

The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs5

MECCA version: 3.3

Date: October 9, 2013.

Selected reactions:

“Tr && G && !S && !Cl && !Br && !I && !Hg”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	394
Aqueous phase:	0
All species:	394

Number of reactions in selected mechanism:

Gas phase (Gnn):	952
Aqueous phase (Ann):	0
Henry (Hnn):	0
Photolysis (Jnn):	102
Heterogeneous (HETnn):	0
Equilibria (EQnn):	0
Isotope exchange (DGnn):	0
Dummy (Dnn):	0
All equations:	1054

This document is part of the electronic supplement to our article
“Observation and modelling of HO_x radicals in a boreal forest”
in ACP (2013), available at:

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

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.2E-11 * EXP(70./temp)$	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34 * ((temp/300.)^{(-2.4)} * cair)$	Sander et al. (2003)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	$k_3rd(temp, cair, 5.7E-32, 1.6, 7.5E-11, 0., 0.6)$	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + LOHOX$	$1.7E-12 * EXP(-940./temp)$	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H + LOHOX$	$2.8E-12 * EXP(-1800./temp)$	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + POHOX$	$1.E-14 * EXP(-490./temp)$	Sander et al. (2003)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + LOHOX$	$4.8E-11 * EXP(250./temp)$	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2 OH + 2 POHOX + 2 POHPR$	$2.2E-10$	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2 + LOHOX$	$2.9E-12 * EXP(-160./temp)$	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$1.8E-11 * EXP(110./temp)$	Sander et al. (2003)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12 * EXP(-1500./temp)$	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13 * EXP(-2450./temp)$	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11 * EXP(170./temp)$	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k_NO3_NO2 / (3.E-27 * EXP(10990./temp))$	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO + LONOX$	$k_3rd(temp, cair, 7.E-31, 2.6, 3.6E-11, 0.1, 0.6)$	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH + PONOX$	$3.5E-12 * EXP(250./temp)$	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3 + LONOX$	$k_3rd(temp, cair, 1.48E-30, 3., 2.58E-11, 0., 0.6)$	Mollner et al. (2010)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2003)
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2 + PONOX$	$3.5E-12$	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O + LONOX$	$1.8E-11 * EXP(-390./temp)$	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3 + LONOX$	k_HN03_OH	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k_NO2_HO2 / (2.1E-27 * EXP(10900./temp))$	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O + LONOX$	$1.3E-12 * EXP(380./temp)$	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O + POHORG$	$1.85E-20 * EXP(2.82 * log(temp) - 987./temp)$	Atkinson (2003)
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2 + POHORG$	$7.3E-12 * EXP(-620./temp)$	Sander et al. (2003)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	$4.1E-13 * EXP(750./temp) / (1.+1./497.7 * EXP(1160./temp))$	Sander et al. (2003)*

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

#	labels	reaction	rate coefficient	reference
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$4.1\text{E}-13*\text{EXP}(750./\text{temp})/(1.+497.7*\text{EXP}(-1160./\text{temp}))$	Sander et al. (2003)*
G4104	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2003)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E}-12$	Atkinson et al. (1999)
G4106a	StTrG	$\text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.*\text{R02}*9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+1./26.2*\text{EXP}(1130./\text{temp}))$	Sander et al. (2003)
G4106b	StTrG	$\text{CH}_3\text{O}_2 \rightarrow .5 \text{ HCHO} + .5 \text{ CH}_3\text{OH}$	$2.*\text{R02}*9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+26.2*\text{EXP}(-1130./\text{temp}))$	Sander et al. (2003)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .6 \text{ CH}_3\text{O}_2 + .4 \text{ HCHO} + .4 \text{ OH} + \text{H}_2\text{O} + .4 \text{ POHORG} + \text{POHORG}$	$k_{\text{CH3OOH_OH}}$	see note
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2 + \text{POHORG}$	$9.52\text{E}-18*\text{EXP}(2.03*\log(\text{temp})+636./\text{temp})$	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. (2003)*
G4110	StTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2 + \text{POHORG}$	$1.57\text{E}-13 + \text{cair}*3.54\text{E}-33$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O} + \text{POHORG}$	$4.5\text{E}-13$	IUPAC (2013)
G4112e	TrGC	$\text{HCHO} + \text{HO}_2 \rightarrow \text{HOCH}_2\text{O}_2$	$7.7\text{E}-15*\text{EXP}(625./\text{temp})$	IUPAC (2013)
G4113e	TrGC	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$2.1\text{E}12*\text{EXP}(-7000./\text{temp})$	IUPAC (2013)
G4114e	TrGC	$\text{HOCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .5 \text{ HOCH}_2\text{OOH} + .5 \text{ HCOOH} + .2 \text{ OH} + .2 \text{ HO}_2 + .3 \text{ H}_2\text{O} + .2 \text{ POHORG}$	$5.6\text{E}-15*\text{EXP}(2300./\text{temp})$	Jenkin et al. (2007)
G4115e	TrGC	$\text{HOCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$2.8\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2003)
G4116e	TrGC	$\text{HOCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCOOH}$	$1.2\text{E}-12$	see note
G4117e	TrGC	$\text{HOCH}_2\text{O}_2 \rightarrow \text{HCOOH} + .62 \text{ HO}_2$	$1.4\text{E}-12*\text{R02}$	see note
G4118e	TrGC	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{HOCH}_2\text{O}_2 + \text{H}_2\text{O} + \text{POHORG}$	$0.6*k_{\text{CH3OOH_OH}} + k_{\text{rohro}}$	see note
G4119e	TrGC	$\text{HOCH}_2\text{OOH} + \text{OH} \rightarrow \text{OH} + \text{HCOOH} + \text{H}_2\text{O} + \text{POHORG} + \text{POHORG}$	$ks*fsoh*fsooh$	see note
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O} + \text{POHORG}$	$1.49\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201e	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + .63 \text{ CO} + .13 \text{ HO}_2 + 0.37 \text{ HOCH}_2\text{OOH} + .13 \text{ OH} + .13 \text{ POHORG}$	$1.2\text{E}-14*\text{EXP}(-2630./\text{temp})$	Sander et al. (2003)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O} + \text{POHORG}$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 1.\text{E}-28, 0.8, 8.8\text{E}-12, 0., 0.6)$	Sander et al. (2003)
G4203	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. (2003)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E}-12*\text{EXP}(365./\text{temp})$	Sander et al. (2003)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E}-12$	Atkinson et al. (1999)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 \rightarrow .98 \text{ CH}_3\text{CHO} + .38 \text{ HO}_2 + .02 \text{ HOCH}_2\text{CH}_2\text{O}_2$	$3.1\text{E}-13*\text{R02}$	Rickard and Pascoe (2009)*
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .43 \text{ C}_2\text{H}_5\text{O}_2 + .43 \text{ H}_2\text{O} + .57 \text{ CH}_3\text{CHO} + .57 \text{ OH} + .57 \text{ POHORG} + \text{POHORG}$	$0.6*k_{\text{CH3OOH_OH}} + 8.01\text{E}-12$	see note

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

#	labels	reaction	rate coefficient	reference
G4208ea	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O} + \text{POHORG}$	4.4E-12*EXP(365./temp)*0.95	Atkinson et al. (2006)
G4208eb	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow .84 + .1 \text{ HCHO} + .1 \text{ CO} + .06 \text{ GLYOX}$ + .16 OH + H ₂ O + .16 POHORG + POHORG	4.4E-12*EXP(365./temp)*0.05	Atkinson et al. (2006)
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HNO}_3$	KNO3AL	Sander et al. (2003)
G4210e	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{H}_2\text{O} + \text{POHORG}$	4.2E-14*exp(850./temp)	IUPAC (2013)
G4211et1	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{POHORG}$	KAPH02*0.70	Taraborrelli (2013a)*
G4211et2	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C(O)OOH}$	KAPH02*0.12	Taraborrelli (2013a)*
G4211et3	TrGC	$\text{CH}_3\text{C(O)OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	KAPH02*0.18	Taraborrelli (2013a)*
G4212	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{NO}_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
G4213	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_CH3C03_N02	Tyndall et al. (2001)
G4214	TrGNC	$\text{CH}_3\text{C(O)OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2 + \text{CO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4217	TrGC	$\text{CH}_3\text{C(O)OO} \rightarrow .7 \text{ CH}_3\text{O}_2 + .7 \text{ CO}_2 + .3 \text{ CH}_3\text{COOH}$	1.00E-11*R02	Rickard and Pascoe (2009)
G4218	TrGC	$\text{CH}_3\text{C(O)OOH} + \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{H}_2\text{O} + \text{POHORG}$	0.6*k_CH300H_OH	Rickard and Pascoe (2009)*
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{CO} + \text{NO}_2 + \text{H}_2\text{O} + \text{POHORG}$	9.50E-13*EXP(-650./temp)	Rickard and Pascoe (2009)
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C(O)OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2003)*
G4223e	TrGC	$\text{HOCH}_2\text{CHO} + \text{OH} \rightarrow .84 + .16 + .2 \text{ HO}_2 + \text{H}_2\text{O} + \text{POHORG}$	8.00E-12	Rickard and Pascoe (2009)
G4224e	TrGNC	$\text{HOCH}_2\text{CHO} + \text{NO}_3 \rightarrow + \text{HNO}_3$	KNO3AL	Rickard and Pascoe (2009)
G4255et2	TrGC	$\rightarrow \text{HOCH}_2\text{CO}_3$	KDEC*.97	Taraborrelli (2013a)*
G4255et3	TrGC	$\rightarrow \text{OH} + \text{HCHO} + \text{CO} + \text{POHORG}$	KDEC*.03	Taraborrelli (2013a)*
G4256et2	TrGC	$\rightarrow \text{GLYOX} + \text{HO}_2$	KDEC	Taraborrelli (2013a)
G4225	TrGC	$\text{HOCH}_2\text{CO}_3 \rightarrow .7 \text{ HCHO} + .7 \text{ CO}_2 + .7 \text{ HO}_2 + .3 \text{ HOCH}_2\text{CO}_2\text{H}$	1.00E-11*R02	Rickard and Pascoe (2009)
G4226ea	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{OH} + \text{CO}_2 + \text{POHORG}$	KAPH02*rco3_oh	Taraborrelli (2013a)*
G4226eb	TrGC	$\text{HOCH}_2\text{CO}_3 + \text{HO}_2 \rightarrow \text{HOCH}_2\text{CO}_3\text{H}$	KAPH02*rco3_ooh	Taraborrelli (2013a)*
G4226ec	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 (2013a)*
G4227	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KAPNO	Rickard and Pascoe (2009)
G4228	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO}_2 \rightarrow \text{PHAN}$	k_CH3C03_N02	Rickard and Pascoe (2009)
G4229	TrGNC	$\text{HOCH}_2\text{CO}_3 + \text{NO}_3 \rightarrow \text{NO}_2 + \text{HO}_2 + \text{HCHO} + \text{CO}_2$	KR02N03*1.60	Rickard and Pascoe (2009)
G4230e	TrGC	$\text{HOCH}_2\text{CO}_2\text{H} + \text{OH} \rightarrow .09 \text{ HCHO} + .09 \text{ CO}_2 + .91 \text{ HCOCO}_2\text{H} + \text{HO}_2 + \text{H}_2\text{O} + \text{POHORG}$	kco2h+ks*fsoh*fco2h	Taraborrelli (2013a)
G4231ea	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{H}_2\text{O} + \text{POHORG}$	0.6*k_CH300H_OH	Taraborrelli (2013a)
G4231eb	TrGC	$\text{HOCH}_2\text{CO}_3\text{H} + \text{OH} \rightarrow \text{HCOCO}_3\text{H} + \text{HO}_2 + \text{POHORG}$	ks*fsoh*fco2h	Taraborrelli (2013a)
G4232	TrGNC	$\text{PHAN} \rightarrow \text{HOCH}_2\text{CO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4233	TrGNC	PHAN + OH → HCHO + CO + NO ₂ + H ₂ O	1.12E-12	Rickard and Pascoe (2009)
G4234e	TrGC	GLYOX + OH → 1.2 CO + .6 HO ₂ + .4 + H ₂ O + POHORG	3.1E-12*EXP(340./temp)	IUPAC (2013)
G4235e	TrGNC	GLYOX + NO ₃ → 1.2 CO + .6 HO ₂ + .4 + HNO ₃	KNO3AL	Rickard and Pascoe (2009)
G4235et2	TrGNC	→ 1.5 CO + .5 HO ₂ + .5 OH + .5 CO ₂ + .5 POHORG	KDEC	Taraborrelli (2013a)
G4236	TrGC	HCOCO ₃ → .7 CO + .7 HO ₂ + .7 CO ₂ + .3 HCOCO ₂ H	1.00E-11*R02	Rickard and Pascoe (2009)
G4237e	TrGC	HCOCO ₃ + HO ₂ → HO ₂ + CO + CO ₂ + OH + POHORG	KAPH02	Feierabend et al. (2008), Taraborrelli (2013a)
G4238	TrGNC	HCOCO ₃ + NO → HO ₂ + CO + NO ₂ + CO ₂	KAPNO	Rickard and Pascoe (2009)
G4239	TrGNC	HCOCO ₃ + NO ₃ → HO ₂ + CO + NO ₂ + CO ₂	KR02N03*1.60	Rickard and Pascoe (2009)
G4239t2	TrGNC	HCOCO ₃ + NO ₂ → HO ₂ + CO + NO ₃ + CO ₂	k_CH3C03_N02	Orlando and Tyndall (2001), Taraborrelli (2013a)*
G4240	TrGC	HCOCO ₂ H + OH → CO + HO ₂ + CO ₂ + H ₂ O + POHORG	kco2h+kt*fo*fco2h	Taraborrelli (2013a)
G4241	TrGC	HCOCO ₃ H + OH → .2 HCOCO ₃ + .8 CO + .8 OH + .8 CO ₂ + H ₂ O + POHORG + .8 POHORG	0.6*k_CH300H_OH+kt*fo*fco2h	Taraborrelli (2013a)
G4242	TrGC	HOCH ₂ CH ₂ O ₂ → .6 HOCH ₂ CH ₂ O + .2 HOCH ₂ CHO + .2 ETHGLY	2.00E-12*R02	Rickard and Pascoe (2009)
G4244	TrGC	HOCH ₂ CH ₂ O ₂ + HO ₂ → HYETHO2H	2.00E-13*EXP(1250./temp)	Rickard and Pascoe (2009)
G4243	TrGNC	HOCH ₂ CH ₂ O ₂ + NO → .24875 HO ₂ + .4975 HCHO + .74625 HOCH ₂ CH ₂ O + .995 NO ₂ + .005 ETHOHNO3	KR02NO	Orlando et al. (1998)
G4245	TrGNC	ETHOHNO3 + OH → .93 + .93 HO ₂ + .07 HOCH ₂ CHO + .07 NO ₂ + H ₂ O + POHORG	ks*(fsoh*fch2ono2+fono2*fpch2oh)+krohro	Taraborrelli (2013a)
G4246a	TrGC	HYETHO2H + OH → HOCH ₂ CH ₂ O ₂ + H ₂ O + POHORG	0.6*k_CH300H_OH	Rickard and Pascoe (2009)
G4246b	TrGC	HYETHO2H + OH → HOCH ₂ CHO + OH + H ₂ O + POHORG + POHORG	ks*fsooh*fpch2oh	Taraborrelli (2013a)
G4246c	TrGC	HYETHO2H + OH → + HO ₂ + H ₂ O	ks*fsoh*fpch2oh+krohro	Taraborrelli (2013a)
G4247a	TrGC	HOCH ₂ CH ₂ O → HO ₂ + HOCH ₂ CHO	6.00E-14*EXP(-550./temp)*C(ind_02)	Orlando et al. (1998)
G4247b	TrGC	HOCH ₂ CH ₂ O → HO ₂ + HCHO + HCHO	9.50E+13*EXP(-5988./temp)	Orlando et al. (1998)
G4248	TrGC	ETHGLY + OH → HOCH ₂ CHO + HO ₂ + H ₂ O + POHORG	2*ks*fsoh*fpch2oh+2*krohro	Taraborrelli (2013a)
G4249e	TrGC	→ 0.6 HCHO + 0.6 CO + 0.6 HO ₂ + 0.2 GLYOX + 0.2 HOCH ₂ CHO	2.00E-12*R02	Taraborrelli (2013a)
G4250e	TrGC	+ HO ₂ → 0.85 + 0.15 HCHO + 0.15 CO + 0.15 HO ₂ + 0.15 OH + .15 POHORG	KR02H02*0.387	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4251e	TrGC	+ NO → NO ₂ + HCHO + CO + HO ₂	KR02NO	Taraborrelli (2013a)
G4252e	TrGC	+ NO ₃ → HCHO + CO + HO ₂ + NO ₂	KR02N03	Taraborrelli (2013a)
G4253e	TrGC	+ OH → .71 OH + .31 HCHO + .31 CO + .40 GLYOX + .29 + .71 POHORG + POHORG	0.6*k_CH300H_OH+ks*fsooh*fcho+.8*8.E-12	Taraborrelli (2013a)
G4254e	TrGNC	+ NO ₃ → OH + HCHO + CO + HNO ₃ + POHORG	KN03AL	Rickard and Pascoe (2009)
G4257e	TrGC	+ OH → HCHO + CO ₂ + NO ₂ + H ₂ O + POHORG	1.E-11	Paulot et al. (2009a), Taraborrelli (2013a)
G4258e	TrGNC	+ NO → NO ₂ + OH + HCHO + CO ₂ + POHORG	KAPNO	Taraborrelli (2013a)
G4259e	TrGNC	+ NO ₃ → NO ₂ + OH + HCHO + CO ₂ + POHORG	KR02N03*1.60	Taraborrelli (2013a)
G4260e	TrGC	+ HO ₂ → 2 OH + HCHO + CO ₂ + 2 POHORG	KAPH02*rco3_oh	Taraborrelli (2013a)
G4260et2	TrGC	+ HO ₂ →	KAPH02*rco3_ooh	Taraborrelli (2013a)*
G4260et3	TrGC	+ HO ₂ → + O ₃	KAPH02*rco3_o3	Taraborrelli (2013a)*
G4261e	TrGC	→ .7 OH + .7 HCHO + .7 CO ₂ + .3 + .7 POHORG	1.00E-11*R02	Taraborrelli (2013a)
G4262e	TrGC	+ OH → + H ₂ O + POHORG	2.*0.6*k_CH300H_OH	Taraborrelli (2013a)
G4263e	TrGC	+ OH → HCOCO ₃ H + OH + H ₂ O + POHORG + POHORG	ks*fsooh*fco2h	Taraborrelli (2013a)
G4265e	TrGC	+ OH → HCOCO ₂ H + OH + H ₂ O + POHORG + POHORG	ks*fsooh*fco2h+kco2h	Taraborrelli (2013a)
G4266e	TrGC	+ OH → .6 HCHO + .6 HO ₂ + .6 CO + .4 + POHORG	2.8E-12*exp(510./temp)	Baulch et al. (2005), Taraborrelli (2013a)*
G4267e	TrGC	+ OH → CH ₃ COOH + OH + POHORG + POHORG	kt*ftooh*ftoh + krohro	Taraborrelli (2013a)
G4268e	TrGC	+ OH → + POHORG	0.6*k_CH300H_OH	Taraborrelli (2013a)
G4269e	TrGC	→ CH ₃ CHO + HO ₂	3.46E12*EXP(-12500./(1.98*temp))	Hermans et al. (2005), Taraborrelli (2013a)
G4270e	TrGC	CH ₃ CHO + HO ₂ →	3.46E12*EXP(-12500./(1.98*temp))/(6.34E26*EXP(-14700./(1.98*temp)))	Hermans et al. (2005), Taraborrelli (2013a)
G4271e	TrGC	+ HO ₂ → .5 + .3 CH ₃ COOH + .2 CH ₃ O ₂ + .2 HCOOH + .2 OH	5.6E-15*EXP(2300./temp)	Taraborrelli (2013a)
G4272e	TrGC	→ CH ₃ O ₂ + HCOOH + OH	1.4E-12*R02	Taraborrelli (2013a)
G4273e	TrGC	+ NO → CH ₃ O ₂ + HCOOH + OH + NO ₂	KR02NO	Taraborrelli (2013a)
G4300	TrGC	C ₃ H ₈ + OH → .736 iC ₃ H ₇ O ₂ + .264 C ₂ H ₅ O ₂ + .264 CO ₂ + .264 HO ₂ + H ₂ O + POHORG	1.55E-17*temp*temp*EXP(-61./temp)	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G4301et2	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .0855 + .4389 \text{CH}_3\text{CHO} + .4389 \text{H}_2\text{O}_2 + .0456 \text{CH}_3\text{COOH} + .285 + .0855 \text{CH}_4 + .0855 \text{CO}_2 + .0342 + .0513 \text{CH}_3\text{OH} + .0228 \text{CH}_3\text{C(O)OO} + .57 \text{HCHO} + .2709 \text{CO} + .0688 \text{HO}_2 + .1591 \text{HOCH}_2\text{OOH} + .43 \text{CH}_3\text{CHO} + .3766 \text{OH} + .3766 \text{POHORG}$	$6.5\text{E}-15*\text{EXP}(-1900./\text{temp})$	Taraborrelli (2013a)
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{HYPROPO2} + \text{POHORG}$	$k_3\text{rd}(\text{temp}, \text{cair}, 8.\text{E}-27, 3.5, 3.\text{E}-11, 0., 0.5)$	Atkinson et al. (1999)
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{PRONO3BO2}$	$4.6\text{E}-13*\text{EXP}(-1155./\text{temp})$	Atkinson et al. (1999)
G4304	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)*
G4305	TrGNC	$\text{iC}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow .96 \text{CH}_3\text{COCH}_3 + .96 \text{HO}_2 + .96 \text{NO}_2 + .04 \text{iC}_3\text{H}_7\text{ONO}_2$	$2.7\text{E}-12*\text{EXP}(360./\text{temp})$	Atkinson et al. (1999)
G4306	TrGC	$\text{iC}_3\text{H}_7\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{HO}_2$	$4.\text{E}-14*\text{R02}$	Rickard and Pascoe (2009)*
G4307	TrGC	$\text{iC}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .27 \text{iC}_3\text{H}_7\text{O}_2 + .73 \text{CH}_3\text{COCH}_3 + .73 \text{OH} + \text{H}_2\text{O} + .73 \text{POHORG} + \text{POHORG}$	$1.66\text{E}-11 + 0.6*k_{\text{CH3OOH}}_{\text{OH}}$	Rickard and Pascoe (2009)*
G4311	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O} + \text{POHORG}$	$1.33\text{E}-13+3.82\text{E}-11*\text{EXP}(-2000./\text{temp})$	Sander et al. (2003)
G4312e	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow .15 \text{OH} + .15 \text{CH}_3\text{C(O)OO} + .15 \text{HCHO} + .85 \text{CH}_3\text{COCH}_2\text{O}_2\text{H} + .15 \text{POHORG}$	$8.6\text{E}-13*\text{EXP}(700./\text{temp})$	Taraborrelli (2013a)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{NO}_2$	$2.9\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2003)
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 \rightarrow .6 \text{CH}_3\text{C(O)OO} + .6 \text{HCHO} + .2 \text{MGLYOX} + .2 \text{CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E}-13*\text{EXP}(500./\text{temp})*2.*\text{R02}$	Tyndall et al. (2001)
G4321	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4315a	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O} + \text{POHORG}$	$0.6*k_{\text{CH3OOH}}_{\text{OH}}$	Rickard and Pascoe (2009)*
G4315b	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow \text{MGLYOX} + \text{OH} + \text{H}_2\text{O} + \text{POHORG} + \text{POHORG}$	$ks*fsooh*fco$	Taraborrelli (2013a)
G4316e	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow + \text{H}_2\text{O} + \text{POHORG}$	$1.60\text{E}-12*\text{EXP}(305./\text{temp})$	Taraborrelli (2013a)
G4336ea	TrGC	$\rightarrow \text{MGLYOX} + \text{HO}_2$	0.8485	Taraborrelli (2013a)
G4317e	TrGC	$\text{MGLYOX} + \text{OH} \rightarrow .4 \text{CH}_3\text{O}_2 + .6 \text{CH}_3\text{C(O)OO} + 1.4 \text{CO} + \text{POHORG}$	$1.9\text{E}-12*\text{EXP}(575./\text{temp})$	Baeza-Romero et al. (2007),IUPAC (2013)
G4331	TrGNC	$\text{MGLYOX} + \text{NO}_3 \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO} + \text{HNO}_3$	$\text{KN03AL}*2.4$	Rickard and Pascoe (2009)
G4320	TrGNC	$\text{iC}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{POHORG}$	$6.2\text{E}-13*\text{EXP}(-230./\text{temp})$	Atkinson et al. (1999)
G4322	TrGC	$\text{HYPROPO2} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2$	$8.80\text{E}-13*\text{R02}$	Rickard and Pascoe (2009)
G4323	TrGC	$\text{HYPROPO2} + \text{HO}_2 \rightarrow \text{HYPROPO2H}$	$\text{KR02H02}*0.520$	Rickard and Pascoe (2009)
G4324	TrGNC	$\text{HYPROPO2} + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)
G4325	TrGNC	$\text{HYPROPO2} + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4326a	TrGC	HYPROPO2H + OH → HYPROPO2 + POHORG	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G4326b	TrGC	HYPROPO2H + OH → CH ₃ COCH ₂ OH + OH + POHORG + POHORG	ks*fsoh*fpch2oh+kt*fcooh*fpch2oh	Taraborrelli (2013a)
G4327	TrGNC	PRONO3BO2 + HO ₂ → PR2O2HNO3	KR02H02*0.520	Rickard and Pascoe (2009)
G4328	TrGNC	PRONO3BO2 + NO → NOA + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009)
G4329	TrGNC	PRONO3BO2 + NO ₃ → NOA + HO ₂ + NO ₂	KR02N03	Rickard and Pascoe (2009)
G4330a	TrGNC	PR2O2HNO3 + OH → PRONO3BO2 + POHORG	1.90E-12*EXP(190./temp)	Rickard and Pascoe (2009)
G4330b	TrGNC	PR2O2HNO3 + OH → NOA + OH + POHORG + POHORG	kt*fcooh*fch2ono2	Rickard and Pascoe (2009)
G4332	TrGNC	NOA + OH → MGLYOX + NO ₂ + POHORG	ks*fco*fono2+kp*fco	Taraborrelli (2013a)
G4333e	TrGC	HOCH2COCHO + OH → .8609 + .8609 CO + .1391 + .1391 HO ₂ + POHORG	1.9E-12*EXP(575./temp)+ks*fsoh*fco	Taraborrelli (2013a)
G4334e	TrGNC	HOCH2COCHO + NO ₃ → + CO + HNO ₃	KN03AL*2.4	Taraborrelli (2013a)
G4337e	TrGC	+ OH → CH ₃ C(O)OO + H ₂ O + CO ₂ + POHORG	4.9E-14*EXP(276./temp)	Mellouki and Mu (2003), Taraborrelli (2013a)
G4338e	TrGC	→ HCHO +	R02*2.0E-12	Taraborrelli (2013a)
G4339e	TrGC	+ HO ₂ → .15 HCHO + .15 + .15 OH + .85 + .15 POHORG	KR02H02*0.520	Taraborrelli (2013a)
G4340e	TrGC	+ NO → HCHO + + NO ₂	KR02NO	Taraborrelli (2013a)
G4341e	TrGC	+ OH → HOCH2COCHO + OH + POHORG + POHORG	ks*fsooh*fco	Taraborrelli (2013a)
G4342e	TrGC	+ OH → + POHORG	.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4343e	TrGC	+ OH → + HO ₂ + POHORG	0.9295*1.60E-12*EXP(305./temp)	Taraborrelli (2013a)
G4344e	TrGC	→ 0.6 + 0.6 HCHO + 0.2 + 0.2 HOCH2COCHO	2.00E-12*R02	Taraborrelli (2013a)
G4345e	TrGC	+ NO → + HCHO + NO ₂	KR02NO	Taraborrelli (2013a)
G4346e	TrGC	+ HO ₂ → 0.85 + 0.15 + 0.15 HCHO + 0.15 OH + .15 POHORG	KR02H02*0.520	Taraborrelli (2013a)
G4347e	TrGC	+ NO ₃ → + HCHO + NO ₂	KR02N03	Taraborrelli (2013a)
G4348e	TrGC	+ OH → + CO + H ₂ O + POHORG	kt*fco*fco	Taraborrelli (2013a)
G4349e	TrGC	+ OH → + OH + H ₂ O + POHORG + POHORG	ks*fsooh*fco	Taraborrelli (2013a)
G4350e	TrGC	+ OH → + H ₂ O + POHORG	0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4351e	TrGC	+ NO ₃ → + CO + HNO ₃	KN03AL*2.4	Taraborrelli (2013a)
G4352e	TrGC	+ OH → + CO + POHORG	2*kt*fco*fco	Taraborrelli (2013a)
G4353e	TrGC	+ OH → .72 CO + .72 CH ₃ CHO + .72 HO ₂ + .21 + .07 CH ₃ CHO + .07 HO ₂ + .07 CO ₂ + POHORG	7.6E-11	Hatakeyama et al. (1985), Taraborrelli (2013a)*

