ .62 BIACET + .38 HCHO + .38 CO <sub>2</sub> + .38 HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + H <sub>2</sub> O + OH	(.62*k_t*f_tooh*f_co+.38*k_s*f_sooH)	Taraborrelli (2016)
G44023a	TrGCN	LC4H9NO3 + OH $\rightarrow$ MEK + NO <sub>2</sub> + H <sub>2</sub> O	(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 <sub>3</sub> H <sub>7</sub> CHO + NO <sub>2</sub> + H <sub>2</sub> O	(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 <sub>3</sub> COCH <sub>2</sub> OH + CO + NO <sub>2</sub>	3.2E-11	Orlando et al. (2002)
G44025	TrGCN	MPAN $\rightarrow$ MACO3 + NO <sub>2</sub>	k_PAN_M	see note*
G44026	TrGC	LMEKO2 $\rightarrow$ .538 HCHO + .538 CO <sub>2</sub> + .459 HOCH <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> + .079 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + .462 CH <sub>3</sub> C(O) + .462 CH <sub>3</sub> CHO	(.62*k1_R02s0R02+.38*k1_R02p0R02)	Rickard and Pascoe (2009)*
G44027	TrGC	MACR + OH $\rightarrow$ .45 MACO3 + .55 MACRO2	8.E-12*EXP(380./temp)	Orlando et al. (1999b), Taraborrelli (2016)
G44028	TrGC	MACR + O <sub>3</sub> $\rightarrow$ .5481 CO + .1392 HO <sub>2</sub> + .1392 OH + .3219 CH <sub>2</sub> OO + .87 MGLYOX + .13 HCHO + .13 OH + .065 HCOCOCH <sub>2</sub> O <sub>2</sub> + .065 CO + .065 CH <sub>3</sub> C(O)	1.36E-15*EXP(-2112./temp)	Taraborrelli (2016)
G44029	TrGCN	MACR + NO <sub>3</sub> $\rightarrow$ MACO3 + HNO <sub>3</sub>	KN03AL*2.0	Rickard and Pascoe (2009)
G44030a	TrGC	MACO3 $\rightarrow$ CH <sub>3</sub> C(O) + HCHO + CO <sub>2</sub>	k1_R02RC03*0.9	Taraborrelli (2016)
G44030b	TrGC	MACO3 $\rightarrow$ MACO2H	k1_R02RC03*0.1	Taraborrelli (2016)
G44031a	TrGC	MACO3 + HO <sub>2</sub> $\rightarrow$ MACO2 + OH	KAPH02*rc03_oh	Taraborrelli (2016)
G44031b	TrGC	MACO3 + HO <sub>2</sub> $\rightarrow$ MACO3H	KAPH02*rc03_ooh	Taraborrelli (2016)
G44031c	TrGC	MACO3 + HO <sub>2</sub> $\rightarrow$ MACO2H + O <sub>3</sub>	KAPH02*rc03_o3	Taraborrelli (2016)
G44032	TrGCN	MACO3 + NO $\rightarrow$ MACO2 + NO <sub>2</sub>	8.70E-12*EXP(290./temp)	Taraborrelli (2016)
G44033	TrGCN	MACO3 + NO <sub>2</sub> $\rightarrow$ MPAN	k_CH3C03_NO2	Rickard and Pascoe (2009)
G44034	TrGCN	MACO3 + NO <sub>3</sub> $\rightarrow$ MACO2 + NO <sub>2</sub>	KR02N03*1.60	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44035	TrGC	MACRO2 $\rightarrow$ .7 CH <sub>3</sub> COCH <sub>2</sub> OH + .7 HCHO + .7 HO <sub>2</sub> + .3 MACROH	k1_R02t0R02	Rickard and Pascoe (2009)*
G44036a	TrGC	MACRO2 + HO <sub>2</sub> $\rightarrow$ MACRO + OH	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)
G44036b	TrGC	MACRO2 + HO <sub>2</sub> $\rightarrow$ MACROOH	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44037a	TrGCN	MACRO2 + NO $\rightarrow$ MACRO + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(6,3,1,0,0, temp, cair))	Taraborrelli (2016)
G44037b	TrGCN	MACRO2 + NO $\rightarrow$ MACRN	KR02N0*alpha_AN(6,3,1,0,0,temp, cair)	Taraborrelli (2016)
G44038	TrGCN	MACRO2 + NO <sub>3</sub> $\rightarrow$ MACRO + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G44039a	TrGC	MACROOH + OH $\rightarrow$ MACRO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G44039b	TrGC	MACROOH + OH $\rightarrow$ CO + CH <sub>3</sub> COCH <sub>2</sub> OH + OH	k_t*f_o*f_tch2oh*f_alk	Taraborrelli (2016)
G44039c	TrGC	MACROOH + OH $\rightarrow$ CO + MGLYOX + HO <sub>2</sub>	(k_s*f_soh*f_pch2oh + k_rohro)	Taraborrelli (2016)
G44040	TrGC	MACROH + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + CO + HO <sub>2</sub>	k_t*f_o*f_tch2oh*f_alk	Taraborrelli (2016)
G44041	TrGC	MACRO $\rightarrow$ .885 CH <sub>3</sub> COCH <sub>2</sub> OH + .885 CO + .115 MGLYOX + .115 HCHO + HO <sub>2</sub>	KDEC	Taraborrelli (2016)
G44042	TrGC	MACO2H + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + HO <sub>2</sub> + CO <sub>2</sub>	((k_adt+k_adp)*a_co2h+k_co2h)	Taraborrelli (2016)
G44043a	TrGC	MACO3H + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + CO <sub>2</sub> + OH	(k_adt+k_adp)*a_co2h	Taraborrelli (2016)
G44043b	TrGC	MACO3H + OH $\rightarrow$ MACO3	0.6*k_CH300H_OH	Taraborrelli (2016)
G44044	TrGC	LHMKABO2 $\rightarrow$ .024 CO2H3CHO + .072 MGLYOX + .072 HO <sub>2</sub> + .072 HCHO + .5280 CH <sub>3</sub> C(O) + .5280 HOCH <sub>2</sub> CHO + .176 BIACETOH + .2 HO12CO3C4	(.12*k1_R02p0R02+.88*k1_R02s0R02)	Taraborrelli (2016)
G44045a	TrGC	LHMKABO2 + HO <sub>2</sub> $\rightarrow$ OH + HOCH <sub>2</sub> CHO + CH <sub>3</sub> C(O)	KR02H02(4)*.88*rcoch2o2_oh	Taraborrelli (2016)
G44045b	TrGC	LHMKABO2 + HO <sub>2</sub> $\rightarrow$ LHMKABOOH	KR02H02(4)*(.12+.88*rcoch2o2_ooh)	Taraborrelli (2016)
G44046a	TrGCN	LHMKABO2 + NO $\rightarrow$ .12 MGLYOX + .12 HO <sub>2</sub> + .88 HOCH <sub>2</sub> CHO + .88 CH <sub>3</sub> C(O) + .12 HCHO + NO <sub>2</sub>	KR02N0*(1.-(.12*alpha_AN(6,1,0,1,0,temp, cair)+.88*alpha_AN(6,2,1,0,0,temp, cair)))	Taraborrelli (2016)
G44046b	TrGCN	LHMKABO2 + NO $\rightarrow$ MVKNO3	KR02N0*(.12*alpha_AN(6,1,0,1,0,temp, cair)+.88*alpha_AN(6,2,1,0,0,temp, cair))	Taraborrelli (2016)*
G44047	TrGCN	LHMKABO2 + NO <sub>3</sub> $\rightarrow$ .12 MGLYOX + .12 HO <sub>2</sub> + .88 HOCH <sub>2</sub> CHO + .88 CH <sub>3</sub> C(O) + .12 HCHO + .12 HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G44048a	TrGC	LHMKABOOH + OH $\rightarrow$ LHMKABO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G44048b	TrGC	LHMKABOOH + OH $\rightarrow$ .12 CO2H3CHO + .88 BIACETOH + OH	(.12*k_s*f_soh*f_pch2oh+.88*k_t*f_tooh*f_pch2oh*f_co)	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44049a	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	$k_{\text{t*f}_0\text{f}_\text{alk}}$	Taraborrelli (2016)
G44049b	TrGC	$\text{CO}_2\text{H}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{COCOCHO} + \text{HO}_2 + \text{H}_2\text{O}$	$k_{\text{t*f}_\text{co*f}_\text{toh*f}_\text{cho}}$	Taraborrelli (2016)
G44050	TrGCN	$\text{CO}_2\text{H}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3 + \text{HNO}_3$	$\text{KN03AL*4.0}$	Rickard and Pascoe (2009)
G44051	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	$k1_{\text{R02RC03}}$	Taraborrelli (2016)
G44052a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HO}_2 + \text{CO}_2$	$\text{KAPH02*rco3\_oh}$	Taraborrelli (2016)
G44052b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{O}_3$	$\text{KAPH02*rco3\_o3}$	Taraborrelli (2016)
G44052c	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{HO}_2 \rightarrow \text{CO}_2\text{H}_3\text{CO}_3\text{H}$	$\text{KAPH02*rco3\_ooh}$	Taraborrelli (2016)
G44053	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO} \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$\text{KAPNO}$	Taraborrelli (2016)
G44054	TrGCN	$\text{CO}_2\text{H}_3\text{CO}_3 + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{NO}_2 + \text{CO}_2$	$\text{KR02N03*1.60}$	Taraborrelli (2016)
G44055a	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CO}_3$	$0.6*k_{\text{CH300H\_OH}}$	Taraborrelli (2016)
G44055b	TrGC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{OH}$	$(k_{\text{t*f}_\text{co2h*f}_\text{co*f}_\text{toh}})$	Taraborrelli (2016)
G44056	TrGC	$\text{CO}_2\text{H}_3\text{CO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCO}_2\text{H} + \text{HO}_2$	$k_{\text{t*f}_\text{co2h*f}_\text{co*f}_\text{toh}+k_{\text{co2h}}}$	Taraborrelli (2016)
G44057a	TrGC	$\text{HO}_1\text{C}_2\text{O}_3\text{C}_4 + \text{OH} \rightarrow \text{BIACETOH} + \text{HO}_2$	$k_{\text{t*f}_\text{toh*f}_\text{alk*f}_\text{co}}$	Taraborrelli (2016)
G44057b	TrGC	$\text{HO}_1\text{C}_2\text{O}_3\text{C}_4 + \text{OH} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$	$k_{\text{s*f}_\text{soh*f}_\text{alk}}$	Taraborrelli (2016)
G44058	TrGC	$\text{MACO}_2 \rightarrow .65 \text{CH}_3 + .65 \text{CO} + .65 \text{HCHO} + .35 \text{OH} + .35 \text{CH}_3\text{COCH}_2\text{O}_2 + \text{CO}_2$	$\text{KDEC}$	Taraborrelli (2016)
G44059	TrGC	$\text{LHMVKABO}_2 \rightarrow .88 \text{MGLYOX} + .88 \text{HCHO} + .12 \text{HOOCH}_2\text{CHO} + .12 \text{CH}_3\text{C}(\text{O}) + \text{OH}$	$\text{KHSD}$	Taraborrelli (2016)
G44060	TrGC	$\text{MACRO}_2 \rightarrow \text{MGLYOX} + \text{HCHO} + \text{OH}$	$\text{KHSB}$	Taraborrelli (2016)
G44061a	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{MGLYOX} + \text{CO}_2 + \text{HO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{s*f}_\text{sooh*f}_\text{ch2ono2}+k_{\text{rohro}}}$	Taraborrelli (2016)*
G44061b	TrGCN	$\text{MVKNO}_3 + \text{OH} \rightarrow \text{BIACETOH} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t*f}_\text{ono2*f}_\text{co*f}_\text{pch2oh}}$	Taraborrelli (2016)*
G44062a	TrGCN	$\text{MACRN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO}_2 + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{t*f}_0\text{f}_\text{ch2ono2}}$	Taraborrelli (2016)*
G44062b	TrGCN	$\text{MACRN} + \text{OH} \rightarrow \text{MGLYOX} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O}$	$k_{\text{rohro}+k_{\text{s*f}_\text{sooh*f}_\text{ch2ono2}}}$	Taraborrelli (2016)*
G44063	TrGC	$\text{MACRO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{OH} + \text{CO}$	$\text{K14HSAL}$	Taraborrelli (2016)
G44064	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow .9 \text{CH}_3\text{COCHCO} + .1 \text{CH}_3\text{C}(\text{O}) + .01 \text{GLYOX} + .18 \text{CO} + .09 \text{HO}_2 + \text{OH}$	$\text{K15HS24VYNAL}$	Taraborrelli (2016)
G44065	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOHCHCHO}$	$\text{KR02H02(4)}$	Taraborrelli (2016)
G44066	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	$\text{KR02N0}$	Taraborrelli (2016)*
G44067	TrGCN	$\text{EZCH}_3\text{CO}_2\text{CHCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_2$	$\text{kR02N03}$	Taraborrelli (2016)
G44068	TrGC	$\text{EZCH}_3\text{CO}_2\text{CHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO}$	$k1_{\text{R02sOR02}}$	Taraborrelli (2016)
G44069	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCCH}_3\text{CO} + \text{OH}$	$\text{K15HS24VYNAL}$	Taraborrelli (2016)
G44070	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	$\text{KR02N0}$	Taraborrelli (2016)*
G44071	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{HO}_2 \rightarrow \text{HCOCCH}_3\text{CHOOH}$	$\text{KR02H02(4)}$	Taraborrelli (2016)
G44072	TrGCN	$\text{EZCHOCCH}_3\text{CHO}_2 + \text{NO}_3 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_2$	$\text{KR02N03}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44073	TrGC	$\text{EZCHOCCH}_3\text{CHO}_2 \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO}$	k1_R02p0R02	Taraborrelli (2016)
G44074	TrGC	$\text{CH}_3\text{COOHCHCHO} \rightarrow \text{CH}_3\text{COCHO}_2\text{CHO} + \text{OH}$	KHYDEC	Taraborrelli (2016)
G44075	TrGC	$\text{HCOCCH}_3\text{CHOOH} \rightarrow \text{HCOCO}_2\text{CH}_3\text{CHO} + \text{OH}$	KHYDEC	Taraborrelli (2016)
G44076	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G44077	TrGCN	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G44078	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX} + \text{OH}$	KR02H02(4)	Taraborrelli (2016)*
G44079	TrGC	$\text{CH}_3\text{COCHO}_2\text{CHO} \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{GLYOX}$	k1_R02s0R02	Taraborrelli (2016)
G44080	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2$	k1_R02t0R02	Taraborrelli (2016)
G44081	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO} \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G44082	TrGC	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	KR02H02(4)	Taraborrelli (2016)*
G44083	TrGCN	$\text{HCOCO}_2\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Taraborrelli (2016)
G44084	TrGC	$\text{HCOCCH}_3\text{CO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	1E-10*a_cho	Hatakeyama et al. (1985), Taraborrelli (2016)
G44085	TrGC	$\text{CH}_3\text{COCHCO} + \text{OH} \rightarrow \text{CO} + \text{MGLYOX} + \text{HO}_2$	7.6E-11*a_coch3	Hatakeyama et al. (1985), Taraborrelli (2016)*
G44086	TrGCN	$\text{LMEKNO}_3 + \text{OH} \rightarrow .62 \text{ MGLYOX} + .62 \text{ HCHO} + .62 \text{ HO}_2 + .62 \text{ NO}_2 + .38 \text{ CH}_3\text{C}(\text{O}) + .38 \text{ NO}_3\text{CH}_2\text{CHO}$	.62*(k_p*(f_co+f_ch2ono2)) +.38*(k_s*f_ch2ono2*f_co)	Taraborrelli (2016)*
G44087	TrGC	$\text{MEPROPENE} + \text{OH} \rightarrow \text{IBUTOLBO}_2$	9.4E-12*EXP(505./temp)	Atkinson et al. (2006)
G44088a	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_2\text{OO}^*$	2.7E-15*EXP(-1630./temp)*0.33	Atkinson et al. (2006), Taraborrelli (2016)
G44088b	TrGC	$\text{MEPROPENE} + \text{O}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{OH} + \text{HCHO}$	2.7E-15*EXP(-1630./temp)*0.67	Atkinson et al. (2006), Taraborrelli (2016)
G44089	TrGCN	$\text{MEPROPENE} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{NO}_2$	3.4E-13	Atkinson et al. (2006), Taraborrelli (2016)*
G44090	TrGC	$\text{IBUTOLBO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2$	k1_R02t0R02	Taraborrelli (2016)
G44091a	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{IBUTOLBOOH}$	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44091b	TrGC	$\text{IBUTOLBO}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)
G44092a	TrGCN	$\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-alpha_AN(5,3,0,0,0,temp,cair))	Taraborrelli (2016)
G44092b	TrGCN	$\text{IBUTOLBO}_2 + \text{NO} \rightarrow \text{IBUTOLBNO}_3$	KR02N0*alpha_AN(5,3,0,0,0,temp,cair)	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44093	TrGCN	IBUTOLBO2 + NO <sub>3</sub> → CH <sub>3</sub> COCH <sub>3</sub> + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G44094a	TrGC	IBUTOLBOOH + OH → IBUTOLBO2	.6*k_CH300H_OH	Taraborrelli (2016)
G44094b	TrGC	IBUTOLBOOH + OH → CH <sub>3</sub> COCH <sub>3</sub> + HCHO + HO <sub>2</sub>	k_s*f_sooh*f_pch2oh	Taraborrelli (2016)
G44095	TrGCN	IBUTOLBNO3 + OH → CH <sub>3</sub> COCH <sub>3</sub> + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	3.*k_p	Taraborrelli (2016)
G44096	TrGC	BUT1ENE + OH → LBUT1ENO2	6.6E-12*EXP(465./temp)	Atkinson et al. (2006)*
G44097a	TrGC	BUT1ENE + O <sub>3</sub> → HCHO + .5 C <sub>2</sub> H <sub>5</sub> CHO + .5 H <sub>2</sub> O <sub>2</sub> + .5 CH <sub>3</sub> CHO + .5 CO + .5 HO <sub>2</sub>	3.35E-15*EXP(-1745./temp)*.57	Atkinson et al. (2006), Taraborrelli (2016)*
G44097b	TrGC	BUT1ENE + O <sub>3</sub> → C <sub>2</sub> H <sub>5</sub> CHO + CH <sub>2</sub> OO*	3.35E-15*EXP(-1745./temp)*.43	Atkinson et al. (2006), Taraborrelli (2016)*
G44098	TrGCN	BUT1ENE + NO <sub>3</sub> → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + NO <sub>2</sub>	3.2E-13*EXP(-950./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44099	TrGC	LBUT1ENO2 → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + HO <sub>2</sub>	k1_R02s0R02	Taraborrelli (2016)
G44100a	TrGC	LBUT1ENO2 + HO <sub>2</sub> → LBUT1ENOOH	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44100b	TrGC	LBUT1ENO2 + HO <sub>2</sub> → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + HO <sub>2</sub> + OH	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)
G44101a	TrGCN	LBUT1ENO2 + NO → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(5,2,0,0,0,temp,cair))	Taraborrelli (2016)
G44101b	TrGCN	LBUT1ENO2 + NO → LBUT1ENNO3	KR02N0*alpha_AN(5,2,0,0,0,temp,cair)	Taraborrelli (2016)
G44102	TrGCN	LBUT1ENO2 + NO <sub>3</sub> → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G44103a	TrGC	LBUT1ENOOH + OH → LBUT1ENO2	.6*k_CH300H_OH	Taraborrelli (2016)
G44103b	TrGC	LBUT1ENOOH + OH → C <sub>2</sub> H <sub>5</sub> CO <sub>3</sub> + HCHO + HO <sub>2</sub>	k_t*f_tooh*f_pch2oh	Taraborrelli (2016)*
G44104	TrGCN	LBUT1ENNO3 + OH → C <sub>2</sub> H <sub>5</sub> CHO + CO + HO <sub>2</sub> + NO <sub>2</sub>	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 <sub>3</sub> → CH <sub>3</sub> CHO + .16 CH <sub>3</sub> CHOHOH + .50 OH + .50 HCOCH <sub>2</sub> O <sub>2</sub> + .05 CH <sub>2</sub> CO + .09 CH <sub>3</sub> OH + .09 CO + .2 CH <sub>4</sub> + .2 CO <sub>2</sub>	3.2E-15*EXP(-965./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44107	TrGCN	CBUT2ENE + NO <sub>3</sub> → 2 CH <sub>3</sub> CHO + NO <sub>2</sub>	3.5E-13	Atkinson et al. (2006), Taraborrelli (2016)*
G44108	TrGC	TBUT2ENE + OH → BUT2OLO2	1.0E-11*EXP(553./temp)	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G44109	TrGC	TBUT2ENE + O <sub>3</sub> → CH <sub>3</sub> CHO + .16 CH <sub>3</sub> CHOHOOH + .50 OH + .50 HCOCH <sub>2</sub> O <sub>2</sub> + .05 CH <sub>2</sub> CO + .09 CH <sub>3</sub> OH + .09 CO + .2 CH <sub>4</sub> + .2 CO <sub>2</sub>	6.6E-15*EXP(-1060./temp)	Atkinson et al. (2006), Taraborrelli (2016)
G44110	TrGCN	TBUT2ENE + NO <sub>3</sub> → 2 CH <sub>3</sub> CHO + NO <sub>2</sub>	1.78E-12*EXP(-530./temp) +1.28E-14*EXP(570./temp)	Atkinson et al. (2006), Taraborrelli (2016)*
G44111	TrGC	BUT2OLO2 → C <sub>2</sub> H <sub>5</sub> CHO + HCHO + HO <sub>2</sub>	k1_R02s0R02	Taraborrelli (2016)
G44112a	TrGC	BUT2OLO2 + HO <sub>2</sub> → BUT2OLOOH	KR02H02(4)*rcoch2o2_ooh	Taraborrelli (2016)
G44112b	TrGC	BUT2OLO2 + HO <sub>2</sub> → 2 CH <sub>3</sub> CHO + HO <sub>2</sub> + OH	KR02H02(4)*rcoch2o2_oh	Taraborrelli (2016)
G44113a	TrGCN	BUT2OLO2 + NO → 2 CH <sub>3</sub> CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(5,2,0,0,0, temp,cair))	Taraborrelli (2016)
G44113b	TrGCN	BUT2OLO2 + NO → BUT2OLNO3	KR02N0*alpha_AN(5,2,0,0,0,temp, cair)	Taraborrelli (2016)
G44114	TrGCN	BUT2OLO2 + NO <sub>3</sub> → 2 CH <sub>3</sub> CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G44115a	TrGC	BUT2OLOOH + OH → BUT2OLO2	.6*k_CH300H_OH	Taraborrelli (2016)
G44115b	TrGC	BUT2OLOOH + OH → LMEKOOH + HO <sub>2</sub>	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 <sub>2</sub>	k_t*f_toh*f_ch2ono2	Taraborrelli (2016)
G44117	TrGC	BUT2OLO + OH → BIACET + HO <sub>2</sub>	k_t*f_toh*f_co	Taraborrelli (2016)
G44118	TrGC	IPRCHO + OH → IPRCO3 + H <sub>2</sub> O	6.8E-12*EXP(410./temp)	Atkinson et al. (2006)
G44119	TrGCN	IPRCHO + NO <sub>3</sub> → IPRCO3 + HNO <sub>3</sub>	1.67E-12*EXP(-1460./temp)	Atkinson et al. (2006)
G44120	TrGC	IPRCO3 → iC <sub>3</sub> H <sub>7</sub> O <sub>2</sub> + CO <sub>2</sub>	k1_R02RCO3	Rickard and Pascoe (2009)
G44121a	TrGC	IPRCO3 + HO <sub>2</sub> → PERIBUACID	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44121b	TrGC	IPRCO3 + HO <sub>2</sub> → iC <sub>3</sub> H <sub>7</sub> O <sub>2</sub> + CO <sub>2</sub> + OH	KAPH02*(1-rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44122	TrGCN	IPRCO3 + NO <sub>2</sub> → PIPN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44123	TrGCN	IPRCO3 + NO → iC <sub>3</sub> H <sub>7</sub> O <sub>2</sub> + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G44124a	TrGC	PERIBUACID + OH → IPRCO3 + H <sub>2</sub> O	.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44124b	TrGC	PERIBUACID + OH → CH <sub>3</sub> COCH <sub>3</sub> + H <sub>2</sub> O + CO <sub>2</sub>	k_s*f_co2h	Taraborrelli (2016)*
G44125	TrGCN	PIPN → IPRCO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G44126	TrGCN	PIPN + OH → CH <sub>3</sub> COCH <sub>3</sub> + CO <sub>2</sub> + NO <sub>2</sub>	k_s*f_cpan	Taraborrelli (2016)*
G44127	TrGC	MPROPENOL + OH → HCOOH + OH + CH <sub>3</sub> COCH <sub>3</sub>	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44128	TrGC	MPROPENOL + HCOOH → IPRCHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*

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

#	labels	reaction	rate coefficient	reference
G44129	TrGC	IPRCHO + HCOOH $\rightarrow$ MPROPENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44130	TrGC	BUTENOL + OH $\rightarrow$ HCOOH + OH + C <sub>2</sub> H <sub>5</sub> CHO	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G44131	TrGC	BUTENOL + HCOOH $\rightarrow$ C <sub>3</sub> H <sub>7</sub> CHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44132	TrGC	C <sub>3</sub> H <sub>7</sub> CHO + HCOOH $\rightarrow$ BUTENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44133	TrGC	HVMK + OH $\rightarrow$ HCOOH + OH + MGLYOX	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44134	TrGC	HVMK + HCOOH $\rightarrow$ CO <sub>2</sub> C <sub>3</sub> CHO + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44135	TrGC	CO <sub>2</sub> C <sub>3</sub> CHO + HCOOH $\rightarrow$ HVMK + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44136	TrGC	HMAC + OH $\rightarrow$ HCOOH + OH + MGLYOX	8.8E-11	Taraborrelli (2016), So et al. (2014), Messaadia et al. (2015)*
G44137	TrGC	HMAC + HCOOH $\rightarrow$ IBUTDIAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44138	TrGC	IBUTDIAL + HCOOH $\rightarrow$ HMAC + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G44139	TrGC	CO <sub>2</sub> C <sub>3</sub> CHO + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + H <sub>2</sub> O	k_t*f_o*f_alk+k_s*f_cho*f_co	Taraborrelli (2016)*
G44140	TrGCN	CO <sub>2</sub> C <sub>3</sub> CHO + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + HNO <sub>3</sub>	KN03AL*4.0	Taraborrelli (2016)*
G44141	TrGC	IBUTDIAL + OH $\rightarrow$ CH <sub>3</sub> CHO + CO + HO <sub>2</sub> + CO <sub>2</sub> + H <sub>2</sub> O	2.*k_t*f_o*f_alk+k_t*f_cho*f_cho	Taraborrelli (2016)*
G44142	TrGCN	IBUTDIAL + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> CHO + CO + HO <sub>2</sub> + CO <sub>2</sub> + HNO <sub>3</sub>	2.*KN03AL*4.0	Taraborrelli (2016)*
G44200	TrGTerC	CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> $\rightarrow$ CH <sub>3</sub> C(O) + HCHO + CO	k1_R02p0R02	Rickard and Pascoe (2009)
G44201	TrGTerC	CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ CH <sub>3</sub> COCOCH <sub>2</sub> OOH	KR02H02(4)	Rickard and Pascoe (2009)
G44202	TrGTerCN	CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + NO $\rightarrow$ CH <sub>3</sub> C(O) + HCHO + CO + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44203a	TrGTerC	CH <sub>3</sub> COCOCH <sub>2</sub> OOH + OH $\rightarrow$ CH <sub>3</sub> COCOCHO + OH	k_s*f_co*f_sooh	Rickard and Pascoe (2009)*
G44203b	TrGTerC	CH <sub>3</sub> COCOCH <sub>2</sub> OOH + OH $\rightarrow$ CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub>	.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44204	TrGTerC	C44O <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ C44OOH	KR02H02(4)	Rickard and Pascoe (2009)
G44205	TrGTerCN	C44O <sub>2</sub> + NO $\rightarrow$ HCOCH <sub>2</sub> CHO + CO <sub>2</sub> + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44206	TrGTerC	C44O <sub>2</sub> $\rightarrow$ HCOCH <sub>2</sub> CHO + CO <sub>2</sub> + HO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)