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

#	labels	reaction	rate coefficient	reference
G4354e	TrGC	+ OH → CO + + POHORG	1E-10*acho	Hatakeyama et al. (1985), Taraborrelli (2013a)*
G4355e	TrGC	+ OH → CO + + POHORG	7.6E-11*acoch3	Hatakeyama et al. (1985), Taraborrelli (2013a)*
G4400	TrGC	nC ₄ H ₁₀ + OH → LC ₄ H ₉ O ₂ + H ₂ O + POHORG	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)*
G4401	TrGC	LC ₄ H ₉ O ₂ → 0.254 CO ₂ + 0.5552 MEK + 0.5552 HO ₂ + 0.3178 CH ₃ CHO + 0.4448 C ₂ H ₅ O ₂	2.5E-13*R02	Rickard and Pascoe (2009)*
G4402	TrGC	LC ₄ H ₉ O ₂ + HO ₂ → LC ₄ H ₉ OOH	KR02H02*0.625	Rickard and Pascoe (2009)
G4403	TrGNC	LC ₄ H ₉ O ₂ + NO → 0.9172 NO ₂ + 0.233 CO ₂ + 0.5092 MEK + 0.5092 HO ₂ + 0.2915 CH ₃ CHO + 0.408 C ₂ H ₅ O ₂ + 0.0828 LC4H9NO3	KR02NO	Rickard and Pascoe (2009)*
G4404	TrGC	LC ₄ H ₉ OOH + OH → 0.2285796 LC ₄ H ₉ O ₂ + 0.7117253 MEK + 0.1193902 CO ₂ + 0.0596951 C ₂ H ₅ O ₂ + 0.7714204 OH + H ₂ O + .7714204 POHORG + POHORG	2.636E-11	Rickard and Pascoe (2009)*
G4405e	TrGC	MVK + O ₃ → .87 MGLYOX + 0.5481 CO + 0.1392 HO ₂ + 0.1392 OH + 0.3219 HOCH2OOH + .13 HCHO + 0.04680 OH + 0.04680 CO + 0.07280 CH ₃ C(O)OO + .026 CH ₃ CHO + .026 CO ₂ + .026 HCHO + .026 HO ₂ + 0.02402 MGLYOX + 0.02402 H ₂ O ₂ + 0.007176 + 0.1860 POHORG	8.5E-16*EXP(-1520./temp)	Taraborrelli (2013a)
G4406e	TrGC	MVK + OH → LHMVKABO2 + POHORG	2.6E-12*EXP(610./temp)	Taraborrelli (2013a)*
G4413	TrGC	MEK + OH → LMEKO2 + H ₂ O + POHORG	3.24E-18*temp*temp*EXP(414./temp)	Rickard and Pascoe (2009)*
G4414ea	TrGC	LMEKO2 + HO ₂ → LMEKOOH	KR02H02*0.625*rcoch2o2_ooh	Taraborrelli (2013a)
G4414eb	TrGC	LMEKO2 + HO ₂ → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO + OH + POHORG	KR02H02*0.625*rcoch2o2_oh	Taraborrelli (2013a)
G4415	TrGNC	LMEKO2 + NO → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO + NO ₂	KR02NO	Rickard and Pascoe (2009)*
G4416	TrGC	LMEKOOH + OH → 0.40851 CH ₃ COCH ₂ O ₂ + 0.350196 BIACET + 0.807212 OH + 0.048506 C ₂ H ₅ O ₂ + 0.505522 CO ₂ + 0.192788 LMEKO2 + H ₂ O + .807212 POHORG + POHORG	3.786E-11	Rickard and Pascoe (2009)*
G4417	TrGNC	LC4H9NO3 + OH → 0.91423 MEK + 0.08577 C ₂ H ₅ O ₂ + 0.17154 CO ₂ + NO ₂ + H ₂ O + POHORG	9.598E-13	Rickard and Pascoe (2009)*

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

#	labels	reaction	rate coefficient	reference
G4418	TrGNC	MPAN + OH → CH ₃ COCH ₂ OH + CO + NO ₂ + POHORG	3.2E-11	Orlando et al. (2002)
G4419	TrGNC	MPAN → MACO ₃ + NO ₂	k_PAN_M	see note
G4420	TrGC	LMEKO ₂ → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO	1.483E-12*R02	Rickard and Pascoe (2009)*
G4421e	TrGC	MACR + OH → .45 MACO ₃ + .55 MACRO ₂ + POHORG	8.E-12*EXP(380./temp)	Orlando et al. (1999b), Taraborrelli (2013a)
G4422e	TrGC	MACR + O ₃ → 0.5481 CO + 0.1392 HO ₂ + 0.1392 OH + 0.3219 HOCH ₂ OOH + .87 MGLYOX + .13 HCHO + .13 OH + .065 CO + .065 CH ₃ C(O)OO + 0.2692 POHORG	1.36E-15*EXP(-2112./temp)	Taraborrelli (2013a)
G4423	TrGNC	MACR + NO ₃ → MACO ₃ + HNO ₃	KNO3AL*2.0	Rickard and Pascoe (2009)
G4424e	TrGC	MACO ₃ → .7 + .3 MACO ₂ H	1.00E-11*R02	Taraborrelli (2013a)
G4425e	TrGC	MACO ₃ + HO ₂ → + OH + POHORG	KAPHO2*rco3_oh	Taraborrelli (2013a)
G4425et2	TrGC	MACO ₃ + HO ₂ → MACO ₃ H	KAPHO2*rco3_ooh	Taraborrelli (2013a)
G4425et3	TrGC	MACO ₃ + HO ₂ → MACO ₂ H + O ₃	KAPHO2*rco3_o3	Taraborrelli (2013a)
G4426e	TrGNC	MACO ₃ + NO → + NO ₂	8.70E-12*EXP(290./temp)	Taraborrelli (2013a)
G4427	TrGNC	MACO ₃ + NO ₂ → MPAN	k_CH3C03_N02	Rickard and Pascoe (2009)
G4428e	TrGNC	MACO ₃ + NO ₃ → + NO ₂	KR02N03*1.60	Taraborrelli (2013a)
G4429e	TrGC	MACRO ₂ → .7 CH ₃ COCH ₂ OH + .7 HCHO + .7 HO ₂ + .3 MACROH	9.20E-14*R02	Taraborrelli (2013a)
G4430e	TrGC	MACRO ₂ + HO ₂ → + OH + POHORG	KR02H02*0.625*rcoch2o2_oh	Taraborrelli (2013a)
G4430et2	TrGC	MACRO ₂ + HO ₂ → MACROOH	KR02H02*0.625*rcoch2o2_ooh	Taraborrelli (2013a)
G4431e	TrGNC	MACRO ₂ + NO → .85 + .85 NO ₂ + .15	KR02NO	Taraborrelli (2013a)
G4432e	TrGNC	MACRO ₂ + NO ₃ → + NO ₂	KR02N03	Taraborrelli (2013a)
G4433ea	TrGC	MACROOH + OH → MACRO ₂ + POHORG	0.6*k_CH300H_OH	Taraborrelli (2013a)
G4433eb	TrGC	MACROOH + OH → CO + OH + CH ₃ COCH ₂ OH + POHORG + POHORG	kt*fo*ftch2oh*falk	Taraborrelli (2013a)
G4433ec	TrGC	MACROOH + OH → CO + MGLYOX + HO ₂ + POHORG	ks*fsoh*fpch2oh + krohro	Taraborrelli (2013a)
G4434e	TrGC	MACROH + OH → CH ₃ COCH ₂ OH + CO + HO ₂ + POHORG	kt*fo*ftch2oh*falk	Taraborrelli (2013a)
G4434et2	TrGC	→ .885 CH ₃ COCH ₂ OH + .885 CO + .115 MGLYOX + .115 HCHO + HO ₂	KDEC	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4435e	TrGC	MACO2H + OH → CH ₃ COCH ₂ OH + HO ₂ + CO ₂ + POHORG	(kadt+kadp)*aco2h+kco2h	Taraborrelli (2013a)
G4436e	TrGC	MACO3H + OH → CH ₃ COCH ₂ OH + CO ₂ + OH + POHORG + POHORG	0.6*k_CH3OOH_OH+(kadt+kadp)*aco2h	Taraborrelli (2013a)
G4437e	TrGC	LHMVKABO2 → .024 CO2H3CHO + .072 HCHO + .5280 CH ₃ C(O)OO + .5280 HOCH ₂ CHO + .176 BIACETOH + .2 HO12CO3C4	1.014E-12*R02	Taraborrelli (2013a)*
G4438e	TrGC	LHMVKABO2 + HO ₂ → OH + HOCH ₂ CHO + CH ₃ C(O)OO + POHORG	KR02H02*0.625*.88*rcoch2o2_oh	Taraborrelli (2013a)
G4438et2	TrGC	LHMVKABO2 + HO ₂ → LHMVKABOOH	KR02H02*0.625*(.12+.88*rcoch2o2_ooh)	Taraborrelli (2013a)
G4439ea	TrGNC	LHMVKABO2 + NO → .12 CH ₃ C(O)OO + .12 HCHO + NO ₂	KR02NO*(1.-0.11)	Taraborrelli (2013a)*
G4439eb	TrGNC	LHMVKABO2 + NO →	KR02NO*0.11	Taraborrelli (2013a)
G4440e	TrGNC	LHMVKABO2 + NO ₃ → .12 MGLYOX + .88 HOCH ₂ CHO + .88 CH ₃ C(O)OO + .12 HCHO + .12 HO ₂ + NO ₂	KR02N03	Taraborrelli (2013a)*
G4441e	TrGC	LHMVKABOOH + OH → .12 BIACETOH + OH + POHORG + POHORG	0.6*k_CH3OOH_OH+.12*ks*fsooh*fpch2oh+.88*kt*fcooh*fpch2oh*fco	Taraborrelli (2013a)*
G4449e	TrGC	CO2H3CHO + OH → CO2H3CO3 + POHORG	kt*fo*falk	Taraborrelli (2013a)
G4449et2	TrGC	CO2H3CHO + OH → + HO ₂ + H ₂ O + POHORG	kt*fco*fcooh*fcho	Taraborrelli (2013a)
G4450	TrGNC	CO2H3CHO + NO ₃ → CO2H3CO3 + HNO ₃	KNO3AL*4.0	Rickard and Pascoe (2009)
G4451e	TrGC	CO2H3CO3 → + CO ₂	1.00E-11*R02	Taraborrelli (2013a)
G4452e	TrGC	CO2H3CO3 + HO ₂ → OH + CO ₂ + POHORG	KAPH02*rco3_oh	Taraborrelli (2013a)
G4452et2	TrGC	CO2H3CO3 + HO ₂ → + O ₃	KAPH02*rco3_o3	Taraborrelli (2013a)
G4452et3	TrGC	CO2H3CO3 + HO ₂ → CO2H3CO3H	KAPH02*rco3_ooh	Taraborrelli (2013a)
G4453e	TrGNC	CO2H3CO3 + NO → + NO ₂ + CO ₂	KAPNO	Taraborrelli (2013a)
G4454e	TrGNC	CO2H3CO3 + NO ₃ → + NO ₂ + CO ₂	KR02N03*1.60	Taraborrelli (2013a)
G4455	TrGC	CO2H3CO3H + OH → 0.5127 CO2H3CO3 + 0.4873 CH ₃ C(O)OO + 0.4873 CO + 0.4873 CO ₂ + 0.4873 OH + POHORG + 0.4873 POHORG	kt*fco2h*fco*fcooh+0.6*k_CH3OOH_OH	Taraborrelli (2013a)*
G4455t2	TrGC	+ OH → + HO ₂ + POHORG	kt*fco2h*fco*fcooh+kco2h	Taraborrelli (2013a)
G4456a	TrGC	HO12CO3C4 + OH → BIACETOH + HO ₂ + POHORG	kt*fcooh*falk*fco	Taraborrelli (2013a)
G4456b	TrGC	HO12CO3C4 + OH → CO2H3CHO + HO ₂ + POHORG	ks*fsoh*falk	Taraborrelli (2013a)
G4457e	TrGC	→ .65 CH ₃ O ₂ + .65 CO + .65 HCHO + .35 OH + .35 CH ₃ COCH ₂ O ₂ + CO ₂ + .35 POHORG	KDEC	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4458e	TrGC	LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 + .12 CH ₃ C(O)OO + OH + POHORG	KHSD	Taraborrelli (2013a)
G4459e	TrGNC	MACRO2 → MGLYOX + HCHO + OH + POHORG	KHSB	Taraborrelli (2013a)
G4460e	TrGNC	+ OH → .7 MGLYOX + .7 HCOOH + .7 NO ₃ + .3 CO ₂ H3CHO + .3 NO ₂ + H ₂ O + POHORG	5.6E-12	Taraborrelli (2013a)
G4461e	TrGC	+ OH → .08 CH ₃ COOH + .08 HCHO + .15 NO ₃ + .07 HCOOH + .07 MGLYOX + .85 CH ₃ COCH ₂ OH + .85 NO ₃ + .93 CO ₂ + H ₂ O + POHORG	5.E-11	Taraborrelli (2013a)
G4462e	TrGC	→ .9 + .1 CH ₃ C(O)OO + .01 GLYOX + .18 CO + .09 HO ₂ + OH + POHORG	k16HS	Taraborrelli (2013a)*
G4463e	TrGC	→ + OH + POHORG	K16HS	Taraborrelli (2013a)
G4500e	TrGC	C ₅ H ₈ + O ₃ → .3508 MACR + 0.01518 MACO2H + .2440 MVK + .7085 HCHO + .11 HOCH2OOH + .1275 C ₃ H ₆ + .1575 CH ₃ C(O)OO + .0510 CH ₃ O ₂ + 0.2625 HO ₂ + .27 OH + .09482 H ₂ O ₂ + .255 CO ₂ + .522 CO + 0.07182 HCHO + .03618 + .01782 CO + .27 POHORG	1.03E-14*EXP(-1995./temp)	Taraborrelli (2013a)*
G4501e	TrGC	C ₅ H ₈ + OH → .63 + .30 + .07 + POHORG	2.7E-11*EXP(390./temp)*(1.-iseg)	Taraborrelli (2013a)*
G4502	TrGNC	C ₅ H ₈ + NO ₃ → NISOPPO2	3.15E-12*EXP(-450./temp)	Rickard and Pascoe (2009)
G4503e	TrGC	+ O ₂ → LISOPACO2	5.530E-13	Taraborrelli (2013a)*
G4504e	TrGC	+ O ₂ → ISOPBO2	3.E-12	Taraborrelli (2013a)*
G4505e	TrGC	+ O ₂ →	6.780E-13	Taraborrelli (2013a)*
G4506e	TrGC	+ O ₂ → ISOPDO2	3.E-12	Taraborrelli (2013a)*
G4507e	TrGC	LISOPACO2 → + O ₂	3.1E12*exp(-7900./temp)*.6+ 7.8E13*exp(-8600./temp)*.4	Taraborrelli (2013a)*
G4508e	TrGC	ISOPBO2 → + O ₂	3.7E14*exp(-9570./temp) +4.2E14*exp(-9970./temp)	Taraborrelli (2013a)*
G4509e	TrGC	→ + O ₂	5.65E12*exp(-8410./temp)*.42+ 1.4E14*exp(-9110./temp)*.58	Taraborrelli (2013a)*
G4510e	TrGC	ISOPDO2 → + O ₂	5.0E14*exp(-10120./temp) +8.25E14*exp(-10220/temp)	Taraborrelli (2013a)*
G4511e	TrGC	LISOPACO2 → + HO ₂	K16HS	Taraborrelli (2013a)
G4512e	TrGC	→ + HO ₂	K16HS	Taraborrelli (2013a)
G4513et3	TrGC	LISOPACO2 → .9 LHC4ACCHO + .8 HO ₂ + .1 ISOPAOH	2.4E-12*R02 .706*KR02H02	Rickard and Pascoe (2009)
G4514t2	TrGC	LISOPACO2 + HO ₂ → LISOPACOOH		Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4515et2	TrGNC	LISOPACO2 + NO → 0.95 LHC4ACCHO + 0.95 HO2 + 0.95 NO2 + .05 LISOPACNO3	KR02NO	Lockwood et al. (2010), Taraborrelli (2013a)
G4506et3	TrGNC	LISOPACO2 + NO3 → LHC4ACCHO + HO2 + NO2	KR02NO3	Rickard and Pascoe (2009)
G4507et3	TrGC	→ .9 LHC4ACCHO + .8 HO2 + .1 ISOPAOH	2.4E-12*R02	Rickard and Pascoe (2009)
G4511et3	TrGC	+ HO2 → LISOPACOOH	.706*KR02HO2	Rickard and Pascoe (2009)
G4512et3	TrGNC	+ NO → 0.95 LHC4ACCHO + 0.95 HO2 + 0.95 NO2 + .05 LISOPACNO3	KR02NO	Lockwood et al. (2010), Taraborrelli (2013a)
G4513et4	TrGNC	+ NO3 → LHC4ACCHO + HO2 + NO2	KR02NO3	Rickard and Pascoe (2009)
G4514e	TrGC	LISOPACOOH + OH → LISOPACO2 + POHORG	0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4514et2	TrGC	LISOPACOOH + OH → + HO2 + POHORG	ks*fallyl*fsoh	Taraborrelli (2013a)
G4514et3	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH + POHORG + POHORG	ks*fsooh*fallyl+ krohro	Taraborrelli (2013a)
G4514et4	TrGC	LISOPACOOH + OH → + OH + POHORG + POHORG	(kadt+kads)*ach2oh*ach2oo	Taraborrelli (2013a)
G4515	TrGC	ISOPAOH + OH → LHC4ACCHO + HO2 + POHORG	(kadt+kads)*ach2oh*ach2oh+ ks*fsoh*fallyl+ krohro	Taraborrelli (2013a)
G4516e	TrGNC	LISOPACNO3 + OH → + POHORG	9.5E-11	Paulot et al. (2009a), Taraborrelli (2013a)
G4517e	TrGC	ISOPBO2 → .8 MVK + .8 HCHO + .8 HO2 + .2 ISOPBOH	8.E-13*R02	Rickard and Pascoe (2009)
G4518	TrGC	ISOPBO2 + HO2 → ISOPBOOH	.706*KR02HO2	Rickard and Pascoe (2009)
G4519e	TrGNC	ISOPBO2 + NO → .947 MVK + .947 HCHO + .947 HO2 + .947 NO2 + .053 ISOPBNO3	KR02NO	Lockwood et al. (2010), Taraborrelli (2013a)
G4520e	TrGNC	ISOPBO2 + NO3 → MVK + .75 HCHO + .75 HO2 + .25 CH3O2 + NO2	KR02NO3	Rickard and Pascoe (2009)
G4521ea	TrGC	ISOPBOOH + OH → + OH + POHORG + POHORG	(kads+kadp)*ach2oo	Paulot et al. (2009b), Taraborrelli (2013a)
G4521eb	TrGC	ISOPBOOH + OH → ISOPBO2 + POHORG	0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4521ec	TrGC	ISOPBOOH + O3 → 0.1368 MACROOH + 0.1368 H2O2 + 0.2280 HO2 + 0.4332 CH3COCH2OH + 0.2280 CO2 + 0.6384 OH + 0.2052 CO + .57 HCHO + .43 MACROOH + 0.06880 HO2 + 0.06880 OH + 0.2709 CO + 0.1591 HOCH2OOH + 0.7072 POHORG	1.E-17	Taraborrelli (2013a)*
G41911	TrGC	ISOPBOOH + OH → MGLYOX + HOCH2CHO + POHORG	krohro+ks*falk*fsoh	Taraborrelli (2013a)
G4522e	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO2 + .25 CH3O2 + POHORG	ks*falk*fsoh+(kadp+kads)*ach2oh	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4523e	TrGNC	$\text{ISOPBNO}_3 + \text{OH} \rightarrow \text{POHORG}$	1.3E-11	Paulot et al. (2009a), Taraborrelli (2013a)
G4524	TrGC	$\text{ISOPDO}_2 \rightarrow .8 \text{ MACR} + .8 \text{ HCHO} + .8 \text{ HO}_2 + .1 \text{ HCOC}_5 + .1 \text{ ISOPDOH}$	2.9E-12*R02	Rickard and Pascoe (2009)
G4525	TrGC	$\text{ISOPDO}_2 + \text{HO}_2 \rightarrow \text{ISOPDOOH}$.706*KR02H02	Rickard and Pascoe (2009)
G4526e	TrGNC	$\text{ISOPDO}_2 + \text{NO} \rightarrow .85 \text{ MACR} + .85 \text{ HCHO} + .85 \text{ HO}_2 + .85 \text{ NO}_2 + .15 \text{ ISOPDNO}_3$	KR02NO	Lockwood et al. (2010), Taraborrelli (2013a)
G4527	TrGNC	$\text{ISOPDO}_2 + \text{NO}_3 \rightarrow \text{MACR} + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4528ea	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{POHORG} + \text{POHORG}$	(kadt+kadp)*ach2ooh	Paulot et al. (2009b), Taraborrelli (2013a)
G4528eb	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{ISOPDO}_2 + \text{POHORG}$	0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4528ec	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{HCOC}_5 + \text{OH} + \text{POHORG} + \text{POHORG}$	kt*ftooh*fallyl*fpch2oh	Taraborrelli (2013a)
G4528ed	TrGC	$\text{ISOPDOOH} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{GLYOX} + \text{OH} + \text{POHORG} + \text{POHORG}$	ks*fpch2oh*fsoh	Taraborrelli (2013a)
G45222	TrGC	$\text{ISOPDOOH} + \text{O}_3 \rightarrow 1.393 \text{ OH} + 1.393 \text{ POHORG} + \text{BIACETOH} + .67 \text{ HCHO} + 0.05280 \text{ HO}_2 + 0.2079 \text{ CO} + 0.1221 \text{ HOCH}_2\text{OOH}$	1.E-17	Taraborrelli (2013a)*
G4529e	TrGC	$\text{ISOPDOH} + \text{OH} \rightarrow \text{HCOC}_5 + \text{HO}_2 + \text{POHORG}$	2.*krohro+(kt*ftoh*fallyl+ks*fsoh)*fpch2oh+(kadt+kadp)*ach2oh	Taraborrelli (2013a)
G4530e	TrGNC	$\text{ISOPDNO}_3 + \text{OH} \rightarrow \text{POHORG}$	1.3E-11	Paulot et al. (2009a), Taraborrelli (2013a)
G4531	TrGNC	$\text{NISOPO}_2 \rightarrow .8 \text{ NC4CHO} + .6 \text{ HO}_2 + .2 \text{ LISOPACNO}_3$	1.3E-12*R02	Rickard and Pascoe (2009)
G4532	TrGNC	$\text{NISOPO}_2 + \text{HO}_2 \rightarrow \text{NISOPOOH}$.706*KR02H02	Rickard and Pascoe (2009)
G4533	TrGNC	$\text{NISOPO}_2 + \text{NO} \rightarrow \text{NC4CHO} + \text{HO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)
G4534	TrGNC	$\text{NISOPO}_2 + \text{NO}_3 \rightarrow \text{NC4CHO} + \text{HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4535	TrGNC	$\text{NISOPOOH} + \text{OH} \rightarrow \text{NC4CHO} + \text{OH} + \text{POHORG} + \text{POHORG}$	1.03E-10	Rickard and Pascoe (2009)
G4536	TrGNC	$\text{NC4CHO} + \text{OH} \rightarrow \text{LNISO}_3 + \text{POHORG}$	4.16E-11	Rickard and Pascoe (2009)
G4537e	TrGNC	$\text{NC4CHO} + \text{O}_3 \rightarrow .27 \text{ NOA} + .027 \text{ HCOCO}_2\text{H} + .0162 \text{ GLYOX} + .0162 \text{ H}_2\text{O}_2 + .1458 + .0405 \text{ HCOOH} + .0405 \text{ CO} + .8758 \text{ OH} + .8758 \text{ POHORG} + .365 \text{ MGLYOX} + .73 \text{ NO}_2 + 0.7705 \text{ HCHO} + .4055 \text{ CO}_2 + .73 \text{ GLYOX}$	2.40E-17	Taraborrelli (2013a)*
G4538	TrGNC	$\text{NC4CHO} + \text{NO}_3 \rightarrow \text{LNISO}_3 + \text{HNO}_3$	KN03AL*4.25	Rickard and Pascoe (2009)
G4539	TrGNC	$\text{LNISO}_3 + \text{HO}_2 \rightarrow \text{LNISOOH}$.5*.706*KR02H02 + .5*KAPH02	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4540e	TrGNC	$\text{LNISO}_3 + \text{NO} \rightarrow \text{NOA} + .5 + .5 \text{ CO} + .5 \text{ HO}_2 + \text{NO}_2 + .5 \text{ CO}_2$.5*KAPNO +.5*KR02NO	Rickard and Pascoe (2009)
G4541e	TrGNC	$\text{LNISO}_3 + \text{NO}_3 \rightarrow \text{NOA} + .5 + .5 \text{ CO} + .5 \text{ HO}_2 + \text{NO}_2 + .5 \text{ CO}_2$	1.3*KR02N03	Rickard and Pascoe (2009)
G4542	TrGNC	$\text{LNISO}_3 + \text{OH} \rightarrow \text{LNISO}_3 + \text{POHORG}$	2.65E-11	Rickard and Pascoe (2009)
G4543e	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LC578O}_2 + \text{POHORG}$	(kadtertprim+kads)*acho*ach2oh	Taraborrelli (2013a)
G4543et2	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow \text{LHC4ACCO}_3 + \text{POHORG}$	kcho	Taraborrelli (2013a)
G4543et3	TrGC	$\text{LHC4ACCHO} + \text{OH} \rightarrow + \text{HO}_2 + \text{POHORG}$	ks*fsoh*fallyl	Taraborrelli (2013a)
G4544	TrGC	$\text{LHC4ACCHO} + \text{O}_3 \rightarrow .2225 \text{ CH}_3\text{C(O)OO} + .89 \text{ CO} + .0171875 \text{ HOCH}_2\text{CO}_2\text{H} + .075625 \text{ H}_2\text{O}_2 + .0171875 \text{ HCOCO}_2\text{H} + .2775 \text{ CH}_3\text{COCH}_2\text{OH} + .6675 \text{ HO}_2 + .2603125 \text{ GLYOX} + .2225 \text{ HCHO} + .89 \text{ OH} + .2603125 \text{ HOCH}_2\text{CHO} + .5 \text{ MGLYOX} + .89 \text{ POHORG}$	2.40E-17	Rickard and Pascoe (2009)
G4545	TrGNC	$\text{LHC4ACCHO} + \text{NO}_3 \rightarrow \text{LHC4ACCO}_3 + \text{HNO}_3$	KNO3AL*4.25	Rickard and Pascoe (2009)
G4546e	TrGC	$\text{LC578O}_2 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2$	9.20E-14*R02	Rickard and Pascoe (2009)
G4547e	TrGC	$\text{LC578O}_2 + \text{HO}_2 \rightarrow \text{MGLYOX} + \text{HOCH}_2\text{CHO} + \text{OH} + \text{POHORG}$	KR02H02*0.706*rcoch2o2_oh	Rickard and Pascoe (2009)
G4547et2	TrGC	$\text{LC578O}_2 + \text{HO}_2 \rightarrow \text{LC578OOH}$	KR02H02*0.706*rcoch2o2_ooh	Rickard and Pascoe (2009)
G4548e	TrGNC	$\text{LC578O}_2 + \text{NO} \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009)
G4549e	TrGNC	$\text{LC578O}_2 + \text{NO}_3 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 + .75 \text{ HOCH}_2\text{CHO} + .75 \text{ HO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009)
G4586e	TrGC	$\text{LC578O}_2 \rightarrow .25 \text{ CH}_3\text{COCH}_2\text{OH} + .75 \text{ MGLYOX} + .25 \text{ HOCH}_2\text{CHO} + .75 \text{ HOCH}_2\text{CHO} + \text{HO}_2 + \text{OH} + \text{POHORG}$	KHSB	Taraborrelli (2013a)
G4550e	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow \text{LC578O}_2 + \text{POHORG}$	0.6*k_CH300H_OH	Taraborrelli (2013a)*
G4550et2	TrGC	$\text{LC578OOH} + \text{OH} \rightarrow + \text{HO}_2 + \text{POHORG}$	kt*fo*ftch2oh*falk+ kt*ftoh*fpch2oh*fpch2oh+ ks*fsoh*fpch2oh	Taraborrelli (2013a)*
G4551e	TrGC	$\text{LHC4ACCO}_3 \rightarrow .3 \text{ LHC4ACCO}_2\text{H} + .7 \text{ OH} + .35 \text{ MACRO}_2 + .35 \text{ LHMVKABO}_2 + .7 \text{ CO}_2 + .7 \text{ POHORG}$	1.00E-11*R02	Taraborrelli (2013a)*
G4552e	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow 2 \text{ OH} + .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{CO}_2 + 2 \text{ POHORG}$	KAPH02*rco3_oh	Taraborrelli (2013a)*
G4552et2	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow \text{LHC4ACCO}_3\text{H}$	KAPH02*rco3_ooh	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4552et3	TrGC	$\text{LHC4ACCO}_3 + \text{HO}_2 \rightarrow \text{LHC4ACCO}_2\text{H} + \text{O}_3$	KAPHO2*rco3_o3	Taraborrelli (2013a)
G4553e	TrGNC	$\text{LHC4ACCO}_3 + \text{NO} \rightarrow .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{NO}_2 + \text{CO}_2$	KAPNO	Taraborrelli (2013a)*
G4554	TrGNC	$\text{LHC4ACCO}_3 + \text{NO}_2 \rightarrow \text{LC5PAN1719}$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G4555e	TrGNC	$\text{LHC4ACCO}_3 + \text{NO}_3 \rightarrow .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{NO}_2 + \text{CO}_2$	1.6*KR02N03	Taraborrelli (2013a)*
G4556e	TrGC	$\text{LHC4ACCO}_2\text{H} + \text{OH} \rightarrow \text{OH} + .5 \text{ MACRO}_2 + .5 \text{ LHMVKABO}_2 + \text{CO}_2 + \text{POHORG} + \text{POHORG}$	2.52E-11	Taraborrelli (2013a)
G4557	TrGC	$\text{LHC4ACCO}_3\text{H} + \text{OH} \rightarrow \text{LHC4ACCO}_3 + \text{POHORG}$	2.88E-11	Rickard and Pascoe (2009)
G4558	TrGNC	$\text{LC5PAN1719} \rightarrow \text{LHC4ACCO}_3 + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009)
G4559	TrGNC	$\text{LC5PAN1719} + \text{OH} \rightarrow .5 \text{ MACROH} + .5 \text{ HO12CO}_3\text{C}_4 + \text{CO} + \text{NO}_2 + \text{POHORG}$	2.52E-11	Rickard and Pascoe (2009)
G4560a	TrGC	$\text{HCOC}_5 + \text{OH} \rightarrow \text{C59O}_2 + \text{POHORG}$	3.81E-11	Rickard and Pascoe (2009)
G4560eb	TrGC	$\text{HCOC}_5 + \text{O}_3 \rightarrow \text{BIACETO}_2 + .335 \text{ H}_2\text{O}_2 + 0.67 \text{ HCHO} + 0.2079 \text{ CO} + 0.1221 \text{ HOCH}_2\text{OOH} + 0.05280 \text{ OH} + 0.0528 \text{ POHORG}$	7.51E-16*EXP(-1521./temp)	Taraborrelli (2013a)
G4561	TrGC	$\text{C59O}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} +$	9.20E-14*R02	Taraborrelli (2013a)
G4562e	TrGC	$\text{C59O}_2 + \text{HO}_2 \rightarrow \text{OH} + \text{CH}_3\text{COCH}_2\text{OH} + + \text{POHORG}$	KR02H02*0.706*rcoch2o2_oh	Taraborrelli (2013a)
G4562et2	TrGC	$\text{C59O}_2 + \text{HO}_2 \rightarrow \text{C59OOH}$	KR02H02*0.706*rcoch2o2_ooh	Taraborrelli (2013a)
G4563	TrGNC	$\text{C59O}_2 + \text{NO} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + + \text{NO}_2$	KR02NO	Taraborrelli (2013a)
G4564	TrGNC	$\text{C59O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + + \text{NO}_2$	KR02N03	Taraborrelli (2013a)
G4565	TrGC	$\text{C59OOH} + \text{OH} \rightarrow \text{C59O}_2 + \text{POHORG}$	9.7E-12	Taraborrelli (2013a)
G4566e	TrGC	$+ \text{OH} \rightarrow \text{LC578O}_2 + \text{H}_2\text{O} + \text{POHORG}$	5.78E-11*EXP(-400/temp)	Paulot et al. (2009b), Taraborrelli (2013a)
G4567e	TrGC	$\text{ISOPBO}_2 \rightarrow \text{MVK} + \text{HCHO} + \text{OH} + \text{POHORG}$	KHSB	Taraborrelli (2013a)
G4568e	TrGC	$\text{ISOPDO}_2 \rightarrow \text{MACR} + \text{HCHO} + \text{OH} + \text{POHORG}$	KHSD	Taraborrelli (2013a)
G4577ea	TrGC	$+ \text{OH} \rightarrow .6 + .4 + \text{POHORG}$	kadt*acho*ach2ooh	Taraborrelli (2013a)
G4577eb	TrGC	$+ \text{OH} \rightarrow .6 + .4 + \text{POHORG}$	kads*acho*ach2ooh	Taraborrelli (2013a)
G4577e	TrGC	$+ \text{OH} \rightarrow + \text{POHORG}$	kt*f0*falk+0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G4577et2	TrGC	$+ \text{OH} \rightarrow \text{OH} + + \text{POHORG} + \text{POHORG}$	ks*fsooh*fallyl	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G4577et3	TrGC	+ O ₃ → .4672 OH + .2336 + .2336 CO + .2336 CH ₃ C(O)OO + .4672 + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 + .02765 H ₂ O ₂ + .02592 CH ₃ OOH + .02592 CO ₂ + .01037 + .01555 HOCH ₂ OOH + .01555 CO + .006912 + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 + 0.2628 GLYOX + .0972 CH ₃ COCH ₂ O ₂ H + .00972 HCOCO ₂ H + .005832 GLYOX + .005832 H ₂ O ₂ + .05249 OH + .05249 + .01458 HCHO + .01458 CO ₂ + .01458 HCOOH + .01458 CO + 1.104 POHORG	2.4E-17	Taraborrelli (2013a)*
G4578e	TrGC	→ .78 CH ₃ COCH ₂ O ₂ H + .78 + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH + .22 POHORG	8.00E-13*R02	Taraborrelli (2013a)
G4579e	TrGC	+ NO → .78 CH ₃ COCH ₂ O ₂ H + .78 + .22 CO ₂ H ₃ CHO + .22 HCHO + .22 OH + .22 POHORG + NO ₂	KR02NO	Taraborrelli (2013a)
G4580e	TrGC	+ HO ₂ →	KR02H02*0.706	Taraborrelli (2013a)
G4580ea	TrGC	→ CH ₃ COCH ₂ O ₂ H + GLYOX + OH + POHORG	KHSB	Taraborrelli (2013a)
G4581e	TrGC	→ OH + + POHORG	K15HSDHB	Taraborrelli (2013a)
G4581et2	TrGC	+ OH → + OH + POHORG + POHORG	ks*fsooh*fpch2oh	Taraborrelli (2013a)
G4581et3	TrGC	+ OH → CH ₃ COCH ₂ O ₂ H + OH + 2 CO + 2 HO ₂ + POHORG + POHORG	kt*ftoh*fpch2oh*fpch2oh	Taraborrelli (2013a)
G4581et4	TrGC	+ OH → + POHORG	0.6*k_CH30OH_OH	Taraborrelli (2013a)
G4581et6	TrGC	→ MGLYOX + + HO ₂	2.90E-12*R02	Taraborrelli (2013a)
G4581et7	TrGC	+ NO → MGLYOX + + HO ₂ + NO ₂	KR02NO	Taraborrelli (2013a)
G4581et8	TrGC	+ HO ₂ → .5 CH ₃ C(O)OO + .5 CO + .5 MGLYOX + .5 HO ₂ +	KR02H02*0.706	Taraborrelli (2013a)*
G4581et9	TrGC	→ MGLYOX + OH + + POHORG	KHSD	Taraborrelli (2013a)
G4581et10	TrGC	→ .625 MGLYOX + 2 CO + 1.625 HO ₂ + .375 CH ₃ C(O)OO + .375 CO ₂ + OH + POHORG	K15HSDHB	Taraborrelli (2013a)*
G4582e	TrGC	LHC4ACCO3 → + HO ₂	K16HS	Taraborrelli (2013a)
G4583e	TrGC	+ OH → + POHORG	2*kt*f0*falk+(kadt+kads)*acho*acho	Taraborrelli (2013a)
G4584e	TrGC	+ HO ₂ → OH + POHORG + MGLYOX +	KR02H02*0.706*rcoch2o2_oh	Taraborrelli (2013a)
G4584et2	TrGC	+ HO ₂ →	KR02H02*0.706*rcoch2o2_ooh	Taraborrelli (2013a)
G4585e	TrGC	+ NO → NO ₂ + MGLYOX +	KR02NO	Taraborrelli (2013a)
G4585et2	TrGC	→ MGLYOX +	8.00E-13*R02	Taraborrelli (2013a)
G4585et3	TrGC	+ OH → MGLYOX + 2 CO + .5 OH + POHORG + .5 POHORG	2.*kt*f0*ftch2oh*falk+kt*ftoh*fcho*fpch2oh	Taraborrelli (2013a)*