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

#	labels	reaction	rate coefficient	reference
G44207	TrGTerC	$\text{C44OOH} + \text{OH} \rightarrow \text{C44O2}$	7.46E-11	Rickard and Pascoe (2009)
G44208	TrGTerC	$\text{CHOC3COO2} \rightarrow \text{HCOCH2CO3} + \text{HCHO}$	k1_R02p0R02	Rickard and Pascoe (2009)
G44209	TrGTerC	$\text{CHOC3COO2} + \text{HO}_2 \rightarrow \text{C413COOOH}$	KR02H02(4)	Rickard and Pascoe (2009)
G44210	TrGTerCN	$\text{CHOC3COO2} + \text{NO} \rightarrow \text{HCOCH2CO3} + \text{HCHO} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G44211	TrGTerC	$\text{C413COOOH} + \text{OH} \rightarrow \text{CHOC3COO2}$	8.33E-11	Rickard and Pascoe (2009)
G44212	TrGTerC	$\text{C4CODIAL} + \text{OH} \rightarrow \text{C312COCO3}$	3.39E-11	Rickard and Pascoe (2009)
G44213	TrGTerCN	$\text{C4CODIAL} + \text{NO}_3 \rightarrow \text{C312COCO3} + \text{HNO}_3$	2.*KN03AL*4.0	Rickard and Pascoe (2009)
G44214	TrGTerC	$\text{C312COCO3} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G44215a	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{C312COCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44215b	TrGTerC	$\text{C312COCO3} + \text{HO}_2 \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	KAPH02*(1-rco3_ooh)	Rickard and Pascoe (2009)
G44216	TrGTerCN	$\text{C312COCO3} + \text{NO}_2 \rightarrow \text{C312COPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G44217	TrGTerCN	$\text{C312COCO3} + \text{NO} \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G44218	TrGTerC	$\text{C312COCO3H} + \text{OH} \rightarrow \text{C312COCO3}$	1.63E-11	Rickard and Pascoe (2009)
G44219	TrGTerCN	$\text{C312COPAN} \rightarrow \text{C312COCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G44220	TrGTerCN	$\text{C312COPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO} + \text{NO}_2$	1.27E-11	Rickard and Pascoe (2009)
G44221	TrGTerC	$\text{CH}_3\text{COCOCHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)} + 2 \text{CO}$	8.4E-13*EXP(830./temp)	Taraborrelli (2016)*
G44222	TrGTerCN	$\text{CH}_3\text{COCOCHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)} + 2 \text{CO} + \text{HNO}_3$	KN03AL*4.0	Rickard and Pascoe (2009)
G44223	TrGTerC	$\text{IBUTALOH} + \text{OH} \rightarrow \text{IPRHOCO3}$	1.4E-11	Rickard and Pascoe (2009)
G44224a	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44224b	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2016)
G44224c	TrGTerC	$\text{IPRHOCO3} + \text{HO}_2 \rightarrow \text{IPRHOCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44225	TrGTerCN	$\text{IPRHOCO3} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)
G44226	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_2 \rightarrow \text{C4PAN5}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G44227	TrGTerCN	$\text{IPRHOCO3} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G44228a	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2$	k1_R02RC03*0.7	Rickard and Pascoe (2009)
G44228b	TrGTerC	$\text{IPRHOCO3} \rightarrow \text{IPRHOCO2H}$	k1_R02RC03*0.3	Rickard and Pascoe (2009)
G44229	TrGTerC	$\text{IPRHOCO2H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	1.72E-12	Rickard and Pascoe (2009)
G44230	TrGTerC	$\text{OH} + \text{IPRHOCO3H} \rightarrow \text{IPRHOCO3}$	4.80E-12	Rickard and Pascoe (2009)
G44231	TrGTerCN	$\text{C4PAN5} \rightarrow \text{IPRHOCO3} + \text{NO}_2$	K_PAN_M	Rickard and Pascoe (2009)
G44232	TrGTerCN	$\text{C4PAN5} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO} + \text{NO}_2$	4.75E-13	Rickard and Pascoe (2009)
G44233a	TrGTerC	$\text{MBOOO} \rightarrow \text{IPRHOCO2H}$	1.60E-17*C(ind_H20)*(0.08+0.15)	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G44233b	TrGTerC	MBOOO $\rightarrow$ IBUTALOH + H <sub>2</sub> O <sub>2</sub>	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2016)
G44234	TrGTerC	MBOOO + CO $\rightarrow$ IBUTALOH + CO <sub>2</sub>	1.20E-15	Rickard and Pascoe (2009)
G44235	TrGTerCN	MBOOO + NO $\rightarrow$ IBUTALOH + NO <sub>2</sub>	1.00E-14	Rickard and Pascoe (2009)
G44236	TrGTerCN	MBOOO + NO <sub>2</sub> $\rightarrow$ IBUTALOH + NO <sub>3</sub>	1.00E-15	Rickard and Pascoe (2009)
G44400	TrGAroC	MALANHY + OH $\rightarrow$ MALANHYO2	1.4E-12	Rickard and Pascoe (2009)
G44401a	TrGAroC	MALDIALOOH + OH $\rightarrow$ HOCOC4DIAL + OH	1.22E-10	Rickard and Pascoe (2009)
G44401b	TrGAroC	MALDIALOOH + OH $\rightarrow$ MALDIALO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G44402	TrGAroCN	NC4DCO2H + OH $\rightarrow$ MALANHY + NO <sub>2</sub>	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G44403	TrGAroC	CO14O3CO2H + OH $\rightarrow$ HCOCH <sub>2</sub> O <sub>2</sub> + 2 CO <sub>2</sub>	2.19E-11	Rickard and Pascoe (2009)
G44404	TrGAroC	BZFUOOH + OH $\rightarrow$ BZFUO2	3.68E-11	Rickard and Pascoe (2009)
G44405	TrGAroC	HOCOC4DIAL + OH $\rightarrow$ CO2C4DIAL + HO <sub>2</sub>	3.67E-11	Rickard and Pascoe (2009)
G44406a	TrGAroC	MALDIALCO3 + HO <sub>2</sub> $\rightarrow$ MALDALCO2H + O <sub>3</sub>	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44406b	TrGAroC	MALDIALCO3 + HO <sub>2</sub> $\rightarrow$ MALDALCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44406c	TrGAroC	MALDIALCO3 + HO <sub>2</sub> $\rightarrow$ .6 MALANHY + HO <sub>2</sub> + .4 GLYOX + .4 CO + .4 CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)*
G44407	TrGAroCN	MALDIALCO3 + NO $\rightarrow$ .6 MALANHY + HO <sub>2</sub> + .4 GLYOX + .4 CO + .4 CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)*
G44408	TrGAroCN	MALDIALCO3 + NO <sub>2</sub> $\rightarrow$ MALDIALPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G44409	TrGAroCN	MALDIALCO3 + NO <sub>3</sub> $\rightarrow$ .6 MALANHY + HO <sub>2</sub> + .4 GLYOX + .4 CO + .4 CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)*
G44410	TrGAroC	MALDIALCO3 $\rightarrow$ .6 MALANHY + HO <sub>2</sub> + .4 GLYOX + .4 CO + .4 CO <sub>2</sub>	k1_R02RC03	Rickard and Pascoe (2009)*
G44411	TrGAroCN	BZFUONE + NO <sub>3</sub> $\rightarrow$ NBZFUO2	3.00E-13	Rickard and Pascoe (2009)
G44412	TrGAroC	BZFUONE + O <sub>3</sub> $\rightarrow$ .3125 CO14O3CO2H + .1875 CO14O3CHO + .1875 H <sub>2</sub> O <sub>2</sub> + .5 CO + .5 CO <sub>2</sub> + .5 HCOCH <sub>2</sub> O <sub>2</sub> + .5 OH	2.20E-19	see note*
G44413	TrGAroC	BZFUONE + OH $\rightarrow$ BZFUO2	4.45E-11	Rickard and Pascoe (2009)
G44414	TrGAroCN	NBZFUOOH + OH $\rightarrow$ NBZFUO2	6.18E-12	Rickard and Pascoe (2009)
G44415	TrGAroC	MALDALCO3H + OH $\rightarrow$ MALDIALCO3	4.00E-11	Rickard and Pascoe (2009)
G44416	TrGAroC	EPXDLCO2H + OH $\rightarrow$ C3DIALO2 + CO <sub>2</sub>	2.31E-11	Rickard and Pascoe (2009)
G44417a	TrGAroC	EPXDLCO3 + HO <sub>2</sub> $\rightarrow$ C3DIALO2 + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G44417b	TrGAroC	EPXDLCO3 + HO <sub>2</sub> $\rightarrow$ EPXDLCO2H + O <sub>3</sub>	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G44417c	TrGAroC	EPXDLCO3 + HO <sub>2</sub> $\rightarrow$ EPXDLCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G44418	TrGAroCN	EPXDLCO3 + NO $\rightarrow$ C3DIALO2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44419	TrGAroCN	EPXDLCO3 + NO <sub>2</sub> → EPXDLPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G44420	TrGAroCN	EPXDLCO3 + NO <sub>3</sub> → C3DIALO2 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G44421	TrGAroC	EPXDLCO3 → C3DIALO2 + CO <sub>2</sub>	k1_R02RCO3	Rickard and Pascoe (2009)*
G44422	TrGAroC	MALNHYOHCO + OH → CO + CO + CO + CO <sub>2</sub> + HO <sub>2</sub>	5.68E-12	Rickard and Pascoe (2009)
G44423	TrGAroCN	MALDIAL + NO <sub>3</sub> → MALDIALCO3 + HNO <sub>3</sub>	2*KN03AL*2.0	Rickard and Pascoe (2009)
G44424	TrGAroC	MALDIAL + O <sub>3</sub> → 1.0675 GLYOX + .125 HCHO + .1125 HCOCO <sub>2</sub> H + .0675 H <sub>2</sub> O <sub>2</sub> + .82 HO <sub>2</sub> + .57 OH + 1.265 CO + .25 CO <sub>2</sub>	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 <sub>2</sub>	3.70E-11	Rickard and Pascoe (2009)
G44428	TrGAroCN	MALDIALPAN → MALDIALCO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G44429a	TrGAroC	MALANHYO2 + HO <sub>2</sub> → MALANHYOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44429b	TrGAroC	MALANHYO2 + HO <sub>2</sub> → HCOCO <sub>2</sub> HCO3 + CO <sub>2</sub> + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44430	TrGAroCN	MALANHYO2 + NO → HCOCO <sub>2</sub> HCO3 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44431	TrGAroCN	MALANHYO2 + NO <sub>3</sub> → HCOCO <sub>2</sub> HCO3 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G44432	TrGAroC	MALANHYO2 → HCOCO <sub>2</sub> HCO3 + CO <sub>2</sub>	k1_R02s0R02	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 <sub>2</sub>	2.45E-11	Rickard and Pascoe (2009)
G44435a	TrGAroCN	NBZFUO2 + HO <sub>2</sub> → NBZFUOOH	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44435b	TrGAroCN	NBZFUO2 + HO <sub>2</sub> → .5 CO14O3CHO + .5 NO <sub>2</sub> + .5 NBZFUONE + .5 HO <sub>2</sub> + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44436	TrGAroCN	NBZFUO2 + NO → .5 CO14O3CHO + .5 NO <sub>2</sub> + .5 NBZFUONE + .5 HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44437	TrGAroCN	NBZFUO2 + NO <sub>3</sub> → .5 CO14O3CHO + .5 NO <sub>2</sub> + .5 NBZFUONE + .5 HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G44438	TrGAroCN	NBZFUO2 → .5 CO14O3CHO + .5 NO <sub>2</sub> + .5 NBZFUONE + .5 HO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)*
G44439	TrGAroC	MALDALCO2H + OH → .6 MALANHY + HO <sub>2</sub> + .4 GLYOX + .4 CO + .4 CO <sub>2</sub>	3.70E-11	Rickard and Pascoe (2009)*
G44440	TrGAroCN	EPXC4DIAL + NO <sub>3</sub> → EPXDLCO3 + HNO <sub>3</sub>	2*KN03AL*4.0	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G44441	TrGAroC	EPXC4DIAL + OH $\rightarrow$ EPXDLCO3	4.32E-11	Rickard and Pascoe (2009)
G44442a	TrGAroC	MECOACETO2 + HO <sub>2</sub> $\rightarrow$ MECOACEOOH	KR02H02(4)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44442b	TrGAroC	MECOACETO2 + HO <sub>2</sub> $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + CO <sub>2</sub> + OH	KR02H02(4)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G44443	TrGAroCN	MECOACETO2 + NO $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + CO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44444	TrGAroCN	MECOACETO2 + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G44445	TrGAroC	MECOACETO2 $\rightarrow$ CH <sub>3</sub> C(O)OO + HCHO + CO <sub>2</sub>	k1_R02p0R02	Rickard and Pascoe (2009)*
G44446	TrGAroCN	CO14O3CHO + NO <sub>3</sub> $\rightarrow$ CO + HCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + HNO <sub>3</sub>	KN03AL*8.0	Rickard and Pascoe (2009)
G44447	TrGAroC	CO14O3CHO + OH $\rightarrow$ CO + HCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub>	3.44E-11	Rickard and Pascoe (2009)
G44448	TrGAroCN	NBZFUONE + OH $\rightarrow$ BZFUCO + NO <sub>2</sub>	1.16E-12	Rickard and Pascoe (2009)
G44449a	TrGAroC	BZFUO2 + HO <sub>2</sub> $\rightarrow$ BZFUOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44449b	TrGAroC	BZFUO2 + HO <sub>2</sub> $\rightarrow$ CO14O3CHO + HO <sub>2</sub> + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G44450	TrGAroCN	BZFUO2 + NO $\rightarrow$ CO14O3CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44451	TrGAroCN	BZFUO2 + NO <sub>3</sub> $\rightarrow$ CO14O3CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G44452	TrGAroC	BZFUO2 $\rightarrow$ CO14O3CHO + HO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)*
G44453	TrGAroC	BZFUCO + OH $\rightarrow$ CO14O3CHO + HO <sub>2</sub>	1.78E-11	Rickard and Pascoe (2009)
G44456a	TrGAroC	MALDIALO2 + HO <sub>2</sub> $\rightarrow$ MALDIALOOH	KR02H02(4)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
G44456b	TrGAroC	MALDIALO2 + HO <sub>2</sub> $\rightarrow$ GLYOX + GLYOX + HO <sub>2</sub> + OH	KR02H02(4)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)
G44457	TrGAroCN	MALDIALO2 + NO $\rightarrow$ GLYOX + GLYOX + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G44458	TrGAroCN	MALDIALO2 + NO <sub>3</sub> $\rightarrow$ GLYOX + GLYOX + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G44459	TrGAroC	MALDIALO2 $\rightarrow$ GLYOX + GLYOX + HO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)*
G44460	TrGAroCN	EPXDLPAN + OH $\rightarrow$ HCOCOCHO + CO + NO <sub>2</sub>	2.29E-11	Rickard and Pascoe (2009)
G44461	TrGAroCN	EPXDLPAN $\rightarrow$ EPXDLCO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)*
G44462	TrGAroC	MECOACEOOH + OH $\rightarrow$ MECOACETO2	3.59E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45000	TrGC	$\text{C}_5\text{H}_8 + \text{O}_3 \rightarrow .3508 \text{ MACR} + .01518 \text{ MACO2H} + .2440 \text{ MVK} + .7085 \text{ HCHO} + .11 \text{ CH}_2\text{OO} + .1275 \text{ C}_3\text{H}_6 + .1575 \text{ CH}_3\text{C(O)} + .0510 \text{ CH}_3 + .2625 \text{ HO}_2 + .27 \text{ OH} + .09482 \text{ H}_2\text{O}_2 + .255 \text{ CO}_2 + .522 \text{ CO} + .07182 \text{ HCHO} + .03618 \text{ HCOCH}_2\text{O}_2 + .01782 \text{ CO} + 0.05408 \text{ LCARBON}$	$1.03\text{E-}14 \cdot \text{EXP}(-1995./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)
G45001	TrGC	$\text{C}_5\text{H}_8 + \text{OH} \rightarrow .63 \text{ ISOPAB} + .30 \text{ ISOPCD} + .07 \text{ LISOPEFO2}$	$2.7\text{E-}11 \cdot \text{EXP}(390./\text{temp})$	Atkinson et al. (2006), Taraborrelli (2016)
G45002	TrGCN	$\text{C}_5\text{H}_8 + \text{NO}_3 \rightarrow \text{NISOP02}$	$3.0\text{E-}12 \cdot \text{EXP}(-450./\text{temp})$	Atkinson et al. (2006)
G45003a	TrGC	$\text{ISOPAB} + \text{O}_2 \rightarrow \text{LISOPACO2}$	$5.530\text{E-}13$	Taraborrelli (2016)
G45003b	TrGC	$\text{ISOPAB} + \text{O}_2 \rightarrow \text{ISOPBO2}$	$3.\text{E-}12$	Taraborrelli (2016)
G45004a	TrGC	$\text{ISOPCD} + \text{O}_2 \rightarrow \text{LDISOPACO2}$	$6.780\text{E-}13$	Taraborrelli (2016)
G45004b	TrGC	$\text{ISOPCD} + \text{O}_2 \rightarrow \text{ISOPDO2}$	$3.\text{E-}12$	Taraborrelli (2016)
G45005	TrGC	$\text{LISOPACO2} \rightarrow \text{ISOPAB} + \text{O}_2$	$3.1\text{E}12 \cdot \exp(-7900./\text{temp}) \cdot .6 + 7.8\text{E}13 \cdot \exp(-8600./\text{temp}) \cdot .4$	Taraborrelli (2016)
G45006	TrGC	$\text{ISOPBO2} \rightarrow \text{ISOPAB} + \text{O}_2$	$3.7\text{E}14 \cdot \exp(-9570./\text{temp}) + 4.2\text{E}14 \cdot \exp(-9970./\text{temp})$	Taraborrelli (2016)
G45007	TrGC	$\text{LDISOPACO2} \rightarrow \text{ISOPCD} + \text{O}_2$	$5.65\text{E}12 \cdot \exp(-8410./\text{temp}) + 4.2 + 1.4\text{E}14 \cdot \exp(-9110./\text{temp}) \cdot .58$	Taraborrelli (2016)
G45008	TrGC	$\text{ISOPDO2} \rightarrow \text{ISOPCD} + \text{O}_2$	$5.0\text{E}14 \cdot \exp(-10120./\text{temp}) + 8.25\text{E}14 \cdot \exp(-10220./\text{temp})$	Taraborrelli (2016)
G45009a	TrGC	$\text{LISOPACO2} \rightarrow \text{C1ODC2O2C4OOH}$	$\text{K16HSZ14} * 2./3. * (1 - \text{fhpal})$	Taraborrelli (2016)
G45009b	TrGC	$\text{LISOPACO2} \rightarrow \text{ZCODC23DBCOOH} + \text{HO}_2$	$\text{K16HSZ14} * (2./3. * \text{fhpal} + 1./3.)$	Taraborrelli (2016)
G45010a	TrGC	$\text{LDISOPACO2} \rightarrow \text{C1OOHC3O2C4OD}$	$\text{k16HSZ41} * 2./3. * (1 - \text{fhpal})$	Taraborrelli (2016)
G45010b	TrGC	$\text{LDISOPACO2} \rightarrow \text{ZCODC23DBCOOH} + \text{HO}_2$	$\text{k16HSZ41} * (2./3. * \text{fhpal} + 1./3.)$	Taraborrelli (2016)
G45011	TrGC	$\text{LISOPACO2} \rightarrow .9 \text{ LISOPACO} + .1 \text{ ISOPAOH}$	$\text{k1\_R02LISOPACO2}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45012	TrGC	$\text{LISOPACO2} + \text{HO}_2 \rightarrow \text{LISOPACOOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009)
G45013a	TrGCN	$\text{LISOPACO2} + \text{NO} \rightarrow \text{LISOPACO} + \text{NO}_2$	$\text{KR02N0} * (1 - \alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45013b	TrGCN	$\text{LISOPACO2} + \text{NO} \rightarrow \text{LISOPACNO3}$	$\text{KR02N0} * \alpha_{\text{AN}}(6, 1, 0, 0, 0, \text{temp}, \text{cair})$	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45014	TrGCN	$\text{LISOPACO2} + \text{NO}_3 \rightarrow \text{LISOPACO} + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45015	TrGC	LDISOPACO2 $\rightarrow$ .9 LISOPACO + .1 ISOPAOH	k1_R02LISOPACO2	Rickard and Pascoe (2009), Taraborrelli (2016)
G45016	TrGC	LDISOPACO2 + HO <sub>2</sub> $\rightarrow$ LISOPACOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45017a	TrGCN	LDISOPACO2 + NO $\rightarrow$ LISOPACO + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(6,1,0,0,0, temp, cair))	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45017b	TrGCN	LDISOPACO2 + NO $\rightarrow$ LISOPACNO3	KR02N0*alpha_AN(6,1,0,0,0, temp, cair)	Lockwood et al. (2010), Paulot et al. (2009a), Taraborrelli (2016)
G45018	TrGCN	LDISOPACO2 + NO <sub>3</sub> $\rightarrow$ LISOPACO + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G45019a	TrGC	LISOPACOOH + OH $\rightarrow$ LISOPACO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G45019b	TrGC	LISOPACOOH + OH $\rightarrow$ ZCODC23DBCOOH + HO <sub>2</sub>	k_s*f_allyl*f_soh	Taraborrelli (2016)
G45019c	TrGC	LISOPACOOH + OH $\rightarrow$ LHC4ACCHO + OH	(k_s*f_soh*f_allyl+ k_rohro)	Taraborrelli (2016)
G45019d	TrGC	LISOPACOOH + OH $\rightarrow$ LIEPOX + OH	(k_adt+k_ads)*a_ch2oh*a_ch2ooh	Taraborrelli (2016)*
G45020	TrGC	ISOPAOH + OH $\rightarrow$ LHC4ACCHO + HO <sub>2</sub>	(k_adt+k_ads)*a_ch2oh*a_ch2oh+k_s*f_soh*f_allyl+k_rohro	Taraborrelli (2016)
G45021	TrGCN	LISOPACNO3 + OH $\rightarrow$ LISOPACNO3O2	(k_adt+k_ads)*a_ch2ono2*a_ch2oh	Taraborrelli (2016)*
G45022	TrGC	ISOPBO2 $\rightarrow$ .8 MVK + .8 HCHO + .8 HO <sub>2</sub> + .2 ISOPBOH	k1_R02ISOPBO2	Rickard and Pascoe (2009)
G45023a	TrGC	ISOPBO2 + HO <sub>2</sub> $\rightarrow$ ISOPBOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45023b	TrGC	ISOPBO2 + HO <sub>2</sub> $\rightarrow$ MVK + HCHO + HO <sub>2</sub> + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45024a	TrGCN	ISOPBO2 + NO $\rightarrow$ MVK + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(6,3,0,0,0, temp, cair))	Lockwood et al. (2010), Taraborrelli (2016)
G45024b	TrGCN	ISOPBO2 + NO $\rightarrow$ ISOPBNO3	KR02N0*alpha_AN(6,3,0,0,0, temp, cair)	Lockwood et al. (2010), Taraborrelli (2016)
G45025	TrGCN	ISOPBO2 + NO <sub>3</sub> $\rightarrow$ MVK + .75 HCHO + .75 HO <sub>2</sub> + .25 CH <sub>3</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G45026a	TrGC	ISOPBOOH + OH $\rightarrow$ LIEPOX + OH	(k_ads+k_adp)*a_ch2ooh	Paulot et al. (2009b), Taraborrelli (2016)
G45026b	TrGC	ISOPBOOH + OH $\rightarrow$ ISOPBO2	0.6*k_CH300H_OH	Taraborrelli (2016)
G45026c	TrGC	ISOPBOOH + OH $\rightarrow$ MGLYOX + HOCH <sub>2</sub> CHO	k_rohro+k_s*f_alk*f_soh	Taraborrelli (2016)
G45027	TrGC	ISOPBOOH + O <sub>3</sub> $\rightarrow$ .1368 MACROOH + .1368 H <sub>2</sub> O <sub>2</sub> + .2280 HO <sub>2</sub> + .4332 CH <sub>3</sub> COCH <sub>2</sub> OH + .2280 CO <sub>2</sub> + .6384 OH + .2052 CO + .57 HCHO + .43 MACROOH + .06880 HO <sub>2</sub> + .06880 OH + .2709 CO + .1591 CH <sub>2</sub> OO	1.E-17	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45028	TrGC	ISOPBOH + OH $\rightarrow$ MVK + .75 HCHO + .75 HO <sub>2</sub> + .25 CH <sub>3</sub>	$k_{\text{s}}*f_{\text{alk}}*f_{\text{soh}}+(k_{\text{adp}}+k_{\text{ads}})*a_{\text{ch2oh}}$	Taraborrelli (2016)
G45029	TrGCN	ISOPBNO <sub>3</sub> + OH $\rightarrow$ ISOPBDNO <sub>3</sub> O <sub>2</sub>	$(k_{\text{adt}}+k_{\text{adp}})*f_{\text{ch2ono2}}$	Taraborrelli (2016)
G45030	TrGC	ISOPDO <sub>2</sub> $\rightarrow$ .8 MACR + .8 HCHO + .8 HO <sub>2</sub> + .1 HCOC <sub>5</sub> + .1 ISOPDOH	k1_R02ISOPD02	Rickard and Pascoe (2009)
G45031a	TrGC	ISOPDO <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ ISOPDOOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45031b	TrGC	ISOPDO <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ MACR + HCHO + HO <sub>2</sub> + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45032a	TrGCN	ISOPDO <sub>2</sub> + NO $\rightarrow$ MACR + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(6,2,0,0,0,temp,cair))	Lockwood et al. (2010), Taraborrelli (2016)
G45032b	TrGCN	ISOPDO <sub>2</sub> + NO $\rightarrow$ ISOPDNO <sub>3</sub>	KR02N0*alpha_AN(6,2,0,0,0,temp,cair)	Lockwood et al. (2010), Taraborrelli (2016)
G45033	TrGCN	ISOPDO <sub>2</sub> + NO <sub>3</sub> $\rightarrow$ MACR + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G45034a	TrGC	ISOPDOOH + OH $\rightarrow$ LIEPOX + OH	$(k_{\text{adt}}+k_{\text{adp}})*a_{\text{ch2ooh}}$	Paulot et al. (2009b), Taraborrelli (2016)
G45034b	TrGC	ISOPDOOH + OH $\rightarrow$ ISOPDO <sub>2</sub>	0.6*k_CH300H_OH	Taraborrelli (2016)
G45034c	TrGC	ISOPDOOH + OH $\rightarrow$ HCOC <sub>5</sub> + OH	$k_{\text{t}}*f_{\text{tooh}}*f_{\text{allyl}}*f_{\text{pch2oh}}$	Taraborrelli (2016)
G45034d	TrGC	ISOPDOOH + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>2</sub> OH + GLYOX + OH	$k_{\text{s}}*f_{\text{pch2oh}}*f_{\text{soh}}$	Taraborrelli (2016)
G45035	TrGC	ISOPDOOH + O <sub>3</sub> $\rightarrow$ 1.393 OH + BIACETOH + .67 HCHO + .05280 HO <sub>2</sub> + .2079 CO + .1221 CH <sub>2</sub> OO	1.E-17	Taraborrelli (2016)
G45036	TrGC	ISOPDOH + OH $\rightarrow$ HCOC <sub>5</sub> + HO <sub>2</sub>	$2.*k_{\text{rohro}}+(k_{\text{t}}*f_{\text{toh}}*f_{\text{allyl}}+k_{\text{s}}*f_{\text{soh}})*f_{\text{pch2oh}}+(k_{\text{adt}}+k_{\text{adp}})*a_{\text{ch2oh}}$	Taraborrelli (2016)
G45037	TrGCN	ISOPDNO <sub>3</sub> + OH $\rightarrow$ ISOPBDNO <sub>3</sub> O <sub>2</sub>	$(k_{\text{adp}}+k_{\text{ads}})*a_{\text{ch2ono2}}$	Taraborrelli (2016)*
G45038	TrGCN	NISOPO <sub>2</sub> $\rightarrow$ .8 NC <sub>4</sub> CHO + .6 HO <sub>2</sub> + .2 LISOPACNO <sub>3</sub>	k1_R02LISOPAC02	Rickard and Pascoe (2009)
G45039	TrGCN	NISOPO <sub>2</sub> + HO <sub>2</sub> $\rightarrow$ NISOPOOH	KR02H02(5)	Rickard and Pascoe (2009)
G45040	TrGCN	NISOPO <sub>2</sub> + NO $\rightarrow$ NC <sub>4</sub> CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G45041	TrGCN	NISOPO <sub>2</sub> + NO <sub>3</sub> $\rightarrow$ NC <sub>4</sub> CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G45042	TrGCN	NISOPOOH + OH $\rightarrow$ NC <sub>4</sub> CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G45043	TrGCN	NC <sub>4</sub> CHO + OH $\rightarrow$ LNISO <sub>3</sub>	$(k_{\text{adt}}+k_{\text{ads}})*a_{\text{cho}}*a_{\text{ch2ono2}}$	Taraborrelli (2016)*
G45044	TrGCN	NC <sub>4</sub> CHO + O <sub>3</sub> $\rightarrow$ .27 NOA + .027 HCOCO <sub>2</sub> H + .0162 GLYOX + .0162 H <sub>2</sub> O <sub>2</sub> + .1458 HCOCO + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO <sub>2</sub> + 0.7705 HCHO + .4055 CO <sub>2</sub> + .73 GLYOX	2.40E-17	Taraborrelli (2016)
G45045	TrGCN	NC <sub>4</sub> CHO + NO <sub>3</sub> $\rightarrow$ LNISO <sub>3</sub> + HNO <sub>3</sub>	KN03AL*4.25	Rickard and Pascoe (2009)
G45046	TrGCN	LNISO <sub>3</sub> + HO <sub>2</sub> $\rightarrow$ LNISOOH	.5*KR02H02(5) + .5*KAPH02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45047	TrGCN	$\text{LNISO}_3 + \text{NO} \rightarrow \text{NOA} + .5 \text{HOCHCHO} + .5 \text{CO} + .5 \text{HO}_2 + \text{NO}_2 + .5 \text{CO}_2$	$.5 * \text{KAPNO} + .5 * \text{KR02NO}$	Rickard and Pascoe (2009)*
G45048	TrGCN	$\text{LNISO}_3 + \text{NO}_3 \rightarrow \text{NOA} + .5 \text{HOCHCHO} + .5 \text{CO} + .5 \text{HO}_2 + \text{NO}_2 + .5 \text{CO}_2$	$1.3 * \text{KR02NO3}$	Rickard and Pascoe (2009)
G45049	TrGCN	$\text{LNISOOH} + \text{OH} \rightarrow \text{LNISO}_3$	$2.65\text{E}-11$	Rickard and Pascoe (2009)
G45050a	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LC578O2}$	$(\text{k\_adtertprim} + \text{k\_ads}) * \text{a\_cho} * \text{a\_ch2oh}$	Taraborrelli (2016)
G45050b	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$\text{k\_t*f\_o}$	Taraborrelli (2016)
G45050c	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{ZCODC23DBCOD} + \text{HO}_2$	$\text{k\_s*f\_soh*f\_allyl}$	Taraborrelli (2016)
G45051	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow .2225 \text{CH}_3\text{C}(\text{O}) + .89 \text{CO} + .0171875 \text{HOCH}_2\text{CO}_2\text{H} + .075625 \text{H}_2\text{O}_2 + .0171875 \text{HCOCO}_2\text{H} + .2775 \text{CH}_3\text{COCH}_2\text{OH} + .6675 \text{HO}_2 + .2603125 \text{GLYOX} + .2225 \text{HCHO} + .89 \text{OH} + .2603125 \text{HOCH}_2\text{CHO} + .5 \text{MGLYOX}$	$2.40\text{E}-17$	Rickard and Pascoe (2009)
G45052	TrGCN	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO3} + \text{HNO}_3$	$\text{KN03AL} * 4.25$	Rickard and Pascoe (2009)
G45053	TrGC	$\text{LC578O2} \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2$	$\text{k1\_R02t0R02}$	Rickard and Pascoe (2009)
G45054a	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO} + \text{OH}$	$\text{KR02H02(5)*rcoch2o2\_oh}$	Rickard and Pascoe (2009)
G45054b	TrGC	$\text{LC578O2} + \text{HO}_2 \rightarrow \text{LC578OOH}$	$\text{KR02H02(5)*rcoch2o2\_ooh}$	Rickard and Pascoe (2009)
G45055	TrGCN	$\text{LC578O2} + \text{NO} \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{NO}_2$	$\text{KR02NO}$	Rickard and Pascoe (2009)*
G45056	TrGCN	$\text{LC578O2} + \text{NO}_3 \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCHCHO} + .75 \text{HOCH}_2\text{CHO} + .75 \text{HO}_2 + \text{NO}_2$	$\text{KR02NO3}$	Rickard and Pascoe (2009)
G45057	TrGC	$\text{LC578O2} \rightarrow .25 \text{CH}_3\text{COCH}_2\text{OH} + .75 \text{MGLYOX} + .25 \text{HOCH}_2\text{CHO} + .75 \text{HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{KHSB}$	Taraborrelli (2016)
G45058a	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O2}$	$0.6 * \text{k\_CH300H\_OH}$	Taraborrelli (2016)
G45058b	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{C1ODC2OOHC4OD} + \text{HO}_2$	$\text{k\_t*f\_o*f\_tch2oh*f\_alk} + \text{k\_t*f\_toh*f\_pch2oh*f\_pch2oh} + \text{k\_s*f\_soh*f\_pch2oh}$	Taraborrelli (2016)
G45059a	TrGC	$\text{LHC4ACCO3} \rightarrow \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{CO}_2$	$\text{k1\_R02RC03} * 0.9$	Taraborrelli (2016)
G45059b	TrGC	$\text{LHC4ACCO3} \rightarrow \text{LHC4ACCO2H}$	$\text{k1\_R02RC03} * 0.1$	Taraborrelli (2016)
G45060a	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow 2 \text{OH} + .5 \text{MACRO2} + .5 \text{LHMKABO2} + \text{CO}_2$	$\text{KAPH02*rco3\_oh}$	Taraborrelli (2016)
G45060b	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO3H}$	$\text{KAPH02*rco3\_ooh}$	Taraborrelli (2016)