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

#	labels	reaction	rate coefficient	reference
G4587e	TrGC	+ NO → .21 NOA + .21 HOCH ₂ CHO + .21 HO ₂ + .49 HO12CO3C4 + .49 HCHO + .49 NO ₂ + .045 + .045 HCHO + .255 CH ₃ COCH ₂ OH + .255 + .225 H ₂ O ₂ + NO ₂	KR02NO	Taraborrelli (2013a)
G4587et2	TrGC	→ .21 NOA + .21 HOCH ₂ CHO + .21 HO ₂ + .49 HO12CO3C4 + .49 HCHO + .49 NO ₂ + .045 + .045 HCHO + .255 CH ₃ COCH ₂ OH + .255 + .225 H ₂ O ₂	8.00E-13*R02+KR02H02*0.706*c(ind_H02)	Taraborrelli (2013a)
G4587et3	TrGC	+ NO → .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 + .14 + .4 HCHO + .4 HO ₂ + 1.6 NO ₂	KR02NO	Taraborrelli (2013a)
G4587et4	TrGC	→ .6 CH ₃ COCH ₂ OH + .6 HOCH ₂ CHO + .26 + .14 + .4 HCHO + .4 HO ₂ + .6 NO ₂	2.9E-12*R02+KR02H02*0.706*c(ind_H02)	Taraborrelli (2013a)
G4588e	TrGNC	LISOPACNO3 + O ₃ → .8704 OH + .365 HO ₂ + .73 MGLYOX + .4325 + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .4325 NO ₂ + .0891 H ₂ O ₂ + .135 NOA + .0675 + .3866 HOCH ₂ CHO + .0405 CH ₃ OH + .0405 CO + .0054 + .8704 POHORG	4.E-16	Taraborrelli (2013a)
G4599e	TrGC	LISOPACOOH + O ₃ → 1.3272 OH + 0.36986 HO ₂ + .0432 H ₂ O ₂ + 0.23002 CO + .2025 CH ₃ OOH + .01215 HOCH2OOH + 0.3704 HCHO + .00405 CH ₃ OH + .0405 CO ₂ + .1825 + .365 MGLYOX + .3866 + .135 CH ₃ COCH ₂ OH + .0675 GLYOX + .00324 + .3866 HOCH ₂ CHO + .135 CH ₃ COCH ₂ O ₂ H + .0675 + .0054 + 1.3272 POHORG	4.829E-16	Taraborrelli (2013a)
G4598et3	TrGC	+ OH → .62 CO2H3CHO + .62 OH + .62 CO ₂ + .38 MGLYOX + .38 HCOCO ₃ H + .38 HO ₂ + POHORG + .62 POHORG	kadt*acho*aco2h	Taraborrelli (2013a)*
G4598et4	TrGC	+ OH → .62 + 1.24 CO + 1.24 HO ₂ + .38 + .38 CO + .38 HO ₂ + .38 OH + .38 CO ₂ + POHORG + .38 POHORG	kads*acho*aco2h	Taraborrelli (2013a)*
G41311	TrGC	→ .7143 MACR + .2857 MVK + HCHO + HO ₂	2.40E-12*R02	Taraborrelli (2013a)
G41341	TrGC	+ NO → .7143 MACR + .2857 MVK + HCHO + HO ₂ + NO ₂	KR02NO	Taraborrelli (2013a)
G41351t2	TrGC	+ HO ₂ → .7143 MACR + .2857 MVK + HCHO + HO ₂	KR02H02*0.706	Taraborrelli (2013a)
G41361	TrGC	+ NO ₃ → .7143 MACR + .2857 MVK + HCHO + HO ₂ + NO ₂	KR02N03	Taraborrelli (2013a)
G41378	TrGC	→	9.39E9*EXP(-7322/temp)	Taraborrelli (2013a)