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

#	labels	reaction	rate coefficient	reference
G45060c	TrGC	$\text{LHC4ACCO3} + \text{HO}_2 \rightarrow \text{LHC4ACCO2H} + \text{O}_3$	$\text{KAPH02*rc03\_o3}$	Taraborrelli (2016)
G45061	TrGCN	$\text{LHC4ACCO3} + \text{NO} \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	KAPN0	Taraborrelli (2016)
G45062	TrGCN	$\text{LHC4ACCO3} + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	$\text{k\_CH3CO3\_NO2}$	Rickard and Pascoe (2009)
G45063	TrGCN	$\text{LHC4ACCO3} + \text{NO}_3 \rightarrow .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{NO}_2 + \text{CO}_2$	$1.6*\text{KR02NO3}$	Taraborrelli (2016)
G45064a	TrGC	$\text{LHC4ACCO2H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO2} + .5 \text{ LHMVKABO2} + \text{CO}_2$	$2.52\text{E-}11$	Taraborrelli (2016)
G45064b	TrGC	$\text{LHC4ACCO3H} + \text{OH} \rightarrow \text{LHC4ACCO3}$	$2.88\text{E-}11$	Rickard and Pascoe (2009)
G45065	TrGCN	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO3} + \text{NO}_2$	$\text{k\_PAN\_M}$	Rickard and Pascoe (2009)
G45066	TrGCN	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO3C4} + \text{CO} + \text{NO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)
G45067	TrGC	$\text{HCOC5} + \text{OH} \rightarrow \text{C59O2}$	$3.81\text{E-}11$	Rickard and Pascoe (2009)
G45068	TrGC	$\text{HCOC5} + \text{O}_3 \rightarrow \text{BIACETOH} + .335 \text{ H}_2\text{O}_2 + .67 \text{ HCHO} + .2079 \text{ CO} + .1221 \text{ CH}_2\text{OO} + .05280 \text{ OH}$	$7.51\text{E-}16*\text{EXP}(-1521./\text{temp})$	Taraborrelli (2016)
G45069	TrGC	$\text{C59O2} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$\text{k1\_R02t0R02}$	Taraborrelli (2016)
G45070a	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO}$	$\text{KR02H02(5)*rcoch2o2\_oh}$	Taraborrelli (2016)
G45070b	TrGC	$\text{C59O2} + \text{HO}_2 \rightarrow \text{C59OOH}$	$\text{KR02H02(5)*rcoch2o2\_ooh}$	Taraborrelli (2016)
G45071	TrGCN	$\text{C59O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	$\text{KR02NO}$	Taraborrelli (2016)*
G45072	TrGCN	$\text{C59O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{HOCH}_2\text{CO} + \text{NO}_2$	$\text{KR02NO3}$	Taraborrelli (2016)
G45073	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O2}$	$9.7\text{E-}12$	Rickard and Pascoe (2009)
G45074	TrGC	$\text{LIEPOX} + \text{OH} \rightarrow \text{DB1O2} + \text{H}_2\text{O}$	$5.78\text{E-}11*\text{EXP}(-400./\text{temp}) * (1.52/3.+0.98*2./3.)/1.51$	Paulot et al. (2009b), Bates et al. (2014), Taraborrelli (2016)*
G45075	TrGC	$\text{ISOPBO2} \rightarrow \text{MVK} + \text{HCHO} + \text{OH}$	KHSB	Taraborrelli (2016)
G45076	TrGC	$\text{ISOPDO2} \rightarrow \text{MACR} + \text{HCHO} + \text{OH}$	KHSD	Taraborrelli (2016)
G45077a	TrGC	$\text{ZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC2O2C4OOH} + .4 \text{ C1OOHC2O2C4OD}$	$\text{k\_adt*a\_cho*a\_ch2ooh}$	Taraborrelli (2016)
G45077b	TrGC	$\text{ZCODC23DBCOOH} + \text{OH} \rightarrow .6 \text{ C1ODC3O2C4OOH} + .4 \text{ C1OOHC3O2C4OD}$	$\text{k\_ads*a\_cho*a\_ch2ooh}$	Taraborrelli (2016)
G45077c	TrGC	$\text{ZCODC23DBCOOH} + \text{OH} \rightarrow \text{ZCO3HC23DBCOD}$	$\text{k\_t*f\_o*f\_alk}+0.6*\text{k\_CH300H\_OH}$	Taraborrelli (2016)
G45077d	TrGC	$\text{ZCODC23DBCOOH} + \text{OH} \rightarrow \text{ZCODC23DBCOD} + \text{OH}$	$\text{k\_s*f\_sooh*f\_allyl}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45078	TrGC	ZCODOC23DBCOOH + O <sub>3</sub> → .4672 OH + .2336 HCOCOCH <sub>2</sub> O <sub>2</sub> + .2336 CO + .2336 CH <sub>3</sub> C(O) + .4672 HOOCH <sub>2</sub> CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH <sub>2</sub> CHO + .02765 H <sub>2</sub> O <sub>2</sub> + .02592 CH <sub>3</sub> OOH + .02592 CO <sub>2</sub> + .01037 HCOCO + .01555 CH <sub>2</sub> OO + .01555 CO + .006908 HOOCH <sub>2</sub> CO <sub>3</sub> + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH <sub>2</sub> OOH + .2628 GLYOX + .0972 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .00972 HCOCO <sub>2</sub> H + .005832 GLYOX + .005832 H <sub>2</sub> O <sub>2</sub> + .05249 OH + .05249 HCOCO + .01458 HCHO + .01458 CO <sub>2</sub> + .01458 HCOOH + .01458 CO	2.4E-17	Taraborrelli (2016)
G45079	TrGC	C1OOHC2O2C4OD → .78 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .78 HOCHCHO + .22 CO <sub>2</sub> H <sub>3</sub> CHO + .22 HCHO + .22 OH	k1_R02t0R02	Taraborrelli (2016)
G45080	TrGCN	C1OOHC2O2C4OD + NO → .78 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .78 HOCHCHO + .22 CO <sub>2</sub> H <sub>3</sub> CHO + .22 HCHO + .22 OH + NO <sub>2</sub>	KR02N0	Taraborrelli (2016)*
G45081a	TrGC	C1OOHC2O2C4OD + HO <sub>2</sub> → C1OOHC2OOHC4OD	KR02H02(5)*rcoch2o2_ooh	Taraborrelli (2016)
G45081b	TrGC	C1OOHC2O2C4OD + HO <sub>2</sub> → .78 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .78 HOCHCHO + .22 CO <sub>2</sub> H <sub>3</sub> CHO + .22 HCHO + 1.22 OH	KR02H02(5)*rcoch2o2_oh	Taraborrelli (2016)
G45082	TrGC	C1OOHC2O2C4OD → CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + 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)
G45084b	TrGC	C1OOHC2OOHC4OD + OH → CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + 2 CO + 2 HO <sub>2</sub> + OH	k_t*f_toh*f_pch2oh*f_pch2oh	Taraborrelli (2016)
G45084c	TrGC	C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD	0.6*k_CH300H_OH	Taraborrelli (2016)
G45085	TrGC	C1ODC2OOHC4OD + OH → CO <sub>2</sub> H <sub>3</sub> CHO + CO + H <sub>2</sub> O + OH	k_t*f_o*f_tch2oh+k_t*f_toh*f_toh*f_cho	Taraborrelli (2016)
G45086	TrGC	C1ODC3O2C4OOH → MGLYOX + HOOCH <sub>2</sub> CHO + HO <sub>2</sub>	k1_R02s0R02	Taraborrelli (2016)
G45087	TrGCN	C1ODC3O2C4OOH + NO → MGLYOX + HOOCH <sub>2</sub> CHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Taraborrelli (2016)
G45088	TrGC	C1ODC3O2C4OOH + HO <sub>2</sub> → .5 CH <sub>3</sub> C(O) + .5 CO + .5 MGLYOX + .5 HO <sub>2</sub> + HOOCH <sub>2</sub> CO <sub>3</sub>	KR02H02(5)	Taraborrelli (2016)
G45089	TrGC	C1ODC3O2C4OOH → MGLYOX + OH + HOOCH <sub>2</sub> CHO	KHSD	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45090	TrGC	$\text{C1OOHC3O2C4OD} \rightarrow .625 \text{ MGLYOX} + 2 \text{ CO} + 1.625 \text{ HO}_2 + .375 \text{ CH}_3\text{C(O)} + .375 \text{ CO}_2 + \text{OH}$	K15HSDHB	Taraborrelli (2016)
G45091	TrGC	$\text{LHC4ACCO3} \rightarrow \text{ZCO3HC23DBCOD} + \text{HO}_2$	K16HS	Taraborrelli (2016)
G45092a	TrGC	$\text{ZCODC23DBCOD} + \text{OH} \rightarrow \text{C1ODC2O2C4OD}$	$(k_{\text{adt}}+k_{\text{ads}})*a_{\text{cho}}*a_{\text{cho}}$	Taraborrelli (2016)*
G45092b	TrGC	$\text{ZCODC23DBCOD} + \text{OH} \rightarrow \text{ZCO3C23DBCOD}$	$2*k_t*f_o*f_{\text{alk}}$	Taraborrelli (2016)*
G45093	TrGCN	$\text{ZCODC23DBCOD} + \text{NO}_3 \rightarrow \text{ZCO3C23DBCOD} + \text{HNO}_3$	$\text{KN03AL}*4.25*2.$	Taraborrelli (2016)*
G45094a	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{OH} + \text{MGLYOX} + \text{HOCHCHO}$	$\text{KR02H02(5)}*r_{\text{coch2o2\_oh}}$	Taraborrelli (2016)
G45094b	TrGC	$\text{C1ODC2O2C4OD} + \text{HO}_2 \rightarrow \text{C1ODC2OOHC4OD}$	$\text{KR02H02(5)}*r_{\text{coch2o2\_ooh}}$	Taraborrelli (2016)
G45095	TrGCN	$\text{C1ODC2O2C4OD} + \text{NO} \rightarrow \text{NO}_2 + \text{MGLYOX} + \text{HOCHCHO}$	KR02N0	Taraborrelli (2016)*
G45096	TrGC	$\text{C1ODC2O2C4OD} \rightarrow \text{MGLYOX} + \text{HOCHCHO}$	$k1\_R02t0R02$	Taraborrelli (2016)
G45097a	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO}$	$(2*k_t*f_o*f_{\text{tch2oh}}*f_{\text{alk}}+k_t*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$	Taraborrelli (2016)
G45097b	TrGC	$\text{C1ODC2OOHC4OD} + \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + \text{OH}$	$(2*k_t*f_o*f_{\text{tch2oh}}*f_{\text{alk}}+k_t*f_{\text{toh}}*f_{\text{cho}}*f_{\text{pch2oh}})*.5$	Taraborrelli (2016)
G45098	TrGCN	$\text{LISOPACNO3O2} + \text{NO} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2 + \text{NO}_2$	KR02N0	Taraborrelli (2016)*
G45099	TrGCN	$\text{LISOPACNO3O2} \rightarrow .21 \text{ NOA} + .21 \text{ HOCH}_2\text{CHO} + .21 \text{ HO}_2 + .49 \text{ HO12CO3C4} + .49 \text{ HCHO} + .49 \text{ NO}_2 + .045 \text{ MVKNO3} + .045 \text{ HCHO} + .255 \text{ CH}_3\text{COCH}_2\text{OH} + .255 \text{ NO}_3\text{CH}_2\text{CHO} + .225 \text{ H}_2\text{O}_2$	$k1\_R02t0R02+\text{KR02H02(5)}*c(\text{ind\_H02})$	Taraborrelli (2016)
G45100	TrGCN	$\text{ISOPBDNO3O2} + \text{NO} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRN} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + 1.6 \text{ NO}_2$	KR02N0	Taraborrelli (2016)*
G45101	TrGCN	$\text{ISOPBDNO3O2} \rightarrow .6 \text{ CH}_3\text{COCH}_2\text{OH} + .6 \text{ HOCH}_2\text{CHO} + .26 \text{ MACRN} + .14 \text{ MVKNO3} + .4 \text{ HCHO} + .4 \text{ HO}_2 + .6 \text{ NO}_2$	$k1\_R02s0R02+\text{KR02H02(5)}*c(\text{ind\_H02})$	Taraborrelli (2016)
G45102	TrGCN	$\text{LISOPACNO3} + \text{O}_3 \rightarrow .8704 \text{ OH} + .365 \text{ HO}_2 + .73 \text{ MGLYOX} + .4325 \text{ NO}_3\text{CH}_2\text{CHO} + .135 \text{ CH}_3\text{COCH}_2\text{OH} + .0675 \text{ GLYOX} + .4325 \text{ NO}_2 + .0891 \text{ H}_2\text{O}_2 + .135 \text{ NOA} + .0675 \text{ HOCHCHO} + .3866 \text{ HOCH}_2\text{CHO} + .0405 \text{ CH}_3\text{OH} + .0405 \text{ CO} + .0054 \text{ HOCH}_2\text{CO}$	$2.8\text{E}-17$	Feierabend et al. (2008), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45103	TrGC	DB1O2 $\rightarrow$ DB1O2	k1_R02s0R02	Taraborrelli (2016)
G45104a	TrGC	DB1O2 + HO <sub>2</sub> $\rightarrow$ DB1OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)*
G45104b	TrGC	DB1O2 + HO <sub>2</sub> $\rightarrow$ DB1O2 + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45105a	TrGCN	DB1O2 + NO $\rightarrow$ DB1O2 + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair))	Taraborrelli (2016)
G45105b	TrGCN	DB1O2 + NO $\rightarrow$ DB1NO3	KR02N0*alpha_AN(7,2,0,0,0,temp, cair)	Taraborrelli (2016)
G45106	TrGCN	DB1O2 + NO <sub>3</sub> $\rightarrow$ DB1O2 + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G45107	TrGC	DB1O2 $\rightarrow$ DB1O2 + OH	1.E4	Peeters and Nguyen (2012)*
G45108a	TrGC	DB1O2 $\rightarrow$ DB1O2	KDEC*0.72	see note*
G45108b	TrGC	DB1O2 $\rightarrow$ .5 HVMK + .5 HMAc + HCHO + HO <sub>2</sub>	KDEC*0.28	see note*
G45109	TrGC	DB1O2 $\rightarrow$ .48 CH <sub>3</sub> COCH <sub>2</sub> OH + .52 HOCH <sub>2</sub> CHO + .52 MGLYOX + .48 GLYOX + HO <sub>2</sub>	k1_R02s0R02	Taraborrelli (2016)
G45110a	TrGC	DB1O2 + HO <sub>2</sub> $\rightarrow$ DB2OOH	KR02H02(5)*(1.-rchohch2o2_oh)	Taraborrelli (2016)
G45110b	TrGC	DB1O2 + HO <sub>2</sub> $\rightarrow$ .48 CH <sub>3</sub> COCH <sub>2</sub> OH + .52 HOCH <sub>2</sub> CHO + .52 MGLYOX + .48 GLYOX + HO <sub>2</sub> + OH	KR02H02(5)*rchohch2o2_oh	Taraborrelli (2016)
G45111	TrGCN	DB1O2 + NO $\rightarrow$ .48 CH <sub>3</sub> COCH <sub>2</sub> OH + .52 HOCH <sub>2</sub> CHO + .52 MGLYOX + .48 GLYOX + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	see note*
G45112	TrGCN	DB1O2 + NO <sub>3</sub> $\rightarrow$ .48 CH <sub>3</sub> COCH <sub>2</sub> OH + .52 HOCH <sub>2</sub> CHO + .52 MGLYOX + .48 GLYOX + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Taraborrelli (2016)
G45113	TrGC	DB1O2 $\rightarrow$ .48 MACROOH + .52 LHMVKABOOH + CO + OH	K14HSAL	Taraborrelli (2016)
G45114a	TrGC	DB1OOH + OH $\rightarrow$ DB1O2	.6*k_CH300H_OH	Taraborrelli (2016)
G45114b	TrGC	DB1OOH + OH $\rightarrow$ HCOOH + HO <sub>2</sub> + CH <sub>3</sub> COCHO <sub>2</sub> CHO	k_adt	Taraborrelli (2016)*
G45115	TrGC	DB1OOH + HCOOH $\rightarrow$ C1ODC2OOHC4OD + HCOOH	4.67E-26*temp**3.286*EXP(4509./(1.987*temp))	Taraborrelli (2016), daSilva (2010)*
G45116	TrGCN	DB1NO3 + OH $\rightarrow$ HCOOH + NO <sub>2</sub> + CH <sub>3</sub> COCHO <sub>2</sub> CHO	k_adt	Taraborrelli (2016)*
G45117	TrGC	DB2OOH + OH $\rightarrow$ DB1O2	.6*k_CH300H_OH	Taraborrelli (2016)*
G45118	TrGC	LISOPACOOH + O <sub>3</sub> $\rightarrow$ 1.3272 OH + .36986 HO <sub>2</sub> + .0432 H <sub>2</sub> O <sub>2</sub> + .08422 CO + .2025 CH <sub>3</sub> OOH + .01215 CH <sub>2</sub> OO + .3704 HCHO + .00405 CH <sub>3</sub> OH + .0405 CO <sub>2</sub> + .1825 HOCH <sub>2</sub> COCH <sub>2</sub> O <sub>2</sub> + .365 MGLYOX + .3866 HOOCH <sub>2</sub> CHO + .135 CH <sub>3</sub> COCH <sub>2</sub> OH + .0675 GLYOX + .00324 HCOCO + .3866 HOCH <sub>2</sub> CHO + .135 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .0675 HOCHCHO + .0054 HOCH <sub>2</sub> CO	4.829E-16	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45119a	TrGC	$\text{ZCO3HC23DBCOD} + \text{OH} \rightarrow .62 \text{ CO2H3CHO} + .62 \text{ OH} + .62 \text{ CO}_2 + .38 \text{ MGLYOX} + .38 \text{ HCOCO}_3\text{H} + .38 \text{ HO}_2$	$k_{\text{adt}}*a_{\text{cho}}*a_{\text{co2h}}$	Taraborrelli (2016)
G45119b	TrGC	$\text{ZCO3HC23DBCOD} + \text{OH} \rightarrow .62 \text{ CH}_3\text{COCO}_3\text{H} + 1.24 \text{ CO} + 1.24 \text{ HO}_2 + .38 \text{ MGLYOX} + .38 \text{ HO}_2 + .38 \text{ CO} + .38 \text{ HO}_2 + .38 \text{ OH} + .38 \text{ CO}_2$	$k_{\text{ads}}*a_{\text{cho}}*a_{\text{co2h}}$	Taraborrelli (2016)
G45120	TrGC	$\text{LISOPEFO2} \rightarrow \text{LISOPEFO}$	$k1_{\text{R02p0R02}}$	Taraborrelli (2016)
G45121a	TrGCN	$\text{LISOPEFO2} + \text{NO} \rightarrow \text{LISOPEFO} + \text{NO}_2$	$\text{KR02N0}*(1.-\alpha_{\text{AN}}(6,1,0,0,0,\text{temp},\text{cair}))$	Taraborrelli (2016)
G45121b	TrGCN	$\text{LISOPEFO2} + \text{NO} \rightarrow \text{ISOPDNO3}$	$\text{KR02N0}*\alpha_{\text{AN}}(6,1,0,0,0,\text{temp},\text{cair})$	Taraborrelli (2016)*
G45122a	TrGC	$\text{LISOPEFO2} + \text{HO}_2 \rightarrow .7143 \text{ ISOPDOOH} + .2857 \text{ ISOPBOOH}$	$\text{KR02H02}(5)*(1.-\text{rchohch2o2\_oh})$	Taraborrelli (2016)
G45122b	TrGC	$\text{LISOPEFO2} + \text{HO}_2 \rightarrow \text{LISOPEFO} + \text{OH}$	$\text{KR02H02}(5)*\text{rchohch2o2\_oh}$	Taraborrelli (2016)
G45123	TrGCN	$\text{LISOPEFO2} + \text{NO}_3 \rightarrow \text{LISOPEFO} + \text{NO}_2$	$\text{KR02N03}$	Taraborrelli (2016)
G45124	TrGC	$\text{LISOPEFO2} \rightarrow .7143 \text{ MACR} + .2857 \text{ MVK} + \text{HCHO} + \text{OH}$	$.7143*\text{KHSD}+.2857*\text{KHSB}$	Taraborrelli (2016)
G45125	TrGC	$\text{LISOPEFO} \rightarrow .7143 \text{ MACR} + .2857 \text{ MVK} + \text{HCHO} + \text{HO}_2$	$\text{KDEC}$	Taraborrelli (2016)
G45126a	TrGC	$\text{LISOPACO} \rightarrow 3\text{METHYLFURAN} + \text{HO}_2$	$\text{KDEC}*0.37$	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45126b	TrGC	$\text{LISOPACO} \rightarrow .65 \text{ LHC4ACCHO} + .65 \text{ HO}_2 + .35 \text{ DB1O2}$	$\text{KDEC}*(1.-0.37)$	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127a	TrGC	$\text{LISOPACO} \rightarrow 3\text{METHYLFURAN} + \text{HO}_2$	$\text{KDEC}*0.37$	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45127b	TrGC	$\text{LISOPACO} \rightarrow .65 \text{ LHC4ACCHO} + .65 \text{ HO}_2 + .35 \text{ DB1O2}$	$\text{KDEC}*(1.-0.37)$	Taraborrelli (2016), Paulot et al. (2009a), Francisco-Marquez et al. (2003)
G45128	TrGC	$3\text{METHYLFURAN} + \text{OH} \rightarrow \text{L3METHYLFURANO2}$	$3.2\text{E}-11*\text{EXP}(310./\text{temp})$	Taraborrelli (2016)*
G45129	TrGCN	$3\text{METHYLFURAN} + \text{NO}_3 \rightarrow \text{L3METHYLFURANO2} + \text{NO}_2$	$1.9\text{E}-11$	Taraborrelli (2016), Atkinson et al. (2006)*
G45130	TrGC	$\text{L3METHYLFURANO2} \rightarrow \text{ZCODC23DBCOD} + \text{HO}_2$	$k1_{\text{R02s0R02}}$	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45131	TrGCN	L3METHYLFURANO2 + NO → ZCODC23DBCOD + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Taraborrelli (2016)*
G45132	TrGC	L3METHYLFURANO2 + HO <sub>2</sub> → ZCODC23DBCOD + HO <sub>2</sub>	KR02H02(5)	Taraborrelli (2016)*
G45133	TrGC	ZCO3C23DBCOD → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO <sub>2</sub>	k1_R02RC03	Taraborrelli (2016)
G45134a	TrGC	ZCO3C23DBCOD + HO <sub>2</sub> → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Taraborrelli (2016)
G45134b	TrGC	ZCO3C23DBCOD + HO <sub>2</sub> → ZCO3HC23DBCOD	KAPH02*(rco3_ooh+rco3_o3)	Taraborrelli (2016)*
G45135	TrGCN	ZCO3C23DBCOD + NO → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPN0	Taraborrelli (2016)
G45136	TrGCN	ZCO3C23DBCOD + NO <sub>2</sub> → ZCPANC23DBCOD	k_CH3C03_N02	Rickard and Pascoe (2009)
G45137	TrGCN	ZCO3C23DBCOD + NO <sub>3</sub> → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO <sub>2</sub> + NO <sub>2</sub>	1.6*KR02N03	Taraborrelli (2016)
G45138	TrGCN	ZCPANC23DBCOD → ZCO3C23DBCOD + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G45139	TrGCN	ZCPANC23DBCOD + OH → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + CO <sub>2</sub> + NO <sub>2</sub>	2.52E-11	Taraborrelli (2016)*
G45200	TrGTerC	C511O2 → CH <sub>3</sub> C(O) + HCOCH2CHO	k1_R02s0R02	Rickard and Pascoe (2009)
G45201	TrGTerCN	C511O2 + NO → CH <sub>3</sub> C(O) + HCOCH2CHO + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G45202a	TrGTerC	C511O2 + HO <sub>2</sub> → C511OOH	KR02H02(5)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45202b	TrGTerC	C511O2 + HO <sub>2</sub> → CH <sub>3</sub> C(O) + HCOCH2CHO + OH	KR02H02(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 <sub>3</sub> → CO23C4CO3 + HNO <sub>3</sub>	KN03AL*5.5	Rickard and Pascoe (2009)
G45206	TrGTerC	CO23C4CO3 → CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub>	k1_R02RC03	Rickard and Pascoe (2009)
G45207	TrGTerCN	CO23C4CO3 + NO → CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + NO <sub>2</sub>	KAPN0	Rickard and Pascoe (2009)*
G45208	TrGTerCN	CO23C4CO3 + NO <sub>2</sub> → C5PAN9	k_CH3C03_N02	Rickard and Pascoe (2009)
G45209a	TrGTerC	CO23C4CO3 + HO <sub>2</sub> → CO23C4CO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45209b	TrGTerC	CO23C4CO3 + HO <sub>2</sub> → CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45210	TrGTerCN	C5PAN9 → CO23C4CO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G45211	TrGTerCN	C5PAN9 + OH → CH <sub>3</sub> COCOCHO + CO + NO <sub>2</sub>	3.12E-13	Rickard and Pascoe (2009)
G45212	TrGTerC	C512O2 → C513O2	k1_R02pR02	Rickard and Pascoe (2009)
G45213	TrGTerC	C512O2 + HO <sub>2</sub> → C512OOH	KR02H02(5)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45214	TrGTerCN	$\text{C512O2} + \text{NO} \rightarrow \text{C513O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45215	TrGTerC	$\text{C512OOH} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{OH}$	1.01E-10	Rickard and Pascoe (2009)
G45216	TrGTerC	$\text{C513O2} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3$	k1_R02s0R02	Rickard and Pascoe (2009)
G45217	TrGTerCN	$\text{C513O2} + \text{NO} \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45218a	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{C513OOH}$	KR02H02(5)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45218b	TrGTerC	$\text{C513O2} + \text{HO}_2 \rightarrow \text{GLYOX} + \text{HOC}_2\text{H}_4\text{CO}_3 + \text{OH}$	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45219	TrGTerC	$\text{CO13C4CHO} + \text{OH} \rightarrow \text{CHOC3COCO3}$	1.33E-10	Rickard and Pascoe (2009)
G45220	TrGTerCN	$\text{CO13C4CHO} + \text{NO}_3 \rightarrow \text{CHOC3COCO3} + \text{HNO}_3$	2.*KN03AL*5.5	Rickard and Pascoe (2009)
G45221	TrGTerC	$\text{C513OOH} + \text{OH} \rightarrow \text{C513CO} + \text{OH}$	9.23E-11	Rickard and Pascoe (2009)
G45222	TrGTerC	$\text{CHOC3COCO3} \rightarrow \text{CHOC3COO2} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45223	TrGTerC	$\text{CHOC3COCO3} + \text{HO}_2 \rightarrow \text{CHOC3COOOH}$	KAPH02	Rickard and Pascoe (2009)
G45224	TrGTerCN	$\text{CHOC3COCO3} + \text{NO}_2 \rightarrow \text{CHOC3COPAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G45225	TrGTerCN	$\text{CHOC3COCO3} + \text{NO} \rightarrow \text{CHOC3COO2} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)*
G45226	TrGTerC	$\text{C513CO} + \text{OH} \rightarrow \text{HOC}_2\text{H}_4\text{CO}_3 + \text{CO} + \text{CO}$	2.64E-11	Rickard and Pascoe (2009)
G45227	TrGTerC	$\text{C514O2} + \text{HO}_2 \rightarrow \text{C514OOH}$	KR02H02(5)	Rickard and Pascoe (2009)
G45228a	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N0*(1.-alpha_AN(7,2,0,1,0, temp,cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G45228b	TrGTerCN	$\text{C514O2} + \text{NO} \rightarrow \text{C514NO3}$	KR02N0*alpha_AN(7,2,0,1,0,temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45229	TrGTerCN	$\text{C514O2} + \text{NO}_3 \rightarrow \text{CO13C4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G45230	TrGTerC	$\text{C514O2} \rightarrow \text{CO13C4CHO} + \text{HO}_2$	k1_R02sR02	Rickard and Pascoe (2009)
G45231	TrGTerC	$\text{C514OOH} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{OH}$	1.10E-10	Rickard and Pascoe (2009)
G45232	TrGTerCN	$\text{C514NO3} + \text{OH} \rightarrow \text{CO13C4CHO} + \text{NO}_2$	4.33E-11	Rickard and Pascoe (2009)
G45233	TrGTerC	$\text{CHOC3COOOH} + \text{OH} \rightarrow \text{CHOC3COCO3}$	7.55E-11	Rickard and Pascoe (2009)
G45234	TrGTerCN	$\text{CHOC3COPAN} \rightarrow \text{CHOC3COCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G45235	TrGTerCN	$\text{CHOC3COPAN} + \text{OH} \rightarrow \text{C4CODIAL} + \text{CO} + \text{NO}_2$	7.19E-11	Rickard and Pascoe (2009)
G45236	TrGTerC	$\text{MBO} + \text{OH} \rightarrow \text{LMBOABO2}$	8.1E-12*EXP(610./TEMP)	Rickard and Pascoe (2009), Taraborrelli (2016)*
G45237a	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{HCHO} + .16 \text{CH}_3\text{COCH}_3 + .16 \text{HO}_2 + .16 \text{CO} + .16 \text{OH} + .84 \text{MBOOO}$	1.0E-17*0.57	Rickard and Pascoe (2009), Taraborrelli (2016)
G45237b	TrGTerC	$\text{MBO} + \text{O}_3 \rightarrow \text{IBUTALOH} + .63 \text{CO} + .37 \text{HOCH}_2\text{OOH} + .16 \text{OH} + .16 \text{HO}_2$	1.0E-17*0.43	Rickard and Pascoe (2009), Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G45238	TrGTerCN	$\text{MBO} + \text{NO}_3 \rightarrow \text{LNMBOABO}_2$	$4.6\text{E-}14 \cdot \text{EXP}(-400./\text{TEMP})$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45239	TrGTerC	$\text{LMBOABO}_2 + \text{HO}_2 \rightarrow \text{LMBOABOOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45240a	TrGTerCN	$\text{LMBOABO}_2 + \text{NO} \rightarrow \text{LMBOABNO}_3$	$\text{KR02N0} * (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45240b	TrGTerCN	$\text{LMBOABO}_2 + \text{NO} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .67$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45240c	TrGTerCN	$\text{LMBOABO}_2 + \text{NO} \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0} * (1 - (.67 * \alpha_{\text{AN}}(7, 2, 0, 0, 0, \text{temp}, \text{cair}) + .33 * \alpha_{\text{AN}}(7, 1, 0, 0, 0, \text{temp}, \text{cair}))) * .33$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45241a	TrGTerC	$\text{LMBOABO}_2 \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2$	$\text{k1\_R02s0R02} * .67$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45241b	TrGTerC	$\text{LMBOABO}_2 \rightarrow \text{IBUTALOH} + \text{HCHO} + \text{HO}_2$	$\text{k1\_R02p0R02} * .33$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45242a	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{MBOACO}$	$.67 * 2.93\text{E-}11 + .33 * 2.05\text{E-}12$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45242b	TrGTerC	$\text{LMBOABOOH} + \text{OH} \rightarrow \text{LMBOABO}_2$	$.6 * \text{k\_CH300H\_OH}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45243	TrGTerCN	$\text{LMBOABNO}_3 + \text{OH} \rightarrow \text{MBOACO} + \text{NO}_2$	$.67 * 1.75\text{E-}12 + .33 * 2.69\text{E-}12$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45244	TrGTerC	$\text{MBOACO} + \text{OH} \rightarrow \text{MBOCOCO} + \text{HO}_2$	$3.79\text{E-}12$	Rickard and Pascoe (2009)
G45245	TrGTerC	$\text{MBOCOCO} + \text{OH} \rightarrow \text{CO} + \text{IPRHOCO}_3$	$1.38\text{E-}11$	Rickard and Pascoe (2009)
G45246	TrGTerCN	$\text{LNMBOABO}_2 + \text{HO}_2 \rightarrow \text{LNMBOABOOH}$	$\text{KR02H02}(5)$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45247	TrGTerCN	$\text{LNMBOABO}_2 + \text{NO} \rightarrow .65 \text{NO}_3\text{CH}_2\text{CHO} + .65 \text{CH}_3\text{COCH}_3 + .65 \text{HO}_2 + .35 \text{IBUTALOH} + .35 \text{HCHO} + .35 \text{NO}_2 + \text{NO}_2$	$\text{KR02N0}$	Rickard and Pascoe (2009), Taraborrelli (2016)*
G45248	TrGTerCN	$\text{LNMBOABO}_2 + \text{NO}_3 \rightarrow .65 \text{NO}_3\text{CH}_2\text{CHO} + .65 \text{CH}_3\text{COCH}_3 + .65 \text{HO}_2 + .35 \text{IBUTALOH} + .35 \text{HCHO} + .35 \text{NO}_2 + \text{NO}_2$	$\text{KR02N03}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G45249	TrGTerCN	$\text{LNMBOABO}_2 \rightarrow .65 \text{NO}_3\text{CH}_2\text{CHO} + .65 \text{CH}_3\text{COCH}_3 + .65 \text{HO}_2 + .35 \text{IBUTALOH} + .35 \text{HCHO} + .35 \text{NO}_2$	$\text{k1\_R02s0R02}$	Rickard and Pascoe (2009), Taraborrelli (2016)



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

#	labels	reaction	rate coefficient	reference
G45250a	TrGTerCN	LNMBOABOOH + OH $\rightarrow$ .65 C4MCONO3OH + .35 NMBOBOCO	.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45250b	TrGTerCN	LNMBOABOOH + OH $\rightarrow$ LNMBOABO2	.6*k_CH300H_OH	Rickard and Pascoe (2009), Taraborrelli (2016)
G45251	TrGTerCN	NMBOBOCO + OH $\rightarrow$ NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45252a	TrGTerCN	NC4OHCO3 + HO <sub>2</sub> $\rightarrow$ IBUTALOH + CO <sub>2</sub> + NO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45252b	TrGTerCN	NC4OHCO3 + HO <sub>2</sub> $\rightarrow$ NC4OHCO3H	KAPH02*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45253	TrGTerCN	NC4OHCO3 + NO $\rightarrow$ IBUTALOH + CO <sub>2</sub> + NO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G45254	TrGTerCN	NC4OHCO3 + NO <sub>2</sub> $\rightarrow$ NC4OHCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45255	TrGTerCN	NC4OHCO3 + NO <sub>3</sub> $\rightarrow$ IBUTALOH + CO <sub>2</sub> + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G45256	TrGTerCN	NC4OHCO3 $\rightarrow$ IBUTALOH + CO <sub>2</sub> + NO <sub>2</sub>	k1_R02RCO3	Rickard and Pascoe (2009)
G45257	TrGTerCN	NC4OHCO3H + OH $\rightarrow$ NC4OHCO3	4.50E-12	Rickard and Pascoe (2009)
G45258	TrGTerCN	NC4OHCPAN + OH $\rightarrow$ IBUTALOH + CO + NO <sub>2</sub> + NO <sub>2</sub>	1.27E-12	Rickard and Pascoe (2009)
G45259	TrGTerCN	NC4OHCPAN $\rightarrow$ NC4OHCO3 + NO <sub>2</sub>	K_PAN_M	Rickard and Pascoe (2009)
G45260	TrGTerCN	C4MCONO3OH + OH $\rightarrow$ CH <sub>3</sub> COCH <sub>3</sub> + HCHO + CO <sub>2</sub> + NO <sub>2</sub>	1.23E-12	Rickard and Pascoe (2009), Taraborrelli (2016)
G45400	TrGAroCN	NC4MDCO2HN + OH $\rightarrow$ MMALANHY + NO <sub>2</sub>	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G45401	TrGAroCN	C54CO + NO <sub>3</sub> $\rightarrow$ 3 CO + CH <sub>3</sub> C(O)OO + HNO <sub>3</sub>	KN03AL*5.5	Rickard and Pascoe (2009)
G45402	TrGAroC	C54CO + OH $\rightarrow$ 3 CO + CH <sub>3</sub> C(O)OO	1.72E-11	Rickard and Pascoe (2009)
G45403a	TrGAroCN	NTLFUO2 + HO <sub>2</sub> $\rightarrow$ NTLFUOOH	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G45403b	TrGAroCN	NTLFUO2 + HO <sub>2</sub> $\rightarrow$ ACCOMECHO + NO <sub>2</sub> + OH	KR02H02(5)*rcoch2o2_oh	Rickard and Pascoe (2009)
G45404	TrGAroCN	NTLFUO2 + NO $\rightarrow$ ACCOMECHO + NO <sub>2</sub> + NO <sub>2</sub>	KR02NO	Rickard and Pascoe (2009)*
G45405	TrGAroCN	NTLFUO2 + NO <sub>3</sub> $\rightarrow$ ACCOMECHO + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G45406	TrGAroCN	NTLFUO2 $\rightarrow$ ACCOMECHO + NO <sub>2</sub>	k1_R02t0R02	Rickard and Pascoe (2009)*
G45407	TrGAroC	C5134CO2OH + OH $\rightarrow$ C54CO + HO <sub>2</sub>	7.48E-11	Rickard and Pascoe (2009)
G45408	TrGAroCN	C5COO2NO2 + OH $\rightarrow$ MGLYOX + CO + CO + NO <sub>2</sub>	5.43E-11	Rickard and Pascoe (2009)
G45409	TrGAroCN	C5COO2NO2 $\rightarrow$ C5CO14O2 + NO <sub>2</sub>	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 <sub>2</sub> $\rightarrow$ C4CO2DCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45411b	TrGAroC	C4CO2DBCO3 + HO <sub>2</sub> $\rightarrow$ HO <sub>2</sub> + CO + HCOCOCHO + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G45412	TrGAroCN	C4CO2DBCO3 + NO $\rightarrow$ HO <sub>2</sub> + CO + HCOCOCHO + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45413	TrGAroCN	$\text{C4CO2DBCO3} + \text{NO}_2 \rightarrow \text{C4CO2DBPAN}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45414	TrGAroCN	$\text{C4CO2DBCO3} + \text{NO}_3 \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G45415	TrGAroC	$\text{C4CO2DBCO3} \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCOCHO} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G45416	TrGAroC	$\text{MMALANHY} + \text{OH} \rightarrow \text{MMALANHYO2}$	1.50E-12	Rickard and Pascoe (2009)
G45421a	TrGAroC	$\text{MMALANHYO2} + \text{HO}_2 \rightarrow \text{MMALNHYOOH}$	KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45421b	TrGAroC	$\text{MMALANHYO2} + \text{HO}_2 \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{OH}$	KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G45422	TrGAroCN	$\text{MMALANHYO2} + \text{NO} \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45423	TrGAroCN	$\text{MMALANHYO2} + \text{NO}_3 \rightarrow \text{CO2H3CO3} + \text{CO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45424	TrGAroC	$\text{MMALANHYO2} \rightarrow \text{CO2H3CO3} + \text{CO}_2$	k1_R02t0R02	Rickard and Pascoe (2009)*
G45428	TrGAroCN	$\text{C4CO2DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CO}_2 + \text{CO} + \text{NO}_2$	2.74E-11	Rickard and Pascoe (2009)
G45429	TrGAroCN	$\text{C4CO2DBPAN} \rightarrow \text{C4CO2DBCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)*
G45430a	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)*
G45430b	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow \text{C5CO14OH} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G45430c	TrGAroC	$\text{C5CO14O2} + \text{HO}_2 \rightarrow \text{C5CO14OOH}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G45431	TrGAroCN	$\text{C5CO14O2} + \text{NO} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)*
G45432	TrGAroCN	$\text{C5CO14O2} + \text{NO}_2 \rightarrow \text{C5COO2NO2}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45433	TrGAroCN	$\text{C5CO14O2} + \text{NO}_3 \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)*
G45434	TrGAroC	$\text{C5CO14O2} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)*
G45436	TrGAroC	$\text{C5CO14OH} + \text{OH} \rightarrow .83 \text{ MALANHY} + .83 \text{ CH}_3 + .17 \text{ MGLYOX} + .17 \text{ HO}_2 + .17 \text{ CO} + .17 \text{ CO}_2$	5.44E-11	Rickard and Pascoe (2009)*
G45441	TrGAroCN	$\text{C5DICARB} + \text{NO}_3 \rightarrow \text{C5CO14O2} + \text{HNO}_3$	KN03AL*2.75	Rickard and Pascoe (2009)
G45442	TrGAroC	$\text{C5DICARB} + \text{O}_3 \rightarrow .5338 \text{ GLYOX} + .063 \text{ CH}_3\text{CHO} + .348 \text{ CH}_3\text{C(O)OO} + .918 \text{ CO} + .57 \text{ OH} + .473 \text{ HO}_2 + .0563 \text{ CH}_3\text{COCO}_2\text{H} + .5338 \text{ MGLYOX} + .676 \text{ H}_2\text{O}_2 + .063 \text{ HCHO} + .0563 \text{ HCOCO}_2\text{H} + .2465 \text{ CO}_2$	2.00E-18	Rickard and Pascoe (2009)
G45443	TrGAroC	$\text{C5DICARB} + \text{OH} \rightarrow .48 \text{ C5CO14O2} + .52 \text{ C5DICARBO2}$	6.2E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45444	TrGAroC	MC3ODBCO2H + OH $\rightarrow$ .35 GLYOX + .35 CH <sub>3</sub> + .35 CO + .35 CO <sub>2</sub> + .65 MMALANHY + .65 HO <sub>2</sub>	4.38E-11	Rickard and Pascoe (2009)*
G45451	TrGAroCN	TLFUONE + NO <sub>3</sub> $\rightarrow$ NTLFUO2	1.00E-12	Rickard and Pascoe (2009)
G45452	TrGAroC	TLFUONE + O <sub>3</sub> $\rightarrow$ .5 CO + .5 OH + .5 MECOACETO2 + .3125 C24O3CCO2H + .1875 ACCOMECHO + .1875 H <sub>2</sub> O <sub>2</sub>	8.00E-19	see note*
G45453	TrGAroC	TLFUONE + OH $\rightarrow$ TLFUO2	6.90E-11	Rickard and Pascoe (2009)
G45454a	TrGAroC	ACCOMECO3 + HO <sub>2</sub> $\rightarrow$ ACCOMECHO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G45454b	TrGAroC	ACCOMECO3 + HO <sub>2</sub> $\rightarrow$ MECOACETO2 + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G45455	TrGAroCN	ACCOMECO3 + NO $\rightarrow$ MECOACETO2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G45456	TrGAroCN	ACCOMECO3 + NO <sub>2</sub> $\rightarrow$ ACCOMECHAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G45457	TrGAroCN	ACCOMECO3 + NO <sub>3</sub> $\rightarrow$ MECOACETO2 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G45458	TrGAroC	ACCOMECO3 $\rightarrow$ MECOACETO2 + CO <sub>2</sub>	k1_R02RCO3	Rickard and Pascoe (2009)
G45459	TrGAroC	C4CO2DCO3H + OH $\rightarrow$ C4CO2DBC03	3.06E-11	Rickard and Pascoe (2009)
G45464	TrGAroCN	ACCOMETCHO + NO <sub>3</sub> $\rightarrow$ ACCOMECHO3 + HNO <sub>3</sub>	KN03AL*5.5	Rickard and Pascoe (2009)
G45465	TrGAroC	ACCOMETCHO + OH $\rightarrow$ ACCOMECHO3	7.09E-11	Rickard and Pascoe (2009)
G45466	TrGAroC	MMALNHYOOH + OH $\rightarrow$ MMALANHYO2	1.69E-11	Rickard and Pascoe (2009)
G45467a	TrGAroC	C5DICAROOH + OH $\rightarrow$ C5134CO2OH + OH	1.21E-10	Rickard and Pascoe (2009)
G45467b	TrGAroC	C5DICAROOH + OH $\rightarrow$ C5DICARBO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G45468	TrGAroC	C24O3CCO2H + OH $\rightarrow$ MECOACETO2 + CO <sub>2</sub>	8.76E-13	Rickard and Pascoe (2009)
G45469	TrGAroCN	NTLFUOOH + OH $\rightarrow$ NTLFUO2	4.44E-12	Rickard and Pascoe (2009)
G45470	TrGAroCN	ACCOMEPAN + OH $\rightarrow$ METACETHO + CO + CO + NO <sub>2</sub>	1.00E-14	Rickard and Pascoe (2009)
G45471	TrGAroCN	ACCOMEPAN $\rightarrow$ ACCOMECHO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G45476a	TrGAroC	TLFUO2 + HO <sub>2</sub> $\rightarrow$ TLFUOOH	KR02H02(5)*(1-rcoch2o2_oh-rchohch2o2_oh)	Rickard and Pascoe (2009)
G45476b	TrGAroC	TLFUO2 + HO <sub>2</sub> $\rightarrow$ ACCOMECHO + HO <sub>2</sub> + OH	KR02H02(5)*(rcoch2o2_oh+rchohch2o2_oh)	Rickard and Pascoe (2009)*
G45477	TrGAroCN	TLFUO2 + NO $\rightarrow$ ACCOMECHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G45478	TrGAroCN	TLFUO2 + NO <sub>3</sub> $\rightarrow$ ACCOMECHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G45479	TrGAroC	TLFUO2 $\rightarrow$ ACCOMECHO + HO <sub>2</sub>	k1_R02t0R02	Rickard and Pascoe (2009)*
G45480	TrGAroC	C5CO14OOH + OH $\rightarrow$ C5CO14O2	3.59E-12	Rickard and Pascoe (2009)
G45483	TrGAroC	TLFUOOH + OH $\rightarrow$ TLFUO2	2.53E-11	Rickard and Pascoe (2009)
G45485	TrGAroC	ACCOMECO3H + OH $\rightarrow$ ACCOMECHO3	3.59E-12	Rickard and Pascoe (2009)
G45486a	TrGAroC	C5DIALO2 + HO <sub>2</sub> $\rightarrow$ C5DIALOOH	KR02H02(5)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45486b	TrGAroC	$\text{C5DIALO2} + \text{HO}_2 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(5)*rcoch2o2\_oh}$	Rickard and Pascoe (2009)*
G45487	TrGAroCN	$\text{C5DIALO2} + \text{NO} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45488	TrGAroCN	$\text{C5DIALO2} + \text{NO}_3 \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45489	TrGAroC	$\text{C5DIALO2} \rightarrow \text{MALDIAL} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G45490a	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{C5DICAROOH}$	$\text{KR02H02(5)*(rco3\_ooh+rco3\_o3)}$	Rickard and Pascoe (2009)
G45491b	TrGAroC	$\text{C5DICARBO2} + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(5)*rco3\_oh}$	Rickard and Pascoe (2009)*
G45492	TrGAroCN	$\text{C5DICARBO2} + \text{NO} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G45493	TrGAroCN	$\text{C5DICARBO2} + \text{NO}_3 \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G45494	TrGAroC	$\text{C5DICARBO2} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46200a	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO235C6OOH}$	$\text{KR02H02(6)*rcoch2o2\_ooh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G46200b	TrGTerC	$\text{CO235C6O2} + \text{HO}_2 \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$	$\text{KR02H02(6)*rcoch2o2\_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G46201	TrGTerCN	$\text{CO235C6O2} + \text{NO} \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46202	TrGTerC	$\text{CO235C6O2} \rightarrow \text{CO23C4CO3} + \text{HCHO}$	k1_R02p0R02	Rickard and Pascoe (2009)
G46203	TrGTerC	$\text{CO235C6OOH} + \text{OH} \rightarrow \text{CO235C6O2}$	1.01E-11	Rickard and Pascoe (2009)
G46204	TrGTerC	$\text{C614O2} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)
G46205a	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{KR02N0*(1.-alpha\_AN(9,2,0,1,0,temp,cair))}$	Rickard and Pascoe (2009)
G46205b	TrGTerCN	$\text{C614O2} + \text{NO} \rightarrow \text{C614NO3}$	$\text{KR02N0*alpha\_AN(9,2,0,1,0,temp,cair)}$	Rickard and Pascoe (2009)
G46206a	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{C614OOH}$	$\text{KR02H02(6)*(1.-rchohch2o2\_oh)}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G46206b	TrGTerC	$\text{C614O2} + \text{HO}_2 \rightarrow \text{CO23C4CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(6)*rchohch2o2\_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G46207	TrGTerCN	$\text{C614NO3} + \text{OH} \rightarrow \text{C614CO} + \text{NO}_2$	7.11E-12	Rickard and Pascoe (2009)
G46208	TrGTerC	$\text{C614OOH} + \text{OH} \rightarrow \text{C614CO} + \text{OH}$	8.69E-11	Rickard and Pascoe (2009)
G46209	TrGTerC	$\text{C614CO} + \text{OH} \rightarrow \text{CO235C5CHO} + \text{HO}_2$	3.22E-12	Rickard and Pascoe (2009)
G46210	TrGTerC	$\text{CO235C5CHO} + \text{OH} \rightarrow \text{CO23C4CO3} + \text{CO}$	1.33E-11	Rickard and Pascoe (2009)
G46211	TrGTerCN	$\text{CO235C5CHO} + \text{NO}_3 \rightarrow \text{CO23C4CO3} + \text{CO} + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G46400	TrGAroC	$\text{PHENO OH} + \text{OH} \rightarrow \text{PHENO2}$	1.16E-10	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46401	TrGAroC	$\text{C6CO4DB} + \text{OH} \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{CO} + \text{HCOCOCHO}$	7.70E-11	Rickard and Pascoe (2009)
G46402	TrGAroC	$\text{C5CO2DCO3H} + \text{OH} \rightarrow \text{C5CO2DBCO3}$	3.60E-11	Rickard and Pascoe (2009)
G46403	TrGAroCN	$\text{NDNPHENOOH} + \text{OH} \rightarrow \text{NDNPHENO2}$	$0.6 \cdot k_{\text{CH300H\_OH}}$	Rickard and Pascoe (2009)
G46404a	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C615CO2OOH}$	$\text{KR02H02(6)} \cdot (1 - \text{rcoch2o2\_oh})$	Rickard and Pascoe (2009)
G46404b	TrGAroC	$\text{C615CO2O2} + \text{HO}_2 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{KR02H02(6)} \cdot \text{rcoch2o2\_oh}$	Rickard and Pascoe (2009)*
G46405	TrGAroCN	$\text{C615CO2O2} + \text{NO} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46406	TrGAroCN	$\text{C615CO2O2} + \text{NO}_3 \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46407	TrGAroC	$\text{C615CO2O2} \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46408	TrGAroCN	$\text{BZEMUCPAN} + \text{OH} \rightarrow \text{MALDIAL} + \text{CO} + \text{CO}_2 + \text{NO}_2$	4.05E-11	Rickard and Pascoe (2009)
G46409	TrGAroCN	$\text{BZEMUCPAN} \rightarrow \text{BZEMUCCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46410	TrGAroCN	$\text{BZBIPERNO3} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{NO}_2$	7.30E-11	Rickard and Pascoe (2009)
G46411	TrGAroCN	$\text{HOC6H4NO2} + \text{NO}_3 \rightarrow \text{NPHEN1O} + \text{HNO}_3$	9.00E-14	Rickard and Pascoe (2009)
G46412	TrGAroCN	$\text{HOC6H4NO2} + \text{OH} \rightarrow \text{NPHEN1O}$	9.00E-13	Rickard and Pascoe (2009)
G46413a	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NDNPHENOOH}$	$\text{KR02H02(6)} \cdot (1 - \text{rchohch2o2\_oh})$	Rickard and Pascoe (2009)
G46413b	TrGAroCN	$\text{NDNPHENO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	$\text{KR02H02(6)} \cdot \text{rchohch2o2\_oh}$	Rickard and Pascoe (2009)*
G46414	TrGAroCN	$\text{NDNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46415	TrGAroCN	$\text{NDNPHENO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46416	TrGAroCN	$\text{NDNPHENO2} \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2$	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46417	TrGAroC	$\text{PBZQCO} + \text{OH} \rightarrow \text{C5CO2OHCO3}$	6.07E-11	Rickard and Pascoe (2009)
G46418	TrGAroCN	$\text{CATECHOL} + \text{NO}_3 \rightarrow \text{CATEC1O} + \text{HNO}_3$	9.9E-11	Rickard and Pascoe (2009)*
G46419	TrGAroC	$\text{CATECHOL} + \text{O}_3 \rightarrow \text{MALDALCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	9.2E-18	Rickard and Pascoe (2009)
G46420	TrGAroC	$\text{CATECHOL} + \text{OH} \rightarrow \text{CATEC1O}$	1.0E-10	Rickard and Pascoe (2009)
G46421	TrGAroC	$\text{C5COOHCO3H} + \text{OH} \rightarrow \text{C5CO2OHCO3}$	8.01E-11	Rickard and Pascoe (2009)
G46422	TrGAroCN	$\text{NCATECHOL} + \text{NO}_3 \rightarrow \text{NNCATECO2}$	2.60E-12	Rickard and Pascoe (2009)
G46423	TrGAroCN	$\text{NCATECHOL} + \text{OH} \rightarrow \text{NCATECO2}$	3.47E-12	Rickard and Pascoe (2009)
G46424a	TrGAroC	$\text{C5CO2OHCO3} + \text{HO}_2 \rightarrow \text{C5COOHCO3H}$	$\text{KAPH02} \cdot (\text{rco3\_ooh} + \text{rco3\_o3})$	Rickard and Pascoe (2009)
G46424b	TrGAroC	$\text{C5CO2OHCO3} + \text{HO}_2 \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	$\text{KAPH02} \cdot \text{rco3\_oh}$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46425	TrGAroCN	$\text{C5CO2OHCO3} + \text{NO} \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G46426	TrGAroCN	$\text{C5CO2OHCO3} + \text{NO}_2 \rightarrow \text{C5CO2OHPAN}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G46427	TrGAroCN	$\text{C5CO2OHCO3} + \text{NO}_3 \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G46428	TrGAroC	$\text{C5CO2OHCO3} \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2$	k1_R02RC03	Rickard and Pascoe (2009)
G46429	TrGAroCN	$\text{BZEPOXMUC} + \text{NO}_3 \rightarrow \text{BZEMUCCO3} + \text{HNO}_3$	2*KN03AL*2.75	Rickard and Pascoe (2009)
G46430	TrGAroC	$\text{BZEPOXMUC} + \text{O}_3 \rightarrow \text{EPXC4DIAL} + .125 \text{ HCHO} + .1125 \text{ HCOCO}_2\text{H} + .0675 \text{ GLYOX} + .0675 \text{ H}_2\text{O}_2 + .82 \text{ HO}_2 + .57 \text{ OH} + 1.265 \text{ CO} + .25 \text{ CO}_2$	2.00E-18	Rickard and Pascoe (2009)*
G46431	TrGAroC	$\text{BZEPOXMUC} + \text{OH} \rightarrow .31 \text{ BZEMUCCO3} + .69 \text{ BZEMUCO2}$	6.08E-11	Rickard and Pascoe (2009)
G46432a	TrGAroCN	$\text{NCATECO2} + \text{HO}_2 \rightarrow \text{NCATECOOH}$	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46432b	TrGAroCN	$\text{NCATECO2} + \text{HO}_2 \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46433	TrGAroCN	$\text{NCATECO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46434	TrGAroCN	$\text{NCATECO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46435	TrGAroCN	$\text{NCATECO2} \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2$	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46436	TrGAroCN	$\text{NPHEN1OOH} + \text{OH} \rightarrow \text{NPHEN1O2}$	9.00E-13	Rickard and Pascoe (2009)
G46437a	TrGAroCN	$\text{NPHENO2} + \text{HO}_2 \rightarrow \text{NPHENOOH}$	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46437b	TrGAroCN	$\text{NPHENO2} + \text{HO}_2 \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{NO}_2 + \text{OH}$	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46438	TrGAroCN	$\text{NPHENO2} + \text{NO} \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46439	TrGAroCN	$\text{NPHENO2} + \text{NO}_3 \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46440	TrGAroCN	$\text{NPHENO2} \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{NO}_2$	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46441	TrGAroC	$\text{BENZENE} + \text{OH} \rightarrow .352 \text{ BZBIPERO2} + .118 \text{ BZEPOXMUC} + .118 \text{ HO}_2 + .53 \text{ PHENOL} + .53 \text{ HO}_2$	2.3E-12*EXP(-190/TEMP)	Rickard and Pascoe (2009)*
G46442	TrGAroCN	$\text{C5CO2OHPAN} + \text{OH} \rightarrow \text{HOCOC4DIAL} + \text{CO} + \text{CO} + \text{NO}_2$	7.66E-11	Rickard and Pascoe (2009)
G46443	TrGAroCN	$\text{C5CO2OHPAN} \rightarrow \text{C5CO2OHCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46444	TrGAroCN	CATEC1O + NO <sub>2</sub> → NCATECHOL	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46445	TrGAroC	CATEC1O + O <sub>3</sub> → CATEC1O2	k_C6H50_03	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 <sub>2</sub> → NNCATECOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46447b	TrGAroCN	NNCATECO2 + HO <sub>2</sub> → NC4DCO2H + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46448	TrGAroCN	NNCATECO2 + NO → NC4DCO2H + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G46449	TrGAroCN	NNCATECO2 + NO <sub>3</sub> → NC4DCO2H + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G46450	TrGAroCN	NNCATECO2 → NC4DCO2H + HCOCO <sub>2</sub> H + NO <sub>2</sub>	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46451	TrGAroC	BZEMUCCO2H + OH → C5DIALO2 + CO <sub>2</sub>	4.06E-11	Rickard and Pascoe (2009)
G46452	TrGAroCN	NNCATECOOH + OH → NNCATECO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46453	TrGAroCN	NPHEN1O + NO <sub>2</sub> → DNPHEN	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G46454	TrGAroCN	NPHEN1O + O <sub>3</sub> → NPHEN1O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G46455	TrGAroCN	DNPHEN + NO <sub>3</sub> → NDNPHENO2	2.25E-15	Rickard and Pascoe (2009)
G46456	TrGAroCN	DNPHEN + OH → DNPHENO2	3.00E-14	Rickard and Pascoe (2009)
G46457	TrGAroCN	PHENOL + NO <sub>3</sub> → .742 C6H5O + .742 HNO <sub>3</sub> + .258 NPHENO2	3.8E-12	Rickard and Pascoe (2009)*
G46458	TrGAroC	PHENOL + OH → .06 C6H5O + .8 CATECHOL + .8 HO <sub>2</sub> + .14 PHENO2	4.7E-13*EXP(1220/TEMP)	Rickard and Pascoe (2009)*
G46459	TrGAroCN	PBZQONE + NO <sub>3</sub> → NBZQO2	3.00E-13	Rickard and Pascoe (2009)
G46460	TrGAroC	PBZQONE + OH → PBZQO2	4.6E-12	Rickard and Pascoe (2009)
G46461a	TrGAroC	PHENO2 + HO <sub>2</sub> → PHENO2OH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46461b	TrGAroC	PHENO2 + HO <sub>2</sub> → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO <sub>2</sub> + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G46462	TrGAroCN	PHENO2 + NO → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G46463	TrGAroCN	PHENO2 + NO <sub>3</sub> → .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G46464	TrGAroC	PHENO2 $\rightarrow$ .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO <sub>2</sub>	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G46465	TrGAroC	C615CO2OOH + OH $\rightarrow$ C6125CO + OH	9.42E-11	Rickard and Pascoe (2009)
G46466a	TrGAroC	C5CO2DBCO3 + HO <sub>2</sub> $\rightarrow$ C5CO2DCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G46466b	TrGAroC	C5CO2DBCO3 + HO <sub>2</sub> $\rightarrow$ CH <sub>3</sub> C(O) + HCOCOCHO + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46467	TrGAroCN	C5CO2DBCO3 + NO $\rightarrow$ CH <sub>3</sub> C(O) + HCOCOCHO + CO <sub>2</sub> + NO <sub>2</sub>	KAPN0	Rickard and Pascoe (2009)
G46468	TrGAroCN	C5CO2DBCO3 + NO <sub>2</sub> $\rightarrow$ C5CO2DBPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)*
G46469	TrGAroCN	C5CO2DBCO3 + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> C(O) + HCOCOCHO + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G46470	TrGAroC	C5CO2DBCO3 $\rightarrow$ CH <sub>3</sub> C(O) + HCOCOCHO + CO <sub>2</sub>	k1_R02RCO3	Rickard and Pascoe (2009)
G46471	TrGAroCN	NPHEN1O2 + HO <sub>2</sub> $\rightarrow$ NPHEN1OOH	KR02H02(6)	Rickard and Pascoe (2009)
G46472a	TrGAroCN	NPHEN1O2 + NO $\rightarrow$ NPHEN1O + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G46472b	TrGAroCN	NPHEN1O2 + NO <sub>2</sub> $\rightarrow$ NPHEN1O + NO <sub>3</sub>	k_C6H5O2_NO2	Jagiella and Zabel (2007)*
G46473	TrGAroCN	NPHEN1O2 + NO <sub>3</sub> $\rightarrow$ NPHEN1O + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G46474	TrGAroCN	NPHEN1O2 $\rightarrow$ NPHEN1O	k1_R02sR02	Rickard and Pascoe (2009)
G46475	TrGAroCN	NPHENOOH + OH $\rightarrow$ NPHENO2	1.07E-10	Rickard and Pascoe (2009)
G46476	TrGAroCN	C6H5O + NO <sub>2</sub> $\rightarrow$ HOC6H4NO2	k_C6H5O_NO2	Rickard and Pascoe (2009), Platz et al. (1998)*
G46477	TrGAroC	C6H5O + O <sub>3</sub> $\rightarrow$ C6H5O2	k_C6H5O_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G46478	TrGAroCN	NCATECOOH + OH $\rightarrow$ NCATECO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46479	TrGAroC	PBZQOOH + OH $\rightarrow$ PBZQCO + OH	1.23E-10	Rickard and Pascoe (2009)
G46480a	TrGAroC	PBZQO2 + HO <sub>2</sub> $\rightarrow$ PBZQOOH	KR02H02(6)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46480b	TrGAroC	PBZQO2 + HO <sub>2</sub> $\rightarrow$ C5CO2OHCO3 + OH	KR02H02(6)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G46481	TrGAroCN	PBZQO2 + NO $\rightarrow$ C5CO2OHCO3 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G46482	TrGAroCN	PBZQO2 + NO <sub>3</sub> $\rightarrow$ C5CO2OHCO3 + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G46483	TrGAroC	PBZQO2 $\rightarrow$ C5CO2OHCO3	k1_R02sOR02	Rickard and Pascoe (2009)*
G46484	TrGAroC	BZOBIPEROH + OH $\rightarrow$ MALDIALCO3 + GLYOX	8.16E-11	Rickard and Pascoe (2009)
G46485a	TrGAroCN	DNPHENO2 + HO <sub>2</sub> $\rightarrow$ DNPHENOOH	KR02H02(6)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G46485b	TrGAroCN	DNPHENO2 + HO <sub>2</sub> $\rightarrow$ NC4DCO2H + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	KR02H02(6)*rchohch2o2_oh	Rickard and Pascoe (2009)*