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

#	labels	reaction	rate coefficient	reference
G41341t2	TrGC	$\rightarrow .7143 \text{ MACR} + .2857 \text{ MVK} + \text{HCHO} + \text{OH} + \text{POHORG}$.7143*KHSD+.2857*KHSB	Taraborrelli (2013a)
G413112	TrGC	$\rightarrow + \text{HO}_2$	8.00E-13*R02	Taraborrelli (2013a)
G413416	TrGC	$+ \text{NO} \rightarrow + \text{HO}_2 + \text{NO}_2$	KR02NO	Taraborrelli (2013a)*
G413519	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2*0.706	Taraborrelli (2013a)
G413618	TrGC	$+ \text{NO}_3 \rightarrow + \text{HO}_2 + \text{NO}_2$	KR02N03	Taraborrelli (2013a)
G413417	TrGC	$\rightarrow + \text{OH} + \text{POHORG}$	KHSB	Taraborrelli (2013a)
G413619	TrGC	$+ \text{OH} \rightarrow + \text{POHORG}$	0.6*k_CH3OOH_OH	Taraborrelli (2013a)
G413621	TrGC	$+ \text{OH} \rightarrow \text{MGLYOX} + 2 \text{ CO} + 2 \text{ HO}_2 + \text{POHORG}$	kt*ftho*falk*fpch2oh	Taraborrelli (2013a)*
G413622	TrGC	$+ \text{OH} \rightarrow .8405 \text{ HCHO} + .8405 \text{ OH} + .8405 \text{ CO2H3CHO} + .1595 + .1595 \text{ HO}_2 + \text{POHORG} + .8405 \text{ POHORG}$	ks*fsoh*falk+ks*fsooh*falk	Taraborrelli (2013a)
G4136	TrGC	$+ \text{OH} \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO}_2 + 2 \text{ HCHO} + \text{POHORG}$	kt*fo*ftch2oh	Taraborrelli (2013a)*
G413610	TrGC	$+ \text{OH} \rightarrow \text{GLYOX} + \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{POHORG}$	ks*fcho*fsooh	Taraborrelli (2013a)
G41361t2	TrGC	$+ \text{OH} \rightarrow \text{MGLYOX} + \text{GLYOX} + \text{HO}_2 + \text{POHORG}$	ks*fco*fsooh	Taraborrelli (2013a)
G45mbo1	TrGC	$+ \text{OH} \rightarrow$	8.1E-12*EXP(610/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo2	TrGC	$+ \text{O}_3 \rightarrow \text{HCHO} + .16 \text{ CH}_3\text{COCH}_3 + .16 \text{ HO}_2 + .16 \text{ CO} + .16 \text{ OH} + .84$	1.0E-17*0.57	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo3	TrGC	$+ \text{O}_3 \rightarrow + .63 \text{ CO} + .37 \text{ HOCH}_2\text{OOH} + .16 \text{ OH} + .16 \text{ HO}_2$	1.0E-17*0.43	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo4	TrGC	$+ \text{NO}_3 \rightarrow$	4.6E-14*EXP(-400/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo5	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo6	TrGC	$+ \text{NO} \rightarrow$	KR02NO*(0.064+0.026)/2.	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo7	TrGC	$+ \text{NO} \rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{NO}_2$	KR02NO*(0.936+0.974)/2.*.67	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo8	TrGC	$+ \text{NO} \rightarrow + \text{HCHO} + \text{HO}_2 + \text{NO}_2$	KR02NO*(0.936+0.974)/2.*.33	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo9	TrGC	$\rightarrow \text{HOCH}_2\text{CHO} + \text{CH}_3\text{COCH}_3 + \text{HO}_2$	8.8E-13*R02*.67	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo10	TrGC	$\rightarrow + \text{HCHO} + \text{HO}_2$	8.8E-13*R02*.33	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G45mbo11	TrGC	+ OH → + OH	.67*2.93E-11+.33*2.05E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G45mbo12	TrGC	+ OH →	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo13	TrGC	+ hν → HOCH ₂ CHO + CH ₃ COCH ₃ + HO ₂ + OH	1.14*jx(ip_CH3OOH)*.67	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo14	TrGC	+ hν → + HCHO + HO ₂ + OH	1.14*jx(ip_CH3OOH)*.33	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo15	TrGC	+ OH → + NO ₂	.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G45mbo16	TrGC	+ OH → + HO ₂	3.79E-12	Rickard and Pascoe (2009)
G45mbo17	TrGC	+ hν → HCHO + HO ₂ +	J_ACETOL	Rickard and Pascoe (2009)
G45mbo18	TrGC	+ OH → CO +	1.38E-11	Rickard and Pascoe (2009)
G45mbo19	TrGC	+ hν → CO + HO ₂ +	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
G45mbo20	TrGC	+ OH →	1.4E-11	Rickard and Pascoe (2009)
G45mbo21	TrGC	+ hν → CH ₃ COCH ₃ + HO ₂ + HO ₂ + CO	J_ACETOL	Rickard and Pascoe (2009)
G45mbo22	TrGC	+ HO ₂ → CH ₃ COCH ₃ + HO ₂ + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo23	TrGC	+ HO ₂ → + O ₃	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo24	TrGC	+ HO ₂ →	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo25	TrGC	+ NO → CH ₃ COCH ₃ + HO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G45mbo26	TrGC	+ NO ₂ →	k_CH3C03_N02	Rickard and Pascoe (2009)
G45mbo27	TrGC	+ NO ₃ → CH ₃ COCH ₃ + HO ₂ + NO ₂	KR02N03*.1.74	Rickard and Pascoe (2009)
G45mbo28	TrGC	→ CH ₃ COCH ₃ + HO ₂	1.00E-11*R02*0.7	Rickard and Pascoe (2009)
G45mbo29	TrGC	→	1.00E-11*R02*0.3	Rickard and Pascoe (2009)
G45mbo30	TrGC	+ OH → CH ₃ COCH ₃ + HO ₂	1.72E-12	Rickard and Pascoe (2009)
G45mbo31	TrGC	+ hν → CH ₃ COCH ₃ + HO ₂ + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)
G45mbo32	TrGC	OH + →	4.80E-12	Rickard and Pascoe (2009)
G45mbo33	TrGC	→ + NO ₂	K_PAN_M	Rickard and Pascoe (2009)
G45mbo34	TrGC	+ OH → CH ₃ COCH ₃ + CO + NO ₂	4.75E-13	Rickard and Pascoe (2009)
G45mbo35	TrGC	+ HO ₂ →	KR02HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G45mbo36	TrGC	+ NO → .65 + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 + .35 HCHO + .35 NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo37	TrGC	+ NO ₃ → .65 + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 + .35 HCHO + .35 NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo38	TrGC	→ .65 + .65 CH ₃ COCH ₃ + .65 HO ₂ + .35 + .35 HCHO + .35 NO ₂	8.8E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo39	TrGC	+ OH → .65 + .35 + OH	.65*4.89E-12+35*2.52E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo40	TrGC	+ OH →	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo41	TrGC	+ hν → + CH ₃ COCH ₃ + HO ₂ + OH	1.14*jx(ip_CH3OOH)*.65	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo42	TrGC	+ hν → + HCHO + NO ₂ + OH	1.14*jx(ip_CH3OOH)*.35	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo43	TrGC	+ OH → CH ₃ COCH ₃ + HCHO + CO ₂ + NO ₂	1.23E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G45mbo44	TrGC	+ OH →	4.26E-12	Rickard and Pascoe (2009)
G45mbo45	TrGC	+ HO ₂ → + NO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo46	TrGC	+ HO ₂ →	KAPH02*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo47	TrGC	+ NO → + NO ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009)
G45mbo48	TrGC	+ NO ₂ →	k_CH3C03_N02	Rickard and Pascoe (2009)
G45mbo49	TrGC	+ NO ₃ → + NO ₂ + NO ₂	KR02NO3*1.74	Rickard and Pascoe (2009)
G45mbo50	TrGC	→ + NO ₂	1.00E-11*R02	Rickard and Pascoe (2009)
G45mbo51	TrGC	+ OH →	4.50E-12	Rickard and Pascoe (2009)
G45mbo52	TrGC	→ + NO ₂ + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)
G45mbo53	TrGC	+ OH → + CO + NO ₂ + NO ₂	1.27E-12	Rickard and Pascoe (2009)
G45mbo54	TrGC	→ + NO ₂	K_PAN_M	Rickard and Pascoe (2009)
G45mbo55	TrGC	→	1.60E-17*C(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo56	TrGC	→ + H ₂ O ₂	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2013b)
G45mbo57	TrGC	+ CO →	1.20E-15	Rickard and Pascoe (2009)
G45mbo58	TrGC	+ NO → + NO ₂	1.00E-14	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45mbo59	TrGC	+ NO ₂ → + NO ₃	1.00E-15	Rickard and Pascoe (2009)
G45mbo60	TrGC	+ SO ₂ → + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009)
G410apin1	TrGC	+ OH →	1.47E-11*EXP(467/TEMP)*(50+.25)	Vereecken et al. (2007), Taraborrelli (2013b)*
G410apin2	TrGC	+ OH → + HO ₂	1.47E-11*EXP(467/TEMP)*.25*.60	Vereecken et al. (2007), Taraborrelli (2013b)*
G410apin3	TrGC	+ OH →	1.47E-11*EXP(467/TEMP)*.25*.40	Vereecken et al. (2007), Taraborrelli (2013b)*
G410apin4	TrGC	+ NO → + HO ₂	KR02NO*0.770	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin5	TrGC	+ NO →	KR02NO*0.230	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin6	TrGC	+ HO ₂ →	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin7	TrGC	→ + HO ₂	R02*(.33*9.20E-14+.67*8.80E-13)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin9	TrGC	+ OH → .33 + .67	.33*1.83E-11+.67*3.28E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin10	TrGC	+ hν → + HO ₂ + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin11	TrGC	+ OH → .33 + .67 + NO ₂	.33*5.50E-12+.67*3.64E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin12	TrGC	+ OH →	(kads+kadt)*acoch3	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin13	TrGC	+ hν → + OH	1.14*jx(ip_CH300H)	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin14	TrGC	+ NO → + HO ₂ + NO ₂	KR02NO	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin15	TrGC	+ HO ₂ →	KR02HO2*0.914	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin16	TrGC	→ + HO ₂	R02*9.20E-14	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin17	TrGC	+ OH → LCARBON	1E-11	Vereecken et al. (2007), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apin18	TrGC	+ hν → LCARBON + OH	1.14*jx(ip_CH300H)	Vereecken et al. (2007), Taraborrelli (2013b)
G410apin18t2	TrGC	+ OH →	4.20E-11*0.772	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin19	TrGC	+ OH →	4.20E-11*0.228	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin20	TrGC	→ + CO + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin21	TrGC	+ NO ₃ → + HNO ₃	3.80E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apin	TrGC	→ 0.3 + 0.7	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint2	TrGC	+ HO ₂ →	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint3	TrGC	+ HO ₂ → + O ₃	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint4	TrGC	+ HO ₂ → + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint5	TrGC	+ NO ₂ →	k_CH3CO3_N02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint6	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint7	TrGC	+ NO ₃ → + NO ₂	KR02N03*1.60	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint8	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint9	TrGC	+ OH → + CO + NO ₂	3.66E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint10	TrGC	→	1.30E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint11	TrGC	+ NO →	KR02NO*0.157	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint12	TrGC	+ HO ₂ →	KR02HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint13	TrGC	+ NO → + NO ₂	KR02NO*0.843	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint14	TrGC	+ hν → + NO ₂	J_IC3H7NO3+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint15	TrGC	+ OH → + NO ₂	2.88E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint16	TrGC	+ hν → + OH	1.14*jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint17	TrGC	+ OH →	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint18	TrGC	+ OH → + OH	1.30E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint19	TrGC	→	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint20	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint21	TrGC	+ HO ₂ →	KR02HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint22	TrGC	+ hν → + OH	1.14*jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint23	TrGC	+ OH →	1.05E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint24	TrGC	→ + CH ₃ COCH ₃	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint25	TrGC	+ NO →	KR02NO*0.118	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint26	TrGC	+ NO → + CH ₃ COCH ₃ + NO ₂	KR02NO*0.882	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint27	TrGC	+ HO ₂ →	KR02HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint28	TrGC	+ hν → + CH ₃ COCH ₃ + OH	1.14*jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint29	TrGC	+ OH →	2.05E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint30	TrGC	+ OH →	6.65E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint31	TrGC	+ hν → + HO ₂	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint32	TrGC	+ OH →	2.64E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint33	TrGC	+ hν → + CO + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint34	TrGC	+ NO ₃ → + HNO ₃	KNO3AL*8.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint35	TrGC	+ hν → + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint36	TrGC	+ OH →	9.73E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint37	TrGC	→	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint38	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint39	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint40	TrGC	+ HO ₂ →	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint41	TrGC	+ HO ₂ → + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint42	TrGC	→	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint43	TrGC	+ HO ₂ →	KR02HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint44	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint45	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint46	TrGC	+ OH → + CO + NO ₂	6.60E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint47	TrGC	$\rightarrow + \text{OH}$	1.14*jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint48	TrGC	$+ \text{OH} \rightarrow$	1.02E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint49	TrGC	$+ h\nu \rightarrow + \text{OH}$	1.14*jx(ip_CH300H)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint50	TrGC	$+ \text{OH} \rightarrow$	1.29E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint51	TrGC	$\rightarrow + \text{CH}_3\text{COCH}_3$	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint52	TrGC	$+ \text{NO} \rightarrow + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint53	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint54	TrGC	$+ h\nu \rightarrow + \text{CH}_3\text{COCH}_3 + \text{OH}$	1.14*jx(ip_CH300H)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint55	TrGC	$+ \text{OH} \rightarrow$	3.45E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint56	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint57	TrGC	$+ \text{NO} \rightarrow$	KR02NO*0.050	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint58	TrGC	$+ \text{NO} \rightarrow + \text{NO}_2$	KR02NO*0.950	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint59	TrGC	\rightarrow	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint60	TrGC	$+ \text{OH} \rightarrow$	2.75E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint61	TrGC	$+ h\nu \rightarrow + \text{OH}$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint62	TrGC	$+ \text{OH} \rightarrow + \text{CH}_3\text{COCH}_3 + \text{NO}_2$	2.25E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint63	TrGC	$+ h\nu \rightarrow + \text{NO}_2$	J_IC3H7N03+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint64	TrGC	+ HO ₂ →	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint65	TrGC	+ NO →	KR02NO*0.125	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint66	TrGC	+ NO → + CH ₃ COCH ₃ + NO ₂	KR02NO*0.875	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint67	TrGC	→ + CH ₃ COCH ₃	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint68	TrGC	+ OH →	8.01E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint69	TrGC	+ hν → + CH ₃ COCH ₃ + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint70	TrGC	+ OH → + CH ₃ COCH ₃ + NO ₂	7.03E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint71	TrGC	+ hν → + CH ₃ COCH ₃ + NO ₂	J_IC3H7NO3+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint72	TrGC	+ NO ₃ → + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint73	TrGC	+ OH →	6.70E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint74	TrGC	+ hν → + CH ₃ C(O)OO	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint75	TrGC	+ HO ₂ →	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint76	TrGC	+ HO ₂ → + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint77	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint78	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint79	TrGC	→	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint80	TrGC	+ OH →	4.75E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint81	TrGC	+ h ν → + OH	1.14*jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint82	TrGC	+ HO ₂ →	KR02HO2*0.770	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint83	TrGC	+ NO → + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint84	TrGC	→ + HCHO	2.00E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint85	TrGC	+ OH → + CO + NO ₂	8.83E-13	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint86	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint87	TrGC	+ OH →	1.01E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint88	TrGC	+ h ν → + HCHO + OH	1.14*jx(ip_CH300H)+ 2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint89	TrGC	+ HO ₂ →	KR02HO2*0.820	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint90	TrGC	+ NO → + CH ₃ C(O)OO + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint91	TrGC	→ + CH ₃ C(O)OO	8.80E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint92	TrGC	+ OH → + OH	1.20E-10	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint93	TrGC	+ h ν → + CH ₃ C(O)OO + OH	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint94	TrGC	→ CH ₃ C(O)OO +	8.80E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint95	TrGC	+ NO → CH ₃ C(O)OO + + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint96	TrGC	+ HO ₂ →	KR02HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint97	TrGC	+ h ν → CH ₃ C(O)OO + + OH	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint98	TrGC	+ OH →	7.49E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint99	TrGC	+ OH →	4.29E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint100	TrGC	+ hν → + HO ₂ + CO	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint101	TrGC	+ NO ₃ → + HNO ₃	2*KN03AL*2.4	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint102	TrGC	→ + HCHO + HO ₂	8.80E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint103	TrGC	+ NO →	KR02NO*0.098	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint104	TrGC	+ NO → + HCHO + HO ₂ + NO ₂	KR02NO*0.902	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint105	TrGC	+ HO ₂ →	KR02HO2*0.770	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint106	TrGC	+ hν → + HCHO + HO ₂ + NO ₂	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint107	TrGC	+ OH → + NO ₂	7.11E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint108	TrGC	+ hν → + HCHO + HO ₂ + OH	1.14*jx(ip_CH300H)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint109	TrGC	+ OH → + OH	8.69E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint110	TrGC	+ hν → + HOCH ₂ CO ₃	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint111	TrGC	+ OH → + HO ₂	3.22E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint112	TrGC	→ CH ₃ C(O)OO + HCHO + CO	2.00E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint113	TrGC	+ HO ₂ →	KR02HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint114	TrGC	+ NO → CH ₃ C(O)OO + HCHO + CO + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint115	TrGC	+ OH → + OH	ks*fco*fsooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint116	TrGC	+ OH →	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint117	TrGC	+ hν → + OH + HO ₂	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint118	TrGC	+ hν → CH ₃ C(O)OO + CO + OH + HCHO	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint119	TrGC	+ hν → CH ₃ C(O)OO + HCOCO ₃	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint120	TrGC	+ OH → + CO	1.33E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint121	TrGC	+ hν → + CO + HO ₂	jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint122	TrGC	+ NO ₃ → + CO + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint123	TrGC	+ OH →	6.65E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint124	TrGC	+ hν → + HO ₂ + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint125	TrGC	+ hν → CH ₃ C(O)OO +	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint126	TrGC	+ NO ₃ → + HNO ₃	KN03AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint127	TrGC	→	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint128	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint129	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint130	TrGC	+ HO ₂ →	KAPH02*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint131	TrGC	+ HO ₂ → + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint132	TrGC	+ h ν → + OH	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint133	TrGC	+ h ν →	4.23E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint134	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint135	TrGC	+ OH → + CO + NO ₂	3.12E-13	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint136	TrGC	→ 0.7 + 0.3	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint137	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint138	TrGC	+ NO ₂ →	k_CH3C03_N02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint139	TrGC	+ HO ₂ →	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint140	TrGC	+ HO ₂ → + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint141	TrGC	+ HO ₂ → + CO ₂ + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint142	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint143	TrGC	+ OH → GLYOX + CO + NO ₂	2.10E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint144	TrGC	+ OH →	2.14E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint145	TrGC	+ h ν → + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint146	TrGC	+ O ₃ →	1.01E-15*EXP(-732/TEMP)*.50*.18	Capouet et al. (2008)
G410apint147	TrGC	+ O ₃ →	1.01E-15*EXP(-732/TEMP)*.50*.16	Capouet et al. (2008)
G410apint148	TrGC	+ O ₃ → OH + + CO + HO ₂	1.01E-15*EXP(-732/TEMP)*.50*.66	Capouet et al. (2008)
G410apint149	TrGC	+ O ₃ →	1.01E-15*EXP(-732/TEMP)*.50*.12	Capouet et al. (2008)
G410apint150	TrGC	+ O ₃ → OH +	1.01E-15*EXP(-732/TEMP)*.50*(.22+.66)	Capouet et al. (2008)*
G410apint151	TrGC	→ + H ₂ O ₂	1.00E-17*c(ind_H2O)	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint152	TrGC	+ CO →	1.20E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint153	TrGC	+ NO → + NO ₂	1.00E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint154	TrGC	+ NO ₂ → + NO ₃	1.00E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint155	TrGC	+ SO ₂ → + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint156	TrGC	→	1.00E-17*c(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint157	TrGC	→ + H ₂ O ₂	1.00E-17*c(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint158	TrGC	+ CO →	1.20E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint159	TrGC	+ NO → + NO ₂	1.00E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint160	TrGC	+ NO ₂ → + NO ₃	1.00E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint161	TrGC	+ SO ₂ → + H ₂ SO ₄	7.00E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint162	TrGC	→ + HCHO	2.00E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint163	TrGC	+ NO → + HCHO + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint164	TrGC	+ HO ₂ →	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint165	TrGC	→ + HCHO + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CH0)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint166	TrGC	+ OH → + OH	5.47E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint167	TrGC	+ hν → + HCHO + OH	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint168	TrGC	+ OH → + CO	5.47E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint169	TrGC	+ $h\nu \rightarrow + CO + HO_2$	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint170	TrGC	$\rightarrow .56 + .14 + 0.3$	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint171	TrGC	+ $HO_2 \rightarrow$	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint172	TrGC	+ $HO_2 \rightarrow + O_3$	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint173	TrGC	+ $HO_2 \rightarrow .80 + 0.20 + OH$	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint174	TrGC	+ $NO_2 \rightarrow$	k_CH3CO3_N02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint175	TrGC	+ $NO \rightarrow 0.80 + 0.20 + NO_2$	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint176	TrGC	+ $OH \rightarrow 0.80 + 0.20$	2.69E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint177	TrGC	+ $h\nu \rightarrow 0.80 + 0.20 + HO_2$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint178	TrGC	$\rightarrow 0.80 + 0.20 + OH$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint179	TrGC	+ $OH \rightarrow$	3.00E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint180	TrGC	$\rightarrow + NO_2$	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint181	TrGC	+ $OH \rightarrow CH_3COCH_3 + + CO + NO_2$	2.52E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint182	TrGC	$\rightarrow 0.7 + 0.3$	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint183	TrGC	+ $HO_2 \rightarrow$	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint184	TrGC	+ $HO_2 \rightarrow + O_3$	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint185	TrGC	+ $HO_2 \rightarrow + OH$	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint186	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint187	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint188	TrGC	+ OH →	7.29E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint189	TrGC	→	1.30E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint190	TrGC	+ HO ₂ →	KR02HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint191	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint192	TrGC	+ hν → + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint193	TrGC	+ OH →	1.04E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint194	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint195	TrGC	+ OH → + CO + NO ₂	6.77E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint196	TrGC	→	9.20E-14*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint197	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint198	TrGC	+ HO ₂ →	KR02HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint199	TrGC	+ hν → + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint200	TrGC	+ OH →	1.09E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint201	TrGC	→ CH ₃ COCH ₃ +	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint202	TrGC	+ NO → CH ₃ COCH ₃ + + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)*

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

#	labels	reaction	rate coefficient	reference
G410apint203	TrGC	+ HO ₂ →	KR02H02*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint204	TrGC	+ hν → CH ₃ COCH ₃ + + OH	1.14*jx(ip_CH300H)+jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint205	TrGC	+ OH →	1.86E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint206	TrGC	+ NO ₃ → + HNO ₃	KN03AL*8.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint207	TrGC	+ OH →	2.63E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint208	TrGC	→ + CO + HO ₂	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint209	TrGC	+ HO ₂ →	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint210	TrGC	+ HO ₂ → + OH	KAPH02*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint211	TrGC	+ HO ₂ → + O ₃	KAPH02*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint212	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint213	TrGC	+ NO ₂ →	k_CH3C03_N02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint214	TrGC	+ NO ₃ → + NO ₂	KR02N03*1.74	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint215	TrGC	→	1.00E-11*R02*0.7	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint216	TrGC	→	1.00E-11*R02*0.3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint217	TrGC	+ HO ₂ →	KR02H02*0.820	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint218	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint219	TrGC	→	1.30E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint220	TrGC	+ OH →	9.65E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint221	TrGC	+ hν → + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint222	TrGC	+ OH →	6.57E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint223	TrGC	+ OH → + CO + NO ₂	2.96E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint224	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint225	TrGC	+ OH →	1.27E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint226	TrGC	+ hν → + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint227	TrGC	+ HO ₂ →	KR02HO2*0.820	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint228	TrGC	+ NO → CH ₃ COCH ₃ + + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint229	TrGC	→ CH ₃ COCH ₃ +	6.70E-15*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint230	TrGC	+ OH →	3.31E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint231	TrGC	+ hν → CH ₃ COCH ₃ + + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint232	TrGC	+ HO ₂ →	KR02HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint233	TrGC	+ NO → + HO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint234	TrGC	→ + HO ₂	8.80E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint235	TrGC	+ OH →	7.46E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint236	TrGC	+ hν → + HO ₂ + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint237	TrGC	\rightarrow	1.30E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint238	TrGC	$+ \text{HO}_2 \rightarrow$	KR02H02*0.706	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint239	TrGC	$+ \text{NO} \rightarrow + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint240	TrGC	$+ h\nu \rightarrow + \text{OH}$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint241	TrGC	$+ \text{OH} \rightarrow + \text{OH}$	1.01E-10	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint242	TrGC	$\rightarrow \text{GLYOX} +$	8.80E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint243	TrGC	$+ \text{NO} \rightarrow \text{GLYOX} + + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint244	TrGC	$+ \text{HO}_2 \rightarrow$	KR02H02*0.706	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint245	TrGC	$+ \text{OH} \rightarrow$	1.33E-10	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint246	TrGC	$+ h\nu \rightarrow + \text{CO} + \text{HO}_2$	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint247	TrGC	$+ \text{NO}_3 \rightarrow + \text{HNO}_3$	2*KN03AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint248	TrGC	$+ h\nu \rightarrow \text{GLYOX} + + \text{OH}$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint249	TrGC	$+ \text{OH} \rightarrow + \text{OH}$	9.23E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint250	TrGC	\rightarrow	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint251	TrGC	$+ \text{HO}_2 \rightarrow$	KAPH02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint252	TrGC	$+ \text{NO}_2 \rightarrow$	k_CH3C03_N02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint253	TrGC	$+ \text{NO} \rightarrow + \text{NO}_2$	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint254	TrGC	$\rightarrow + \text{HCHO}$	2.00E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint255	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint256	TrGC	$+ \text{NO} \rightarrow + \text{HCHO} + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint257	TrGC	$+ \text{OH} \rightarrow + \text{CO} + \text{CO}$	2.64E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint258	TrGC	$+ h\nu \rightarrow + \text{HO}_2 + \text{CO} + \text{CO}$	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint259	TrGC	$+ \text{OH} \rightarrow$	8.33E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint260	TrGC	$+ h\nu \rightarrow + \text{HCHO} + \text{OH}$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO) +J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint261	TrGC	$+ \text{OH} \rightarrow$	7.55E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint262	TrGC	$+ h\nu \rightarrow + \text{OH}$	1.14*jx(ip_CH300H)+jx(ip_HOCH2CHO) +J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint263	TrGC	$\rightarrow + \text{NO}_2$	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint264	TrGC	$+ \text{OH} \rightarrow + \text{CO} + \text{NO}_2$	7.19E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint265	TrGC	$+ \text{OH} \rightarrow$	3.39E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint266	TrGC	$+ h\nu \rightarrow + \text{HO}_2 + \text{CO}$	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint267	TrGC	$+ h\nu \rightarrow + \text{HO}_2 + \text{CO}$	jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint268	TrGC	$+ \text{NO}_3 \rightarrow + \text{HNO}_3$	2*KNO3AL*4.0	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint269	TrGC	\rightarrow	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint270	TrGC	$+ \text{HO}_2 \rightarrow$	KAPH02*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint271	TrGC	+ HO ₂ → + OH	KAPHO2*(1-rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint272	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint273	TrGC	+ NO → + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint274	TrGC	+ OH →	1.63E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint275	TrGC	+ hν → + OH	1.14*jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint276	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint277	TrGC	+ OH → + CO + NO ₂	1.27E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410apint278	TrGC	→ 0.7 HOCH ₂ CH ₂ O ₂ + 0.3	1.00E-11*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint279	TrGC	+ NO → HOCH ₂ CH ₂ O ₂ + NO ₂	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint280	TrGC	+ HO ₂ →	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint281	TrGC	+ HO ₂ → HOCH ₂ CH ₂ O ₂ + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint282	TrGC	+ HO ₂ → + O ₃	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint283	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint284	TrGC	+ OH → HOCH ₂ CH ₂ O ₂	1.39E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint285	TrGC	+ OH →	1.73E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint286	TrGC	+ hν → HOCH ₂ CH ₂ O ₂ + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint287	TrGC	→ + NO ₂	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410apint288	TrGC	+ OH → HOCH ₂ CHO + CO + NO ₂	4.51E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint289	TrGC	+ NO ₃ →	1.2E-12*EXP(490./temp)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint290	TrGC	→ + NO ₂	(.65*6.70E-15+.35*2.50E-13)*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint291	TrGC	+ NO → + NO ₂ + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint292	TrGC	+ HO ₂ →	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint293	TrGC	+ NO ₃ → + NO ₂ + NO ₂	KR02NO3	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint294	TrGC	+ hν → + NO ₂ + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint295	TrGC	+ OH →	.65*6.87E-12+.35*1.23E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)*
G410bpint	TrGC	+ OH →	1.47E-11*EXP(467/TEMP)*(0.8326*0.3+0.068)/(0.8326+0.068)	Vereecken and Peeters (2012)*
G410bpint2	TrGC	+ OH →	1.47E-11*EXP(467/TEMP)*0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012)*
G410bpint3	TrGC	+ HO ₂ →	KR02HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint4	TrGC	+ NO →	KR02NO*0.240	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint5	TrGC	+ NO → + HCHO + HO ₂ + NO ₂	KR02NO*0.760	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint6	TrGC	→ + HCHO + HO ₂	9.20E-14*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint7	TrGC	+ OH →	1.33E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint8	TrGC	+ hν → + HCHO + HO ₂ + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint9	TrGC	+ OH → + HCHO + NO ₂	4.70E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410bpint10	TrGC	+ NO → + CH ₃ COCH ₃ + NO ₂	KR02NO*0.892	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint11	TrGC	+ NO →	KR02NO*0.108	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint12	TrGC	+ HO ₂ →	KR02HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint13	TrGC	→ + CH ₃ COCH ₃	1.60E-13*R02	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint14	TrGC	→	5.68E10*exp(-8745/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2013b)*
G410bpint15	TrGC	+ NO → + NO ₂	KR02NO*0.890	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint16	TrGC	+ NO →	KR02NO*0.110	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint17	TrGC	+ HO ₂ →	KR02HO2*0.820	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint18	TrGC	→	2.50E-13*R02	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint19	TrGC	→ + HO ₂	5.7E10*exp(-2949/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2013b)*
G410bpint20	TrGC	→ + OH	9.17E10*exp(-8706/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2013b)*
G410bpint21	TrGC	+ NO → + NO ₂	KR02NO*0.747	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint22	TrGC	+ NO →	KR02NO*0.253	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint23	TrGC	+ HO ₂ →	KR02HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint24	TrGC	→	8.80E-13*R02	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint25	TrGC	+ NO → + NO ₂	KR02NO*0.893	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint26	TrGC	+ NO →	KR02NO*0.107	Vereecken and Peeters (2012), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410bpint27	TrGC	+ HO ₂ →	KR02HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint28	TrGC	→	5.00E-12*R02	Vereecken and Peeters (2012), Taraborrelli (2013b)
G410bpint29	TrGC	+ OH →	1.55E-11	Lewis et al. (2005), Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint30	TrGC	+ HO ₂ →	KR02HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint31	TrGC	+ NO → + NO ₂	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint32	TrGC	→	2.00E-12*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint33	TrGC	+ OH → + OH	2.63E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint34	TrGC	+ hν → + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint35	TrGC	+ OH →	3.07E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint36	TrGC	+ O ₃ → + .63 CO + .37 HOCH2OOH + .16 OH + .16 HO ₂	1.5E-17*.051/(1-.027)	Nguyen et al. (2009), Taraborrelli (2013b)
G410bpint37	TrGC	+ O ₃ →	1.5E-17*.368/(1-.027)	Nguyen et al. (2009), Taraborrelli (2013b)
G410bpint38	TrGC	+ O ₃ → + OH	1.5E-17*.283/(1-.027)	Nguyen et al. (2009), Taraborrelli (2013b)
G410bpint40	TrGC	+ O ₃ → + CO ₂	1.5E-17*(.104+.167)/(1-.027)	Nguyen et al. (2009), Taraborrelli (2013b)*
G410bpint41	TrGC	+ OH →	3.04E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint42	TrGC	+ HO ₂ →	KR02HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint43	TrGC	+ NO →	KR02NO*0.138	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint44	TrGC	+ NO → + NO ₂	KR02NO*0.862	Rickard and Pascoe (2009), Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410bpint45	TrGC	\rightarrow	2.50E-13*R02	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint46	TrGC	$+ \text{OH} \rightarrow + \text{OH}$	1.62E-11	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint47	TrGC	$+ h\nu \rightarrow + \text{OH}$	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint48	TrGC	$+ \text{OH} \rightarrow + \text{NO}_2$	1.84E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint49	TrGC	$\rightarrow + \text{NO}_2$	J_IC3H7N03	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint50	TrGC	$+ \text{OH} \rightarrow$	3.94E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint51	TrGC	$\rightarrow + \text{H}_2\text{O}_2$	6.00E-18*c(ind_H20)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint52	TrGC	$+ \text{CO} \rightarrow$	1.2E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint53	TrGC	$+ \text{NO} \rightarrow + \text{NO}_2$	1.E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint54	TrGC	$+ \text{NO}_2 \rightarrow + \text{NO}_3$	1.E-15	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint55	TrGC	$+ \text{SO}_2 \rightarrow + \text{H}_2\text{SO}_4$	7.E-14	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint56	TrGC	$+ \text{NO}_3 \rightarrow$	2.51E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint57	TrGC	$+ \text{HO}_2 \rightarrow$	KR02H02*0.914	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint58	TrGC	$+ \text{NO} \rightarrow + \text{HCHO} + \text{NO}_2 + \text{NO}_2$	KR02NO	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint59	TrGC	$+ \text{NO}_3 \rightarrow + \text{HCHO} + \text{NO}_2 + \text{NO}_2$	KR02N03	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint60	TrGC	$\rightarrow + \text{HCHO} + \text{NO}_2$	9.20E-14*R02*0.7	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint61	TrGC	\rightarrow	9.20E-14*R02*0.3	Rickard and Pascoe (2009), Taraborrelli (2013b)*

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

#	labels	reaction	rate coefficient	reference
G410bpint62	TrGC	+ OH →	9.58E-12	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410bpint63	TrGC	+ hν → + HCHO + NO ₂ + OH	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009), Taraborrelli (2013b)
G410apint296	TrGC	+ OH →	8.7E-11*(.50+.25)	Wolfe et al. (2011), Taraborrelli (2013b)*
G410apint297	TrGC	+ OH → + HO ₂	8.7E-11*.25*.60	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint298	TrGC	+ OH →	8.7E-11*.25*.40	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint299	TrGC	+ O ₃ →	2.E-16*.50*.18	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint300	TrGC	+ O ₃ →	2.E-16*.50*.16	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint301	TrGC	+ O ₃ → OH + + CO + HO ₂	2.E-16*.50*.66	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint302	TrGC	+ O ₃ →	2.E-16*.50*.12	Wolfe et al. (2011), Taraborrelli (2013b)
G410apint303	TrGC	+ O ₃ → OH +	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Taraborrelli (2013b)*
G410apint304	TrGC	+ NO ₃ →	9.5E-12	Wolfe et al. (2011), Taraborrelli (2013b)
G410myrc	TrGC	+ OH → + POHORG	9.19E-12*exp(1071./temp)*0.64	Hites and Turner (2009), Orlando et al. (2000), Taraborrelli (2013b)
G410myrct2	TrGC	+ OH → + POHORG	9.19E-12*exp(1071./temp)*0.36	Hites and Turner (2009), Orlando et al. (2000), Taraborrelli (2013b)
G410myrct3	TrGC	+ O ₃ → .25 CH ₃ COCH ₃ + .75 OH + .75 CH ₃ COCH ₂ O ₂ + + .75 POHORG	4.7E-16	Atkinson and Arey (2003), Taraborrelli (2013b)
G410myrct4	TrGNC	+ NO ₃ →	1.1E-11	Atkinson and Arey (2003), Taraborrelli (2013b)
G410myrct5	TrGC	→ CH ₃ COCH ₃ + HO ₂ +	8.E-13*R02	Taraborrelli (2013b)
G410myrct6	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410myrct7	TrGCN	+ NO → .80 CH ₃ COCH ₃ + .80 HO ₂ + .80 + .80 NO ₂ + .20	KR02NO	Taraborrelli (2013b)*
G410myrct8	TrGCJ	+ hν → CH ₃ COCH ₃ + OH + HO ₂ + + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410myrct9	TrGC	+ OH → + POHORG	1.55E-10	Baker et al. (2004), Taraborrelli (2013b)
G410myrct10	TrGC	+ NO ₃ → CH ₃ COCH ₃ + + NISOPO2	4.7E-13	Baker et al. (2004), Taraborrelli (2013b)
G410myrct11	TrGC	+ OH → iC ₃ H ₇ ONO ₂ + + POHORG	1.55E-10	see note
G410myrct12	TrGC	→	1.E-12*R02	Taraborrelli (2013b)
G410myrct13	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410myrct14	TrGC	+ NO → .8 + .8 NO ₂ + .2	KR02NO	Taraborrelli (2013b)
G410myrct15	TrGC	→ + HO ₂	K16HS	Taraborrelli (2013b)
G410myrct16	TrGC	→ CH ₃ COCH ₃ + + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO ₂	KDEC	Taraborrelli (2013b)
G410myrct17	TrGC	+ OH → CH ₃ COCH ₃ + HO ₂ + + ISOPBNO3 + POHORG	kadt+kads	Taraborrelli (2013b)
G410myrct18	TrGC	+ hν → + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410myrct19	TrGC	+ OH → + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH + CH ₃ COCH ₃ + HO ₂ + POHORG	kadt+kads	Taraborrelli (2013b)
G410myrct20	TrGCJ	+ hν → OH + + HO ₂ + POHORG	J_HPALD	Taraborrelli (2013b)
G410myrct21	TrGC	+ OH → + HO ₂ + CH ₃ COCH ₃ + POHORG	kadt+kads	Taraborrelli (2013b)
G410myrct22	TrGC	+ OH → + + HCHO + GLYOX + HO ₂ + POHORG	(kadt+kads)*acho*ach2ooh	Taraborrelli (2013b)
G410myrct23	TrGC	+ O ₃ → + .25 CH ₃ COCH ₃ + .75 OH + .75 CH ₃ COCH ₂ O ₂ + .75 POHORG	4.7E-16	Taraborrelli (2013b)
G410myrct24	TrGC	+ OH → + + POHORG	1.55E-10	Baker et al. (2004), Taraborrelli (2013b)
G410myrct25	TrGC	+ NO ₃ → + NISOPO2	4.7E-13	Baker et al. (2004), Taraborrelli (2013b)
G410myrct26	TrGC	→	1.E-12*R02	Taraborrelli (2013b)
G410myrct27	TrGC	+ HO ₂ → + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH	KR02HO2	Taraborrelli (2013b)
G410myrct28	TrGC	+ NO → .8 + .8 NO ₂ + .2 + .2 ISOPBNO3	KR02NO	Taraborrelli (2013b)
G410myrct29	TrGC	→ + HO ₂	K16HS	Taraborrelli (2013b)
G410myrct30	TrGC	→ + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO ₂	KDEC	Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410myrct31	TrGCJ	+ hν → + OH + + HO ₂ + POHORG	J_HPALD	Taraborrelli (2013b)
G410myrct32	TrGC	+ OH → + .3 + .2 + .3 + .2 + POHORG	(kad _t +kad _s)*ach ₀ *ach _{200h}	Taraborrelli (2013b)
G410myrct33	TrGC	→	1.E-12*R02	Taraborrelli (2013b)
G410myrct34	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410myrct35	TrGC	+ NO → .8 + .8 NO ₂ + .2 CH ₃ COCH ₃ + .2 + .2 ISOPBNO3	KR02NO	Taraborrelli (2013b)
G410myrct36	TrGC	→ + HO ₂	K16HS	Taraborrelli (2013b)
G410myrct37	TrGC	→ CH ₃ COCH ₃ + + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO ₂ + OH + POHORG	KDEC	Taraborrelli (2013b)
G410myrct38	TrGCJ	+ hν → + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410myrct39	TrGCJ	+ hν → CH ₃ COCH ₃ + HO ₂ + + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410myrct40	TrGCJ	+ hν → CH ₃ COCH ₃ + OH + + OH + + HO ₂ + 2 POHORG	J_HPALD	Taraborrelli (2013b)
G410myrct41	TrGC	+ OH → CH ₃ COCH ₃ + OH + + .3 + .2 + .3 + .2 + POHORG + POHORG	(kad _t +kad _s)*ach ₀ *ach _{200h}	Taraborrelli (2013b)
G410myrct42	TrGC	+ OH → + H ₂ O + POHORG	4.4E-12*EXP(365./temp)	Taraborrelli (2013b)*
G410myrct43	TrGC	+ hν → HCHO + HO ₂ + HO ₂ + CO	jx(ip_CH3CHO)	Taraborrelli (2013b)
G410myrct44	TrGC	+ NO ₃ → HNO ₃ +	KNO3AL	Taraborrelli (2013b)
G410myrct45	TrGC	→ HCHO + HO ₂ + CO ₂	1.00E-11*0.7*R02	Taraborrelli (2013b)
G410myrct46	TrGC	→	1.00E-11*0.3*R02	Taraborrelli (2013b)
G410myrct47	TrGC	+ HO ₂ → OH + HCHO + HO ₂ + CO ₂ + POHORG	KAPH02*0.44	Taraborrelli (2013b)
G410myrct48	TrGC	+ HO ₂ →	KAPH02*0.41	Taraborrelli (2013b)
G410myrct49	TrGC	+ HO ₂ → + O ₃	KAPH02*0.15	Taraborrelli (2013b)
G410myrct50	TrGC	+ NO ₂ →	k_CH3CO3_NO2	Taraborrelli (2013b)
G410myrct51	TrGC	+ NO → NO ₂ + HCHO + HO ₂ + CO ₂	KAPNO	Taraborrelli (2013b)
G410myrct52	TrGC	+ NO ₃ → NO ₂ + HCHO + HO ₂ + CO ₂	KR02NO3*1.60	Taraborrelli (2013b)
G410myrct53	TrGC	+ OH → HCHO + HO ₂ + CO ₂ + POHORG	4.2E-14*exp(850./temp)	Taraborrelli (2013b)*
G410myrct54	TrGC	+ hν → HCHO + HO ₂ + OH + CO ₂ + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410myrct55	TrGC	+ OH → + H ₂ O + POHORG	0.6*k_CH300H_OH	Taraborrelli (2013b)
G410myrct56	TrGC	→ + NO ₂	k_PAN_M	Taraborrelli (2013b)
G410myrct57	TrGC	+ OH → HCHO + CO + NO ₂ + POHORG	9.50E-13*EXP(-650./temp)	Taraborrelli (2013b)
G410afarn	TrGC	+ OH → + POHORG	2.7E-11*EXP(390./temp)	Taraborrelli (2013b)*
G410afarnt2	TrGC	+ OH → + POHORG	2.*1.9E-11*exp(450./temp)	Taraborrelli (2013b)*