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

#	labels	reaction	rate coefficient	reference
G46486	TrGAroCN	$\text{DNPHENO2} + \text{NO} \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2$ + $\text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46487	TrGAroCN	$\text{DNPHENO2} + \text{NO}_3 \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2$ + $\text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46488	TrGAroCN	$\text{DNPHENO2} \rightarrow \text{NC4DCO2H} + \text{HCOCO2H} + \text{NO}_2$	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G46489	TrGAroC	$\text{BZBIPEROOH} + \text{OH} \rightarrow \text{BZOBIPEROH} + \text{OH}$	9.77E-11	Rickard and Pascoe (2009)
G46490a	TrGAroC	$\text{BZEMUCO2} + \text{HO}_2 \rightarrow \text{BZEMUCOOH}$	KR02H02(6)	Rickard and Pascoe (2009)
G46490b	TrGAroC	$\text{BZEMUCO2} + \text{HO}_2 \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5$ $\text{HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{OH}$	KR02H02(6)	Rickard and Pascoe (2009)*
G46491a	TrGAroCN	$\text{BZEMUCO2} + \text{NO} \rightarrow \text{BZEMUCNO3}$	KR02N0*alpha_AN(10,2,0,1,0, temp,cair)	Rickard and Pascoe (2009)
G46491b	TrGAroCN	$\text{BZEMUCO2} + \text{NO} \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5$ $\text{HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{NO}_2$	KR02N0*(1.-alpha_AN(10,2,0,1,0, temp,cair))	Rickard and Pascoe (2009)*
G46492	TrGAroCN	$\text{BZEMUCO2} + \text{NO}_3 \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5$ $\text{HO}_2 + .5 \text{ C3DIALO2} + .5 \text{ C32OH13CO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46493	TrGAroC	$\text{BZEMUCO2} \rightarrow .5 \text{ EPXC4DIAL} + .5 \text{ GLYOX} + .5 \text{ HO}_2 +$ $.5 \text{ C3DIALO2} + .5 \text{ C32OH13CO}$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46494	TrGAroCN	$\text{C5CO2DBPAN} + \text{OH} \rightarrow \text{HCOCOCHO} + \text{CH}_3\text{CHO} + \text{CO}_2$ + $\text{NO}_2$	3.28E-11	Rickard and Pascoe (2009)
G46495	TrGAroCN	$\text{C5CO2DBPAN} \rightarrow \text{C5CO2DBCO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G46496	TrGAroCN	$\text{NBZQOOH} + \text{OH} \rightarrow \text{NBZQO2}$	6.68E-11	Rickard and Pascoe (2009)
G46497	TrGAroC	$\text{CATEC1OOH} + \text{OH} \rightarrow \text{CATEC1O2}$	.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46498	TrGAroC	$\text{C6125CO} + \text{OH} \rightarrow \text{C5CO14O2} + \text{CO}$	6.45E-11	Rickard and Pascoe (2009)
G46499a	TrGAroCN	$\text{NBZQO2} + \text{HO}_2 \rightarrow \text{NBZQOOH}$	KR02H02(6)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G46499b	TrGAroCN	$\text{NBZQO2} + \text{HO}_2 \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$	KR02H02(6)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G46500	TrGAroCN	$\text{NBZQO2} + \text{NO} \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G46501	TrGAroCN	$\text{NBZQO2} + \text{NO}_3 \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)*
G46502	TrGAroCN	$\text{NBZQO2} \rightarrow \text{C6CO4DB} + \text{NO}_2$	k1_R02s0R02	Rickard and Pascoe (2009)*
G46503	TrGAroCN	$\text{DNPHENO2} + \text{OH} \rightarrow \text{DNPHENO2}$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G46504	TrGAroC	$\text{CATEC1O2} + \text{HO}_2 \rightarrow \text{CATEC1OOH}$	KR02H02(6)	Rickard and Pascoe (2009)
G46505a	TrGAroCN	$\text{CATEC1O2} + \text{NO} \rightarrow \text{CATEC1O} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G46505b	TrGAroCN	$\text{CATEC1O2} + \text{NO}_2 \rightarrow \text{CATEC1O} + \text{NO}_3$	K_C6H502_N02	Jagiella and Zabel (2007)*
G46506	TrGAroCN	$\text{CATEC1O2} + \text{NO}_3 \rightarrow \text{CATEC1O} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G46507	TrGAroC	$\text{CATEC1O2} \rightarrow \text{CATEC1O}$	k1_R02s0R02	Rickard and Pascoe (2009)
G46508	TrGAroC	$\text{BZEMUCCO3H} + \text{OH} \rightarrow \text{BZEMUCCO3}$	4.37E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G46509	TrGAroC	$\text{C6H5OOH} + \text{OH} \rightarrow \text{C6H5O2}$	3.60E-12	Rickard and Pascoe (2009)
G46510	TrGAroC	$\text{BZEMUCOOH} + \text{OH} \rightarrow \text{BZEMUCCO} + \text{OH}$	1.31E-10	Rickard and Pascoe (2009)
G46511a	TrGAroC	$\text{BZEMUCCO3} + \text{HO}_2 \rightarrow \text{BZEMUCCO2H} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G46511b	TrGAroC	$\text{BZEMUCCO3} + \text{HO}_2 \rightarrow \text{BZEMUCCO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G46511c	TrGAroC	$\text{BZEMUCCO3} + \text{HO}_2 \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G46512	TrGAroCN	$\text{BZEMUCCO3} + \text{NO} \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G46513	TrGAroCN	$\text{BZEMUCCO3} + \text{NO}_2 \rightarrow \text{BZEMUCPAN}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G46514	TrGAroCN	$\text{BZEMUCCO3} + \text{NO}_3 \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G46515	TrGAroC	$\text{BZEMUCCO3} \rightarrow \text{C5DIALO2} + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)*
G46516	TrGAroC	$\text{C6H5O2} + \text{HO}_2 \rightarrow \text{C6H5OOH}$	KR02H02(6)	Rickard and Pascoe (2009)
G46517a	TrGAroCN	$\text{C6H5O2} + \text{NO} \rightarrow \text{C6H5O} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)
G46517b	TrGAroCN	$\text{C6H5O2} + \text{NO}_2 \rightarrow \text{C6H5O} + \text{NO}_3$	K_C6H5O2_NO2	Jagiella and Zabel (2007)*
G46518	TrGAroCN	$\text{C6H5O2} + \text{NO}_3 \rightarrow \text{C6H5O} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G46519	TrGAroC	$\text{C6H5O2} \rightarrow \text{C6H5O}$	k1_R02sR02	Rickard and Pascoe (2009)
G46521	TrGAroCN	$\text{BZEMUCNO3} + \text{OH} \rightarrow \text{BZEMUCCO} + \text{NO}_2$	4.38E-11	Rickard and Pascoe (2009)
G46522a	TrGAroC	$\text{BZBIPERO2} + \text{HO}_2 \rightarrow \text{BZBIPEROOH}$	KR02H02(6)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G46522b	TrGAroC	$\text{BZBIPERO2} + \text{HO}_2 \rightarrow \text{OH} + \text{GLYOX} + \text{HO}_2 + .5$ $\text{BZFUONE} + .5 \text{BZFUONE}$	KR02H02(6)*rbipero2_oh	Rickard and Pascoe (2009), Bird- sall et al. (2010)*
G46523a	TrGAroCN	$\text{BZBIPERO2} + \text{NO} \rightarrow \text{BZBIPERNO3}$	KR02N0*alpha_AN(9,2,0,0,1,temp, cair)	Rickard and Pascoe (2009)
G46523b	TrGAroCN	$\text{BZBIPERO2} + \text{NO} \rightarrow \text{NO}_2 + \text{GLYOX} + \text{HO}_2 + .5$ $\text{BZFUONE} + .5 \text{BZFUONE}$	KR02N0*(1.-alpha_AN(9,2,0,0,1, temp,cair))	Rickard and Pascoe (2009)*
G46524	TrGAroCN	$\text{BZBIPERO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{GLYOX} + \text{HO}_2 + .5$ $\text{BZFUONE} + .5 \text{BZFUONE}$	KR02N03	Rickard and Pascoe (2009)*
G46525	TrGAroC	$\text{BZBIPERO2} \rightarrow \text{GLYOX} + \text{HO}_2 + \text{BZFUONE}$	k1_R02sOR02	Rickard and Pascoe (2009)*
G47200	TrGTerCN	$\text{CO235C6CHO} + \text{NO}_3 \rightarrow \text{CO235C6CO3} + \text{HNO}_3$	KN03AL*5.5	Rickard and Pascoe (2009)
G47201	TrGTerC	$\text{CO235C6CHO} + \text{OH} \rightarrow \text{CO235C6CO3}$	6.70E-11	Rickard and Pascoe (2009)
G47202a	TrGTerC	$\text{CO235C6CO3} + \text{HO}_2 \rightarrow \text{C235C6CO3H}$	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47202b	TrGTerC	$\text{CO235C6CO3} + \text{HO}_2 \rightarrow \text{CO235C6O2} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47203	TrGTerCN	$\text{CO235C6CO3} + \text{NO} \rightarrow \text{CO235C6O2} + \text{CO}_2 + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009)
G47204	TrGTerCN	$\text{CO235C6CO3} + \text{NO}_2 \rightarrow \text{C7PAN3}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G47205	TrGTerC	$\text{CO235C6CO3} \rightarrow \text{CO235C6O2} + \text{CO}_2$	k1_R02RCO3	Rickard and Pascoe (2009)
G47206	TrGTerC	$\text{C235C6CO3H} + \text{OH} \rightarrow \text{CO235C6CO3}$	4.75E-12	Rickard and Pascoe (2009)
G47207	TrGTerCN	$\text{C7PAN3} + \text{OH} \rightarrow \text{CO235C5CHO} + \text{CO} + \text{NO}_2$	8.83E-13	Rickard and Pascoe (2009)
G47208	TrGTerCN	$\text{C7PAN3} \rightarrow \text{CO235C6CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47209a	TrGTerC	$C716O2 + HO_2 \rightarrow C716OOH$	$KR02H02(7)*rcoch2o2\_ooh$	Rickard and Pascoe (2009), Taraborrelli (2016)
G47209b	TrGTerC	$C716O2 + HO_2 \rightarrow CO13C4CHO + CH_3C(O) + OH$	$KR02H02(7)*rcoch2o2\_oh$	Rickard and Pascoe (2009), Taraborrelli (2016)
G47210	TrGTerCN	$C716O2 + NO \rightarrow CO13C4CHO + CH_3C(O) + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G47211	TrGTerC	$C716O2 \rightarrow CO13C4CHO + CH_3C(O)$	k1_R02s0R02	Rickard and Pascoe (2009)
G47212	TrGTerC	$C716OOH + OH \rightarrow CO235C6CHO + OH$	1.20E-10	Rickard and Pascoe (2009)
G47213	TrGTerC	$C721O2 + HO_2 \rightarrow C721OOH$	KR02H02(7)	Rickard and Pascoe (2009)
G47214	TrGTerCN	$C721O2 + NO \rightarrow C722O2 + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G47215	TrGTerC	$C721O2 \rightarrow C722O2$	k1_R02pR02	Rickard and Pascoe (2009)
G47216	TrGTerC	$C721OOH + OH \rightarrow C721O2$	1.27E-11	Rickard and Pascoe (2009)
G47217	TrGTerC	$C722O2 + HO_2 \rightarrow C722OOH$	KR02H02(7)	Rickard and Pascoe (2009)
G47218	TrGTerCN	$C722O2 + NO \rightarrow CH_3COCH_3 + C44O2 + NO_2$	KR02N0	Rickard and Pascoe (2009)*
G47219	TrGTerC	$C722O2 \rightarrow CH_3COCH_3 + C44O2$	k1_R02tR02	Rickard and Pascoe (2009)
G47220	TrGTerC	$C722OOH + OH \rightarrow C722O2$	3.31E-11	Rickard and Pascoe (2009)
G47221	TrGTerC	$ROO6R3O2 \rightarrow ROO6R5O2$	$5.68E10*EXP(-8745./TEMP)$	Vereecken and Peeters (2012)
G47222	TrGTerCN	$ROO6R3O2 + NO \rightarrow ROO6R3O + NO_2$	KR02N0	Vereecken and Peeters (2012)*
G47223	TrGTerC	$ROO6R3O2 + HO_2 \rightarrow 7\text{ L CARBON}$	KR02H02(7)	Vereecken and Peeters (2012)*
G47224	TrGTerC	$ROO6R3O2 \rightarrow ROO6R3O$	k1_R02sR02	Vereecken and Peeters (2012)
G47225	TrGTerC	$ROO6R3O \rightarrow 7\text{ L CARBON} + HO_2$	$5.7E10*EXP(-2949./TEMP)$	Vereecken and Peeters (2012)*
G47226	TrGTerC	$ROO6R5O2 \rightarrow 7\text{ L CARBON} + OH$	$9.17E10*EXP(-8706./TEMP)$	Vereecken and Peeters (2012)*
G47400	TrGAroC	$TOLUENE + OH \rightarrow .07\text{ C6H5CH2O2} + .18\text{ CRESOL} + .18\text{ HO}_2 + .65\text{ TLBIPERO2} + .10\text{ TLEPOXMUC} + .10\text{ HO}_2$	$1.8E-12*EXP(340/TEMP)$	Rickard and Pascoe (2009)*
G47401	TrGAroC	$C6H5CH2O2 + HO_2 \rightarrow C6H5CH2OOH$	$1.5E-13*EXP(1310/TEMP)$	Rickard and Pascoe (2009)
G47402a	TrGAroCN	$C6H5CH2O2 + NO \rightarrow C6H5CH2NO3$	$KR02N0*\alpha\_AN(7,1,0,0,0,temp, cair)$	Rickard and Pascoe (2009)*
G47402b	TrGAroCN	$C6H5CH2O2 + NO \rightarrow BENZAL + HO_2 + NO_2$	$KR02N0*(1.-\alpha\_AN(7,1,0,0,0,temp, cair))$	Rickard and Pascoe (2009)*
G47403	TrGAroCN	$C6H5CH2O2 + NO_3 \rightarrow BENZAL + HO_2 + NO_2$	KR02N03	Rickard and Pascoe (2009)*
G47404	TrGAroC	$C6H5CH2O2 \rightarrow BENZAL + HO_2$	$2*(k\_CH302*2.4E-14*EXP(1620./TEMP))*0.5*R02$	Rickard and Pascoe (2009)*
G47405	TrGAroCN	$CRESOL + NO_3 \rightarrow .103\text{ CRESO2} + .103\text{ HNO}_3 + .506\text{ NCRESO2} + .391\text{ TOL1O} + .391\text{ HNO}_3$	1.4E-11	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47406	TrGAroC	CRESOL + OH $\rightarrow$ .2 CRESO2 + .727 MCATECHOL + .727 HO <sub>2</sub> + .073 TOL1O	4.65E-11	Rickard and Pascoe (2009)*
G47407a	TrGAroC	TLBIPERO2 + HO <sub>2</sub> $\rightarrow$ TLBIPEROOH	KR02H02(7)*(1.-rbipero2_oh)	Rickard and Pascoe (2009)
G47407b	TrGAroC	TLBIPERO2 + HO <sub>2</sub> $\rightarrow$ OH + .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KR02H02(7)*rbipero2_oh	Rickard and Pascoe (2009), Bird-sall et al. (2010)*
G47408a	TrGAroCN	TLBIPERO2 + NO $\rightarrow$ NO <sub>2</sub> + .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KR02N0*(1.-alpha_AN(11,2,0,0,1,temp,cair))	Rickard and Pascoe (2009)*
G47408b	TrGAroCN	TLBIPERO2 + NO $\rightarrow$ TLBIPERNO3	KR02N0*alpha_AN(11,2,0,0,1,temp,cair)	Rickard and Pascoe (2009)*
G47409	TrGAroCN	TLBIPERO2 + NO <sub>3</sub> $\rightarrow$ NO <sub>2</sub> + .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	KR02N03	Rickard and Pascoe (2009)*
G47410	TrGAroC	TLBIPERO2 $\rightarrow$ .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL	k1_R02s0R02	Rickard and Pascoe (2009)*
G47411	TrGAroCN	TLEPOXMUC + NO <sub>3</sub> $\rightarrow$ TLEMUCCO3 + HNO <sub>3</sub>	KN03AL*2.75	Rickard and Pascoe (2009)
G47412	TrGAroC	TLEPOXMUC + O <sub>3</sub> $\rightarrow$ EPXC4DIAL + .125 CH <sub>3</sub> CHO + .695 CH <sub>3</sub> C(O) + .57 CO + .57 OH + .125 HO <sub>2</sub> + .1125 CH <sub>3</sub> COCO <sub>2</sub> H + .0675 MGLYOX + .0675 H <sub>2</sub> O <sub>2</sub> + .25 CO <sub>2</sub>	5.00E-18	Rickard and Pascoe (2009)*
G47413	TrGAroC	TLEPOXMUC + OH $\rightarrow$ .31 TLEMUCCO3 + .69 TLEMUCO2	7.99E-11	Rickard and Pascoe (2009)*
G47414	TrGAroC	C6H5CH2OOH + OH $\rightarrow$ BENZAL + OH	2.05E-11	Rickard and Pascoe (2009)
G47415	TrGAroCN	C6H5CH2NO3 + OH $\rightarrow$ BENZAL + NO <sub>2</sub>	6.03E-12	Rickard and Pascoe (2009)
G47416	TrGAroCN	BENZAL + NO <sub>3</sub> $\rightarrow$ C6H5CO3 + HNO <sub>3</sub>	2.40E-15	Rickard and Pascoe (2009)
G47417	TrGAroC	BENZAL + OH $\rightarrow$ C6H5CO3	5.9E-12*EXP(225/TEMP)	Rickard and Pascoe (2009)
G47418a	TrGAroC	CRESO2 + HO <sub>2</sub> $\rightarrow$ CRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47418b	TrGAroC	CRESO2 + HO <sub>2</sub> $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47419	TrGAroCN	CRESO2 + NO $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47420	TrGAroCN	CRESO2 + NO <sub>3</sub> $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47421	TrGAroC	CRESO2 $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47422a	TrGAroCN	NCRESO2 + HO <sub>2</sub> $\rightarrow$ NCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47422b	TrGAroCN	NCRESO2 + HO <sub>2</sub> $\rightarrow$ C5CO14OH + GLYOX + NO <sub>2</sub> + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47423	TrGAroCN	NCRESO2 + NO $\rightarrow$ C5CO14OH + GLYOX + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47424	TrGAroCN	NCRESO2 + NO <sub>3</sub> $\rightarrow$ C5CO14OH + GLYOX + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47425	TrGAroCN	NCRESO2 $\rightarrow$ C5CO14OH + GLYOX + NO <sub>2</sub>	k1_R02ISOPD02	Rickard and Pascoe (2009)*
G47426	TrGAroCN	TOL1O + NO <sub>2</sub> $\rightarrow$ TOL1OHNO2	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)*
G47427	TrGAroC	TOL1O + O <sub>3</sub> $\rightarrow$ OXYL1O2	k_C6H50_O3	Rickard and Pascoe (2009), Tao and Li (1999)
G47428	TrGAroCN	MCATECHOL + NO <sub>3</sub> $\rightarrow$ MCATEC1O + HNO <sub>3</sub>	1.7E-10*1.0	Rickard and Pascoe (2009)
G47429	TrGAroC	MCATECHOL + O <sub>3</sub> $\rightarrow$ MC3ODBCO2H + HCOCO <sub>2</sub> H + HO <sub>2</sub> + OH	2.8E-17	Rickard and Pascoe (2009)*
G47430	TrGAroC	MCATECHOL + OH $\rightarrow$ MCATEC1O	2.0E-10*1.0	Rickard and Pascoe (2009)
G47431	TrGAroC	TLBIPEROOH + OH $\rightarrow$ TLOBIPEROH + OH	9.64E-11	Rickard and Pascoe (2009)
G47432	TrGAroCN	TLBIPERNO3 + OH $\rightarrow$ TLOBIPEROH + NO <sub>2</sub>	7.16E-11	Rickard and Pascoe (2009)
G47433	TrGAroC	TLOBIPEROH + OH $\rightarrow$ C5CO14O2 + GLYOX	7.99E-11	Rickard and Pascoe (2009)
G47434a	TrGAroC	TLEMUCCO3 + HO <sub>2</sub> $\rightarrow$ C615CO2O2 + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47434b	TrGAroC	TLEMUCCO3 + HO <sub>2</sub> $\rightarrow$ TLEMUCCO2H + O <sub>3</sub>	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G47434c	TrGAroC	TLEMUCCO3 + HO <sub>2</sub> $\rightarrow$ TLEMUCCO3H	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G47435	TrGAroCN	TLEMUCCO3 + NO $\rightarrow$ C615CO2O2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G47436	TrGAroCN	TLEMUCCO3 + NO <sub>2</sub> $\rightarrow$ TLEMUCPAN	k_CH3C03_N02	Rickard and Pascoe (2009)*
G47437	TrGAroCN	TLEMUCCO3 + NO <sub>3</sub> $\rightarrow$ C615CO2O2 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G47438	TrGAroC	TLEMUCCO3 $\rightarrow$ C615CO2O2 + CO <sub>2</sub>	k1_R02RC03	Rickard and Pascoe (2009)*
G47439a	TrGAroC	TLEMUCO2 + HO <sub>2</sub> $\rightarrow$ TLEMUCOOH	KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47439b	TrGAroC	TLEMUCO2 + HO <sub>2</sub> $\rightarrow$ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO <sub>2</sub> + OH	KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G47440a	TrGAroCN	TLEMUCO2 + NO $\rightarrow$ TLEMUCNO3	KR02N0*alpha_AN(11,2,1,0,0,temp,cair)	Rickard and Pascoe (2009)
G47440b	TrGAroCN	TLEMUCO2 + NO $\rightarrow$ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(11,2,1,0,0,temp,cair))	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G47441	TrGAroCN	TLEMUCO2 + NO <sub>3</sub> → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47442	TrGAroC	TLEMUCO2 → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)*
G47443a	TrGAroC	C6H5CO3 + HO <sub>2</sub> → C6H5CO3H	1.1E-11*EXP(364./temp)*0.65	Roth et al. (2010)
G47443b	TrGAroC	C6H5CO3 + HO <sub>2</sub> → C6H5O2 + CO <sub>2</sub> + OH	1.1E-11*EXP(364./temp)*0.20	Roth et al. (2010)
G47443c	TrGAroC	C6H5CO3 + HO <sub>2</sub> → PHCOOH + O <sub>3</sub>	1.1E-11*EXP(364./temp)*0.15	Roth et al. (2010)
G47444	TrGAroCN	C6H5CO3 + NO → C6H5O2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G47445	TrGAroCN	C6H5CO3 + NO <sub>2</sub> → PBZN	k_CH3CO3_N02	Rickard and Pascoe (2009)*
G47446	TrGAroCN	C6H5CO3 + NO <sub>3</sub> → C6H5O2 + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G47447	TrGAroC	C6H5CO3 → C6H5O2 + CO <sub>2</sub>	k1_R02RC03	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 <sub>3</sub> → NCRES1O + HNO <sub>3</sub>	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 <sub>2</sub> → OXYL1OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47453	TrGAroCN	OXYL1O2 + NO → TOL1O + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G47454	TrGAroCN	OXYL1O2 + NO <sub>2</sub> → TOL1O + NO <sub>3</sub>	K_C6H5O2_N02	Jagiella and Zabel (2007)*
G47455	TrGAroCN	OXYL1O2 + NO <sub>3</sub> → TOL1O + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G47456	TrGAroC	OXYL1O2 → TOL1O	k1_R02sR02	Rickard and Pascoe (2009)
G47457	TrGAroCN	MCATEC1O + NO <sub>2</sub> → MNCATECH	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47458	TrGAroC	MCATEC1O + O <sub>3</sub> → MCATEC1O2	k_C6H50_03	Rickard and Pascoe (2009), Tao and Li (1999)
G47459	TrGAroC	TLEMUCCO2H + OH → C615CO2O2 + CO <sub>2</sub>	5.98E-11	Rickard and Pascoe (2009)
G47460	TrGAroC	TLEMUCCO3H + OH → TLEMUCCO3	6.29E-11	Rickard and Pascoe (2009)
G47461	TrGAroCN	TLEMUCPAN + OH → C5DICARB + CO + CO <sub>2</sub> + NO <sub>2</sub>	5.96E-11	Rickard and Pascoe (2009)
G47462	TrGAroCN	TLEMUCPAN → TLEMUCCO3 + NO <sub>2</sub>	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 <sub>2</sub>	3.06E-11	Rickard and Pascoe (2009)
G47465	TrGAroC	TLEMUCCO + OH → CH <sub>3</sub> C(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 <sub>2</sub>	1.10E-12	Rickard and Pascoe (2009)
G47468	TrGAroCN	PBZN + OH → C6H5OOH + CO + NO <sub>2</sub>	1.06E-12	Rickard and Pascoe (2009)
G47469	TrGAroCN	PBZN → C6H5CO3 + NO <sub>2</sub>	k_PAN_M*0.67	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47470	TrGAroCN	PTLQONE + NO <sub>3</sub> → NPTLQO2	1.00E-12	Rickard and Pascoe (2009)
G47471	TrGAroC	PTLQONE + OH → PTLQO2	2.3E-11	Rickard and Pascoe (2009)
G47472	TrGAroCN	NCRES1O + NO <sub>2</sub> → DNCRES	k_C6H50_N02	Rickard and Pascoe (2009), Platz et al. (1998)
G47473	TrGAroCN	NCRES1O + O <sub>3</sub> → NCRES1O2	k_C6H50_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 <sub>3</sub> → MNNCATECO2	5.03E-12	Rickard and Pascoe (2009)
G47476	TrGAroCN	MNCATECH + OH → MNCATECO2	6.83E-12	Rickard and Pascoe (2009)
G47477	TrGAroC	MCATEC1O2 + HO <sub>2</sub> → MCATEC1OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47478	TrGAroCN	MCATEC1O2 + NO → MCATEC1O + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G47479	TrGAroCN	MCATEC1O2 + NO <sub>2</sub> → MCATEC1O + NO <sub>3</sub>	K_C6H502_N02	Jagiella and Zabel (2007)*
G47480	TrGAroCN	MCATEC1O2 + NO <sub>3</sub> → MCATEC1O + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G47481	TrGAroC	MCATEC1O2 → MCATEC1O	k1_R02s0R02	Rickard and Pascoe (2009)
G47482a	TrGAroCN	NPTLQO2 + HO <sub>2</sub> → NPTLQOOH	KR02H02(7)*(1-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47482b	TrGAroCN	NPTLQO2 + HO <sub>2</sub> → C7CO4DB + NO <sub>2</sub> + OH	KR02H02(7)*rcoch2o2_oh	Rickard and Pascoe (2009)*
G47483	TrGAroCN	NPTLQO2 + NO → C7CO4DB + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47484	TrGAroCN	NPTLQO2 + NO <sub>3</sub> → C7CO4DB + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47485	TrGAroCN	NPTLQO2 → C7CO4DB + NO <sub>2</sub>	k1_R02s0R02	Rickard and Pascoe (2009)*
G47486a	TrGAroC	PTLQO2 + HO <sub>2</sub> → PTLQOOH	KR02H02(7)*(1-rchohch2o2_oh-rcoch2o2_oh)	Rickard and Pascoe (2009)
G47486b	TrGAroC	PTLQO2 + HO <sub>2</sub> → C6CO2OHCO3 + OH	KR02H02(7)*(rchohch2o2_oh+rcoch2o2_oh)	Rickard and Pascoe (2009)*
G47487	TrGAroCN	PTLQO2 + NO → C6CO2OHCO3 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47488	TrGAroCN	PTLQO2 + NO <sub>3</sub> → C6CO2OHCO3 + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47489	TrGAroC	PTLQO2 → C6CO2OHCO3	k1_R02s0R02	Rickard and Pascoe (2009)*
G47490	TrGAroCN	DNCRES + NO <sub>3</sub> → NDNCRESO2	7.83E-15	Rickard and Pascoe (2009)
G47491	TrGAroCN	DNCRES + OH → DNCRESO2	5.10E-14	Rickard and Pascoe (2009)
G47492	TrGAroCN	NCRES1O2 + HO <sub>2</sub> → NCRES1OOH	KR02H02(7)	Rickard and Pascoe (2009)
G47493	TrGAroCN	NCRES1O2 + NO → NCRES1O + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)
G47494	TrGAroCN	NCRES1O2 + NO <sub>2</sub> → NCRES1O + NO <sub>3</sub>	K_C6H502_N02	Jagiella and Zabel (2007)*
G47495	TrGAroCN	NCRES1O2 + NO <sub>3</sub> → NCRES1O + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G47496	TrGAroCN	NCRES1O2 → NCRES1O	k1_R02sR02	Rickard and Pascoe (2009)
G47497a	TrGAroCN	MNNCATECO2 + HO <sub>2</sub> → MNNCATCOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G47497b	TrGAroCN	MNNCATECO <sub>2</sub> + HO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47498	TrGAroCN	MNNCATECO <sub>2</sub> + NO → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47499	TrGAroCN	MNNCATECO <sub>2</sub> + NO <sub>3</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47500	TrGAroCN	MNNCATECO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub>	k1_R02IS0PD02	Rickard and Pascoe (2009)
G47501a	TrGAroCN	MNCATECO <sub>2</sub> + HO <sub>2</sub> → MNCATECOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47501b	TrGAroCN	MNCATECO <sub>2</sub> + HO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + HO <sub>2</sub> + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47502	TrGAroCN	MNCATECO <sub>2</sub> + NO → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47503	TrGAroCN	MNCATECO <sub>2</sub> + NO <sub>3</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + HO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47504	TrGAroCN	MNCATECO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + HO <sub>2</sub>	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47505	TrGAroC	MCATEC1OOH + OH → MCATEC1O2	2.05E-10	Rickard and Pascoe (2009)
G47506	TrGAroCN	NPTLQOOH + OH → NPTLQO2	8.56E-11	Rickard and Pascoe (2009)
G47507	TrGAroC	PTLQOOH + OH → PTLQCO + OH	1.42E-10	Rickard and Pascoe (2009)
G47508	TrGAroC	PTLQCO + OH → C6CO2OHCO3	7.95E-11	Rickard and Pascoe (2009)
G47509a	TrGAroCN	NDNCRESO <sub>2</sub> + HO <sub>2</sub> → NDNCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47509b	TrGAroCN	NDNCRESO <sub>2</sub> + HO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HNO <sub>3</sub> + 2 CO + NO <sub>2</sub> + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47510	TrGAroCN	NDNCRESO <sub>2</sub> + NO → NC <sub>4</sub> MDCO <sub>2</sub> HN + HNO <sub>3</sub> + 2 CO + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47511	TrGAroCN	NDNCRESO <sub>2</sub> + NO <sub>3</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HNO <sub>3</sub> + 2 CO + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47512	TrGAroCN	NDNCRESO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HNO <sub>3</sub> + 2 CO + NO <sub>2</sub>	k1_R02IS0PD02	Rickard and Pascoe (2009)*
G47513a	TrGAroCN	DNCRESO <sub>2</sub> + HO <sub>2</sub> → DNCRESOOH	KR02H02(7)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G47513b	TrGAroCN	DNCRESO <sub>2</sub> + HO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	KR02H02(7)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G47514	TrGAroCN	DNCRESO <sub>2</sub> + NO → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G47515	TrGAroCN	DNCRESO <sub>2</sub> + NO <sub>3</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)*
G47516	TrGAroCN	DNCRESO <sub>2</sub> → NC <sub>4</sub> MDCO <sub>2</sub> HN + HCOCO <sub>2</sub> H + NO <sub>2</sub>	k1_R02IS0PD02	Rickard and Pascoe (2009)*



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

#	labels	reaction	rate coefficient	reference
G47517	TrGAroCN	NCRES1OOH + OH $\rightarrow$ NCRES1O2	1.53E-12	Rickard and Pascoe (2009)
G47518	TrGAroCN	MNNCATCOOH + OH $\rightarrow$ MNNCATECO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47519	TrGAroCN	MNCATECOOH + OH $\rightarrow$ MNCATECO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47520	TrGAroC	C7CO4DB + OH $\rightarrow$ CO + CO + CH <sub>3</sub> C(O) + HCOCOCHO	9.58E-11	Rickard and Pascoe (2009)
G47521a	TrGAroC	C6CO2OHCO3 + HO <sub>2</sub> $\rightarrow$ C5134CO2OH + HO <sub>2</sub> + CO + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G47521b	TrGAroC	C6CO2OHCO3 + HO <sub>2</sub> $\rightarrow$ C6COOHCO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G47522	TrGAroCN	C6CO2OHCO3 + NO $\rightarrow$ C5134CO2OH + HO <sub>2</sub> + CO + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G47523	TrGAroCN	C6CO2OHCO3 + NO <sub>2</sub> $\rightarrow$ C6CO2OHPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G47524	TrGAroCN	C6CO2OHCO3 + NO <sub>3</sub> $\rightarrow$ C5134CO2OH + HO <sub>2</sub> + CO + CO <sub>2</sub> + NO <sub>2</sub>	KR02N03*1.74	Rickard and Pascoe (2009)
G47525	TrGAroC	C6CO2OHCO3 $\rightarrow$ C5134CO2OH + HO <sub>2</sub> + CO + CO <sub>2</sub>	k1_R02RC03	Rickard and Pascoe (2009)
G47526	TrGAroCN	NDNCRESOOH + OH $\rightarrow$ NDNCRESO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47527	TrGAroCN	DNCRESOOH + OH $\rightarrow$ DNCRESO2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G47528	TrGAroC	C6COOHCO3H + OH $\rightarrow$ C6CO2OHCO3	9.29E-11	Rickard and Pascoe (2009)
G47529	TrGAroCN	C6CO2OHPAN + OH $\rightarrow$ C5134CO2OH + CO + CO + NO <sub>2</sub>	8.96E-11	Rickard and Pascoe (2009)
G47530	TrGAroCN	C6CO2OHPAN $\rightarrow$ C6CO2OHCO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G48200	TrGTerC	C85O2 $\rightarrow$ C86O2	k1_R02tR02	Rickard and Pascoe (2009)
G48201	TrGTerC	C85O2 + HO <sub>2</sub> $\rightarrow$ C85OOH	KR02H02(8)	Rickard and Pascoe (2009)
G48202	TrGTerCN	C85O2 + NO $\rightarrow$ C86O2 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G48203	TrGTerC	C85OOH + OH $\rightarrow$ C85O2	1.29E-11	Rickard and Pascoe (2009)
G48204	TrGTerC	C86O2 $\rightarrow$ C511O2 + CH <sub>3</sub> COCH <sub>3</sub>	k1_R02tR02	Rickard and Pascoe (2009)
G48205	TrGTerCN	C86O2 + NO $\rightarrow$ C511O2 + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G48206	TrGTerC	C86O2 + HO <sub>2</sub> $\rightarrow$ C86OOH	KR02H02(8)	Rickard and Pascoe (2009)
G48207	TrGTerC	C86OOH + OH $\rightarrow$ C86O2	3.45E-11	Rickard and Pascoe (2009)
G48208	TrGTerC	C811O2 $\rightarrow$ C812O2	k1_R02pR02	Rickard and Pascoe (2009)
G48209	TrGTerC	C811O2 + HO <sub>2</sub> $\rightarrow$ 8 LCARBON	KR02H02(8)	Rickard and Pascoe (2009)
G48210	TrGTerCN	C811O2 + NO $\rightarrow$ C812O2 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G48211	TrGTerC	C812O2 $\rightarrow$ C813O2	k1_R02t0R02	Rickard and Pascoe (2009)
G48212	TrGTerCN	C812O2 + NO $\rightarrow$ C813O2 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G48213	TrGTerC	C812O2 + HO <sub>2</sub> $\rightarrow$ C812OOH	KR02H02(8)	Rickard and Pascoe (2009)
G48214	TrGTerC	C812OOH + OH $\rightarrow$ C812O2	1.09E-11	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48215	TrGTerC	$\text{C813O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G48216	TrGTerCN	$\text{C813O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C512O2} + \text{NO}_2$	KR02N0	Rickard and Pascoe (2009)*
G48217	TrGTerC	$\text{C813O2} + \text{HO}_2 \rightarrow \text{C813OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48218	TrGTerC	$\text{C813OOH} + \text{OH} \rightarrow \text{C813O2}$	1.86E-11	Rickard and Pascoe (2009)
G48219	TrGTerCN	$\text{C721CHO} + \text{NO}_3 \rightarrow \text{C721CO3} + \text{HNO}_3$	KN03AL*8.5	Rickard and Pascoe (2009)
G48220	TrGTerC	$\text{C721CHO} + \text{OH} \rightarrow \text{C721CO3}$	2.63E-11	Rickard and Pascoe (2009)
G48221a	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721CO3H}$	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G48221b	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{C721O2} + \text{CO}_2 + \text{OH}$	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G48221c	TrGTerC	$\text{C721CO3} + \text{HO}_2 \rightarrow \text{NORPINIC} + \text{O}_3$	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G48222	TrGTerCN	$\text{C721CO3} + \text{NO} \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KAPN0	Rickard and Pascoe (2009)*
G48223	TrGTerCN	$\text{C721CO3} + \text{NO}_2 \rightarrow \text{C721PAN}$	k_CH3CO3_N02	Rickard and Pascoe (2009)
G48224	TrGTerCN	$\text{C721CO3} + \text{NO}_3 \rightarrow \text{C721O2} + \text{CO}_2 + \text{NO}_2$	KR02N03*1.74	Rickard and Pascoe (2009)
G48225	TrGTerC	$\text{C721CO3} \rightarrow \text{C721O2} + \text{CO}_2$	k1_R02RC03*0.9	Taraborrelli (2016)
G48226	TrGTerC	$\text{C721CO3} \rightarrow \text{NORPINIC}$	k1_R02RC03*0.1	Taraborrelli (2016)
G48227	TrGTerC	$\text{C721CO3H} + \text{OH} \rightarrow \text{C721CO3}$	9.65E-12	Rickard and Pascoe (2009)
G48228	TrGTerC	$\text{NORPINIC} + \text{OH} \rightarrow \text{C721O2} + \text{CO}_2$	6.57E-12	Rickard and Pascoe (2009)
G48229	TrGTerCN	$\text{C721PAN} + \text{OH} \rightarrow \text{C721OOH} + \text{CO} + \text{NO}_2$	2.96E-12	Rickard and Pascoe (2009)
G48230	TrGTerCN	$\text{C721PAN} \rightarrow \text{C721CO3} + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G48231	TrGTerC	$\text{C8BC} + \text{OH} \rightarrow \text{C8BCO2}$	3.04E-12	Rickard and Pascoe (2009)
G48232	TrGTerC	$\text{C8BCO2} + \text{HO}_2 \rightarrow \text{C8BCOOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48233a	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C89O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(8,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48233b	TrGTerCN	$\text{C8BCO2} + \text{NO} \rightarrow \text{C8BCNO3}$	KR02N0*alpha_AN(8,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48234	TrGTerC	$\text{C8BCO2} \rightarrow \text{C89O2}$	k1_R02sR02	Rickard and Pascoe (2009)
G48235	TrGTerC	$\text{C8BCOOH} + \text{OH} \rightarrow \text{C8BCCO} + \text{OH}$	1.62E-11	Rickard and Pascoe (2009)
G48236	TrGTerCN	$\text{C8BCNO3} + \text{OH} \rightarrow \text{C8BCCO} + \text{NO}_2$	1.84E-12	Rickard and Pascoe (2009)
G48237	TrGTerC	$\text{C8BCCO} + \text{OH} \rightarrow \text{C89O2}$	3.94E-12	Rickard and Pascoe (2009)
G48238	TrGTerC	$\text{C89O2} + \text{HO}_2 \rightarrow \text{C89OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48239a	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C810O2} + \text{NO}_2$	KR02N0*(1.-alpha_AN(7,2,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48239b	TrGTerCN	$\text{C89O2} + \text{NO} \rightarrow \text{C89NO3}$	KR02N0*alpha_AN(7,2,0,0,0,temp, cair)	Rickard and Pascoe (2009)
G48240	TrGTerCN	$\text{C89O2} + \text{NO}_3 \rightarrow \text{C810O2} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G48241	TrGTerC	$\text{C89O2} \rightarrow \text{C810O2}$	k1_R02tR02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G48242	TrGTerC	$\text{C89OOH} + \text{OH} \rightarrow \text{C89O2}$	3.61E-11	Rickard and Pascoe (2009)
G48243	TrGTerCN	$\text{C89NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	2.56E-11	Rickard and Pascoe (2009)
G48244	TrGTerC	$\text{C810O2} + \text{HO}_2 \rightarrow \text{C810OOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48245a	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KR02N0*(1-alpha_AN(10,3,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G48245b	TrGTerCN	$\text{C810O2} + \text{NO} \rightarrow \text{C810NO3}$	KR02N0*alpha_AN(10,3,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G48246	TrGTerCN	$\text{C810O2} + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G48247	TrGTerC	$\text{C810O2} \rightarrow \text{CH}_3\text{COCH}_3 + \text{C514O2}$	k1_R02tR02	Rickard and Pascoe (2009)
G48248	TrGTerC	$\text{C810OOH} + \text{OH} \rightarrow \text{C810O2}$	8.35E-11	Rickard and Pascoe (2009)
G48249	TrGTerCN	$\text{C810NO3} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{NO}_2$	4.96E-11	Rickard and Pascoe (2009)
G48400a	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLEPOXMUC} + \text{HO}_2 + \text{LCARBON}$	0.401E-11	Rickard and Pascoe (2009)*
G48400b	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{C6H5CH2O2} + \text{LCARBON}$	0.101E-11	Rickard and Pascoe (2009)*
G48400c	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{CRESOL} + \text{LCARBON}$	0.261E-11	Rickard and Pascoe (2009)*
G48400d	TrGAroC	$\text{LXYL} + \text{OH} \rightarrow \text{TLBIPERO2} + \text{HO}_2 + \text{LCARBON}$	0.932E-11	Rickard and Pascoe (2009)*
G48401	TrGAroCN	$\text{LXYL} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	3.9E-16	Rickard and Pascoe (2009)*
G48402	TrGAroC	$\text{EBENZ} + \text{OH} \rightarrow .10 \text{ TLEPOXMUC} + .07 \text{ C6H5CH2O2} + .18 \text{ CRESOL} + .65 \text{ TLBIPERO2} + .28 \text{ HO}_2 + \text{LCARBON}$	7.00E-12	Rickard and Pascoe (2009)*
G48403	TrGAroCN	$\text{EBENZ} + \text{NO}_3 \rightarrow \text{C6H5CH2O2} + \text{HNO}_3 + \text{LCARBON}$	1.20E-16	Rickard and Pascoe (2009)*
G48404	TrGAroCN	$\text{STYRENE} + \text{NO}_3 \rightarrow \text{NSTYRENO2}$	1.50E-12	Rickard and Pascoe (2009)
G48405	TrGAroC	$\text{STYRENE} + \text{O}_3 \rightarrow .545 \text{ HCHO} + .1 \text{ BENZENE} + .28 \text{ C6H5O2} + .56 \text{ CO} + .36 \text{ OH} + .28 \text{ HO}_2 + .075 \text{ PHCOOH} + .545 \text{ BENZAL} + .09 \text{ H}_2\text{O}_2 + .075 \text{ HCOOH} + .2 \text{ CO}_2$	1.70E-17	Rickard and Pascoe (2009)*
G48406	TrGAroC	$\text{STYRENE} + \text{OH} \rightarrow \text{STYRENO2}$	5.80E-11	Rickard and Pascoe (2009)
G48407	TrGAroCN	$\text{NSTYRENO2} + \text{HO}_2 \rightarrow \text{NSTYRENOOH}$	KR02H02(8)	Rickard and Pascoe (2009)
G48408	TrGAroCN	$\text{NSTYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N0	Rickard and Pascoe (2009)*
G48409	TrGAroCN	$\text{NSTYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N03	Rickard and Pascoe (2009)*
G48410	TrGAroCN	$\text{NSTYRENO2} \rightarrow \text{NO}_2 + \text{HCHO} + \text{BENZAL}$	k1_R02sR02	Rickard and Pascoe (2009)*
G48411	TrGAroCN	$\text{NSTYRENOOH} + \text{OH} \rightarrow \text{NSTYRENO2}$	6.16E-11	Rickard and Pascoe (2009)
G48412a	TrGAroC	$\text{STYRENO2} + \text{HO}_2 \rightarrow \text{STYRENOOH}$	KR02H02(8)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009)
G48412b	TrGAroC	$\text{STYRENO2} + \text{HO}_2 \rightarrow \text{HO}_2 + \text{OH} + \text{HCHO} + \text{BENZAL}$	KR02H02(8)*rchohch2o2_oh	Rickard and Pascoe (2009)*
G48413	TrGAroCN	$\text{STYRENO2} + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N0	Rickard and Pascoe (2009)*
G48414	TrGAroCN	$\text{STYRENO2} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	KR02N03	Rickard and Pascoe (2009)*
G48415	TrGAroC	$\text{STYRENO2} \rightarrow \text{HO}_2 + \text{HCHO} + \text{BENZAL}$	k1_R02sR02	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G48416	TrGAroC	STYRENOOH + OH $\rightarrow$ STYRENO2	6.16E-11	Rickard and Pascoe (2009)
G49200	TrGTerC	C96O2 $\rightarrow$ C97O2	k1_R02pR02	Rickard and Pascoe (2009)
G49201	TrGTerC	C96O2 + HO <sub>2</sub> $\rightarrow$ C96OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49202a	TrGTerCN	C96O2 + NO $\rightarrow$ C97O2 + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(10,1,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49202b	TrGTerCN	C96O2 + NO $\rightarrow$ C96NO3	KR02N0*alpha_AN(10,1,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49203	TrGTerCN	C96NO3 + OH $\rightarrow$ NORPINAL + NO <sub>2</sub>	2.88E-12	Rickard and Pascoe (2009)
G49204a	TrGTerC	C96OOH + OH $\rightarrow$ C96O2	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G49205b	TrGTerC	C96OOH + OH $\rightarrow$ NORPINAL + OH	1.30E-11	Rickard and Pascoe (2009)
G49206	TrGTerC	C97O2 $\rightarrow$ C98O2	k1_R02tR02	Rickard and Pascoe (2009)
G49207	TrGTerCN	C97O2 + NO $\rightarrow$ C98O2 + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G49208a	TrGTerC	C97O2 + HO <sub>2</sub> $\rightarrow$ C97OOH	KR02H02(9)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49208b	TrGTerC	C97O2 + HO <sub>2</sub> $\rightarrow$ C98O2 + OH	KR02H02(9)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G49209	TrGTerC	C97OOH + OH $\rightarrow$ C97O2	1.05E-11	Rickard and Pascoe (2009)
G49210	TrGTerC	C98O2 $\rightarrow$ C614O2 + CH <sub>3</sub> COCH <sub>3</sub>	k1_R02tR02	Rickard and Pascoe (2009)
G49211a	TrGTerCN	C98O2 + NO $\rightarrow$ C614O2 + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp, cair))	Rickard and Pascoe (2009)
G49211b	TrGTerCN	C98O2 + NO $\rightarrow$ 9 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp, cair)	Rickard and Pascoe (2009)
G49212	TrGTerC	C98O2 + HO <sub>2</sub> $\rightarrow$ C98OOH	KR02H02(9)	Rickard and Pascoe (2009)
G49213	TrGTerC	C98OOH + OH $\rightarrow$ C98O2	2.05E-11	Rickard and Pascoe (2009)
G49214	TrGTerC	NORPINAL + OH $\rightarrow$ C85CO3	2.64E-11	Rickard and Pascoe (2009)
G49215	TrGTerCN	NORPINAL + NO <sub>3</sub> $\rightarrow$ C85CO3 + HNO <sub>3</sub>	KN03AL*8.5	Rickard and Pascoe (2009)
G49216	TrGTerC	C85CO3 $\rightarrow$ C85O2 + CO <sub>2</sub>	k1_R02RC03	Rickard and Pascoe (2009)
G49217	TrGTerCN	C85CO3 + NO $\rightarrow$ C85O2 + CO <sub>2</sub> + NO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G49218	TrGTerCN	C85CO3 + NO <sub>2</sub> $\rightarrow$ C9PAN2	k_CH3C03_N02	Rickard and Pascoe (2009)
G49219a	TrGTerC	C85CO3 + HO <sub>2</sub> $\rightarrow$ C85CO3H	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009)
G49219b	TrGTerC	C85CO3 + HO <sub>2</sub> $\rightarrow$ C85O2 + CO <sub>2</sub> + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G49220	TrGTerCN	C9PAN2 $\rightarrow$ C85CO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G49221	TrGTerCN	C9PAN2 + OH $\rightarrow$ C85OOH + CO + NO <sub>2</sub>	6.60E-12	Rickard and Pascoe (2009)
G49222	TrGTerC	C85CO3H + OH $\rightarrow$ C85CO3	1.02E-11	Rickard and Pascoe (2009)
G49223a	TrGTerC	C89CO3 $\rightarrow$ .8 C811CO3 + .2 C89O2 + .2 CO <sub>2</sub>	k1_R02RC03*0.9	Taraborrelli (2016)

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

#	labels	reaction	rate coefficient	reference
G49223b	TrGTerC	$\text{C89CO3} \rightarrow \text{C89CO2H}$	$\text{k1\_R02RC03*0.1}$	Taraborrelli (2016)
G49224a	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO3H}$	$\text{KAPH02*rc03\_ooh}$	Rickard and Pascoe (2009)
G49224b	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow \text{C89CO2H} + \text{O}_3$	$\text{KAPH02*rc03\_o3}$	Rickard and Pascoe (2009)
G49224c	TrGTerC	$\text{C89CO3} + \text{HO}_2 \rightarrow .80 \text{ C811CO3} + .20 \text{ C89O2} + .2 \text{ CO}_2 + \text{OH}$	$\text{KAPH02*rc03\_oh}$	Rickard and Pascoe (2009)
G49225	TrGTerCN	$\text{C89CO3} + \text{NO}_2 \rightarrow \text{C89PAN}$	$\text{k\_CH3C03\_N02}$	Rickard and Pascoe (2009)
G49226	TrGTerCN	$\text{C89CO3} + \text{NO} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2 + \text{NO}_2$	$\text{KAPNO}$	Rickard and Pascoe (2009)
G49227	TrGTerC	$\text{C89CO2H} + \text{OH} \rightarrow .8 \text{ C811CO3} + .2 \text{ C89O2} + .2 \text{ CO}_2$	$2.69\text{E-}11$	Rickard and Pascoe (2009)
G49228	TrGTerC	$\text{C89CO3H} + \text{OH} \rightarrow \text{C89CO3}$	$3.00\text{E-}11$	Rickard and Pascoe (2009)
G49229	TrGTerCN	$\text{C89PAN} \rightarrow \text{C89CO3} + \text{NO}_2$	$\text{k\_PAN\_M}$	Rickard and Pascoe (2009)
G49230	TrGTerCN	$\text{C89PAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{CO13C4CHO} + \text{CO} + \text{NO}_2$	$2.52\text{E-}11$	Rickard and Pascoe (2009)
G49231a	TrGTerC	$\text{C811CO3} \rightarrow \text{C811O2} + \text{CO}_2$	$\text{k1\_R02RC03*0.9}$	Taraborrelli (2016)
G49231b	TrGTerC	$\text{C811CO3} \rightarrow \text{PINIC}$	$\text{k1\_R02RC03*0.1}$	Taraborrelli (2016)
G49232a	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811CO3H}$	$\text{KAPH02*rc03\_ooh}$	Rickard and Pascoe (2009)
G49232b	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{PINIC} + \text{O}_3$	$\text{KAPH02*rc03\_o3}$	Rickard and Pascoe (2009)
G49232c	TrGTerC	$\text{C811CO3} + \text{HO}_2 \rightarrow \text{C811O2} + \text{CO}_2 + \text{OH}$	$\text{KAPH02*rc03\_oh}$	Rickard and Pascoe (2009)
G49233	TrGTerCN	$\text{C811CO3} + \text{NO} \rightarrow \text{C811O2} + \text{CO}_2 + \text{NO}_2$	$\text{KAPNO}$	Rickard and Pascoe (2009)
G49234	TrGTerCN	$\text{C811CO3} + \text{NO}_2 \rightarrow \text{C811PAN}$	$\text{k\_CH3C03\_N02}$	Rickard and Pascoe (2009)
G49235	TrGTerC	$\text{PINIC} + \text{OH} \rightarrow \text{C811O2} + \text{CO}_2$	$7.29\text{E-}12$	Rickard and Pascoe (2009)
G49236	TrGTerC	$\text{NOPINONE} + \text{OH} \rightarrow \text{NOPINDO2}$	$1.55\text{E-}11$	Capouet et al. (2008), Rickard and Pascoe (2009)
G49237a	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{NOPINDOOH}$	$\text{KR02H02(9)*rc0ch2o2\_ooh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G49237b	TrGTerC	$\text{NOPINDO2} + \text{HO}_2 \rightarrow \text{C89CO3} + \text{OH}$	$\text{KR02H02(9)*rc0ch2o2\_oh}$	Rickard and Pascoe (2009), Taraborrelli (2016)
G49238	TrGTerCN	$\text{NOPINDO2} + \text{NO} \rightarrow \text{C89CO3} + \text{NO}_2$	$\text{KR02NO}$	Rickard and Pascoe (2009)*
G49239	TrGTerC	$\text{NOPINDO2} \rightarrow \text{C89CO3}$	$\text{k1\_R02p0R02}$	Rickard and Pascoe (2009)
G49240	TrGTerC	$\text{NOPINDOOH} \rightarrow \text{NOPINDCO}$	$2.63\text{E-}11$	Rickard and Pascoe (2009)
G49241	TrGTerC	$\text{NOPINDCO} + \text{OH} \rightarrow \text{C89CO3}$	$3.07\text{E-}12$	Rickard and Pascoe (2009)
G49242	TrGTerC	$\text{NOPINOO} \rightarrow \text{NOPINONE} + \text{H}_2\text{O}_2$	$6.00\text{E-}18*\text{c(ind\_H20)}$	Rickard and Pascoe (2009)
G49243	TrGTerC	$\text{NOPINOO} + \text{CO} \rightarrow \text{NOPINONE} + \text{CO}_2$	$1.2\text{E-}15$	Rickard and Pascoe (2009)
G49244	TrGTerCN	$\text{NOPINOO} + \text{NO} \rightarrow \text{NOPINONE} + \text{NO}_2$	$1.\text{E-}14$	Rickard and Pascoe (2009)
G49245	TrGTerCN	$\text{NOPINOO} + \text{NO}_2 \rightarrow \text{NOPINONE} + \text{NO}_3$	$1.\text{E-}15$	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G49246	TrGTerC	NORPINENOL + OH $\rightarrow$ HCOOH + OH + C86O2	k_CH2CHOH_OH_HCOOH	Taraborrelli (2016), So et al. (2014)*
G49247	TrGTerC	NORPINENOL + HCOOH $\rightarrow$ NORPINAL + HCOOH	k_CH2CHOH_HCOOH	Taraborrelli (2016), daSilva (2010)*
G49248	TrGTerC	NORPINAL + HCOOH $\rightarrow$ NORPINENOL + HCOOH	k_ALD_HCOOH	Taraborrelli (2016), daSilva (2010)*
G49249	TrGTerC	C811CO3H + OH $\rightarrow$ C811CO3	1.04E-11	Rickard and Pascoe (2009)
G49250	TrGTerCN	C811PAN $\rightarrow$ C811CO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G49251	TrGTerCN	C811PAN + OH $\rightarrow$ C721CHO + CO + NO <sub>2</sub>	6.77E-12	Rickard and Pascoe (2009)
G49400a	TrGAroC	LTMB + OH $\rightarrow$ TLEPOXMUC + HO <sub>2</sub> + 2 LCARBON	0.827E-11	Rickard and Pascoe (2009)*
G49400b	TrGAroC	LTMB + OH $\rightarrow$ C6H5CH2O2 + 2 LCARBON	0.189E-11	Rickard and Pascoe (2009)*
G49400c	TrGAroC	LTMB + OH $\rightarrow$ CRESOL + 2 LCARBON	0.141E-11	Rickard and Pascoe (2009)*
G49400d	TrGAroC	LTMB + OH $\rightarrow$ TLBIPERO2 + HO <sub>2</sub> + 2 LCARBON	2.917E-11	Rickard and Pascoe (2009)*
G49401	TrGAroCN	LTMB + NO <sub>3</sub> $\rightarrow$ C6H5CH2O2 + HNO <sub>3</sub> + 2 LCARBON	1.52E-15	Rickard and Pascoe (2009)*
G40200	TrGTerC	APINENE + OH $\rightarrow$ .75 LAPINABO2 + .15 MENTHEN6ONE + .15 HO <sub>2</sub> + .10 ROO6R1O2	1.2E-11*EXP(440./TEMP)	Atkinson et al. (2006)*
G40201a	TrGTerCN	LAPINABO2 + NO $\rightarrow$ PINAL + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(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 $\rightarrow$ LAPINABNO3	KR02N0*(.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 <sub>2</sub> $\rightarrow$ LAPINABOOH	KR02H02(10)*(1-rchohch2o2_oh)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40202b	TrGTerC	LAPINABO2 + HO <sub>2</sub> $\rightarrow$ PINAL + HO <sub>2</sub> + OH	KR02H02(10)*rchohch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40203	TrGTerC	LAPINABO2 $\rightarrow$ PINAL + HO <sub>2</sub>	R02*(0.65*k1_R02tOR02+.35*k1_R02sOR02)	Rickard and Pascoe (2009)*
G40204	TrGTerC	LAPINABOOH + OH $\rightarrow$ .35 LAPINABO2 + .65 C96CO3	2.77E-11	Rickard and Pascoe (2009)*
G40205	TrGTerCN	LAPINABNO3 + OH $\rightarrow$ .35 PINAL + .65 C96CO3 + NO <sub>2</sub>	4.29E-12	Rickard and Pascoe (2009)*
G40206	TrGTerC	MENTHEN6ONE + OH $\rightarrow$ OHMENTHEN6ONEO2	6.46E-11	Vereecken et al. (2007)*
G40207	TrGTerCN	OHMENTHEN6ONEO2 + NO $\rightarrow$ 2OHMENTHEN6ONE + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Vereecken et al. (2007)*
G40208	TrGTerC	OHMENTHEN6ONEO2 + HO <sub>2</sub> $\rightarrow$ 2OHMENTHEN6ONE	KR02H02(10)	Vereecken et al. (2007)
G40209	TrGTerC	OHMENTHEN6ONEO2 $\rightarrow$ 2OHMENTHEN6ONE + HO <sub>2</sub>	k1_R02tOR02	Vereecken et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G40210	TrGTerC	2OHMENTHEN6ONE + OH $\rightarrow$ 10 LCARBON	1E-11	Vereecken et al. (2007)
G40211	TrGTerC	PINAL + OH $\rightarrow$ .772 C96CO3 + .228 PINALO2	5.2E-12*EXP(600./TEMP)	T. J. Wallington et al. (2014)*
G40212	TrGTerCN	PINAL + NO <sub>3</sub> $\rightarrow$ C96CO3 + HNO <sub>3</sub>	2.0E-14	T. J. Wallington et al. (2014)*
G40213a	TrGTerC	C96CO3 $\rightarrow$ C96O2 + CO <sub>2</sub>	k1_R02RC03*0.9	Rickard and Pascoe (2009)
G40213b	TrGTerC	C96CO3 $\rightarrow$ PINONIC	k1_R02RC03*0.1	Rickard and Pascoe (2009)
G40214a	TrGTerC	C96CO3 + HO <sub>2</sub> $\rightarrow$ PERPINONIC	KAPH02*rco3_ooh	Rickard and Pascoe (2009)
G40214b	TrGTerC	C96CO3 + HO <sub>2</sub> $\rightarrow$ PINONIC + O <sub>3</sub>	KAPH02*rco3_o3	Rickard and Pascoe (2009)
G40214c	TrGTerC	C96CO3 + HO <sub>2</sub> $\rightarrow$ C96O2 + OH + CO <sub>2</sub>	KAPH02*rco3_oh	Rickard and Pascoe (2009)
G40215	TrGTerCN	C96CO3 + NO <sub>2</sub> $\rightarrow$ C10PAN2	k_CH3C03_NO2	Rickard and Pascoe (2009)
G40216	TrGTerCN	C96CO3 + NO $\rightarrow$ C96O2 + NO <sub>2</sub> + CO <sub>2</sub>	KAPNO	Rickard and Pascoe (2009)
G40217	TrGTerCN	C96CO3 + NO <sub>3</sub> $\rightarrow$ C96O2 + NO <sub>2</sub> + CO <sub>2</sub>	KR02N03*1.60	Rickard and Pascoe (2009)
G40218	TrGTerCN	C10PAN2 $\rightarrow$ C96CO3 + NO <sub>2</sub>	k_PAN_M	Rickard and Pascoe (2009)
G40219	TrGTerCN	C10PAN2 + OH $\rightarrow$ NORPINAL + CO + NO <sub>2</sub>	3.66E-12	Rickard and Pascoe (2009)
G40220	TrGTerC	PINONIC + OH $\rightarrow$ C96O2 + CO <sub>2</sub>	6.65E-12	Rickard and Pascoe (2009)
G40221	TrGTerC	PERPINONIC + OH $\rightarrow$ C96CO3	9.73E-12	Rickard and Pascoe (2009)
G40222	TrGTerC	PINALO2 + HO <sub>2</sub> $\rightarrow$ PINALOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40223a	TrGTerCN	PINALO2 + NO $\rightarrow$ C106O2 + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(12,3,0,1,0, temp, cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G40223b	TrGTerCN	PINALO2 + NO $\rightarrow$ PINALNO3	KR02N0*alpha_AN(12,3,0,1,0, temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40224	TrGTerC	PINALO2 $\rightarrow$ C106O2	k1_R02tR02	Rickard and Pascoe (2009)
G40225	TrGTerC	PINALOOH + OH $\rightarrow$ PINALO2	2.75E-11	Rickard and Pascoe (2009)
G40226	TrGTerCN	PINALNO3 + OH $\rightarrow$ CO235C6CHO + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	2.25E-11	Rickard and Pascoe (2009)
G40227	TrGTerC	C106O2 + HO <sub>2</sub> $\rightarrow$ C106OOH	KR02H02(10)	Rickard and Pascoe (2009)
G40228a	TrGTerCN	C106O2 + NO $\rightarrow$ C716O2 + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	KR02N0*0.875*(1.-alpha_AN(13,3,0,0,0, temp, cair))	Rickard and Pascoe (2009), Taraborrelli (2016)
G40228b	TrGTerCN	C106O2 + NO $\rightarrow$ C106NO3	KR02N0*0.875*alpha_AN(13,3,0,0,0, temp, cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40229	TrGTerC	C106O2 $\rightarrow$ C716O2 + CH <sub>3</sub> COCH <sub>3</sub>	k1_R02tR02	Rickard and Pascoe (2009)
G40230	TrGTerC	C106OOH + OH $\rightarrow$ C106O2	8.01E-11	Rickard and Pascoe (2009)
G40231	TrGTerCN	C106NO3 + OH $\rightarrow$ CO235C6CHO + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	7.03E-11	Rickard and Pascoe (2009)
G40232	TrGTerC	APINENE + O <sub>3</sub> $\rightarrow$ .09 APINBOO + .08 PINONIC + .77 OH + .33 NORPINAL + .33 CO + .33 HO <sub>2</sub> + .06 APINAOO + .44 C109O2	8.05E-16*EXP(-640./TEMP)	T. J. Wallington et al. (2014)*

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

#	labels	reaction	rate coefficient	reference
G40233	TrGTerC	APINAOO $\rightarrow$ PINAL + H <sub>2</sub> O <sub>2</sub>	1.00E-17*c(ind_H20)	Rickard and Pascoe (2009)
G40234	TrGTerC	APINAOO + CO $\rightarrow$ PINAL + CO <sub>2</sub>	1.20E-15	Rickard and Pascoe (2009)
G40235	TrGTerCN	APINAOO + NO $\rightarrow$ PINAL + NO <sub>2</sub>	1.00E-14	Rickard and Pascoe (2009)
G40236	TrGTerCN	APINAOO + NO <sub>2</sub> $\rightarrow$ PINAL + NO <sub>3</sub>	1.00E-15	Rickard and Pascoe (2009)
G40237a	TrGTerC	APINBOO $\rightarrow$ PINONIC	1.00E-17*c(ind_H20)*(0.08+0.15)	Rickard and Pascoe (2009)
G40237b	TrGTerC	APINBOO $\rightarrow$ PINAL + H <sub>2</sub> O <sub>2</sub>	1.00E-17*c(ind_H20)*0.77	Rickard and Pascoe (2009)
G40238	TrGTerC	APINBOO + CO $\rightarrow$ PINAL + CO <sub>2</sub>	1.20E-15	Rickard and Pascoe (2009)
G40239	TrGTerCN	APINBOO + NO $\rightarrow$ PINAL + NO <sub>2</sub>	1.00E-14	Rickard and Pascoe (2009)
G40240	TrGTerCN	APINBOO + NO <sub>2</sub> $\rightarrow$ PINAL + NO <sub>3</sub>	1.00E-15	Rickard and Pascoe (2009)
G40241	TrGTerC	C109O2 $\rightarrow$ C89CO3 + HCHO	k1_R02p0R02	Rickard and Pascoe (2009)
G40242	TrGTerCN	C109O2 + NO $\rightarrow$ C89CO3 + HCHO + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G40243a	TrGTerC	C109O2 + HO <sub>2</sub> $\rightarrow$ C109OOH	KR02H02(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40243b	TrGTerC	C109O2 + HO <sub>2</sub> $\rightarrow$ C89CO3 + HCHO + OH	KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40244	TrGTerC	C109OOH + OH $\rightarrow$ C109CO + OH	5.47E-11	Rickard and Pascoe (2009)
G40245	TrGTerC	C109CO + OH $\rightarrow$ C89CO3 + CO	5.47E-11	Rickard and Pascoe (2009)
G40246	TrGTerCN	APINENE + NO <sub>3</sub> $\rightarrow$ LNAPINABO2	1.2E-12*EXP(490./temp)	T. J. Wallington et al. (2014)*
G40247	TrGTerCN	LNAPINABO2 $\rightarrow$ PINAL + NO <sub>2</sub>	(0.65*k1_R02tR02 + 0.35*k1_R02sR02)	Rickard and Pascoe (2009)
G40248	TrGTerCN	LNAPINABO2 + NO $\rightarrow$ PINAL + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*
G40249	TrGTerCN	LNAPINABO2 + HO <sub>2</sub> $\rightarrow$ LNAPINABOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40250	TrGTerCN	LNAPINABO2 + NO <sub>3</sub> $\rightarrow$ PINAL + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G40251	TrGTerCN	LNAPINABOOH + OH $\rightarrow$ LNAPINABO2	(.65*6.87E-12+.35*1.23E-11)	Rickard and Pascoe (2009)
G40252a	TrGTerC	BPINENE + OH $\rightarrow$ BPINAO2	1.47E-11*EXP(467./TEMP) *(0.8326*0.3+0.068)/(0.8326+0.068)	Gill and Hites (2002)*
G40252b	TrGTerC	BPINENE + OH $\rightarrow$ ROO6R1O2	1.47E-11*EXP(467./TEMP) *0.8326*0.7/(0.8326+0.068)	Gill and Hites (2002)*
G40253a	TrGTerC	BPINAO2 + HO <sub>2</sub> $\rightarrow$ BPINAOOH	KR02H02(10)*rcoch2o2_ooh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40253b	TrGTerC	BPINAO2 + HO <sub>2</sub> $\rightarrow$ NOPINONE + HCHO + HO <sub>2</sub> + OH	KR02H02(10)*rcoch2o2_oh	Rickard and Pascoe (2009), Taraborrelli (2016)
G40254a	TrGTerCN	BPINAO2 + NO $\rightarrow$ NOPINONE + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(11,3,0,0,0, temp, cair))	Rickard and Pascoe (2009), Taraborrelli (2016)