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

#	labels	reaction	rate coefficient	reference
G410afarnt3	TrGC	+ O ₃ → + .25 CH ₃ COCH ₃ + .75 OH + .75 CH ₃ COCH ₂ O ₂ + .75 POHORG	6.51E-15*exp(-829./temp)	Taraborrelli (2013b)*
G410afarnt4	TrGC	+ O ₃ → + + .75 OH + .75 POHORG	6.51E-15*exp(-829./temp)	Taraborrelli (2013b)*
G410afarnt5	TrGNC	+ NO ₃ →	2E-12+2*9.37E-12	Taraborrelli (2013b)*
G410afarnt6	TrGC	→	8.E-13*R02	Taraborrelli (2013b)
G410afarnt7	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410afarnt8	TrGC	+ NO → .75 + .75 NO ₂ + .25	KR02NO	Taraborrelli (2013b)
G410afarnt9	TrGCJ	+ hν → + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410afarnt10	TrGC	+ OH → + + POHORG	2.7E-11*EXP(390./temp)	Taraborrelli (2013b)
G410afarnt11	TrGC	+ OH → .5 + .5 + + POHORG	2.*1.9E-11*exp(450./temp)	Taraborrelli (2013b)
G410afarnt12	TrGC	→ .5 + .5 + .5 + .5 CH ₃ COCH ₃ + HO ₂	KDEC	Taraborrelli (2013b)
G410afarnt13	TrGC	→	1.E-12*R02	Taraborrelli (2013b)
G410afarnt14	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410afarnt15	TrGC	+ NO → .75 + .75 NO ₂ + .25	KR02NO	Taraborrelli (2013b)
G410afarnt16	TrGC	→ + HO ₂ +	K16HS	Taraborrelli (2013b)
G410afarnt17	TrGC	→ +	KDEC	Taraborrelli (2013b)
G410afarnt18	TrGC	+ OH → + HO ₂ + ISOPBNO ₃ + POHORG	kadt+kads	Taraborrelli (2013b)
G410afarnt19	TrGC	+ hν → + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410afarnt20	TrGC	+ OH → + + POHORG	kadt+kads	Taraborrelli (2013b)
G410afarnt21	TrGC	+ O ₃ → + + .75 OH + .75 POHORG	2.*6.51E-15*exp(-829./temp)	Taraborrelli (2013b)*
G410afarnt22	TrGC	+ OH → + POHORG	1.9E-11*exp(450./temp)	Taraborrelli (2013b)*
G410afarnt23	TrGC	+ OH → + POHORG	2.7E-11*EXP(390./temp)	Taraborrelli (2013b)*
G410afarnt24	TrGC	+ O ₃ → + + .75 OH + .75 POHORG	6.51E-15*exp(-829./temp)	Taraborrelli (2013b)*
G410afarnt25	TrGNC	+ NO ₃ →	2E-12	Taraborrelli (2013b)*
G410afarnt26	TrGNC	+ NO ₃ →	9.37E-12	Taraborrelli (2013b)*
G410afarnt27	TrGC	→	8.E-13*R02	Taraborrelli (2013b)
G410afarnt28	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410afarnt29	TrGC	+ NO → .75 + .75 NO ₂ + .25	KR02NO	Taraborrelli (2013b)
G410afarnt30	TrGCJ	+ hν → + OH + POHORG	1.14*jx(ip_CH300H)	Taraborrelli (2013b)
G410afarnt31	TrGC	+ OH → + HO ₂ + + POHORG	2.7E-11*EXP(390./temp)	Taraborrelli (2013b)*
G410afarnt32	TrGC	+ OH → + + POHORG	1.9E-11*exp(450./temp)	Taraborrelli (2013b)*
G410afarnt33	TrGC	→ + + HO ₂	KDEC	Taraborrelli (2013b)
G410afarnt34	TrGC	→	1.E-12*R02	Taraborrelli (2013b)
G410afarnt35	TrGC	+ HO ₂ →	KR02HO2	Taraborrelli (2013b)
G410afarnt36	TrGC	+ NO → .75 + .75 NO ₂ + .25	KR02NO	Taraborrelli (2013b)

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

#	labels	reaction	rate coefficient	reference
G410afarnt37	TrGC	$\rightarrow + + \text{HO}_2 +$	K16HS	Taraborrelli (2013b)
G410afarnt38	TrGC	$\rightarrow +$	KDEC	Taraborrelli (2013b)
G410afarnt39	TrGC	$+ \text{OH} \rightarrow + \text{HO}_2 + \text{ISOPBNO}_3 + \text{POHORG}$	kadt+kads	Taraborrelli (2013b)
G410afarnt40	TrGC	$+ h\nu \rightarrow + \text{OH} + \text{POHORG}$	$1.14 * jx(ip_{\text{CH3OOH}})$	Taraborrelli (2013b)
G410afarnt41	TrGC	$+ \text{OH} \rightarrow + + \text{POHORG}$	kadt+kads	Taraborrelli (2013b)
G410afarnt42	TrGC	$+ \text{O}_3 \rightarrow + + .75 \text{ OH} + .75 \text{ POHORG}$	$6.51E-15 * \exp(-829./\text{temp})$	Taraborrelli (2013b)
G410afarnt43	TrGC	$+ \text{OH} \rightarrow + \text{POHORG}$	$1.37E-10$	Smith et al. (1996), Taraborrelli (2013b)*
G410afarnt44	TrGC	$+ \text{O}_3 \rightarrow .25 \text{ CH}_3\text{COCH}_3 + .125 + .25 \text{ GLYOX}$ $+ .25 \text{ CH}_3\text{COCH}_2\text{O}_2 + .125 \text{ H}_2\text{O}_2 + .75 \text{ OH} + .75 \text{ CH}_3\text{COCH}_2\text{O}_2 + .75 + .75 \text{ POHORG}$	$3.9E-16$	Grosjean et al. (1996), Taraborrelli (2013b)*
G410afarnt45	TrGC	$+ \text{NO}_3 \rightarrow$	$7E-12$	Smith et al. (1996), Taraborrelli (2013b)
G410afarnt46	TrGC	$\rightarrow \text{CH}_3\text{COCH}_3 + + \text{HO}_2$	$8.E-13 * R02$	Taraborrelli (2013b)
G410afarnt47	TrGC	$+ \text{HO}_2 \rightarrow$	KR02HO2	Taraborrelli (2013b)
G410afarnt48	TrGC	$+ \text{NO} \rightarrow .25 + .75 \text{ CH}_3\text{COCH}_3 + .75 + .75 \text{ HO}_2 + .75 \text{ NO}_2$	KR02NO	Taraborrelli (2013b)
G410afarnt49	TrGC	$+ \text{OH} \rightarrow + \text{POHORG}$	$0.6 * k_{\text{CH3OOH_OH}}$	Taraborrelli (2013b)
G410afarnt50	TrGC	$+ \text{OH} \rightarrow + \text{HO}_2 + \text{POHORG}$	$kt * ftoh * falk * falk$	Taraborrelli (2013b)
G410afarnt51	TrGCJ	$+ h\nu \rightarrow \text{CH}_3\text{COCH}_3 + + \text{OH} + \text{POHORG}$	$1.14 * jx(ip_{\text{CH3OOH}})$	Taraborrelli (2013b)
G410afarnt52	TrGCJ	$+ h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{CH}_3\text{COCH}_2\text{O}_2 + + \text{OH} + \text{POHORG}$	$1.14 * jx(ip_{\text{CH3OOH}}) + 2.77 * jx(ip_{\text{HOCH2CHO}})$	Taraborrelli (2013b)*
G410afarnt53	TrGC	$+ \text{OH} \rightarrow + \text{HO}_2 + \text{POHORG}$	$kt * ftoh * falk * fch2ono2$	Taraborrelli (2013b)
G410afarnt54	TrGC	$+ h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{CH}_3\text{COCH}_2\text{O}_2 +$	$2.84 * J_{\text{IC3H7N03}}$	Taraborrelli (2013b)
G410afarnt55	TrGC	$+ \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + + \text{POHORG}$	$2.E-11$	Fruekilde et al. (1997), Taraborrelli (2013b)*
G410afarnt56	TrGCJ	$+ h\nu \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + + \text{HO}_2$	$jx(ip_{\text{CH3CHO}}) + jx(ip_{\text{CH3COCH3}})$	Taraborrelli (2013b)

*Notes:

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

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

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

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

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

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

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

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

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

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

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

G2110: The rate coefficient is: $k_HO2_HO2 = (1.5E-12 * EXP(19./temp) + 1.7E-33 * EXP(1000./temp) * cair) * (1 + 1.4E-21 * EXP(2200./temp)) * C(ind_$

$H2O))$. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

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.

G3206: The rate coefficient is: $k_HN3_OH = 2.4E-14 * EXP(460./temp) + 1. / (1. / (6.5E-34 * EXP(1335./temp) * cair) + 1. / (2.7E-17 * EXP(2199./temp)))$

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

G4107: The rate coefficient is: $k_CH3OOH_OH = 3.8E-12 * EXP(200./temp)$.

G4109: The same temperature dependence assumed as for $CH_3CHO + NO_3$.

G4206: The product C_2H_5OH , which reacts only with OH , is substituted by its degradation products $\approx 0.1 HOCH_2CH_2O_2 + 0.9 CH_3CHO + 0.9 HO_2$.

G4207: The rate constant $8.01E-12$ is for the H abstraction in alpha to the $-OOH$ group (Rickard and Pascoe, 2009) and $0.6 * k_CH3OOH_OH$ is for the $C_2H_5O_2$ channel. The branching ratios are calculated from the terms of the rate coefficient at 298 K.

G4218: The rate coefficient is the same as for the CH_3O_2 channel in G4107 ($CH_3OOH + OH$).

G4221: The rate coefficient is $k_PAN_M = k_CH3C03_NO2 / 9.E-29 * EXP(-14000./temp)$, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G4300: The product $NC3H7O2$ is substituted with its degradation products $C_2H_5O_2 + CO_2 + HO_2$.

G4304: The value for the generic $RO_2 + HO_2$ reaction from Atkinson (1997) is used here.

G4306: The MCM (Rickard and Pascoe, 2009) products are $0.2 IPOPOL + 0.2 CH_3COCH_3 + 0.6 IC3H7O$. IPOPOL and IC3H7O are substituted with their degradation products. We assume IPOPOL to be oxidized entirely to $CH_3COCH_3 + HO_2$ by OH . $IC3H7O + O_2$ produces the same products.

G4307: Analogous to G4207 for both rate coefficient and branching ratios.

G4400: $LC_4H_9O_2$ represents $0.127 NC4H9O2 + 0.873 SC4H9O2$.

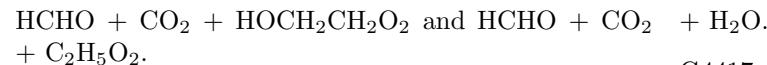
G4401: $NC4H9O$ and $SC4H9O$ are substituted with $2 CO_2 + C_2H_5O_2$ and $0.636 MEK + HO_2$ and $0.364 CH_3CHO + C_2H_5O_2$, respectively. The stoichiometric coefficients on the right side are weighted averages.

G4403: The alkyl nitrate yield is the weighted average yield for the two isomers forming from $NC4H9O2$ and $SC4H9O2$.

G4404: The product distribution is the weighted average of the single isomer hydroperoxides. It is calculated from the rate constants of single channels and the ratio of the isomers $NC4H9O2$ and $SC4H9O2$. The overall rate constant for this reaction is calculated as weighted average of the channels rate constants. The relative weight of the products from $NC4H9OOH$ and $SC4H9OOH$ are then 0.0887 and 0.9113. The channels producing RO_2 are given the rate coefficient $0.6 * k_CH3OOH_OH$ as for G4107. For $NC4H9OOH$ the products are $0.327 NC4H9O2 + 0.673 C3H7CHO + 0.673 OH$. $C3H7CHO$ is then substituted with $2 CO_2 + C_2H_5O_2$. Hence, $0.327 NC4H9O2 + 1.346 CO_2 + 0.673 C_2H_5O_2 + 0.673 OH$. For $SC4H9OOH$ the products are $0.219 SC4H9O2 + 0.781 MEK + 0.781 OH$.

G4413: $LMEKO2$ represents $0.459 MEKAO2 + 0.462 MEKBO2 + 0.079 MEKCO2$.

G4415: Alkyl nitrate formation is neglected. The products of $MEKAO$ and $MEKCO$ are substituted with



G4416: LMEKOOH is assumed having the composition 0.459 MEKAOOH + 0.462 MEKBOOH + 0.079 MEKCOOH. MEKAOOH + OH gives 0.89 CO₂C₃CHO + 0.89 OH + 0.11 MEKAO₂ + H₂O. CO₂C₃CHO is substituted with CH₃COCH₂O₂ + CO₂ and the products become 0.89 CH₃COCH₂O₂ + 0.89 CO₂ + 0.89 OH + 0.11 MEKAO₂ + H₂O. MEKBOOH + OH gives 0.758 BIACET + 0.758 OH + 0.242 MEKBO₂ + H₂O. MEKCOOH + OH gives 0.614 EGLYOX + 0.614 OH + 0.386 MEKCO₂ + H₂O. EGLYOX is substituted with C₂H₅O₂ + 2 CO₂ and the products become 0.614 C₂H₅O₂ + 1.228 CO₂ + 0.614 OH + 0.386 MEKCO₂ + H₂O.

G4417: The rate coefficient is the combination of the ones for the two isomers weighted by the relative abundances for NC4H₉NO₃ and SC4H₉NO₃, respectively. Product distribution is calculated accordingly.

NC4H₉NO₃ + OH gives C3H₇CHO + NO₂ + H₂O with C3H₇CHO being substituted with 2 CO₂ + C₂H₅O₂. After substitution is obtained 2 CO₂ + C₂H₅O₂ + NO₂ + H₂O. SC4H₉NO₃ + OH gives MEK + NO₂ + H₂O For the product distribution NC4H₉NO₃ and SC4H₉NO₃ account for 0.08577 and 0.91423, respectively.

G4419: The same value as for PAN is assumed.

G4420: Products are as in G4415. Only the main channels for each isomer are considered. Rate constant is the weighted average for the isomers.