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

#	labels	reaction	rate coefficient	reference
G40254b	TrGTerCN	BPINAO2 + NO → BPINANO3	KR02N0*alpha_AN(11,3,0,0,0, temp,cair)	Rickard and Pascoe (2009), Taraborrelli (2016)
G40255	TrGTerC	BPINAO2 → NOPINONE + HCHO + HO <sub>2</sub>	k1_R02t0R02	Rickard and Pascoe (2009)
G40256	TrGTerC	BPINAOOH + OH → BPINAO2	1.33E-11	Rickard and Pascoe (2009)
G40257	TrGTerCN	BPINANO3 + OH → NOPINONE + HCHO + NO <sub>2</sub>	4.70E-12	Rickard and Pascoe (2009)
G40258a	TrGTerCN	ROO6R1O2 + NO → ROO6R3O2 + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(13,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40258b	TrGTerCN	ROO6R1O2 + NO → ROO6R1NO3	KR02N0*alpha_AN(13,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40259	TrGTerC	ROO6R1O2 + HO <sub>2</sub> → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40260	TrGTerC	ROO6R1O2 → ROO6R3O2 + CH <sub>3</sub> COCH <sub>3</sub>	k1_R02t0R02	Vereecken and Peeters (2012)
G40261a	TrGTerCN	RO6R1O2 + NO → RO6R3O2 + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40261b	TrGTerCN	RO6R1O2 + NO → RO6R1NO3	KR02N0*alpha_AN(12,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40262	TrGTerC	RO6R1O2 + HO <sub>2</sub> → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)*
G40263	TrGTerC	RO6R1O2 → RO6R3O2	k1_R02s0R02	Vereecken and Peeters (2012)
G40264a	TrGTerCN	RO6R3O2 + NO → 9 LCARBON + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	KR02N0*(1.-alpha_AN(12,3,0,0,0, temp,cair))	Vereecken and Peeters (2012)
G40264b	TrGTerCN	RO6R3O2 + NO → 10 LCARBON + LNITROGEN	KR02N0*alpha_AN(12,3,0,0,0, temp,cair)	Vereecken and Peeters (2012)
G40265	TrGTerC	RO6R3O2 + HO <sub>2</sub> → 10 LCARBON	KR02H02(10)	Vereecken and Peeters (2012)
G40266	TrGTerC	RO6R3O2 → 9 LCARBON + HCHO + HO <sub>2</sub>	k1_R02sR02	Vereecken and Peeters (2012)*
G40267a	TrGTerC	BPINENE + O <sub>3</sub> → NOPINONE + .63 CO + .37 CH <sub>2</sub> OO + .16 OH + .16 HO <sub>2</sub>	1.35E-15*EXP(-1270./TEMP) * .051/(1-.027)	T. J. Wallington et al. (2014)*
G40267b	TrGTerC	BPINENE + O <sub>3</sub> → NOPINOO + CO <sub>2</sub>	1.35E-15*EXP(-1270./TEMP) * .368/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40267c	TrGTerC	BPINENE + O <sub>3</sub> → NOPINDO2 + CO <sub>2</sub> + OH	1.35E-15*EXP(-1270./TEMP) * .283/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40267d	TrGTerC	BPINENE + O <sub>3</sub> → C8BC + 2 CO <sub>2</sub>	1.35E-15*EXP(-1270./TEMP) * (.104+.167)/(1-.027)	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40268	TrGTerCN	BPINENE + NO <sub>3</sub> → LNBPINABO2	2.51E-12	T. J. Wallington et al. (2014)*
G40269	TrGTerCN	LNBPINABO2 + HO <sub>2</sub> → LNBPINABOOH	KR02H02(10)	Rickard and Pascoe (2009)
G40270	TrGTerCN	LNBPINABO2 + NO → NOPINONE + HCHO + NO <sub>2</sub> + NO <sub>2</sub>	KR02N0	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G40271	TrGTerCN	LNBPINABO2 + NO <sub>3</sub> → NOPINONE + HCHO + NO <sub>2</sub> + NO <sub>2</sub>	KR02N03	Rickard and Pascoe (2009)
G40272a	TrGTerCN	LNBPINABO2 → NOPINONE + HCHO + NO <sub>2</sub>	k1_R02tR02*0.7	Rickard and Pascoe (2009)
G40272b	TrGTerCN	LNBPINABO2 → BPINANO3	k1_R02tR02*0.3	Rickard and Pascoe (2009)
G40273	TrGTerCN	LNBPINABOOH + OH → LNBPINABO2	9.58E-12	Rickard and Pascoe (2009)
G40274	TrGTerCN	ROO6R1NO3 + OH → ROO6R3O2 + CH <sub>3</sub> COCH <sub>3</sub> + NO <sub>2</sub>	9.16E-13	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40275	TrGTerCN	RO6R1NO3 + OH → 9 LCARBON + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	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 <sub>2</sub>	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 <sub>3</sub> → APINBOO	2.E-16*.50*.18	Wolfe et al. (2011), Taraborrelli (2016)
G40280b	TrGC	CARENE + O <sub>3</sub> → PINONIC	2.E-16*.50*.16	Wolfe et al. (2011), Taraborrelli (2016)
G40280c	TrGC	CARENE + O <sub>3</sub> → OH + NORPINAL + CO + HO <sub>2</sub>	2.E-16*.50*.66	Wolfe et al. (2011), Taraborrelli (2016)
G40280d	TrGC	CARENE + O <sub>3</sub> → APINAOO	2.E-16*.50*.12	Wolfe et al. (2011), Taraborrelli (2016)
G40280e	TrGC	CARENE + O <sub>3</sub> → OH + C109O2	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Taraborrelli (2016)
G40281	TrGCN	CARENE + NO <sub>3</sub> → 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)*

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

#	labels	reaction	rate coefficient	reference
G40282b	TrGTerC	SABINENE + OH $\rightarrow$ ROO6R1O2	$1.47\text{E-}11 \cdot \text{EXP}(467./\text{TEMP})$ $\cdot 0.8326 \cdot 0.7 / (0.8326 + 0.068)$	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40283a	TrGTerC	SABINENE + O <sub>3</sub> $\rightarrow$ NOPINONE + .63 CO + .37 HOCH <sub>2</sub> OOH + .16 OH + .16 HO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.051 / (1 - .027)$	T. J. Wallington et al. (2014)*
G40283b	TrGTerC	SABINENE + O <sub>3</sub> $\rightarrow$ NOPINOO + CO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.368 / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40283c	TrGTerC	SABINENE + O <sub>3</sub> $\rightarrow$ NOPINDO2 + CO <sub>2</sub> + OH	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.283 / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40283d	TrGTerC	SABINENE + O <sub>3</sub> $\rightarrow$ C8BC + 2 CO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot (.104 + .167) / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40284	TrGTerCN	SABINENE + NO <sub>3</sub> $\rightarrow$ LNBPINABO2	$2.51\text{E-}12$	T. J. Wallington et al. (2014)*
G40285a	TrGTerC	CAMPHENE + OH $\rightarrow$ BPINAO2	$1.47\text{E-}11 \cdot \text{EXP}(467./\text{TEMP})$ $\cdot (0.8326 \cdot 0.3 + 0.068) / (0.8326 + 0.068)$	Gill and Hites (2002)*
G40285b	TrGTerC	CAMPHENE + OH $\rightarrow$ ROO6R1O2	$1.47\text{E-}11 \cdot \text{EXP}(467./\text{TEMP})$ $\cdot 0.8326 \cdot 0.7 / (0.8326 + 0.068)$	Vereecken and Peeters (2012), Gill and Hites (2002)*
G40286a	TrGTerC	CAMPHENE + O <sub>3</sub> $\rightarrow$ NOPINONE + .63 CO + .37 HOCH <sub>2</sub> OOH + .16 OH + .16 HO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.051 / (1 - .027)$	T. J. Wallington et al. (2014)*
G40286b	TrGTerC	CAMPHENE + O <sub>3</sub> $\rightarrow$ NOPINOO + CO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.368 / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40286c	TrGTerC	CAMPHENE + O <sub>3</sub> $\rightarrow$ NOPINDO2 + CO <sub>2</sub> + OH	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot 0.283 / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40286d	TrGTerC	CAMPHENE + O <sub>3</sub> $\rightarrow$ C8BC + 2 CO <sub>2</sub>	$1.35\text{E-}15 \cdot \text{EXP}(-1270./\text{TEMP})$ $\cdot (.104 + .167) / (1 - .027)$	Nguyen et al. (2009), T. J. Wallington et al. (2014)
G40287	TrGTerCN	CAMPHENE + NO <sub>3</sub> $\rightarrow$ LNBPINABO2	$2.51\text{E-}12$	T. J. Wallington et al. (2014)*
G40400	TrGAroC	LHAROM + OH $\rightarrow$ .14 TLEPOXMUC + .03 C6H5CH2O2 + .04 CRESOL + .79 TLBIPERO2 + .18 HO <sub>2</sub> + 4 LCARBON	$5.67\text{E-}11$	Rickard and Pascoe (2009)*
G40401	TrGAroCN	LHAROM + NO <sub>3</sub> $\rightarrow$ C6H5CH2O2 + HNO <sub>3</sub> + 4 LCARBON	$2.60\text{E-}15$	Rickard and Pascoe (2009)*
G9200	StTrGS	SO <sub>2</sub> + OH $\rightarrow$ H <sub>2</sub> SO <sub>4</sub> + HO <sub>2</sub>	$k\_3\text{rd}(\text{temp}, \text{cair}, 3.3\text{E-}31, 4.3,$ $1.6\text{E-}12, 0., 0.6)$	Sander et al. (2011)
G9400a	TrGCS	DMS + OH $\rightarrow$ CH <sub>3</sub> SO <sub>2</sub> + HCHO	$1.13\text{E-}11 \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	DMS + OH $\rightarrow$ DMSO + HO <sub>2</sub>	$k\_DMS\_OH$	Atkinson et al. (2004)*
G9401	TrGCNS	DMS + NO <sub>3</sub> $\rightarrow$ CH <sub>3</sub> SO <sub>2</sub> + HNO <sub>3</sub> + HCHO	$1.9\text{E-}13 \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)

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

#	labels	reaction	rate coefficient	reference
G9402	TrGCS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{ SO}_2 + \text{HCHO} + .6 \text{ CH}_3 + .4 \text{ HO}_2 + .4 \text{ CH}_3\text{SO}_3\text{H}$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3$	$1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	5.E-11	Barone et al. (1995)
G9408	StTrGS	$\text{CH}_2\text{OO} + \text{SO}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HCHO}$	k_CH200_S02	Welz et al. (2012), Stone et al. (2014)*
G9409	TrGTerCS	$\text{NOPINOO} + \text{SO}_2 \rightarrow \text{NOPINONE} + \text{H}_2\text{SO}_4$	7.E-14	Rickard and Pascoe (2009)
G9410	TrGTerCS	$\text{APINAOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G9411	TrGTerCS	$\text{APINBOO} + \text{SO}_2 \rightarrow \text{PINAL} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G9412	TrGTerCS	$\text{MBOOO} + \text{SO}_2 \rightarrow \text{IBUTALOH} + \text{H}_2\text{SO}_4$	7.00E-14	Rickard and Pascoe (2009)
G0070dCM	StTrG	$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{OOH}$	4.0/(680*100)	see general notes*
G0055dUJ	StTrGC	$\text{C511OOH} \rightarrow \text{C511OOHDummy}$	4.0/(680*100)	see general notes*
G0056dUJ	StTrGC	$\text{C512OOH} \rightarrow \text{C512OOHDummy}$	4.0/(680*100)	see general notes*
G0057dUJ	StTrGC	$\text{C513OOH} \rightarrow \text{C513OOHDummy}$	4.0/(680*100)	see general notes*
G0026dUJ	StTrGC	$\text{ISOPBOOH} \rightarrow \text{ISOPBOOHDummy}$	4.0/(680*100)	see general notes*
G0028dUJ	StTrGC	$\text{ISOPDOOH} \rightarrow \text{ISOPDOOHDummy}$	4.0/(680*100)	see general notes*
G0024dUJ	StTrGC	$\text{C59OOH} \rightarrow \text{C59OOHDummy}$	4.0/(680*100)	see general notes*
G0070dUJ	StTrGC	$\text{C85OOH} \rightarrow \text{C85OOHDummy}$	4.0/(680*100)	see general notes*
G0071dUJ	StTrGC	$\text{C86OOH} \rightarrow \text{C86OOHDummy}$	4.0/(680*100)	see general notes*
G0068dUJ	StTrGC	$\text{C812OOH} \rightarrow \text{C812OOHDummy}$	4.0/(680*100)	see general notes*
G0069dUJ	StTrGC	$\text{C813OOH} \rightarrow \text{C813OOHDummy}$	4.0/(680*100)	see general notes*
G0076dUJ	StTrGC	$\text{C96OOH} \rightarrow \text{C96OOHDummy}$	4.0/(680*100)	see general notes*
G0077dUJ	StTrGC	$\text{C97OOH} \rightarrow \text{C97OOHDummy}$	4.0/(680*100)	see general notes*
G0079dUJ	StTrGC	$\text{C98OOH} \rightarrow \text{C98OOHDummy}$	4.0/(680*100)	see general notes*
G0124dUJ	StTrGC	$\text{PINALOOH} \rightarrow \text{PINALOOHDummy}$	4.0/(680*100)	see general notes*
G0044dUJ	StTrGC	$\text{C106OOH} \rightarrow \text{C106OOHDummy}$	4.0/(680*100)	see general notes*
G0042dUJ	StTrGC	$\text{BPINAOOH} \rightarrow \text{BPINAOOHDummy}$	4.0/(680*100)	see general notes*
G0045dUJ	StTrGC	$\text{C109OOH} \rightarrow \text{C109OOHDummy}$	4.0/(680*100)	see general notes*
G0009dUJ	StTrG	$\text{HCOOH} \rightarrow \text{HCOOHDummy}$	0.3/(680*100)	see general notes*
G0010dUJ	StTrG	$\text{HOCH}_2\text{OOH} \rightarrow \text{HOCH}_2\text{OOHDummy}$	4.0/(680*100)	see general notes*
G0011dUJ	StTrGC	$\text{C}_2\text{H}_5\text{OOH} \rightarrow \text{C}_2\text{H}_5\text{OOHDummy}$	4.0/(680*100)	see general notes*
G0081dUJ	StTrGC	$\text{CH}_3\text{CHOHOOH} \rightarrow \text{CH}_3\text{CHOHOOHDummy}$	4.0/(680*100)	see general notes*
G0121dUJ	StTrGC	$\text{NOPINDOOH} \rightarrow \text{NOPINDOOHDummy}$	4.0/(680*100)	see general notes*
G0074dUJ	StTrGC	$\text{C8BCOOH} \rightarrow \text{C8BCOOHDummy}$	4.0/(680*100)	see general notes*

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

#	labels	reaction	rate coefficient	reference
G0062dUJ	StTrGC	C721OOH $\rightarrow$ C721OOHDummy	4.0/(680*100)	see general notes*
G0064dUJ	StTrGC	C722OOH $\rightarrow$ C722OOHDummy	4.0/(680*100)	see general notes*
G0085dUJ	StTrGC	CO235C6OOH $\rightarrow$ CO235C6OOHDummy	4.0/(680*100)	see general notes*
G0060dUJ	StTrGC	C614OOH $\rightarrow$ C614OOHDummy	4.0/(680*100)	see general notes*
G0052dUJ	StTrGC	C413COOOH $\rightarrow$ C413COOOHDummy	4.0/(680*100)	see general notes*
G0053dUJ	StTrGC	C44OOH $\rightarrow$ C44OOHDummy	4.0/(680*100)	see general notes*
G0021dUJ	StTrGC	MACROOH $\rightarrow$ MACROOHDummy	4.0/(680*100)	see general notes*
G0083dUJ	StTrGC	CHOC3COOOH $\rightarrow$ CHOC3COOOHDummy	4.0/(680*100)	see general notes*
G0094dUJ	StTrGC	LAPINABOOH $\rightarrow$ LAPINABOOHDummy	4.0/(680*100)	see general notes*
G0013dUJ	StTrGCN	PAN $\rightarrow$ PANDummy	0.2/(680*100)	see general notes*
G0005dUJ	StTrGN	NO <sub>3</sub> $\rightarrow$ NO <sub>3</sub> Dummy	4/(680*100)	see general notes*
G0006dUJ	StTrGN	HNO <sub>3</sub> $\rightarrow$ HNO <sub>3</sub> Dummy	4/(680*100)	see general notes*
G3116uj	StTrGC	MVK $\rightarrow$ MVKDummy	1/(680*100)	see general notes*
G3116ujb	StTrGC	MACR $\rightarrow$ MACRDummy	1/(680*100)	see general notes*
G3119uj	StTrGC	PINAL $\rightarrow$ PINALDummy	0.6/(680*100)	see general notes*

## General notes

### Three-body reactions

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

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

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

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

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

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

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

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

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

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

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

### RO<sub>2</sub> self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as  $k^{1\text{st}} = 2 \times \sqrt{k_{\text{self}} \times k_{\text{CH3O2}}} \times [\text{RO}_2]$  where  $k_{\text{self}}$  = second-order rate coefficient of the self reaction of the organic peroxy radical,  $k_{\text{CH3O2}}$  = second-order rate coefficient of the self reaction of  $\text{CH}_3\text{O}_2$ , and  $[\text{RO}_2]$  = sum of the concentrations of all organic peroxy radicals.

### Deposition of peroxides

The value of  $4.0/(680 \times 100)$  is based on deposition velocities for peroxides obtained by ?. The PBL height of 680 m is based on 120 hour FlexPart (<https://www.flexpart.eu>) backtrajectory simulations. The deposition of PAN is based on ?.

## Specific notes

G2110: The rate coefficient is: `k_HO2_HO2 = (3.0E-13*EXP(460./temp)+2.1E-33*EXP(920./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. 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  $\text{Kc} [\text{molec}^{-1} \text{cm}^3] = \text{Kp} \times \text{R} \times \text{T} / \text{NA}$ , where  $\text{R}$  is  $82.05736 [\text{cm}^3 \text{atm K}^{-1} \text{mol}^{-1}]$ .

G2118: Assuming fast equilibrium.

G3109: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.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 recommended value at 298K.

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

G4130a: SAR for H-abstraction by OH.

G4130b: SAR for H-abstraction by OH.

G4132: SAR for H-abstraction by OH.

G4133: Lower limit of the rate constant. Products uncertain but  $\text{CH}_3\text{OH}$  can be excluded because of a likely high energy barrier (L. Vereecken, pers. comm.).  $\text{CH}_2\text{OO}$  production cannot be excluded.

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

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

G4136: Average of two measurements.

G4137: Upper limit.

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

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

G4142: High-pressure limit.

G4143: Generic estimate for reaction with alcohols.

G4144: Generic estimate for reaction with  $\text{RO}_2$ .

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

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

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

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

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

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

G4164: Upper limit. Dominant pathway under atmospheric conditions.

G42001: The product distribution is from Rickard and Pascoe (2009), after substitution of the energized Criegee intermediate,  $\text{CH}_2\text{OO}$ , by its decomposition products and reaction of the stabilized CI with the water dimer.

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

G42013: The rate coefficient is:  $k_{\text{CH}_3\text{CO}_3\text{NO}_2} = k_{3\text{rd}}(\text{temp}, \text{cair}, 9.7\text{E}-29, 5.6, 9.3\text{E}-12, 1.5, 0.6)$ .

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

G42021: The rate coefficient is  $k_{\text{PAN}_M} = k_{\text{CH}_3\text{CO}_3\text{NO}_2}/9.9\text{E}-29 \cdot \exp(-14000./\text{temp})$ , 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  $\text{HOCH}_2\text{CH}_2\text{O}$  in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are  $2 \text{HCHO} + \text{HO}_2$ .

G42051a: Same as for the  $\text{CH}_3\text{O}_2$  channel in G4107:  $\text{CH}_3\text{OOH} + \text{OH}$ .

G42058b: The aldehydic H is assumed to be like the analogous H of  $\text{HOCH}_2\text{CHO}$ .

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

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

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

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

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

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

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

G42085a: Uncertainties on the kinetics at pressures  $< 0.1 \text{ bar}$ .

G42085b: Channel proposed by Hynes and Wine 1991,  $\text{OH} + \text{HCHO} + \text{HOCN}$ , could not be confirmed by

Tyndall et al. (2001b). There is no alternative mechanism at the moment. Products assumed to be  $\text{OH} + \text{CH}_3\text{CO}_3 + \text{NO}$

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

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

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

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

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

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  $\text{RO}_2 + \text{HO}_2$  reaction from Atkinson (1997) is used here.

G43008: The value for the generic  $\text{RO}_2 + \text{HO}_2$  reaction from Atkinson (1997) is used here.

G43011: Strong positive deviation of  $k$  below 240 K compared to the expression recommended by JPL (Sander et al., 2011).

G43015a: The same value as for G4107 ( $\text{CH}_3\text{OOH} + \text{OH}$ ) is used, multiplied by the branching ratio of the  $\text{CH}_3\text{O}_2$  channel.

G43028: Alkyl nitrate formation neglected. (also not considered in MCM).

G43037: Alkyl nitrate formation neglected. (also not considered in MCM).

G43040a: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43040b: Rate coefficient estimated with SAR (Taraborrelli, 2010).

G43044: Alkyl nitrate formation neglected.

G43045c: Rate coefficient assumed to equal to the one of hydroxyacetone (ACETOL) for this channel.

G43048: Using the high-pressure limit.

G43049: The pressure fall-off between 1000 and 100 mbar is only 3% (Kirchner et al., 1999).

G43050: Value for  $\text{CH}_3\text{O}_2\text{NO}_2 + \text{OH}$ , H-abstraction enhanced by the  $\text{CH}_3\text{CO}$ -group by  $f_{\text{co}}$ .

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

G43052: Only major H-abstraction channel considered.

G43059: Products approximated with the major end-product  $\text{CH}_3\text{CHO}$ .

G43060b: Products approximated with the major end-product  $\text{CH}_3\text{CHO}$ .

G43061: Products approximated with the likely end-product  $\text{CH}_3\text{CHO}$ .

G43065: As for  $\text{HCOCO}_3$ .

G43070a: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43070b: Branching ratios estimated with SAR for H-abstraction rate constants by OH.

G43071a: Only this channel considered as the intermediate radical is likely more stable than  $\text{CHCH}(\text{OH})_2$ .

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

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

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

G43223: Products simplified

G43419:  $\text{KDEC C3DIALO} \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2$

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

G43421: Permutation reaction (minor channels removed).

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

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

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

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

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

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

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

G44018: LHMVKABO2 is  $0.12 \text{ HMVKA02} + 0.88 \text{ HMVKBO2}$ .

G44019: LMEKO2 represents  $0.62 \text{ MEKBO2} + 0.38 \text{ MEKAO2}$ .

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

G44023a: Products from H-abstraction from the tertiary carbon bearing the  $\text{ONO}_2$  group.

G44023b: Products from H-abstraction from the secondary carbon bearing the  $\text{ONO}_2$  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  $\text{RO}_2$ .

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  $\text{CH}_3\text{CHCO}$  from Hatakeyama et al. (1985) adjusted.

G44086: Simplified product distribution.



G44089: The nitrated RO<sub>2</sub> is replaced by its products upon reaction with NO.

G44096: Both LBUT1ENO2 isomers mostly C<sub>2</sub>H<sub>5</sub>CHO.

G44097a: Branching ratios according to Rickard et al. (1999). CH<sub>3</sub>CHO<sub>2</sub>CHO is replaced with its major products CH<sub>3</sub>CHO + CO + HO<sub>2</sub>.

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

G44098: The nitrated RO<sub>2</sub> is replaced by its products upon reaction with NO.

G44103b: MEKCOH replaced by its major oxidation products.

G44104: Carbonyl nitrate replaced by its major oxidation products.

G44106: CH<sub>3</sub>CHOOA products as from C<sub>3</sub>H<sub>6</sub> + O<sub>3</sub> reaction.

G44107: The nitrated RO<sub>2</sub> is replaced by its products upon reaction with NO.

G44110: The nitrated RO<sub>2</sub> 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)<sub>2</sub>.

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)<sub>2</sub>.

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)<sub>2</sub>.

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)<sub>2</sub>.

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 NC<sub>4</sub>DCO<sub>2</sub> → MALANHY + NO<sub>2</sub>

G44406c: KDEC MALDIALCO<sub>2</sub> → .6 MALANHY + HO<sub>2</sub> + .4 GLYOX + .4 CO + .4 CO<sub>2</sub>

G44407: KDEC MALDIALCO<sub>2</sub> → .6 MALANHY + HO<sub>2</sub> + .4 GLYOX + .4 CO + .4 CO<sub>2</sub>

G44409: KDEC MALDIALCO<sub>2</sub> → .6 MALANHY + HO<sub>2</sub> + .4 GLYOX + .4 CO + .4 CO<sub>2</sub>

G44410: KDEC MALDIALCO<sub>2</sub> → .6 MALANHY + HO<sub>2</sub> + .4 GLYOX + .4 CO + .4 CO<sub>2</sub>

G44412: KDEC BZFUONOOA → .5 BZFUONOO + .5 CO + .5 CO<sub>2</sub> + .5 HCOCH<sub>2</sub>O<sub>2</sub> + .5 OH and BZFUONOO → .625 CO<sub>14</sub>O<sub>3</sub>CO<sub>2</sub>H + .375 CO<sub>14</sub>O<sub>3</sub>CHO + .375 H<sub>2</sub>O<sub>2</sub>

G44421: Only major channel.

G44424: KDEC: GLYOOA → .125 HCHO + .18 GLYOO + 0.82 HO<sub>2</sub> + .57 OH + 1.265 CO + .25 CO<sub>2</sub> and H<sub>2</sub>O substitution GLYOO → .625 HCOCO<sub>2</sub>H + .375 GLYOX + .375 H<sub>2</sub>O<sub>2</sub>

G44425: Merged equations.

G44430: KDEC MALANHYO → HCOCO<sub>2</sub>HCO<sub>3</sub>

G44431: KDEC MALANHYO → HCOCO<sub>2</sub>HCO<sub>3</sub>

G44432: Only major channel. KDEC MALANHYO → HCOCO<sub>2</sub>HCO<sub>3</sub>

G44436: KDEC NBZFUO → .5 CO<sub>14</sub>O<sub>3</sub>CHO + .5 NO<sub>2</sub> + .5 NBZFUONE + .5 HO<sub>2</sub>

G44437: KDEC NBZFUO → .5 CO<sub>14</sub>O<sub>3</sub>CHO + .5 NO<sub>2</sub> + .5 NBZFUONE + .5 HO<sub>2</sub>

G44438: KDEC NBZFUO → .5 CO<sub>14</sub>O<sub>3</sub>CHO + .5 NO<sub>2</sub> + .5 NBZFUONE + .5 HO<sub>2</sub> and RO<sub>2</sub> Only major channel.

G44439: KDEC MALDIALCO<sub>2</sub> → .6 MALANHY + HO<sub>2</sub> + .4 GLYOX + .4 CO + .4 CO<sub>2</sub>

G44443: KDEC MECOACETO → CH<sub>3</sub>CO<sub>3</sub> + HCHO

G44444: KDEC MECOACETO → CH<sub>3</sub>CO<sub>3</sub> + HCHO

G44445: KDEC MECOACETO → CH<sub>3</sub>CO<sub>3</sub> + HCHO

G44450: KDEC BZFUO → CO<sub>14</sub>O<sub>3</sub>CHO + HO<sub>2</sub>

G44451: KDEC BZFUO → CO<sub>14</sub>O<sub>3</sub>CHO + HO<sub>2</sub>

G44452: KDEC BZFUO → CO<sub>14</sub>O<sub>3</sub>CHO + HO<sub>2</sub>. Only major channel.

G44457: KDEC MALDIALO  $\rightarrow$  GLYOX + GLYOX + HO2

G44458: KDEC MALDIALO  $\rightarrow$  GLYOX + GLYOX + HO2

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

G44461: KBPAN  $\rightarrow$  k.PAN\_M

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

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

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

G45040: Alkyl nitrate formation neglected.

G45043: Old MCM rate constant 4.16E-11.

G45047: Alkyl nitrate formation neglected.

G45055: Alkyl nitrate formation neglected.

G45071: Alkyl nitrate formation neglected.

G45074: Formic acid production consistent with results of Bates et al. (2014). Here, the high yields of formic acid and hydroxycarbonyls at low NO from oxidation of cis-beta-LIEPOX (the most abundant isomer) are approximated with the production of DB1O which undergo both the Dibble double H-transfer to DB2O2 and HOCH2 elimination yielding HVMK and HMAK (keto-vinyl alcohol potentially arising from decomposition of the alkoxy radical resulting from the ring opening after H-abstraction). The rate constant is from Paulot et al. (2009b) and adjusted based on Bates et al. (2014) that determined the single rate constants for the cis- and trans- beta isomer.

G45080: Alkyl nitrate formation neglected.

G45092a: ZCODC23DBCOD = CM4DIAL in MCM only from aromatics.

G45092b: Only one acyl peroxy radical considered.

G45093: Two aldehydic sites reacting with NO<sub>3</sub> 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<sub>2</sub> 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<sub>2</sub>-to-RO conversion (skipped here), yields the HOCHOH fragment which in turn reacts with O<sub>2</sub> forming HCOOH + HO<sub>2</sub>. Along CH<sub>3</sub>COCHOHCHO should be produced but not in the mechanism. Only CH<sub>3</sub>COCHO<sub>2</sub>CHO. The rate constant is consistent with predictions by Ganzeveld et al. (2006) for ENOL. OH-addition to the OH-bearing carbon is considered the dominant channel as it is already for the ENOL (Ganzeveld et al., 2006).

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

G45116: As for DB1OOH + OH.

G45117: Additional sinks for DB2OOH are neglected.

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

G45128: Rate constant by Liljegren and Stevens (2013). A lumped RO<sub>2</sub> 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<sub>2</sub> production for mass conservation.

G45131: Alkyl nitrate formation neglected.

G45132: Hydroperoxide formation neglected.

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

G45139: ZCPANC23DBCOD is assumed to react like LC5PAN1719.

G45201: Alkyl nitrate formation neglected.

G45207: Alkyl nitrate formation neglected.

G45214: Alkyl nitrate formation neglected.

G45217: Alkyl nitrate formation neglected.

G45225: Alkyl nitrate formation neglected.

G45236: LMBOABO2 = .67 MBOAO2 + .33 MBOBO2

G45247: Alkyl nitrate formation neglected.

G45400: KDEC NC4MDCO2  $\rightarrow$  MMALANHY + NO2

G45404: KDEC NTLFUO  $\rightarrow$  ACCOMECHO + NO2

G45405: KDEC NTLFUO  $\rightarrow$  ACCOMECHO + NO2

G45406: KDEC NTLFUO  $\rightarrow$  ACCOMECHO

G45409: KBPAN  $\rightarrow$  k.PAN\_M(renaming)

G45413: KFPAN  $\rightarrow$  k.CH3CO3.NO2 (renaming)

G45422: KDEC MMALANHYO  $\rightarrow$  CO2H3CO3

G45423: KDEC MMALANHYO  $\rightarrow$  CO2H3CO3

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

G45429: KBPAN  $\rightarrow$  k.PAN\_M (renamed)

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

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

G45432: KFPAN  $\rightarrow$  k.CH3CO3.NO2 (renaming)

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

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

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

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

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

G45456: KFPAN  $\rightarrow$  k.CH3CO3.NO2 (renaming)

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

G45477: KDEC NTLFUO  $\rightarrow$  ACCOMECHO + NO2

G45478: KDEC NTLFUO  $\rightarrow$  ACCOMECHO + NO2

G45479: KDEC NTLFUO  $\rightarrow$  ACCOMECHO + NO2

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

G45487: KDEC C5DIALO  $\rightarrow$  MALDIAL

G45488: KDEC C5DIALO  $\rightarrow$  MALDIAL

G45489: KDEC C5DIALO  $\rightarrow$  MALDIAL

G45491b: Reactions with KRO2HO2.

G45492: MGLYOX + GLYOX + HO2 from KDEC substitution

G45493: MGLYOX + GLYOX + HO2 from KDEC substitution

G45494: Permutation reaction (minor channels removed).

G46201: Alkyl nitrate formation neglected.

G46404b: Reactions with KRO2HO2 and KDEC C615CO2O  $\rightarrow$  C5DICARB + CO + HO2.

G46405: KDEC C615CO2O  $\rightarrow$  C5DICARB + CO + HO2

G46406: KDEC C615CO2O  $\rightarrow$  C5DICARB + CO + HO2

G46407: Only major channel.

G46413b: Reactions with KRO2HO2 and KDEC NDNPHENO  $\rightarrow$  NC4DCO2H + HNO3 + CO + CO + NO2.

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

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

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

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

G46426: KFPAN  $\rightarrow$  k.CH3CO3.NO2

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

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

G46433: KDEC NCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + HO2

G46434: KDEC NCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + HO2

G46435: KDEC NCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + HO2

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

G46438: KDEC NPHENO  $\rightarrow$  MALDALCO2H + GLYOX + NO2

G46439: KDEC NPHENO  $\rightarrow$  MALDALCO2H + GLYOX + NO2

G46440: KDEC NPHENO  $\rightarrow$  MALDALCO2H + GLYOX + NO2

G46441: Merged equations.

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

G46448: KDEC NNCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + NO2

G46449: KDEC NNCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + NO2

G46450: KDEC NNCATECO  $\rightarrow$  NC4DCO2H + HCOCO2H + NO2

G46457: Merged equations.

G46458: Merged equations.

G46461b: Reactions with KRO2HO2 and KDEC PHENO  $\rightarrow$  .71 MALDALCO2H + .71 GLYOX + .29 PBZQONE + HO2

G46462: KDEC PHENO  $\rightarrow$  .71 MALDALCO<sub>2</sub>H + .71 GLYOX + .29 PBZQONE + HO<sub>2</sub>

G46463: KDEC PHENO  $\rightarrow$  .71 MALDALCO<sub>2</sub>H + .71 GLYOX + .29 PBZQONE + HO<sub>2</sub>

G46464: KDEC PHENO  $\rightarrow$  .71 MALDALCO<sub>2</sub>H + .71 GLYOX + .29 PBZQONE + HO<sub>2</sub> and Only major channel.

G46468: KFPAN  $\rightarrow$  k\_CH<sub>3</sub>CO<sub>3</sub>\_NO<sub>2</sub>

G46472b: new channel

G46476: HOC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub> is a nitro-phenol

G46480b: Reactions with KRO<sub>2</sub>HO<sub>2</sub> and KDEC PBZQO  $\rightarrow$  C<sub>5</sub>CO<sub>2</sub>OHCO<sub>3</sub>

G46481: KDEC PBZQO  $\rightarrow$  C<sub>5</sub>CO<sub>2</sub>OHCO<sub>3</sub>

G46482: KDEC PBZQO  $\rightarrow$  C<sub>5</sub>CO<sub>2</sub>OHCO<sub>3</sub>

G46483: KDEC PBZQO  $\rightarrow$  C<sub>5</sub>CO<sub>2</sub>OHCO<sub>3</sub> and Only major channel.

G46485b: Reactions with KRO<sub>2</sub>HO<sub>2</sub> and KDEC DNPHENO  $\rightarrow$  NC<sub>4</sub>DCO<sub>2</sub>H + HCOCO<sub>2</sub>H + NO<sub>2</sub>

G46486: KDEC DNPHENO  $\rightarrow$  NC<sub>4</sub>DCO<sub>2</sub>H + HCOCO<sub>2</sub>H + NO<sub>2</sub>

G46487: KDEC DNPHENO  $\rightarrow$  NC<sub>4</sub>DCO<sub>2</sub>H + HCOCO<sub>2</sub>H + NO<sub>2</sub>

G46488: KDEC DNPHENO  $\rightarrow$  NC<sub>4</sub>DCO<sub>2</sub>H + HCOCO<sub>2</sub>H + NO<sub>2</sub>

G46490b: Reactions with KRO<sub>2</sub>HO<sub>2</sub> and KDEC BZEMUCO  $\rightarrow$  .5 EPXC<sub>4</sub>DIAL + .5 GLYOX + .5 HO<sub>2</sub> + .5 C<sub>3</sub>DIALO<sub>2</sub> + .5 C<sub>3</sub>OH<sub>13</sub>CO.

G46491b: KDEC BZEMUCO  $\rightarrow$  .5 EPXC<sub>4</sub>DIAL + .5 GLYOX + .5 HO<sub>2</sub> + .5 C<sub>3</sub>DIALO<sub>2</sub> + .5 C<sub>3</sub>OH<sub>13</sub>CO.

G46492: KDEC BZEMUCO  $\rightarrow$  .5 EPXC<sub>4</sub>DIAL + .5 GLYOX + .5 HO<sub>2</sub> + .5 C<sub>3</sub>DIALO<sub>2</sub> + .5 C<sub>3</sub>OH<sub>13</sub>CO

G46493: KDEC BZEMUCO  $\rightarrow$  .5 EPXC<sub>4</sub>DIAL + .5 GLYOX + .5 HO<sub>2</sub> + .5 C<sub>3</sub>DIALO<sub>2</sub> + .5 C<sub>3</sub>OH<sub>13</sub>CO and Only major channel.

G46499b: Reactions with KRO<sub>2</sub>HO<sub>2</sub> and KDEC NBZQO  $\rightarrow$  C<sub>6</sub>CO<sub>4</sub>DB + NO<sub>2</sub>.

G46500: KDEC NBZQO  $\rightarrow$  C<sub>6</sub>CO<sub>4</sub>DB + NO<sub>2</sub>

G46501: KDEC NBZQO  $\rightarrow$  C<sub>6</sub>CO<sub>4</sub>DB + NO<sub>2</sub>

G46502: KDEC NBZQO  $\rightarrow$  C<sub>6</sub>CO<sub>4</sub>DB + NO<sub>2</sub>

G46505b: New channel.

G46515: Only major channel.

G46517b: New channel.

G46522b: In analogy to TLBIPERO<sub>2</sub> from toluene (Birdsall et al., 2010).

G46523b: KDEC BZBIPERO  $\rightarrow$  GLYOX + HO<sub>2</sub> + .5 BZFUONE + .5 BZFUONE

G46524: KDEC BZBIPERO  $\rightarrow$  GLYOX + HO<sub>2</sub> + .5 BZFUONE + .5 BZFUONE

G46525: KDEC BZBIPERO  $\rightarrow$  GLYOX + HO<sub>2</sub> + .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: ROO<sub>6</sub>R<sub>3</sub>OOH produced but no sink for it.

G47225: ROO<sub>6</sub>R<sub>4</sub>P produced but no sink for it.

G47226: ROO<sub>6</sub>R<sub>5</sub>P produced but no sink for it

G47400: Merged.

G47402a: KROPRIM\*O<sub>2</sub> fast reaction C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>O = BENZAL + HO<sub>2</sub>.

G47402b: KROPRIM\*O<sub>2</sub> fast reaction C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>O = BENZAL + HO<sub>2</sub>.

G47403: KROPRIM\*O<sub>2</sub> fast reaction C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>O = BENZAL + HO<sub>2</sub>.

G47404: KROPRIM\*O<sub>2</sub> fast reaction C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>O = BENZAL + HO<sub>2</sub>. C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>OH replaced with its oxidation product BENZAL.

G47405: Merged.

G47406: Merged.

G47407b: According to Birdsall et al. (2010), the branching ratio rbipero<sub>2\_oh</sub> is set to 0.40 in order to take into account the OH-recycling and summed yield of butendial and methylbutendial.

G47408a: KDEC TLBIPERO  $\rightarrow$  .6 GLYOX + .4 MGLYOX + HO<sub>2</sub> + .2 ZCODC<sub>23</sub>DBCOD + .2 C<sub>5</sub>DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47408b: KDEC TLBIPERO  $\rightarrow$  .6 GLYOX + .4 MGLYOX + HO<sub>2</sub> + .2 ZCODC<sub>23</sub>DB COD + .2 C<sub>5</sub>DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47409: KDEC TLBIPERO  $\rightarrow$  .6 GLYOX + .4 MGLYOX + HO<sub>2</sub> + .2 ZCODC<sub>23</sub>DB COD + .2 C<sub>5</sub>DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47410: Only major channel and KDEC TLBIPERO  $\rightarrow$  .6 GLYOX + .4 MGLYOX + HO<sub>2</sub> + .2 ZCODC<sub>23</sub>DB COD + .2 C<sub>5</sub>DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL

G47412: KDEC MGLOOB  $\rightarrow$  .125 CH<sub>3</sub>CHO + .695 CH<sub>3</sub>CO + .57 CO + .57 OH + .125 HO<sub>2</sub> + .18 MGLOO + .25 CO<sub>2</sub>

G47413: Merged.

G47418b: Reactions with KRO<sub>2</sub>HO<sub>2</sub> and KDEC CRESO  $\rightarrow$  .68 C<sub>5</sub>CO<sub>14</sub>OH + .68 GLYOX + HO<sub>2</sub> + .32 PTLQONE.