G4455: CH₃COCOCO₃H assumed to photolysis quickly and give CH₃CO₃ + CO + CO₂ + OH

G45222: HYBIACETOAA approximated to yield BIACETOAH only, CH₃COCHOOHCH₂OH's main reaction with OH yields BIACETOAH recycling OH =_i substitution with BIACETOAH

G413621: PEROXYRINGC₂OOHC₃OD substituted

G4136: CH₃COCH₂OOCH₂CO₃ -_i CH₃CO₃ + CO₂ + 2 HCHO

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	O ₂ + hν → O(³ P) + O(³ P)	jx(ip_02)	see note
J1001a	StTrGJ	O ₃ + hν → O(¹ D)	jx(ip_01D)	see note
J1001b	StTrGJ	O ₃ + hν → O(³ P)	jx(ip_03P)	see note
J2101	StTrGJ	H ₂ O ₂ + hν → 2 OH + 2 POHOX	JX(ip_H2O2)	see note
J3101	StTrGNJ	NO ₂ + hν → NO + O(³ P)	jx(ip_N02)	see note
J3103a	StTrGNJ	NO ₃ + hν → NO ₂ + O(³ P)	jx(ip_N020)	see note
J3103b	StTrGNJ	NO ₃ + hν → NO	jx(ip_N002)	see note
J3104a	StTrGNJ	N ₂ O ₅ + hν → NO ₂ + NO ₃	jx(ip_N205)	see note
J3200	TrGJ	HONO + hν → NO + OH + PONOX	JX(ip_HONO)	see note
J3201	StTrGNJ	HNO ₃ + hν → NO ₂ + OH + PONOX	JX(ip_HN03)	see note
J3202	StTrGNJ	HNO ₄ + hν → .667 NO ₂ + .667 HO ₂ + .333 NO ₃ + .333 OH + .333 PONOX	JX(ip_HN04)	see note
J4100e	StTrGJ	CH ₃ OOH + hν → HCHO + OH + HO ₂ + POHORG	1.14*jx(ip_CH3OOH)	see note
J4101a	StTrGJ	HCHO + hν → H ₂ + CO	jx(ip_COH2)	see note
J4101b	StTrGJ	HCHO + hν → H + CO + HO ₂	jx(ip_CHOH)	see note
J4104e	StTrGJ	HOCH ₂ OOH + hν → OH + HO ₂ + HCOOH + POHORG	1.14*jx(ip_CH3OOH)	see note
J4200e	TrGCJ	C ₂ H ₅ OOH + hν → CH ₃ CHO + HO ₂ + OH + POHORG	1.14*jx(ip_CH3OOH)	see note
J4201	TrGCJ	CH ₃ CHO + hν → CH ₃ O ₂ + HO ₂ + CO	jx(ip_CH3CHO)	see note
J4202e	TrGCJ	CH ₃ C(O)OOH + hν → CH ₃ O ₂ + OH + CO ₂ + POHORG	1.14*jx(ip_CH3C03H)	see note
J4204e	TrGNCJ	PAN + hν → .6 CH ₃ C(O)OO + .6 NO ₂ + .4 CH ₃ O ₂ + .4 CO ₂ + .4 NO ₃	jx(ip_PAN)	see note
J4205ae	TrGCJ	HOCH ₂ CHO + hν → HCHO + 2 HO ₂ + CO	jx(ip_HOCH2CHO)*0.70	Taraborrelli (2013a)
J4205be	TrGCJ	HOCH ₂ CHO + hν → 1.16 OH + .84 + .1 HCHO + .1 CO + .06 GLYOX + 1.16 POHORG	jx(ip_HOCH2CHO)*0.15	Taraborrelli (2013a)
J4205ce	TrGCJ	HOCH ₂ CHO + hν → CH ₃ OH + CO	jx(ip_HOCH2CHO)*0.15	Taraborrelli (2013a)
J4206e	TrGCJ	+ hν → OH + HCHO + CO + HO ₂ + POHORG	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Taraborrelli (2013a)
J4206et2	TrGCJ	HOCH ₂ CO ₃ H + hν → HCHO + HO ₂ + OH + CO ₂ + POHORG	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4207	TrGCJ	PHAN + hν → HOCH ₂ CO ₃ + NO ₂	jx(ip_PAN)	see note
J4208	TrGCJ	GLYOX + hν → 2 CO + 2 HO ₂	jx(ip_GLYOX)	see note
J4209	TrGNCJ	HCOCO ₂ H + hν → 2 HO ₂ + CO + CO ₂	jx(ip_MGLYOX)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4210e	TrGNCJ	$\text{HCOCO}_3\text{H} + h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{OH} + \text{CO}_2 + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)} + \text{jx(ip_HOCH}_2\text{CHO)}$	Rickard and Pascoe (2009)*
J4211e	TrGCJ	$\text{HYETHO}_2\text{H} + h\nu \rightarrow \text{HOCH}_2\text{CH}_2\text{O} + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Rickard and Pascoe (2009)*
J4212	TrGCJ	$\text{ETHOHN}_3 + h\nu \rightarrow \text{HO}_2 + 2 \text{HCHO} + \text{NO}_2$	J_IC3H7N_3	see note
J4213e	TrGCJ	$+ h\nu \rightarrow \text{OH} + \text{HCHO} + \text{CO}_2 + \text{OH} + 2 \text{POHORG}$	$2*1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4214e	TrGC	$+ h\nu \rightarrow \text{OH} + \text{HCHO} + \text{HO}_2 + \text{CO}_2 + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4215e	TrGC	$+ h\nu \rightarrow .4 \text{CO}_2 + .8 \text{H} + .34 \text{CO} + .34 \text{OH} + .34 \text{HO}_2 + .16 \text{HCHO} + .16 \text{O}^{(3}\text{P)} + .1 \text{HCOOH} + \text{CO} + .34 \text{POHORG}$	$\text{J_ketene}* 0.36$	Taraborrelli (2013a)
J4216e	TrGC	$+ h\nu \rightarrow \text{CH}_3\text{O}_2 + \text{HCOOH} + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4217e	TrGCJ	$+ h\nu \rightarrow \text{HO}_2 + \text{CO} + \text{HCHO} + \text{NO}_2$	$1.59*\text{J_IC3H7N}_3 + \text{jx(ip_CH3COCH}_3)$	Taraborrelli (2013a)
J4300e	TrGCJ	$\text{iC}_3\text{H}_7\text{OOH} + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{HO}_2 + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	von Kuhlmann (2001)*
J4301	TrGCJ	$\text{CH}_3\text{COCH}_3 + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{CH}_3\text{O}_2$	$\text{jx(ip_CH3COCH}_3)$	see note
J4302	TrGCJ	$\text{CH}_3\text{COCH}_2\text{OH} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{HO}_2$	J_ACETOL	see note
J4303	TrGCJ	$\text{MGLYOX} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	see note
J4304e	TrGCJ	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)} + \text{J_ACETOL}$	Taraborrelli (2013a)
J4305e	TrGCJ	$+ h\nu \rightarrow + \text{HCHO} + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)} + \text{J_ACETOL}$	Taraborrelli (2013a)
J4306	TrGNCJ	$\text{iC}_3\text{H}_7\text{ONO}_2 + h\nu \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2 + \text{HO}_2$	J_IC3H7N_3	von Kuhlmann et al. (2003)*
J4307	TrGCJ	$\text{NOA} + h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{HCHO} + \text{NO}_2$	$\text{J_IC3H7N}_3 + \text{jx(ip_CH3COCH}_3)$	see note
J4309e	TrGCJ	$\text{HYPROPO}_2\text{H} + h\nu \rightarrow \text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4310e	TrGNCJ	$\text{PR}_2\text{O}_2\text{HNO}_3 + h\nu \rightarrow \text{NOA} + \text{HO}_2 + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4311e	TrGCJ	$\text{HOCH}_2\text{COCHO} + h\nu \rightarrow + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Taraborrelli (2013a)
J4312e	TrGCJ	$+ h\nu \rightarrow .5 \text{CH}_3\text{CHO} + .8 \text{CO}_2 + .4 \text{CH}_3\text{C(O)OO} + .3 \text{HO}_2 + .1 \text{CH}_3\text{COOH} + .1 \text{OH} + .2 \text{CO} + .1 \text{POHORG}$	jx(ip_MGLYOX)	Taraborrelli (2013a)
J4313e	TrGCJ	$+ h\nu \rightarrow + \text{HCHO} + \text{OH} + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)} + \text{J_ACETOL}$	Taraborrelli (2013a)
J4314e	TrGCJ	$+ h\nu \rightarrow + \text{CO} + \text{HO}_2$	jx(ip_MGLYOX)	Taraborrelli (2013a)
J4315e	TrGCJ	$+ h\nu \rightarrow + \text{HO}_2 + \text{CO}$	$2*\text{jx(ip_MGLYOX)}$	Taraborrelli (2013a)
J4316e	TrGC	$+ h\nu \rightarrow \text{CH}_3\text{C(O)OO} + \text{OH} + \text{POHORG} + \text{CO}_2$	$\text{jx(ip_MGLYOX)} + 1.14*\text{jx(ip_CH3OOH)}$	Taraborrelli (2013a)
J4317e	TrGC	$+ h\nu \rightarrow \text{C}_2\text{H}_4 + \text{CO}$	$\text{J_ketene}*0.36*2.$	Taraborrelli (2013a)*
J4400e	TrGCJ	$\text{LC}_4\text{H}_9\text{OOH} + h\nu \rightarrow \text{OH} + 0.254 \text{CO}_2 + 0.5552 \text{MEK} + 0.5552 \text{HO}_2 + 0.3178 \text{CH}_3\text{CHO} + 0.4448 \text{C}_2\text{H}_5\text{O}_2 + \text{POHORG}$	$1.14*\text{jx(ip_CH3OOH)}$	Rickard and Pascoe (2009)*
J4401	TrGCJ	$\text{MVK} + h\nu \rightarrow \text{C}_3\text{H}_6 + \text{CO}$	jx(ip_MVK)	Taraborrelli (2013a)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4403	TrGCJ	MEK + hν → CH ₃ C(O)OO + C ₂ H ₅ O ₂	0.42*jx(ip_CHOH)	von Kuhlmann et al. (2003)*
J4404e	TrGCJ	LMEKOOH + hν → 0.538 HCHO + 0.538 CO ₂ + 0.459 HOCH ₂ CH ₂ O ₂ + 0.079 C ₂ H ₅ O ₂ + 0.462 CH ₃ C(O)OO + 0.462 CH ₃ CHO + OH + POHORG	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)*
J4405	TrGCJ	BIACET + hν → 2 CH ₃ C(O)OO	2.15*jx(ip_MGLYOX)	see note
J4406	TrGNCJ	LC4H9NO ₃ + hν → NO ₂ + 0.254 CO ₂ + 0.5552 MEK + 0.5552 HO ₂ + 0.3178 CH ₃ CHO + 0.4448 C ₂ H ₅ O ₂	J_IC3H7NO ₃	see note
J4407e	TrGNCJ	MPAN + hν → .6 MACO ₃ + .6 NO ₂ + .4 + .4 NO ₃	jx(ip_PAN)	Taraborrelli (2013a)*
J4409e	TrGCJ	CO ₂ H ₃ CO ₃ H + hν → + OH + CO ₂ + POHORG	1.14*jx(ip_CH3OOH)	Taraborrelli (2013a)
J4410	TrGCJ	CO ₂ H ₃ CO ₃ H + hν → CH ₃ C(O)OO + HO ₂ + HCOCO ₃ H	J_ACETOL	Rickard and Pascoe (2009)*
J4410t2	TrGCJ	+ hν → CH ₃ C(O)OO + HCOCO ₂ H + HO ₂	J_ACETOL	Taraborrelli (2013a)
J4411	TrGCJ	MACR + hν → .5 MACO ₃ + .5 + .5 CO + HO ₂	jx(ip_MACR)	see note
J4412e	TrGCJ	MACROOH + hν → + OH + POHORG	1.14*jx(ip_CH3OOH)+ 2.77*jx(ip_HOCH ₂ CHO)	see note
J4414	TrGCJ	MACROH + hν → CH ₃ COCH ₂ OH + CO + HO ₂ + HO ₂	2.77*jx(ip_HOCH ₂ CHO)	see note
J4415e	TrGCJ	MACO ₃ H + hν → + OH + POHORG	1.14*jx(ip_CH3OOH)	Taraborrelli (2013a)
J4416e	TrGCJ	LHMVKABOOH + hν → .12 + .88 CH ₃ C(O)OO + .88 HOCH ₂ CHO + .12 HCHO + OH + POHORG	1.14*jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2013a)
J4418e	TrGCJ	CO ₂ H ₃ CHO + hν → + CO + HO ₂	jx(ip_HOCH ₂ CHO)+J_ACETOL	Taraborrelli (2013a)
J4419	TrGCJ	HO ₁₂ CO ₃ C ₄ + hν → CH ₃ C(O)OO + HOCH ₂ CHO + HO ₂	J_ACETOL	Rickard and Pascoe (2009)*
J4420e	TrGCJ	BIACETO _H + hν → CH ₃ C(O)OO +	2.15*jx(ip_MGLYOX)	Taraborrelli (2013a)
J4421e	TrGC	+ hν → .5 OH + .25 + .25 CH ₃ C(O)OO + .5 + .5 CO + .5 POHORG	J_KETENE	Taraborrelli (2013a)
J4422e	TrGC	+ hν → .0192 + .1848 H ₂ O ₂ + .2208 MGLYOX + .36 OH + .36 CO + .56 CH ₃ C(O)OO + .2 CH ₃ CHO + .2 CO ₂ + .2 HCHO + .2 HO ₂ + .36 POHORG	J_KETENE*0.5	Taraborrelli (2013a)
J4422et2	TrGC	+ hν → + CO	J_KETENE*0.5	Taraborrelli (2013a)
J4423e	TrGCJ	+ hν → CH ₃ C(O)OO + CO + CO + HO ₂	jx(ip_MGLYOX)	Taraborrelli (2013a)
J4424e	TrGCJ	+ hν → CH ₃ C(O)OO +	2.15*jx(ip_MGLYOX)	Taraborrelli (2013a)
J4424et2	TrGC	+ hν → CH ₃ C(O)OO + CO + CO ₂ + HO ₂	3.15*jx(ip_MGLYOX)	Taraborrelli (2013a)
J4502et2	TrGCJ	LISOPACOOH + hν → LHC4ACCHO + HO ₂ + OH + POHORG	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4503et2	TrGNCJ	LISOPACNO3 + hν → LHC4ACCHO + HO ₂ + NO ₂	0.59*J_IC3H7N03	see note
J4504e	TrGCJ	ISOPBOOH + hν → MVK + HCHO + HO ₂ + OH + POHORG	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4505e	TrGNCJ	ISOPBNO3 + hν → MVK + HCHO + HO ₂ + NO ₂	2.84*J_IC3H7N03	see note
J4506e	TrGCJ	ISOPDOOH + hν → MACR + HCHO + HO ₂ + OH + POHORG	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4507	TrGNCJ	ISOPDNO3 + hν → MACR + HCHO + HO ₂ + NO ₂	J_IC3H7N03	see note
J4508e	TrGNCJ	NISOPOOH + hν → NC4CHO + HO ₂ + OH + POHORG	1.14*jx(ip_CH300H)	Rickard and Pascoe (2009)*
J4509	TrGNCJ	NC4CHO + hν → NOA + 2 CO + 2 HO ₂	jx(ip_MACR)	see note
J4510e	TrGNCJ	LNISOOH + hν → NOA + OH + .5 CO + .5 HO ₂ + .5 CO ₂ + POHORG	1.14*jx(ip_CH300H)	Taraborrelli et al. (2009)*
J4511e	TrGCJ	LHC4ACCHO + hν → .5 LHC4ACCO3 + .5 HO ₂ + .5 OH + .25 MACRO2 + .25 LHMVKABO2 + .5 POHORG	jx(ip_MACR)	Taraborrelli (2013a)*
J4512e	TrGCJ	LC578OOH + hν → .25 CH ₃ COCH ₂ OH + .75 MGLYOX + .25 HOCH ₂ CHO + .75 HO ₂ + OH + POHORG	1.14*jx(ip_CH300H) + 2.77*jx(ip_HOCH2CHO)	Taraborrelli (2013a)
J4513e	TrGCJ	LHC4ACCO3H + hν → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + 2 POHORG + CO ₂	J_HPALD	Taraborrelli (2013a)*
J4514	TrGNCJ	LC5PAN1719 + hν → .6 LHC4ACCO3 + .6 NO ₂ + .2 MACRO2 + .2 LHMVKABO2 + .4 CO ₂ + .4 NO ₃	jx(ip_PAN)	see note
J4515e	TrGCJ	HCOC5 + hν → +	0.5*jx(ip_MVK)	Taraborrelli (2013a)
J4516e	TrGCJ	C59OOH + hν → CH ₃ COCH ₂ OH + OH + POHORG	J_ACETOL+1.14*jx(ip_CH300H)	Taraborrelli (2013a)
J4517e	TrGCJ	+ hν → LHC4ACCO3 + OH + POHORG	J_HPALD	Taraborrelli (2013a)
J4518e	TrGCJ	+ hν → .62 + .38 + OH + CO ₂ + POHORG	J_HPALD	Taraborrelli (2013a)
J4519e	TrGCJ	+ hν → CH ₃ COCH ₂ O ₂ H + OH + 2 CO + HO ₂ + POHORG	2.77*jx(IP_HOCH2CHO)	Taraborrelli (2013a)
J4520e	TrGCJ	+ hν → .5 CH ₃ COCH ₂ O ₂ H + .5 CO ₂ H3CHO + .5 HCHO + 1.5 OH + 1.5 POHORG	2.*1.14*jx(IP_CH300H)	Taraborrelli (2013a)
J4523e	TrGCJ	+ hν → MGLYOX + OH + POHORG	1.14*jx(IP_CH300H)	Taraborrelli (2013a)
J4524e	TrGCJ	+ hν → CO ₂ H3CHO + CO + HO ₂ + OH + POHORG	2.*2.77*jx(IP_HOCH2CHO)	Taraborrelli (2013a)*
J4525	TrGCJ	+ hν → + HO ₂ + OH + POHORG	1.14*jx(IP_CH300H)	Taraborrelli (2013a)
J4526	TrGCJ	+ hν → HCHO + OH + HO ₂ + CO ₂ H3CHO + POHORG	1.14*jx(IP_CH300H)	Taraborrelli (2013a)*
J4525e	TrGCJ	+ hν → .5 + .5 CO + HO ₂ + OH + POHORG	jx(ip_NO2)*0.1*0.5	Taraborrelli (2013a)
J4526e	TrGCJ	+ hν → CH ₃ C(O)OO + HCHO + GLYOX + HO ₂	1.14*jx(IP_CH300H)+J_ACETOL	Taraborrelli (2013a)
J4527e	TrGCJ	+ hν → CH ₃ C(O)OO + HCHO + HCHO + CO + HO ₂	jx(ip_HOCH2CHO)	Taraborrelli (2013a)

*Notes:

J-values are calculated with an external module and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:

J(11) → jx(ip_COH2)
J(12) → jx(ip_CHOH)
J(15) → jx(ip_HOCH2CHO)
J(18) → jx(ip_MACR)
J(22) → jx(ip_ACETOL)
J(23)+J(24) → jx(ip_MVK)
J(31)+J(32)+J(33) → jx(ip_GLYOX)
J(34) → jx(ip_MGLYOX)
J(41) → jx(ip_CH3OOH)
J(53) → J(iC₃H₇ONO₂)
J(54) → J(iC₃H₇ONO₂)
J(55) → J(iC₃H₇ONO₂)
J(56)+J(57) → jx(ip_NOA)

J4207: It is assumed that J(PHAN) is the same as J(PAN).

J4212: It is assumed that J(ETHOHO3) is the same as J(iC₃H₇ONO₂).

J4302: Following von Kuhlmann et al. (2003), we use J(CH₃COCH₂OH) = 0.11*jx(ip_CHOH). As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a).

J4306: Following von Kuhlmann et al. (2003), we use J(iC₃H₇ONO₂) = 3.7*jx(ip_PAN).

J4307: NOA contains the cromophores of both CH₃COCH₃ and a nitrate group. It is assumed here that the J values are additive, i.e.: J(NOA) = J(CH₃COCH₃) + J(iC₃H₇ONO₂).

J4401: Romero et al(2005)

J4406: It is assumed that J(LC4H9NO3) is the same as J(iC₃H₇ONO₂).

J4407: It is assumed that J(MPAN) is the same as J(PAN).

J4405: It is assumed that J(BIACET) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4414: It is assumed that J(MACROH) is 2.77 times larger than J(HOCH₂CHO), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4505: It is assumed that J(ISOPBNO3) = 2.84 × J(iC₃H₇ONO₂), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4509: It is assumed that J(NC4CHO) is the same as J(MACR).

J4514: It is assumed that J(LC5PAN1719) is the same as J(PAN).

J4526: decomposition of a dialkoxy radical

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