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

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

G47421: KDEC CRESO  $\rightarrow$  .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE and Only major channel.

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

G47423: KDEC NCRESO  $\rightarrow$  C5CO14OH + GLYOX + NO2

G47424: KDEC NCRESO  $\rightarrow$  C5CO14OH + GLYOX + NO2

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

G47426: TOL1OHNO2 is a nitro-phenol

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

G47436: KFPAN  $\rightarrow$  k\_CH3CO3\_NO2

G47438: Only major channel.

G47439b: Reactions with KRO2HO2 and KDEC TLEMUCO  $\rightarrow$  .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2

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

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

G47442: KDEC TLEMUCO  $\rightarrow$  .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2 and Only major channel.

G47445: KFPAN  $\rightarrow$  k\_CH3CO3\_NO2

G47447: Only major channel.

G47454: New channel.

G47479: New channel.

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

G47483: KDEC NPTLQO  $\rightarrow$  C7CO4DB + NO2

G47484: KDEC NPTLQO  $\rightarrow$  C7CO4DB + NO2

G47485: KDEC NPTLQO  $\rightarrow$  C7CO4DB + NO2

G47486b: Reactions with KRO2HO2 and KDEC PTLQO  $\rightarrow$  C6CO2OHCO3

G47487: KDEC PTLQO  $\rightarrow$  C6CO2OHCO3

G47488: KDEC PTLQO  $\rightarrow$  C6CO2OHCO3

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

G47494: New channel.

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

G47498: KDEC MNCATECO  $\rightarrow$  NC4MDCO2H + HCOCO2H + NO2

G47499: KDEC MNCATECO  $\rightarrow$  NC4MDCO2H + HCOCO2H + NO2

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

G47502: KDEC MNCATECO  $\rightarrow$  NC4MDCO2H + HCOCO2H + HO2

G47503: KDEC MNCATECO  $\rightarrow$  NC4MDCO2H + HCOCO2H + HO2

G47504: KDEC MNCATECO  $\rightarrow$  NC4MDCO2H + HCOCO2H + HO2

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

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

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

G47512: KDEC NDNCRESO  $\rightarrow$  NC4MDCO2H + HNO3 + CO + CO + NO2

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

G47514: KDEC DNCRESO  $\rightarrow$  NC4MDCO2H + HCOCO2H + NO2

G47515: KDEC DNCRESO  $\rightarrow$  NC4MDCO2H + HCOCO2H + NO2

G47516: KDEC DNCRESO  $\rightarrow$  NC4MDCO2H + HCOCO2H + NO2

G48202: Alkyl nitrate formation neglected.

G48205: Alkyl nitrate formation neglected.

G48210: Alkyl nitrate formation neglected.

G48212: Alkyl nitrate formation neglected.

G48216: Alkyl nitrate formation neglected.

G48222: Alkyl nitrate formation neglected.

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

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

G48400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal

to  $(1.36\text{E-}11*0.16 + 2.31\text{E-}11*0.17 + 1.43\text{E-}11*0.12)/3$ , 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  $(1.36\text{E-}11*0.55 + 2.31\text{E-}11*0.50 + 1.43\text{E-}11*0.625)/3$ , 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  $k=(4.10\text{E-}16+2.60\text{E-}16+5.00\text{E-}16)/3 = 3.9\text{E-}16$ .

G48402: merged under same rate constant

G48403: Same products as for toluene

G48405:  $\text{KDEC CH}_2\text{OOb} \rightarrow .24 \text{ CH}_2\text{OO} + .40 \text{ CO} + .36 \text{ HO}_2 + .36 \text{ CO} + .36 \text{ OH}$  and  $\text{H}_2\text{O}_{\text{subs}} \text{PHCHOO} \rightarrow .625 \text{ PHCOOH} + .375 \text{ BENZAL} + .375 \text{ H}_2\text{O}_2 + .2 \text{ CO}_2$

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

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

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

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

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

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

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

G49207: Alkyl nitrate formation neglected.

G49238: Alkyl nitrate formation neglected.

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

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

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

G49400a: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to  $(3.27\text{E-}11*0.21 + 3.25\text{E-}11*0.30 + 5.67\text{E-}11*0.14)/3$ , where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400b: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to  $(3.27\text{E-}11*0.06 + 3.25\text{E-}11*0.06 + 5.67\text{E-}11*0.03)/3$ , where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400c: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to  $(3.27\text{E-}11*0.03 + 3.25\text{E-}11*0.03 + 5.67\text{E-}11*.04)/3$ , where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49400d: Same products as for toluene. Assuming a 1:1:1 proportion in xylenes emissions the analogous toluene product is produced with a rate constant equal to  $(3.27\text{E-}11*0.70 + 3.25\text{E-}11*0.61 + 5.67\text{E-}11*0.79)/3$ , where k and coefficients are for the single isomers 1,2,3-, 1,3,4- and 1,3,5- from MCM.

G49401: Same products as for toluene. The rate constant is the average of m, p, o  $k=(1.90+1.80+0.88)\text{E-}15/3=1.52\text{E-}15$ .

G40200: Products from Vereecken et al. (2007).  $\text{LAP-INABO}_2 = .65 \text{ APINAO}_2 + .35 \text{ APINBO}_2$

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

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

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

G40206: SAR-estimated rate constant,  $(k_{\text{ads}}+k_{\text{adt}})*\text{acoch}_3 = 6.46\text{E-}11$  where  $k_{\text{ads}} = 3.0\text{E-}11$ ,  $k_{\text{adt}} = 5.5\text{E-}11$ ,  $\text{acoch}_3 = 0.76$

G40207: Alkyl nitrate formation neglected.

G40211: Products from Rickard and Pascoe (2009).

G40212: Products from Rickard and Pascoe (2009).

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

G40242: Alkyl nitrate formation neglected.

G40246: Products from Rickard and Pascoe (2009).

G40248: Alkyl nitrate formation neglected.

G40252a: Products from Vereecken and Peeters (2012).

G40252b: Products from Vereecken and Peeters (2012).

G40259:  $\text{ROO}_6\text{R1OOH}$  is produced but no sink for it.

G40262:  $\text{RO}_6\text{R1OOH}$  is produced but no sink for it.

G40266: Rate constant modified according to MCM protocol.

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

G40268: Products from Rickard and Pascoe (2009).

G40270: Alkyl nitrate neglected.

G40274: As for  $\text{RO}_6\text{R1NO}_3$  in G4085.

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

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).

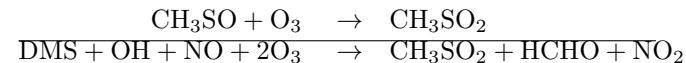
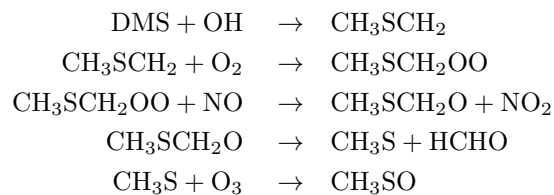
G40286a: Products from Nguyen et al. (2009).

G40287: Products from Rickard and Pascoe (2009).

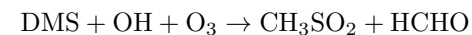
G40400: DIET35TOL(from MCM) as representative of higher aromatics

G40401: Same products as for toluene.

G9400a: For the abstraction path, the assumed reaction sequence (omitting H<sub>2</sub>O and O<sub>2</sub> as products) according to Yin et al. (1990) is:



Neglecting the effect on O<sub>3</sub> and NO<sub>x</sub>, the remaining reaction is:



.

G9400b: For the addition path, the rate coefficient is:  $k_{\text{DMS\_OH}} = 1.0\text{E-}39 \cdot \text{EXP}(5820./\text{temp}) \cdot \text{C}(\text{ind\_02}) / (1.+5.0\text{E-}30 \cdot \text{EXP}(6280./\text{temp}) \cdot \text{C}(\text{ind\_02}))$ .

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

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_02)	Sander et al. (2014)
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	jx(ip_01D)	Sander et al. (2014)
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	jx(ip_03P)	Sander et al. (2014)
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	jx(ip_H202)	Sander et al. (2014)
J3101	UpStTrGJN	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_N02)	Sander et al. (2014)
J3103a	UpStTrGJN	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGJN	$NO_3 + h\nu \rightarrow NO + O_2$	jx(ip_N002)	Sander et al. (2014)
J3104	StTrGJN	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N205)	Sander et al. (2014)
J3200	TrGJN	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	Sander et al. (2014)
J3201	StTrGJN	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HNO3)	Sander et al. (2014)
J3202	StTrGJN	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	jx(ip_HNO4)	Sander et al. (2014)
J41000	StTrGJ	$CH_3OOH + h\nu \rightarrow CH_3O + OH$	jx(ip_CH300H)	Sander et al. (2014)
J41001a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	jx(ip_COH2)	Sander et al. (2014)
J41001b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	jx(ip_CHOH)	Sander et al. (2014)
J41004	StTrGJN	$CH_3ONO + h\nu \rightarrow CH_3O + NO$	jx(ip_CH3ON0)	Sander et al. (2014)
J41005	StTrGJN	$CH_3ONO_2 + h\nu \rightarrow CH_3O + NO_2$	jx(ip_CH3NO3)	Sander et al. (2014)
J41006	StTrGJN	$CH_3O_2NO_2 + h\nu \rightarrow .667 NO_2 + .667 CH_3O_2 + .333 NO_3 + .333 CH_3O$	jx(ip_CH302NO2)	Sander et al. (2014)*
J41007	StTrGJ	$HOCH_2OOH + h\nu \rightarrow HCOOH + OH + HO_2$	jx(ip_CH300H)	Sander et al. (2014)
J41008	StTrGJ	$CH_3O_2 + h\nu \rightarrow HCHO + OH$	jx(ip_CH302)	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_CH302NO2)	Sander et al. (2014)
J42000	TrGJC	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH300H)	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	$HOCH_2CHO + h\nu \rightarrow OH + HCOCH_2O_2$	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_CH300H)	Rickard and Pascoe (2009)



Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J42007	TrGJCN	PHAN + $h\nu \rightarrow .7 \text{ HOCH}_2\text{CO} + .7 \text{ NO}_2 + .3 \text{ HCHO} + .3 \text{ HO}_2$ + $.3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	see note*
J42008	TrGJC	GLYOX + $h\nu \rightarrow 2 \text{ CO} + 2 \text{ HO}_2$	jx(ip_GLYOX)	Sander et al. (2014)
J42009	TrGJC	HCOCO <sub>2</sub> H + $h\nu \rightarrow 2 \text{ HO}_2 + \text{CO} + \text{CO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J42010	TrGJC	HCOCO <sub>3</sub> H + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J42011	TrGJC	HYETHO <sub>2</sub> H + $h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J42012	TrGJCN	ETHOHNO <sub>3</sub> + $h\nu \rightarrow \text{HO}_2 + 2 \text{ HCHO} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)
J42013	TrGJC	HOCH <sub>2</sub> CO <sub>3</sub> H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH}$	2*jx(ip_CH300H)	Taraborrelli (2016)
J42014	TrGC	HOCH <sub>2</sub> CO <sub>2</sub> H + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2$	jx(ip_CH300H)	Taraborrelli (2016)
J42015	TrGC	CH <sub>2</sub> CO + $h\nu \rightarrow .4 \text{ CO}_2 + .8 \text{ H} + .34 \text{ CO} + .34 \text{ OH} + .34 \text{ HO}_2$ + $.16 \text{ HCHO} + .16 \text{ O}(^3\text{P}) + .1 \text{ HCOOH} + \text{CO}$	J_ketene* 0.36	Taraborrelli (2016)
J42016	TrGC	CH <sub>3</sub> CHOHO <sub>2</sub> OH + $h\nu \rightarrow \text{CH}_3 + \text{HCOOH} + \text{OH}$	jx(ip_CH300H)	Taraborrelli (2016)
J42017	TrGJCN	NO <sub>3</sub> CH <sub>2</sub> CHO + $h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	(jx(ip_C2H5N03)+jx(ip_CH3CHO)) *(jx(ip_NOA)+1E-10)/(0.59*J_ IC3H7N03+jx(ip_CH3COCH3)+1E-10)	Taraborrelli (2016)*
J42018	TrGJC	HOCH <sub>2</sub> CHO + $h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{HO}_2$	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Taraborrelli (2016)
J42019	TrGJCN	C <sub>2</sub> H <sub>5</sub> ONO <sub>2</sub> + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	jx(ip_C2H5N03)	Taraborrelli (2016)
J42020	TrGJCN	NO <sub>3</sub> CH <sub>2</sub> CHO + $h\nu \rightarrow .7 \text{ NO}_3\text{CH}_2\text{CO}_3 + .7 \text{ NO}_2 + .3 \text{ HCHO} +$ $.3 \text{ NO}_2 + .3 \text{ CO}_2 + .3 \text{ NO}_3$	jx(ip_PAN)	Taraborrelli (2016)*
J42021	StTrGJCN	C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> NO <sub>2</sub> + $h\nu \rightarrow .667 \text{ NO}_2 + .667 \text{ C}_2\text{H}_5\text{O}_2 + .333 \text{ NO}_3 +$ $.333 \text{ CH}_3\text{CHO} + .333 \text{ HO}_2$	jx(ip_CH302N02)	Taraborrelli (2016)*
J43000	TrGJC	iC <sub>3</sub> H <sub>7</sub> OOH + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	von Kuhlmann (2001)
J43001	TrGJC	CH <sub>3</sub> COCH <sub>3</sub> + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{CH}_3$	jx(ip_CH3COCH3)	Sander et al. (2014)
J43002	TrGJC	CH <sub>3</sub> COCH <sub>2</sub> OH + $h\nu \rightarrow .5 \text{ CH}_3\text{C(O)} + .5 \text{ HCHO} + .5 \text{ HO}_2 + .5$ $\text{HOCH}_2\text{CO} + .5 \text{ CH}_3$	J_ACETOL	Sander et al. (2011)*
J43003	TrGJC	MGLYOX + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Sander et al. (2014)
J43004	TrGJC	CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009)
J43005	TrGJC	HOCH <sub>2</sub> COCH <sub>2</sub> O <sub>2</sub> H + $h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+J_ACETOL	Taraborrelli (2016)
J43006	TrGJCN	iC <sub>3</sub> H <sub>7</sub> ONO <sub>2</sub> + $h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	J_IC3H7N03	von Kuhlmann et al. (2003)*
J43007	TrGJCN	NOA + $h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCHO} + \text{NO}_2$	jx(ip_NOA)	Barnes et al. (1993)
J43009	TrGJC	HYPROPO <sub>2</sub> H + $h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43010	TrGJCN	PR <sub>2</sub> O <sub>2</sub> HNO <sub>3</sub> + $h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH}$	jx(ip_CH300H)	Rickard and Pascoe (2009)
J43011	TrGJC	HOCH <sub>2</sub> COCHO + $h\nu \rightarrow \text{HOCH}_2\text{CO} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J43012	TrGJC	HCOCOCH <sub>2</sub> O <sub>2</sub> H + $h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	jx(ip_CH300H)+J_ACETOL	Taraborrelli (2016)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J43013	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J43014	TrGJTerC	$\text{HCOCH}_2\text{CHO} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) * 2.$	Rickard and Pascoe (2009)
J43015	TrGJTerC	$\text{HCOCH}_2\text{CO}_2\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{HO}_2$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J43016	TrGJTerC	$\text{HOC}_2\text{H}_4\text{CO}_3\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J43017	TrGJC	$\text{HCOCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{HO}_2 + \text{CO}$	$2 * \text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J43018	TrGJC	$\text{CH}_3\text{COCO}_2\text{H} + h\nu \rightarrow .32 \text{CH}_3\text{CHO} + .16 \text{CH}_2\text{CHOH} + .54 \text{CO}_2 + .38 \text{CH}_3\text{C}(\text{O}) + .38 \text{HO}_2 + .38 \text{CO}_2 + .07 \text{CH}_3\text{COOH} + .07 \text{CO} + .05 \text{CH}_3\text{C}(\text{O}) + .05 \text{CO} + .05 \text{OH}$	$\text{JX}(\text{IP\_CH3COCOC}_2\text{H})$	Sander et al. (2011), Taraborrelli (2016)*
J43019	TrGC	$\text{CH}_3\text{COCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{CO}_2$	$\text{JX}(\text{IP\_MGLYOX}) + \text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J43020	TrGC	$\text{CH}_3\text{CHCO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{J\_ketene} * 0.36 * 2.$	Taraborrelli (2016)
J43021	TrGCN	$\text{PROPOLNO}_3 + h\nu \rightarrow \text{HOCH}_2\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{J\_IC3H7N03}$	Taraborrelli (2016)
J43022	TrGCN	$\text{CH}_3\text{COCH}_2\text{OONO}_2 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{NO}_3$	$\text{jx}(\text{ip\_CH302N02}) + \text{jx}(\text{ip\_CH3COC}_3\text{H})$	Taraborrelli (2016)
J43023	TrGJC	$\text{C}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	von Kuhlmann (2001)
J43024	TrGJCN	$\text{C}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{NO}_2 + \text{HO}_2$	$0.59 * \text{J\_IC3H7N03}$	see note*
J43025a	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{HCO})$	see note*
J43025b	TrGJC	$\text{C}_2\text{H}_5\text{CHO} + h\nu \rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$	Andrews et al. (2012), Taraborrelli (2016)*
J43026	TrGJCN	$\text{PPN} + h\nu \rightarrow .7 \text{C}_2\text{H}_5\text{CO}_3 + .7 \text{NO}_2 + .3 \text{C}_2\text{H}_5\text{O}_2 + .3 \text{CO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip\_PAN})$	Sander et al. (2014), Sander et al. (2011)
J43027	TrGJC	$\text{C}_2\text{H}_5\text{CO}_3\text{H} + h\nu \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	von Kuhlmann (2001)
J43028a	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HOOCH}_2\text{CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J43028b	TrGJC	$\text{HCOCOCH}_2\text{OOH} + h\nu \rightarrow \text{HCOCO} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) + \text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J43200	TrGJTerC	$\text{HCOCH}_2\text{CO}_3\text{H} + h\nu \rightarrow \text{HCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) + \text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J43400	TrGJAroC	$\text{C3DIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) * 2 + \text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J43401	TrGJAroC	$\text{C32OH13CO} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) * 2$	Rickard and Pascoe (2009)
J43402	TrGJAroC	$\text{HCOCOHCOC}_3\text{H} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J44000a	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{jx}(\text{ip\_CH300H}) * (\text{k\_p} / (\text{k\_p} + \text{k\_s}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
J44000b	TrGJC	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + .636 \text{MEK} + .636 \text{HO}_2 + .364 \text{CH}_3\text{CHO} + .364 \text{C}_2\text{H}_5\text{O}_2$	$\text{jx}(\text{ip\_CH300H}) * (\text{k\_s} / (\text{k\_p} + \text{k\_s}))$	Rickard and Pascoe (2009), Taraborrelli (2016)
J44001	TrGJC	$\text{MVK} + h\nu \rightarrow .5 \text{C}_3\text{H}_6 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + \text{CO} + .5 \text{HO}_2$	$\text{jx}(\text{ip\_MVK})$	Sander et al. (2014)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44002	TrGJC	MEK + $h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{C}_2\text{H}_5\text{O}_2$	$0.42 \cdot \text{jx}(\text{ip\_CHOH})$	von Kuhlmann et al. (2003)
J44003	TrGJC	$\text{LMEKOOH} + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO} + .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + 0.42 \cdot \text{jx}(\text{ip\_CHOH})$	Taraborrelli (2016)
J44004	TrGJC	$\text{BIACET} + h\nu \rightarrow 2 \text{CH}_3\text{C}(\text{O})$	$2.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	see note*
J44005a	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{C}_3\text{H}_7\text{CHO} + \text{HO}_2$	$\text{J\_IC3H7N03} \cdot (\text{k\_p} / (\text{k\_p} + \text{k\_s}))$	see note*
J44005b	TrGJCN	$\text{LC4H9NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{MEK} + \text{HO}_2$	$\text{J\_IC3H7N03} \cdot (\text{k\_s} / (\text{k\_p} + \text{k\_s}))$	see note*
J44006	TrGJCN	$\text{MPAN} + h\nu \rightarrow .7 \text{MACO}_3 + .7 \text{NO}_2 + .3 \text{MACO}_2 + .3 \text{NO}_3$	$\text{jx}(\text{ip\_PAN})$	see note*
J44007a	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{MGLYOX} + \text{HO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J44007b	TrGJC	$\text{CO}_2\text{H}_3\text{CO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HO}_2 + \text{HCOCO}_3\text{H}$	$\text{J\_ACETOL}$	Rickard and Pascoe (2009)
J44008	TrGJC	$\text{MACR} + h\nu \rightarrow .5 \text{MACO}_3 + .5 \text{CH}_3\text{C}(\text{O}) + .5 \text{HCHO} + .5 \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MACR})$	Sander et al. (2014)
J44009	TrGJC	$\text{MACROOH} + h\nu \rightarrow \text{MACRO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + 2.77 \cdot \text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Taraborrelli (2016)*
J44010	TrGJC	$\text{MACROH} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$2.77 \cdot \text{jx}(\text{ip\_HOCH}_2\text{CHO})$	see note*
J44011	TrGJC	$\text{MACO}_3\text{H} + h\nu \rightarrow \text{MACO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44012	TrGJC	$\text{LHMVKABOOH} + h\nu \rightarrow .12 \text{MGLYOX} + .12 \text{HO}_2 + .88 \text{CH}_3\text{C}(\text{O}) + .88 \text{HOCH}_2\text{CHO} + .12 \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + \text{J\_ACETOL}$	Taraborrelli (2016)
J44013	TrGJC	$\text{CO}_2\text{H}_3\text{CHO} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + \text{HO}_2 + \text{HO}_2$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO}) + \text{J\_ACETOL}$	Taraborrelli (2016)
J44014	TrGJC	$\text{HO}_2\text{CO}_3\text{C}_4 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{HO}_2$	$\text{J\_ACETOL}$	Rickard and Pascoe (2009)
J44015	TrGJC	$\text{BIACETOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	$2.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	see note*
J44016	TrGC	$\text{HCOCCH}_3\text{CO} + h\nu \rightarrow .5 \text{OH} + .5 \text{CH}_3\text{CHO} + \text{CO} + .5 \text{CH}_3\text{CHCO} + .5 \text{CO}$	$\text{J\_KETENE}$	Taraborrelli (2016)
J44017a	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow .0192 \text{CH}_3\text{COCO}_2\text{H} + .1848 \text{H}_2\text{O}_2 + .2208 \text{MGLYOX} + .36 \text{OH} + .36 \text{CO} + .56 \text{CH}_3\text{C}(\text{O}) + .2 \text{CH}_3\text{CHO} + .2 \text{CO}_2 + .2 \text{HCHO} + .2 \text{HO}_2 + \text{CO}$	$\text{J\_KETENE} \cdot 0.5$	Taraborrelli (2016), Rickard and Pascoe (2009)*
J44017b	TrGC	$\text{CH}_3\text{COCHCO} + h\nu \rightarrow \text{CH}_3\text{CHCO} + \text{CO}$	$\text{J\_KETENE} \cdot 0.5$	Taraborrelli (2016)
J44018a	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + 2 \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J44018b	TrGJC	$\text{CH}_3\text{COCOCHO} + h\nu \rightarrow \text{HCOCO} + \text{CH}_3\text{C}(\text{O})$	$2.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J44019	TrGJC	$\text{CH}_3\text{COCOCO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CO} + \text{CO}_2 + \text{HO}_2$	$3.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	Taraborrelli (2016)
J44020a	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{OH} + \text{HCHO} + \text{CO}$	$\text{jx}(\text{ip\_CH300H}) + \text{J\_ACETOL}$	Rickard and Pascoe (2009)
J44020b	TrGJTerC	$\text{CH}_3\text{COCOCH}_2\text{OOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCOCO}$	$2.15 \cdot \text{jx}(\text{ip\_MGLYOX})$	Rickard and Pascoe (2009)
J44021	TrGJTerC	$\text{C44OOH} + h\nu \rightarrow \text{HCOCH}_2\text{CHO} + \text{CO}_2 + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J44022	TrGJTerC	$\text{C413COOOH} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + \text{jx}(\text{ip\_HOCH}_2\text{CHO}) + \text{J\_ACETOL}$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44023a	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J44023b	TrGJTerC	$\text{C4CODIAL} + h\nu \rightarrow \text{HCOCH}_2\text{CO}_3 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_MGLYOX})$	Rickard and Pascoe (2009)
J44024	TrGJTerC	$\text{C312COCO}_3\text{H} + h\nu \rightarrow \text{HCOCOCH}_2\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + \text{jx}(\text{ip\_MGLYOX})$	Rickard and Pascoe (2009)
J44025	TrGJCN	$\text{LMEKNO}_3 + h\nu \rightarrow .62 \text{CH}_3\text{C}(\text{O}) + .62 \text{CH}_3\text{CHO} + .38 \text{HCHO}$ $+ .38 \text{CO}_2 + .38 \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO}_2$	$\text{jx}(\text{ip\_MEKN03})$	Barnes et al. (1993), Taraborrelli (2016)*
J44026	TrGJCN	$\text{MVKNO}_3 + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CHO} + \text{NO}_2$	$\text{jx}(\text{ip\_MEKN03})$	Barnes et al. (1993), Taraborrelli (2016)*
J44027	TrGJCN	$\text{MACRN} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CO} + \text{HO}_2 + \text{NO}_2$	$(2.84 * \text{J\_IC3H7N03} + \text{jx}(\text{ip\_CH3CHO}))$ $* (\text{jx}(\text{ip\_MEKN03}) + 1\text{E-}10) / (\text{J\_}$ $\text{IC3H7N03} + 0.42 * \text{jx}(\text{ip\_CHOH}) + 1\text{E-}10)$	Müller et al. (2014), Taraborrelli (2016)*
J44028	TrGJCN	$\text{TC4H9NO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{NO}_2$	$2.84 * \text{J\_IC3H7N03}$	Taraborrelli (2016)
J44029	TrGJC	$\text{TC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44030	TrGJCN	$\text{IBUTOLBNO}_3 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{J\_IC3H7N03}$	Taraborrelli (2016)
J44031	TrGJC	$\text{IBUTOLBOOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44032	TrGJC	$\text{LBUT1ENOOH} + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44033	TrGJCN	$\text{LBUT1ENNO}_3 + h\nu \rightarrow \text{C}_2\text{H}_5\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$\text{J\_IC3H7N03}$	Taraborrelli (2016)
J44034	TrGJC	$\text{BUT2OLOOH} + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44035	TrGJCN	$\text{BUT2OLNO}_3 + h\nu \rightarrow 2 \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$\text{J\_IC3H7N03}$	Taraborrelli (2016)
J44036	TrGJC	$\text{BUT2OLO} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HOCH}_2\text{CO}$	$\text{J\_ACETOL}$	Taraborrelli (2016)
J44037a	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_C3H7CHO2HCO})$	Taraborrelli (2016)
J44037b	TrGJC	$\text{C}_3\text{H}_7\text{CHO} + h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CH}_2\text{CHOH}$	$\text{jx}(\text{ip\_C3H7CHO2VINY})$	Taraborrelli (2016)*
J44038	TrGJC	$\text{IPRCHO} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_IPRCHO2HCO})$	Taraborrelli (2016)
J44039	TrGJCN	$\text{IC4H9NO}_3 + h\nu \rightarrow \text{IPRCHO} + \text{NO}_2$	$\text{J\_IC3H7N03}$	Taraborrelli (2016)
J44040	TrGJC	$\text{IC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{IPRCHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44041	TrGJC	$\text{PERIBUACID} + h\nu \rightarrow \text{iC}_3\text{H}_7\text{O}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Taraborrelli (2016)
J44042	TrGJCN	$\text{PIPn} + h\nu \rightarrow .7 \text{IPRCO}_3 + .7 \text{NO}_2 + .3 \text{iC}_3\text{H}_7\text{O}_2 + .3 \text{CO}_2 +$ $.3 \text{NO}_3$	$\text{jx}(\text{ip\_PAN})$	Taraborrelli (2016), Sander et al. (2014), Sander et al. (2011)
J44043	TrGJC	$\text{HVMK} + h\nu \rightarrow \text{MGLYOX} + \text{CO} + 2 \text{OH}$	$\text{jx}(\text{ip\_PeDIONE24})$	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J44044	TrGJC	$\text{HMAC} + h\nu \rightarrow \text{HCOCCH}_3\text{CO} + 2 \text{ OH}$	$\text{jx}(\text{ip\_PeDIONE24})$	Taraborrelli (2016), Nakanishi et al. (1977), Messaadia et al. (2015), Yoon et al. (1999)*
J44045a	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{HCO})$	Rickard and Pascoe (2009)
J44045b	TrGJC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HVMK}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{ENOL})$	Andrews et al. (2012), Taraborrelli (2016)
J44046a	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{CO} + \text{HO}_2 + \text{CO}_2 + \text{H}_2\text{O}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{HCO})*2.$	see note*
J44046b	TrGJC	$\text{IBUTDIAL} + h\nu \rightarrow \text{HMAC}$	$\text{jx}(\text{ip\_C}_2\text{H}_5\text{CHO}_2\text{ENOL})*2.$	Andrews et al. (2012), Taraborrelli (2016)
J44200	TrGJTerC	$\text{IBUTALOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{HO}_2 + \text{CO}$	$\text{J\_ACETOL}$	Rickard and Pascoe (2009)
J44201	TrGJTerC	$\text{IPRHOCO}_3\text{H} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J44400a	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{C}_3\text{O}_2\text{H}_3\text{CO} + \text{CO} + \text{OH} + \text{HO}_2$	$\text{jx}(\text{ip\_HOCH}_2\text{CHO})*2$	Rickard and Pascoe (2009)
J44400b	TrGJAroC	$\text{MALDIALOOH} + h\nu \rightarrow \text{GLYOX} + \text{GLYOX} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J44401	TrGJAroC	$\text{BZFUOOH} + h\nu \rightarrow \text{CO}_2\text{C}_3\text{CHO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J44402	TrGJAroC	$\text{HOCOC}_4\text{DIAL} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_MGLYOX})+\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J44403	TrGJAroCN	$\text{NBZFUOOH} + h\nu \rightarrow .5 \text{ CO}_2\text{C}_3\text{CHO} + .5 \text{ NO}_2 + .5 \text{ NBZFUONE} + .5 \text{ HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J44404a	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_MACR})$	Rickard and Pascoe (2009)
J44404b	TrGJAroC	$\text{MALDALCO}_3\text{H} + h\nu \rightarrow .6 \text{ MALANHY} + \text{HO}_2 + .4 \text{ GLYOX} + .4 \text{ CO} + .4 \text{ CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J44405	TrGJAroC	$\text{EPXDLCO}_2\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO}_2 + \text{HO}_2$	$2.77*\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J44406	TrGJAroC	$\text{MALDIAL} + h\nu \rightarrow .4 \text{ BZFUONE} + .6 \text{ MALDIALCO}_3 + .6 \text{ HO}_2$	$\text{jx}(\text{ip\_NO}_2)*0.14$	Rickard and Pascoe (2009)
J44407	TrGJAroC	$\text{MALANHYOOH} + h\nu \rightarrow \text{HCOCOHCO}_3 + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J44408	TrGJAroC	$\text{EPXDLCO}_3\text{H} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{OH} + \text{CO}_2$	$\text{jx}(\text{ip\_CH300H})+2.77*\text{jx}(\text{ip\_HOCH}_2\text{CHO})$	Rickard and Pascoe (2009)
J44409	TrGJAroC	$\text{CO}_2\text{C}_4\text{DIAL} + h\nu \rightarrow \text{CO} + \text{CO} + \text{HO}_2 + \text{HO}_2 + \text{CO} + \text{CO}$	$\text{jx}(\text{ip\_MGLYOX})*2$	Rickard and Pascoe (2009)
J44410	TrGJAroC	$\text{MALDALCO}_2\text{H} + h\nu \rightarrow \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{CO} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_MACR})$	Rickard and Pascoe (2009)
J44411	TrGJAroC	$\text{EPXC}_4\text{DIAL} + h\nu \rightarrow \text{C}_3\text{DIALO}_2 + \text{CO} + \text{HO}_2$	$2.77*\text{jx}(\text{ip\_HOCH}_2\text{CHO})*2$	Rickard and Pascoe (2009)
J44412	TrGJAroC	$\text{CO}_2\text{C}_3\text{CHO} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCOCH}_2\text{O}_2 + \text{CO}_2$	$\text{jx}(\text{ip\_MGLYOX})$	Rickard and Pascoe (2009)
J44414	TrGJAroC	$\text{MECOACEOOH} + h\nu \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{HCHO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45002	TrGJC	LISOPACOOH + $h\nu$ → LISOPACO + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45003	TrGJCN	LISOPACNO3 + $h\nu$ → LISOPACO + NO <sub>2</sub>	0.59*J_IC3H7N03	see note*
J45004	TrGJC	ISOPBOOH + $h\nu$ → MVK + HCHO + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45005	TrGJCN	ISOPBNO3 + $h\nu$ → MVK + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	2.84*J_IC3H7N03	see note*
J45006	TrGJC	ISOPDOOH + $h\nu$ → MACR + HCHO + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45007	TrGJCN	ISOPDNO3 + $h\nu$ → MACR + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	J_IC3H7N03	see note*
J45008	TrGJCN	NISOPOOH + $h\nu$ → NC4CHO + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45009	TrGJCN	NC4CHO + $h\nu$ → LHC4ACCO3 + NO <sub>2</sub>	(.59*J_IC3H7N03+jx(ip_MACR)) *(jx(ip_MEKN03)+1E-10)/(J_IC3H7N03+0.42*jx(ip_CHOH)+1E-10)	Müller et al. (2014), Taraborrelli (2016)*
J45010	TrGJCN	LNISOOH + $h\nu$ → NOA + OH + .5 HOCHCHO + .5 CO + .5 HO <sub>2</sub> + .5 CO <sub>2</sub>	jx(ip_CH300H)	Taraborrelli et al. (2009), Taraborrelli (2016)
J45011	TrGJC	LHC4ACCHO + $h\nu$ → .5 LHC4ACCO3 + .5 HO <sub>2</sub> + .5 CO + .5 OH + .25 MACRO2 + .25 LHMVKABO2	jx(ip_MACR)	Taraborrelli (2016)
J45012	TrGJC	LC578OOH + $h\nu$ → .25 CH <sub>3</sub> COCH <sub>2</sub> OH + .75 MGLYOX + .25 HOCHCHO + .75 HOCH <sub>2</sub> CHO + .75 HO <sub>2</sub> + OH	jx(ip_CH300H)+ 2.77*jx(ip_HOCH2CHO)	Taraborrelli (2016)
J45013	TrGJC	LHC4ACCO3H + $h\nu$ → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO <sub>2</sub>	J_HPALD	Taraborrelli (2016)
J45014	TrGJCN	LC5PAN1719 + $h\nu$ → .7 LHC4ACCO3 + .7 NO <sub>2</sub> + .15 MACRO2 + .15 LHMVKABO2 + .3 CO <sub>2</sub> + .3 NO <sub>3</sub>	jx(ip_PAN)	Taraborrelli (2016)
J45015	TrGJC	HCOC5 + $h\nu$ → .65 CH <sub>3</sub> + .65 CO + .65 HCHO + .35 OH + .35 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> + HOCH2CO	0.5*jx(ip_MVK)	Taraborrelli (2016)*
J45016	TrGJC	C59OOH + $h\nu$ → CH <sub>3</sub> COCH <sub>2</sub> OH + HOCH2CO + OH	J_ACETOL+jx(ip_CH300H)	Taraborrelli (2016)
J45017	TrGJTerC	C511OOH + $h\nu$ → CH <sub>3</sub> C(O) + HCOCH2CHO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018a	TrGJTerC	CO23C4CHO + $h\nu$ → CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + HO <sub>2</sub> + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45018b	TrGJTerC	CO23C4CHO + $h\nu$ → CH <sub>3</sub> C(O) + HCOCH2CO3	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45019	TrGJTerC	CO23C4CO3H + $h\nu$ → CH <sub>3</sub> COCOCH <sub>2</sub> O <sub>2</sub> + CO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45020	TrGJTerC	C512OOH + $h\nu$ → C513O2 + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45021	TrGJTerC	CO13C4CHO + $h\nu$ → CHOC3COO2 + CO + HO <sub>2</sub>	jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45022	TrGJTerC	C513OOH + $h\nu$ → GLYOX + HOC <sub>2</sub> H <sub>4</sub> CO <sub>3</sub> + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45023	TrGJTerC	C513CO + $h\nu$ → HOC <sub>2</sub> H <sub>4</sub> CO <sub>3</sub> + HO <sub>2</sub> + CO + CO	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45024	TrGJTerC	C514OOH + $h\nu$ → CO13C4CHO + HO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)
J45025	TrGJTerCN	C514NO3 + $h\nu$ → CO13C4CHO + HO <sub>2</sub> + NO <sub>2</sub>	J_IC3H7N03+jx(ip_HOCH2CHO)*2.	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45026a	TrGJC	ZCODC23DBCOOH + $h\nu$ → OH + CO + HVMK + OH	J_HPALD*0.6*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026b	TrGJC	ZCODC23DBCOOH + $h\nu$ → OH + CO + CH <sub>3</sub> C(O) + HOCH <sub>2</sub> CHO	J_HPALD*0.6*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026c	TrGJC	ZCODC23DBCOOH + $h\nu$ → OH + CO + HMAc + OH	J_HPALD*0.4*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45026d	TrGJC	ZCODC23DBCOOH + $h\nu$ → OH + CO + CO + CH <sub>3</sub> COCH <sub>2</sub> OH + HO <sub>2</sub>	J_HPALD*0.4*0.5	Taraborrelli (2016), Jenkin et al. (2015), Peeters et al. (2014)
J45027	TrGJC	ZCO3HC23DBCOD + $h\nu$ → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO <sub>2</sub>	J_HPALD	Taraborrelli (2016)
J45028a	TrGJC	C1OOHC2OOHC4OD + $h\nu$ → CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + OH + 2 CO + HO <sub>2</sub>	2.77*JX(IP_HOCH2CHO)	Taraborrelli (2016)
J45028b	TrGJC	C1OOHC2OOHC4OD + $h\nu$ → .5 CH <sub>3</sub> COCH <sub>2</sub> O <sub>2</sub> H + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH	2.*JX(IP_CH300H)	Taraborrelli (2016)
J45029	TrGC	DB1OOH + $h\nu$ → DB1O2 + OH	JX(IP_CH300H)	Taraborrelli (2016)
J45030	TrGC	DB2OOH + $h\nu$ → .48 CH <sub>3</sub> COCH <sub>2</sub> OH + .52 HOCH <sub>2</sub> CHO + .52 MGLYOX + .48 GLYOX + HO <sub>2</sub> + OH	JX(ip_CH300H)	Taraborrelli (2016)
J45031a	TrGJC	C1ODC2OOHC4OD + $h\nu$ → MGLYOX + HOCHCHO + OH	JX(ip_CH300H)	Taraborrelli (2016)
J45031b	TrGJC	C1ODC2OOHC4OD + $h\nu$ → CO2H3CHO + CO + HO <sub>2</sub> + OH	2.*2.77*JX(IP_HOCH2CHO)	Taraborrelli (2016)
J45032	TrGJC	ZCODC23DBCOD + $h\nu$ → .5 CH <sub>3</sub> COCHCO + .5 HCOCCH <sub>3</sub> CO + CO + HO <sub>2</sub> + OH	jx(ip_N02)*0.1*0.5	Taraborrelli (2016)*
J45033	TrGCN	DB1NO3 + $h\nu$ → DB1O2 + NO <sub>2</sub>	J_IC3H7N03	Taraborrelli (2016)
J45034	TrGJTerC	CHOC3COOOH + $h\nu$ → CHOC3COO2 + CO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)
J45200a	TrGJTerC	LMBOABOOH + $h\nu$ → HOCH <sub>2</sub> CHO + CH <sub>3</sub> COCH <sub>3</sub> + HO <sub>2</sub> + OH	jx(ip_CH300H)*.67	Rickard and Pascoe (2009), Taraborrelli (2016)
J45200b	TrGJTerC	LMBOABOOH + $h\nu$ → IBUTALOH + HCHO + HO <sub>2</sub> + OH	jx(ip_CH300H)*.33	Rickard and Pascoe (2009), Taraborrelli (2016)
J45201	TrGJTerC	MBOACO + $h\nu$ → HCHO + HO <sub>2</sub> + IPRHOCO3	J_ACETOL	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J45202	TrGJTerC	MBOCOCO + $h\nu$ → CO + HO <sub>2</sub> + IPRHOCO3	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45203a	TrGJTerCN	LNMB0ABOOH + $h\nu$ → NO <sub>3</sub> CH <sub>2</sub> CHO + CH <sub>3</sub> COCH <sub>3</sub> + HO <sub>2</sub> + OH	jx(ip_CH300H)*.65	Rickard and Pascoe (2009), Taraborrelli (2016)
J45203b	TrGJTerCN	LNMB0ABOOH + $h\nu$ → IBUTALOH + HCHO + NO <sub>2</sub> + OH	jx(ip_CH300H)*.35	Rickard and Pascoe (2009), Taraborrelli (2016)
J45204	TrGJTerCN	NC4OHCO3H + $h\nu$ → IBUTALOH + CO <sub>2</sub> + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45400	TrGJAroC	C54CO + $h\nu$ → HO <sub>2</sub> + CO + CO + CO + CH <sub>3</sub> C(O)	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
J45401	TrGJAroC	C5134CO2OH + $h\nu$ → CH <sub>3</sub> COCOCHO + HO <sub>2</sub> + CO + HO <sub>2</sub>	jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J45402	TrGJAroC	C5DIALOOH + $h\nu$ → MALDIAL + CO + HO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)*
J45406	TrGJAroC	C5CO14OH + $h\nu$ → CH <sub>3</sub> C(O) + HCOCO <sub>2</sub> H + HO <sub>2</sub> + CO	jx(ip_MVK)	Rickard and Pascoe (2009)
J45407	TrGJAroC	C5DICARB + $h\nu$ → .6 C5CO14O2 + .6 HO <sub>2</sub> + .4 TLFUONE	jx(ip_N02)*0.2	Rickard and Pascoe (2009)*
J45408	TrGJAroC	MC3ODBCO2H + $h\nu$ → CH <sub>3</sub> COCO <sub>2</sub> H + HO <sub>2</sub> + CO + HO <sub>2</sub> + CO	jx(ip_MACR)	Rickard and Pascoe (2009)
J45409	TrGJAroC	ACCOMMECHO + $h\nu$ → MECOACETO2 + HO <sub>2</sub> + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J45410	TrGJAroC	MMALNHOOH + $h\nu$ → CO2H3CO3 + CO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45411	TrGJAroC	C5DICAROOH + $h\nu$ → MGLYOX + GLYOX + HO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)*
J45412	TrGJAroCN	NTLFUOOH + $h\nu$ → ACCOMECHO + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45414	TrGJAroC	C5CO14OOH + $h\nu$ → .83 MALANHY + .83 CH <sub>3</sub> + .17 MGLYOX + .17 HO <sub>2</sub> + .17 CO + .17 CO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45415	TrGJAroC	TLFUOOH + $h\nu$ → ACCOMECHO + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J45417	TrGJAroC	ACCOMECO3H + $h\nu$ → MECOACETO2 + CO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J45418	TrGJAroC	C5DIALCO + $h\nu$ → MALDIALCO3 + CO + HO <sub>2</sub>	jx(ip_MGLYOX)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46200	TrGJTerCN	C614NO3 + $h\nu$ → CO23C4CHO + HCHO + HO <sub>2</sub> + NO <sub>2</sub>	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46201	TrGJTerC	C614OOH + $h\nu$ → CO23C4CHO + HCHO + HO <sub>2</sub> + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J46202	TrGJTerC	CO235C5CHO + $h\nu$ → CO23C4CO3 + CO + HO <sub>2</sub>	jx(ip_MGLYOX)	Rickard and Pascoe (2009)



Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46203	TrGJTerC	$\text{CO235C6OOH} + h\nu \rightarrow \text{CO23C4CO3} + \text{HCHO} + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + 2.15 * \text{jx}(\text{ip\_MGLY0X})$	Rickard and Pascoe (2009)
J46400	TrGJAroC	$\text{PHENOOH} + h\nu \rightarrow .71 \text{ MALDALCO2H} + .71 \text{ GLYOX} + .29 \text{ PBZQONE} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46401	TrGJAroC	$\text{C6CO4DB} + h\nu \rightarrow \text{C4CO2DBC03} + \text{HO}_2 + \text{CO}$	$\text{jx}(\text{ip\_MGLY0X}) * 2$	Rickard and Pascoe (2009)
J46402	TrGJAroC	$\text{C5CO2DCO3H} + h\nu \rightarrow \text{CH}_3\text{C(O)} + \text{HCOCOCHO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H}) + \text{jx}(\text{ip\_MGLY0X})$	Rickard and Pascoe (2009)
J46403	TrGJAroCN	$\text{NDNPHEOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HNO}_3 + \text{CO} + \text{CO} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46404	TrGJAroCN	$\text{BZBIPERNO3} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009)*
J46405	TrGJAroCN	$\text{HOC6H4NO2} + h\nu \rightarrow \text{HONO} + \text{CPDKETENE}$	$\text{jx}(\text{ip\_HOC6H4N02})$	Chen et al. (2011)*
J46406	TrGJAroC	$\text{CPDKETENE} + h\nu \rightarrow \text{CO}_2 + \text{CO} + 2 \text{ HO}_2 + \text{MALDIAL}$	J_KETENE	see note*
J46407	TrGJAroC	$\text{C5COOHCO3H} + h\nu \rightarrow \text{HOCOC4DIAL} + \text{HO}_2 + \text{CO} + \text{CO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J46408	TrGJAroC	$\text{BZEPOXMUC} + h\nu \rightarrow .5 \text{ C5DIALO2} + 1.5 \text{ HO}_2 + 1.5 \text{ CO} + .5 \text{ MALDIAL}$	$4.E3 * \text{jx}(\text{ip\_MVK}) * 0.1$	Rickard and Pascoe (2009)
J46409	TrGJAroCN	$\text{NPHEN1OOH} + h\nu \rightarrow \text{NPHEN1O} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J46410	TrGJAroC	$\text{BZEMUCCO} + h\nu \rightarrow \text{HCOCO2HCO3} + \text{C3DIALO2}$	$\text{jx}(\text{ip\_HOCH2CHO}) * 2 + \text{J\_ACETOL}$	Rickard and Pascoe (2009)
J46411	TrGJAroC	$\text{BZEMUCCO2H} + h\nu \rightarrow \text{C5DIALO2} + \text{CO}_2 + \text{HO}_2$	$\text{jx}(\text{ip\_MACR})$	Rickard and Pascoe (2009)
J46412	TrGJAroCN	$\text{NNCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46413	TrGJAroC	$\text{C615CO2OOH} + h\nu \rightarrow \text{C5DICARB} + \text{CO} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_MVK}) + \text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J46414	TrGJAroCN	$\text{NPHEOOH} + h\nu \rightarrow \text{MALDALCO2H} + \text{GLYOX} + \text{OH} + \text{NO}_2$	$\text{J\_IC3H7N03} + \text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J46415	TrGJAroCN	$\text{NCATECOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{HO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46416	TrGJAroC	$\text{PBZQOOH} + h\nu \rightarrow \text{C5CO2OHCO3} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46417	TrGJAroC	$\text{BZOBIPEROH} + h\nu \rightarrow \text{MALDIALCO3} + \text{GLYOX} + \text{HO}_2$	J_ACETOL	Rickard and Pascoe (2009)
J46418	TrGJAroC	$\text{BZBIPEROOH} + h\nu \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{ BZFUONE} + .5 \text{ BZFUONE} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46419	TrGJAroCN	$\text{NBZQOOH} + h\nu \rightarrow \text{C6CO4DB} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*
J46420	TrGJAroC	$\text{CATEC1OOH} + h\nu \rightarrow \text{CATEC1O} + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)
J46421	TrGJAroC	$\text{C6125CO} + h\nu \rightarrow \text{C5CO14O2} + \text{CO} + \text{HO}_2$	$\text{jx}(\text{ip\_MGLY0X}) + \text{jx}(\text{ip\_MVK})$	Rickard and Pascoe (2009)
J46422	TrGJAroCN	$\text{DNPHENOOH} + h\nu \rightarrow \text{NC4DCO2H} + \text{HCOCO}_2\text{H} + \text{NO}_2 + \text{OH}$	$\text{jx}(\text{ip\_CH300H})$	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J46423	TrGJAroC	BZEMUCCO3H + $h\nu$ → C5DIALO2 + CO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)
J46424	TrGJAroC	C6H5OOH + $h\nu$ → C6H5O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J46425	TrGJAroC	BZEMUCOOH + $h\nu$ → .5 EPXC4DIAL + .5 GLYOX + .5 HO <sub>2</sub> + .5 C3DIALO2 + .5 C32OH13CO + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009)*
J46427	TrGJAroCN	BZEMUCNO3 + $h\nu$ → EPXC4DIAL + NO <sub>2</sub> + GLYOX + HO <sub>2</sub>	2.77*jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J46428	TrGJAroCN	DNPEN + $h\nu$ → HONO + NCPDKETENE	jx(ip_HOC6H4NO2)	Taraborrelli (2016)
J46429	TrGJAroCN	NCPDKETENE + $h\nu$ → CO <sub>2</sub> + CO + 2 HO <sub>2</sub> + NC4DCO2H	J_KETENE	see note*
J47200	TrGJTerC	CO235C6CHO + $h\nu$ → CHOC3COCO3 + CH <sub>3</sub> C(O)	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47201	TrGJTerC	C235C6CO3H + $h\nu$ → CO235C6O2 + CO <sub>2</sub> + OH	jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47202	TrGJTerC	C716OOH + $h\nu$ → CO13C4CHO + CH <sub>3</sub> C(O) + OH	jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J47203	TrGJTerC	C721OOH + $h\nu$ → C722O2 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47204	TrGJTerC	C722OOH + $h\nu$ → CH <sub>3</sub> COCH <sub>3</sub> + C44O2 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47400	TrGJAroC	TLEPOXMUC + $h\nu$ → .5 C615CO2O2 + HO <sub>2</sub> + CO + .5 EPXC4DIAL + .5 CH <sub>3</sub> C(O)	4.E3*jx(ip_MVK)*0.1	Rickard and Pascoe (2009)
J47401	TrGJAroC	C6H5CH2OOH + $h\nu$ → BENZAL + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47402	TrGJAroCN	C6H5CH2NO3 + $h\nu$ → BENZAL + HO <sub>2</sub> + NO <sub>2</sub>	0.59*J_IC3H7N03	Rickard and Pascoe (2009)*
J47403	TrGJAroC	BENZAL + $h\nu$ → HO <sub>2</sub> + CO + C6H5O2	jx(ip_BENZAL)	T. J. Wallington et al. (2014)
J47404	TrGJAroC	TLBIPEROOH + $h\nu$ → .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47405	TrGJAroCN	TLBIPERNO3 + $h\nu$ → .6 GLYOX + .4 MGLYOX + HO <sub>2</sub> + .2 ZCODC23DBCOD + .2 C5DICARB + .2 TLFUONE + .2 BZFUONE + .2 MALDIAL + NO <sub>2</sub>	J_IC3H7N03	Rickard and Pascoe (2009)*
J47406	TrGJAroC	TLOBIPEROH + $h\nu$ → C5CO14O2 + GLYOX + HO <sub>2</sub>	J_ACETOL	Rickard and Pascoe (2009)
J47407	TrGJAroC	CRESOOH + $h\nu$ → .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47408a	TrGJAroCN	NCRESOOH + $h\nu$ → .68 C5CO14OH + .68 GLYOX + HO <sub>2</sub> + .32 PTLQONE + OH + NO <sub>2</sub>	J_IC3H7N03	Rickard and Pascoe (2009)*
J47408b	TrGJAroCN	NCRESOOH + $h\nu$ → C5CO14OH + GLYOX + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47409	TrGJAroCN	TOL1OHNO2 + $h\nu$ → HONO + MCPDKETENE	jx(ip_HOPh3Me2NO2)	see note*
J47410	TrGJAroC	TLEMUCCO2H + $h\nu$ → C615CO2O2 + CO <sub>2</sub> + HO <sub>2</sub>	jx(ip_MACR)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J47411	TrGJAroC	TLEMUCCO3H + $h\nu$ → C615CO2O2 + CO <sub>2</sub> + OH	jx(ip_CH300H)+jx(ip_MACR)	Rickard and Pascoe (2009)
J47412	TrGJAroC	TLEMUCOOH + $h\nu$ → .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO <sub>2</sub> + OH	jx(ip_CH300H)+2.77*jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)*
J47413	TrGJAroCN	TLEMUCNO3 + $h\nu$ → EPXC4DIAL + NO <sub>2</sub> + CH <sub>3</sub> C(O) + CO + HO <sub>2</sub>	2.77*jx(ip_HOCH2CHO)+J_ACETOL	Rickard and Pascoe (2009)
J47414	TrGJAroC	TLEMUCCO + $h\nu$ → CH <sub>3</sub> C(O) + EPXC4DIAL + CO + HO <sub>2</sub>	2.77*jx(ip_HOCH2CHO)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009)
J47415	TrGJAroC	C6H5CO3H + $h\nu$ → C6H5O2 + CO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47416	TrGJAroC	OXYL1OOH + $h\nu$ → TOL1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47417	TrGJAroCN	MNCATECH + $h\nu$ → HONO + MCPDKETENE	jx(ip_HOPh3Me2NO2)	see note*
J47418	TrGJAroC	MCPDKETENE + $h\nu$ → CO <sub>2</sub> + CO + 2 HO <sub>2</sub> + ZCODC23DBCOD	J_KETENE	see note*
J47419	TrGJAroCN	DNCRES + $h\nu$ → HONO + MNCPDKETENE	jx(ip_HOPh3Me2NO2)	see note*
J47420	TrGJAroCN	MNCPDKETENE + $h\nu$ → CO <sub>2</sub> + CO + 2 HO <sub>2</sub> + NC4MDCO2HN	J_KETENE	see note*
J47421	TrGJAroC	MCATEC1OOH + $h\nu$ → MCATEC1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47422	TrGJAroCN	NPTLQOOH + $h\nu$ → C7CO4DB + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47423	TrGJAroC	PTLQOOH + $h\nu$ → C6CO2OHCO3 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47424	TrGJAroCN	NCRES1OOH + $h\nu$ → NCRES1O + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J47425	TrGJAroCN	MNNCATCOOH + $h\nu$ → NC4MDCO2HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47426	TrGJAroCN	MNCATECOOH + $h\nu$ → NC4MDCO2HN + HCOCO <sub>2</sub> H + HO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47427	TrGJAroC	C7CO4DB + $h\nu$ → C5CO2DBCO3 + HO <sub>2</sub> + CO	jx(ip_MGLYOX)*2	Rickard and Pascoe (2009)
J47428	TrGJAroCN	NDNCRESOOH + $h\nu$ → NC4MDCO2HN + HNO <sub>3</sub> + CO + CO + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47429	TrGJAroCN	DNCRESOOH + $h\nu$ → NC4MDCO2HN + HCOCO <sub>2</sub> H + NO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)*
J47430	TrGJAroC	C6COOHCO3H + $h\nu$ → C5134CO2OH + HO <sub>2</sub> + CO + CO <sub>2</sub> + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48200	TrGJTerC	C86OOH + $h\nu$ → C511O2 + CH <sub>3</sub> COCH <sub>3</sub> + OH	jx(ip_CH300H)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)
J48201	TrGJTerC	C812OOH + $h\nu$ → C813O2 + OH	jx(ip_CH300H)	Rickard and Pascoe (2009)
J48202	TrGJTerC	C813OOH + $h\nu$ → CH <sub>3</sub> COCH <sub>3</sub> + C512O2 + OH	jx(ip_CH300H)+jx(ip_MGLYOX)	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J48203	TrGJTerC	$C721CHO + h\nu \rightarrow C721O2 + CO + HO_2$	$jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J48204	TrGJTerC	$C721CO3H + h\nu \rightarrow C721O2 + CO_2 + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)
J48205	TrGJTerC	$C8BCOOH + h\nu \rightarrow C89O2 + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)
J48206	TrGJTerC	$C89OOH + h\nu \rightarrow C810O2 + OH$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J48207	TrGJTerCN	$C89NO3 + h\nu \rightarrow C810O2 + NO_2$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J48208	TrGJTerC	$C810OOH + h\nu \rightarrow CH_3COCH_3 + C514O2 + OH$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J48209	TrGJTerCN	$C810NO3 + h\nu \rightarrow CH_3COCH_3 + C514O2 + NO_2$	$2.84*J\_IC3H7N03+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J48210	TrGJTerCN	$C8BCNO3 + h\nu \rightarrow C89O2 + NO_2$	$J\_IC3H7N03$	Rickard and Pascoe (2009)
J48211	TrGJTerC	$C85OOH + h\nu \rightarrow C86O2 + OH$	$jx(ip\_CH300H)+J\_ACETOL$	Rickard and Pascoe (2009)
J48400	TrGJAroC	$STYRENOOH + h\nu \rightarrow HO_2 + HCHO + BENZAL + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)*
J49200	TrGJTerC	$C96OOH + h\nu \rightarrow C97O2 + OH$	$jx(ip\_CH300H)+J\_ACETOL$	Rickard and Pascoe (2009)
J49201	TrGJTerC	$C97OOH + h\nu \rightarrow C98O2 + OH$	$jx(ip\_CH300H)+J\_ACETOL$	Rickard and Pascoe (2009)
J49202	TrGJTerC	$C98OOH + h\nu \rightarrow C614O2 + CH_3COCH_3 + OH$	$(jx(ip\_CH300H)+2.15*jx(ip\_MGLYOX))$	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	$C85CO3H + h\nu \rightarrow C85O2 + CO_2 + OH$	$jx(ip\_CH300H)+J\_ACETOL$	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	$C89CO3H + h\nu \rightarrow .8 C811CO3 + .2 C89O2 + .2 CO_2 + OH$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J49207	TrGJTerC	$C811CO3H + h\nu \rightarrow C811O2 + CO_2 + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)
J49208	TrGJTerC	$NOPINDOOH + h\nu \rightarrow C89CO3 + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)
J40200	TrGJTerC	$LAPINABOOH + h\nu \rightarrow PINAL + HO_2 + OH$	$jx(ip\_CH300H)$	Rickard and Pascoe (2009)
J40201	TrGJTerC	$MENTHEN6ONE + h\nu \rightarrow RO6R1O2 + OH$	$jx(ip\_CH300H)$	Vereecken et al. (2007)
J40202	TrGJTerC	$2OHMENTHEN6ONE + h\nu \rightarrow 10 LCARBON + OH$	$jx(ip\_CH300H)$	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	$PERPINONIC + h\nu \rightarrow C96O2 + CO_2 + OH$	$jx(ip\_CH300H)+J\_ACETOL$	Rickard and Pascoe (2009)
J40205	TrGJTerC	$PINALOOH + h\nu \rightarrow C106O2 + OH$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J40206	TrGJTerCN	$PINALNO3 + h\nu \rightarrow C106O2 + NO_2$	$J\_IC3H7N03+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)
J40207	TrGJTerC	$C106OOH + h\nu \rightarrow C716O2 + CH_3COCH_3 + OH$	$jx(ip\_CH300H)+jx(ip\_HOCH2CHO)$	Rickard and Pascoe (2009)

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J40208	TrGJTerCN	$\text{C106NO}_3 + h\nu \rightarrow \text{C716O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$\text{J\_IC3H7N03} + \text{jx(ip\_HOCH2CHO)}$	Rickard and Pascoe (2009)
J40209	TrGJTerC	$\text{C109OOH} + h\nu \rightarrow \text{C89CO}_3 + \text{HCHO} + \text{OH}$	$\text{jx(ip\_CH300H)} + \text{jx(ip\_HOCH2CHO)}$	Rickard and Pascoe (2009)
J40210	TrGJTerC	$\text{C109CO} + h\nu \rightarrow \text{C89CO}_3 + \text{CO} + \text{HO}_2$	$\text{jx(ip\_MGLYOX)} + \text{jx(ip\_HOCH2CHO)}$	Rickard and Pascoe (2009)
J40211	TrGJTerCN	$\text{LNAPINABOOH} + h\nu \rightarrow \text{PINAL} + \text{NO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)
J40212	TrGJTerC	$\text{BPINAOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{HO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)
J40213	TrGJTerCN	$\text{LNBPINABOOH} + h\nu \rightarrow \text{NOPINONE} + \text{HCHO} + \text{NO}_2 + \text{OH}$	$\text{jx(ip\_CH300H)}$	Rickard and Pascoe (2009)
J40214	TrGJTerCN	$\text{ROO6R1NO}_3 + h\nu \rightarrow \text{ROO6R3O}_2 + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$2.84 * \text{J\_IC3H7N03} + \text{jx(ip\_CH300H)}$	Taraborrelli (2016)
J40215	TrGJTerCN	$\text{RO6R1NO}_3 + h\nu \rightarrow 9 \text{ L CARBON} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$2.84 * \text{J\_IC3H7N03}$	Taraborrelli (2016)

## 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:

$\text{J(11)} \rightarrow \text{jx(ip\_COH2)}$   
 $\text{J(12)} \rightarrow \text{jx(ip\_CHOH)}$   
 $\text{J(15)} \rightarrow \text{jx(ip\_HOCH2CHO)}$   
 $\text{J(18)} \rightarrow \text{jx(ip\_MACR)}$   
 $\text{J(22)} \rightarrow \text{jx(ip\_ACETOL)}$   
 $\text{J(23)} + \text{J(24)} \rightarrow \text{jx(ip\_MVK)}$   
 $\text{J(31)} + \text{J(32)} + \text{J(33)} \rightarrow \text{jx(ip\_GLYOX)}$   
 $\text{J(34)} \rightarrow \text{jx(ip\_MGLYOX)}$   
 $\text{J(41)} \rightarrow \text{jx(ip\_CH300H)}$   
 $\text{J(53)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2\text{)}$   
 $\text{J(54)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2\text{)}$   
 $\text{J(55)} \rightarrow \text{J(iC}_3\text{H}_7\text{ONO}_2\text{)}$   
 $\text{J(56)} + \text{J(57)} \rightarrow \text{jx(ip\_NOA)}$

## Specific notes

J41006: product distribution as for  $\text{HNO}_4$

J42007: It is assumed that  $\text{J(PHAN)}$  is the same as  $\text{J(PAN)}$ .

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

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

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

J43002: Following von Kuhlmann et al. (2003), we use  $\text{J(CH}_3\text{COCH}_2\text{OH)} = 0.11 * \text{jx(ip\_CHOH)}$ . 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  $\text{J(iC}_3\text{H}_7\text{ONO}_2\text{)} = 3.7 * \text{jx(ip\_PAN)}$ .

J43018: One third of the acetaldehyde channel is considered to be  $\text{CH}_2\text{CHOH}$  according to Hjorth (2002) EUPHORE Report.

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

J43025a: Photolysis frequencies very similar to the ones of  $\text{CH}_3\text{CHO}$ .

J43025b: Photolysis frequencies very similar to the ones of  $\text{CH}_3\text{CHO}$ .

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

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

J44005a: It is assumed that  $\text{J(LC}_4\text{H}_9\text{NO}_3\text{)}$  is the same as  $\text{J(iC}_3\text{H}_7\text{ONO}_2\text{)}$ .

J44005b: It is assumed that  $\text{J(LC}_4\text{H}_9\text{NO}_3\text{)}$  is the same as  $\text{J(iC}_3\text{H}_7\text{ONO}_2\text{)}$ .

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

J44009: It is assumed that  $\text{J(MACROOH)}$  is 2.77 times larger than  $\text{J(HOCH}_2\text{CHO)}$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44010: It is assumed that  $\text{J(MACROH)}$  is 2.77 times larger than  $\text{J(HOCH}_2\text{CHO)}$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J44015: It is assumed that  $\text{J(BIACETOH)}$  is 2.15 times larger than  $\text{J(MGLYOX)}$ , consistent with the photolysis

rate coefficients used in the MCM (Rickard and Pascoe, 2009).

**J44017a:** CO-channel yielding  $\text{CH}_3\text{COCH}$  which upon reaction with  $\text{O}_2$  produces an excited Criegee Intermediate assumed to be similar to MGLOOA in MCM. MGLOOA is produced also in other reactions and is substituted by its decomposition products. Furthermore, the stabilized Criegee Intermediate is assumed to solely react with water.

**J44025:** J values only for the secondary nitrate.

**J44026:** Like for LMEKNO3 photolysis

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

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

**J44043:** The resulting vinyl peroxy radical is assumed to mostly form with  $\text{HO}_2$  a labile hydroperoxide (see ketene formation). The products are further simplified.

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

**J44046a:** Simplified oxidation.

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

**J44401:**  $\text{KDEC BZFUO} \rightarrow \text{CO}_2\text{H}_3\text{CHO} + \text{HO}_2$

**J44403:**  $\text{KDEC NBZFUO} \rightarrow .5 \text{CO}_2\text{H}_3\text{CHO} + .5 \text{NO}_2 + .5 \text{NBZFUONE} + .5 \text{HO}_2$

**J44404b:**  $\text{KDEC MALDIALCO}_2 \rightarrow .6 \text{MALANHY} + \text{HO}_2 + .4 \text{GLYOX} + .4 \text{CO}$

**J44407:**  $\text{KDEC MALANHYO} \rightarrow \text{HCOCOHC}_3\text{O}_3$

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

**J45003:** It is assumed that  $\text{J}(\text{LISOPACNO}_3) = 0.59 \times \text{J}(\text{IC}_3\text{H}_7\text{ONO}_2)$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

**J45005:** It is assumed that  $\text{J}(\text{ISOPBNO}_3) = 2.84 \times \text{J}(\text{IC}_3\text{H}_7\text{ONO}_2)$ , consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

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

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

**J45015:** Consistent with the MCM (Rickard and Pascoe, 2009), we assume that  $\text{J}(\text{HCOC}_5)$  is half as large as  $\text{J}(\text{MVK})$ . With exception of  $\text{HOCH}_2\text{CO}$  the products of  $\text{MACO}_2$  decomposition without  $\text{CO}_2$ .

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

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

**J45407:**  $\text{KDEC TLFUONE} \rightarrow .6 \text{C}_5\text{CO}_{14}\text{O}_2 + .6 \text{HO}_2 + .4 \text{TLFUONE}$

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

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

**J45412:**  $\text{KDEC NTLFUO} \rightarrow \text{ACCOMEC}_3\text{O} + \text{NO}_2$

**J45414:**  $\text{KDEC C}_5\text{CO}_{14}\text{CO}_2 \rightarrow .83 \text{MALANHY} + .83 \text{CH}_3 + .17 \text{MGLYOX} + .17 \text{HO}_2 + .17 \text{CO} + .17 \text{CO}_2$

**J45415:**  $\text{KDEC TLFUO} \rightarrow \text{ACCOMEC}_3\text{O} + \text{HO}_2$

**J46400:**  $\text{KDEC PHENO} \rightarrow .71 \text{MALDALCO}_2\text{H} + .71 \text{GLYOX} + .29 \text{PBZQONE} + \text{HO}_2$

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

**J46404:**  $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{BZFUONE} + .5 \text{BZFUONE}$

**J46405:** new channel created for nitrophenol decomposition

**J46406:** new channel created for nitrophenol decomposition

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

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

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

**J46418:**  $\text{KDEC BZBIPERO} \rightarrow \text{GLYOX} + \text{HO}_2 + .5 \text{BZFUONE} + .5 \text{BZFUONE}$

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

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

**J46425:**  $\text{KDEC BZEMUCO} \rightarrow .5 \text{EPXC}_4\text{DIAL} + .5 \text{GLYOX} + .5 \text{HO}_2 + .5 \text{C}_3\text{DIALO}_2 + .5 \text{C}_3\text{OH}_{13}\text{CO}$

**J46429:** new channel

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

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

**J47404:**  $\text{KDEC TLBIPERO} \rightarrow .6 \text{GLYOX} + .4 \text{MGLYOX} + \text{HO}_2 + .2 \text{ZC}_3\text{O}_2\text{C}_2\text{H}_3\text{BCOD} + .2 \text{C}_5\text{DICARB} + .2 \text{TLFUONE} + .2 \text{BZFUONE} + .2 \text{MALDIAL}$

**J47405:**  $\text{KDEC TLBIPERO} \rightarrow .6 \text{GLYOX} + .4 \text{MGLYOX} + \text{HO}_2 + .2 \text{ZC}_3\text{O}_2\text{C}_2\text{H}_3\text{BCOD} + .2 \text{C}_5\text{DICARB} + .2 \text{TLFUONE} + .2 \text{BZFUONE} + .2 \text{MALDIAL}$

**J47407:**  $\text{KDEC CRESO} \rightarrow .68 \text{C}_5\text{CO}_{14}\text{OH} + .68 \text{GLYOX} + \text{HO}_2 + .32 \text{PTLQONE}$

J47408a: KDEC CRESO $\rightarrow$ .68 C5CO14OH + .68 GLYOX + HO2 + .32 PTLQONE	J47418: new channel	J47428: KDEC NDNCRESO $\rightarrow$ NC4MDCO2H + HNO3 + CO + CO + NO2
J47408b: KDEC NCRESO $\rightarrow$ C5CO14OH + GLYOX + NO2	J47419: Using J for 3-methyl-2-nitrophenol.	J47429: KDEC DNCRESO $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2
J47409: Using J for 3-methyl-2-nitrophenol.	J47420: new channel	J48400: KDEC STYRENO $\rightarrow$ HO2 + HCHO + BENZAL
J47412: KDEC TLEMUCO $\rightarrow$ .5 C3DIALO2 + .5 CO2H3CHO + .5 EPXC4DIAL + .5 MGLYOX + .5 HO2	J47422: KDEC NPTLQO $\rightarrow$ C7CO4DB + NO2	J40203b: Substituted vinyl alcohol in analogy to CH <sub>3</sub> CHO photolysis.
J47417: Using J for 3-methyl-2-nitrophenol.	J47423: KDEC PTLQO $\rightarrow$ C6CO2OHCO3	
	J47425: KDEC MNNCATECO $\rightarrow$ NC4MDCO2H + HCOCO2H + NO2	
	J47426: KDEC MNCATECO $\rightarrow$ NC4MDCO2H + HCOCO2H + HO2	

Table 3: Henry’s law coefficients

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
O <sub>2</sub>	$1.3 \times 10^{-3}$	1500.	Wilhelm et al. (1977)
O <sub>3</sub>	$1.2 \times 10^{-2}$	2560.	Chameides (1984)
OH	$3.0 \times 10^1$	4300.	Hanson et al. (1992)
HO <sub>2</sub>	$3.9 \times 10^3$	5900.	Hanson et al. (1992)
H <sub>2</sub> O <sub>2</sub>	$1. \times 10^5$	6338.	Lind and Kok (1994)
H <sub>2</sub> O	BIG	0.	see note
NH <sub>3</sub>	58.	4085.	Chameides (1984)
NO	$1.9 \times 10^{-3}$	1480.	Schwartz and White (1981)
NO <sub>2</sub>	$7.0 \times 10^{-3}$	2500.	Lee and Schwartz (1981)*
NO <sub>3</sub>	2.	2000.	Thomas et al. (1993)
N <sub>2</sub> O <sub>5</sub>	BIG	0.	see note
HONO	$4.9 \times 10^1$	4780.	Schwartz and White (1981)
HNO <sub>3</sub>	$2.45 \times 10^6 / 1.5 \times 10^1$	8694.	Brimblecombe and Clegg (1989)*
HNO <sub>4</sub>	$1.2 \times 10^4$	6900.	Régimbal and Mozurkewich (1997)
CH <sub>3</sub> OH	$2.20 \times 10^2$	5200.	Snider and Dawson (1985)
CH <sub>3</sub> O <sub>2</sub>	6.	5600.	Jacob (1986)*
CH <sub>3</sub> OOH	$3.0 \times 10^2$	5322.	Lind and Kok (1994)
CO <sub>2</sub>	$3.1 \times 10^{-2}$	2423.	Chameides (1984)
HCHO	$7.0 \times 10^3$	6425.	Chameides (1984)
HCOOH	$3.7 \times 10^3$	5700.	Chameides (1984)
CH <sub>3</sub> COOH	$4.1 \times 10^3$	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	6.	5600.	see note
CH <sub>3</sub> CHO	$1.29 \times 10^1$	5890.	Sander et al. (2006)
GLYOX	$4.19 \times 10^5$	7481.	Sander et al. (2011)
HOCH <sub>2</sub> CO <sub>2</sub> H	$2.83 \times 10^4$	4029.	Ip et al. (2009)
HOCH <sub>2</sub> CHO	$4.10 \times 10^4$	4600.	Betterton and Hoffmann (1988)
CH <sub>3</sub> COCH <sub>3</sub>	28.1	5050.	Sander et al. (2006)
MGLYOX	$3.70 \times 10^3$	7500.	Betterton and Hoffmann (1988)
SO <sub>2</sub>	1.2	3120.	Chameides (1984)
H <sub>2</sub> SO <sub>4</sub>	$1. \times 10^{11}$	0.	see note
CH <sub>3</sub> SO <sub>3</sub> H	BIG	0.	see note
DMS	$5.4 \times 10^{-1}$	3500.	Staudinger and Roberts (2001)



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

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
DMSO	$5. \times 10^4$	6425.	De Bruyn et al. (1994)*

## 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:

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

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

## Specific notes

NO<sub>2</sub>: The temperature dependence is from Chameides (1984).

HNO<sub>3</sub>: Calculated using the acidity constant from Davis and de Bruin (1964).

CH<sub>3</sub>O<sub>2</sub>: This value was estimated by Jacob (1986).

C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>: Assumed to be the same as  $K_H(\text{CH}_3\text{O}_2)$ .

H<sub>2</sub>SO<sub>4</sub>: To account for the very high Henry’s law coefficient of H<sub>2</sub>SO<sub>4</sub>, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^\ominus$	$\frac{-\Delta_{\text{obs}}H/R}{K}$	reference
O <sub>2</sub>	0.01	2000.	see note
O <sub>3</sub>	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO <sub>2</sub>	0.5	(default)	Thornton and Abbatt (2005)
H <sub>2</sub> O <sub>2</sub>	0.077	3127.	Worsnop et al. (1989)
H <sub>2</sub> O	0.0	(default)	see note
NH <sub>3</sub>	0.06	(default)	DeMore et al. (1997)*
NO	$5.0 \times 10^{-5}$	(default)	Saastad et al. (1993)*
NO <sub>2</sub>	0.0015	(default)	Ponche et al. (1993)*
NO <sub>3</sub>	0.04	(default)	Rudich et al. (1996)*
N <sub>2</sub> O <sub>5</sub>	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO <sub>3</sub>	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO <sub>4</sub>	(default)	(default)	DeMore et al. (1997)*
CH <sub>3</sub> OH	(default)	(default)	see note
CH <sub>3</sub> O <sub>2</sub>	0.01	2000.	see note
CH <sub>3</sub> OOH	0.0046	3273.	Magi et al. (1997)
CO <sub>2</sub>	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH <sub>3</sub> COOH	$2.0 \times 10^{-2}$	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
C <sub>2</sub> H <sub>5</sub> O <sub>2</sub>	(default)	(default)	see note
CH <sub>3</sub> CHO	$3.0 \times 10^{-2}$	(default)	see note
GLYOX	(default)	(default)	see note
HOCH <sub>2</sub> CO <sub>2</sub> H	(default)	(default)	see note
HOCH <sub>2</sub> CHO	(default)	(default)	see note
CH <sub>3</sub> COCH <sub>3</sub>	$3.72 \times 10^{-3}$	6395.	Davidovits et al. (1995)
MGLYOX	(default)	(default)	see note
SO <sub>2</sub>	0.11	(default)	DeMore et al. (1997)
H <sub>2</sub> SO <sub>4</sub>	0.65	(default)	Pöschl et al. (1998)*
CH <sub>3</sub> SO <sub>3</sub> H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)

## General notes

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

$$\alpha^{\ominus} = 0.1$$

$$-\Delta_{\text{obs}}H/R = 0 \text{ K}$$

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

$$\begin{aligned} \frac{\alpha}{1-\alpha} &= \exp\left(\frac{-\Delta_{\text{obs}}G}{RT}\right) \\ &= \exp\left(\frac{-\Delta_{\text{obs}}H}{RT} + \frac{\Delta_{\text{obs}}S}{R}\right) \end{aligned}$$

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

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

and further:

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

## Specific notes

O<sub>2</sub>: Estimate.

O<sub>3</sub>: Value measured at 292 K.

OH: Value measured at 293 K.

NH<sub>3</sub>: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO<sub>2</sub>: Value measured at 298 K.

NO<sub>3</sub>: Value is a lower limit, measured at 273 K.

N<sub>2</sub>O<sub>5</sub>: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO<sub>3</sub>: Value measured at room temperature. Abbatt and Waschewsky (1998) say  $\gamma > 0.2$ . Here  $\alpha = 0.5$  is used.

HNO<sub>4</sub>: Value measured at 200 K for water ice.

CH<sub>3</sub>O<sub>2</sub>: Estimate.

CO<sub>2</sub>: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>: Estimate.

CH<sub>3</sub>CHO: Using the same estimate as in the CAPRAM 2.4 model ([http://projects.tropos.de/capram/capram\\_24.html](http://projects.tropos.de/capram/capram_24.html)).

H<sub>2</sub>SO<sub>4</sub>: Value measured at 303 K.

Table 5: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
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## 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<sub>2</sub>O<sub>5</sub>, ClNO<sub>3</sub>, or BrNO<sub>3</sub>) and subsequent reaction with H<sub>2</sub>O, Cl<sup>−</sup>, and Br<sup>−</sup> 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,  $k_{\text{mt}}$  = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by  $k_{\text{mt}}$ . The factors only affect the branching between hydrolysis and the halide reac-

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

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
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## General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA\_KHET) and then supplied to the MECCA chemistry (see [www.messy-interface.org](http://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
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Specific notes

Table 8: Aqueous phase reactions

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

## References

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