The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs5`

MECCA version: `3.3`

Date: June 30, 2014.

Selected reactions:
"`Tr && G && !S && !Cl && !Br && !I && !Hg`"

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	395
Aqueous phase:	0
All species:	395

Number of reactions in selected mechanism:

Gas phase (Gnnn):	979
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	102
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	0
Isotope exchange (DGnnn):	0
Dummy (Dnn):	0
All equations:	1081

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	$OH + O_3 \rightarrow HO_2$	1.7E-12*EXP(-940./temp)	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	2.8E-12*EXP(-1800./temp)	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	1.E-14*EXP(-490./temp)	Sander et al. (2003)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	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	$H_2O + O(^1D) \rightarrow 2\ OH$	2.2E-10	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	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	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.E-31,2.6,3.6E-11,0.1,0.6)	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	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	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_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	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*log(temp)-987./temp)	Atkinson (2003)
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	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	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	4.1E-13*EXP(750./temp)/(1.+ 497.7*EXP(-1160./temp))	Sander et al. (2003)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2003)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
G4106a	StTrG	$CH_3O_2 \rightarrow HCHO + HO_2$	2.*RO2*9.5E-14*EXP(390./temp)/(1.+1./ 26.2*EXP(1130./temp))	Sander et al. (2003)
G4106b	StTrG	$CH_3O_2 \rightarrow .5\ HCHO + .5\ CH_3OH$	2.*RO2*9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2003)
G4107	StTrG	$CH_3OOH + OH \rightarrow .6\ CH_3O_2 + .4\ HCHO + .4\ OH + H_2O$	k_CH3OOH_OH	see note
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	9.52E-18*EXP(2.03*log(temp)+636./temp)	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	3.4E-13*EXP(-1900./temp)	Sander et al. (2003)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	1.57E-13 + cair*3.54E-33	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow CO_2 + HO_2 + H_2O$	4.5E-13	IUPAC (2013)
G4112e	TrGC	$HCHO + HO_2 \rightarrow HOCH2O2$	7.7E-15*EXP(625./temp)	IUPAC (2013)
G4113e	TrGC	$HOCH2O2 \rightarrow HCHO + HO_2$	2.E12*EXP(-7000./temp)	IUPAC (2013)
G4114e	TrGC	$HOCH2O2 + HO_2 \rightarrow .5\ HOCH2OOH + .5\ HCOOH + .2\ OH + .2\ HO_2 + .3\ H_2O$	5.6E-15*EXP(2300./temp)	Jenkin et al. (2007)
G4115e	TrGC	$HOCH2O2 + NO \rightarrow NO_2 + HO_2 + HCOOH$	2.8E-12*EXP(300./temp)	Sander et al. (2003)
G4116e	TrGC	$HOCH2O2 + NO_3 \rightarrow NO_2 + HO_2 + HCOOH$	1.2E-12	see note
G4117e	TrGC	$HOCH2O2 \rightarrow HCOOH + .62\ HO_2$	1.4E-12*RO2	see note
G4118e	TrGC	$HOCH2OOH + OH \rightarrow HOCH2O2 + H_2O$	0.6*k_CH3OOH_OH + krohro	see note
G4119e	TrGC	$HOCH2OOH + OH \rightarrow OH + HCOOH + H_2O$	ks*fsoh*fsooh	see note
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	1.49E-17*temp*temp*EXP(-499./temp)	Atkinson (2003)
G4201e	TrGC	$C_2H_4 + O_3 \rightarrow HCHO + .63\ CO + .13\ HO_2 + 0.37\ HOCH2OOH + .13\ OH$	1.2E-14*EXP(-2630./temp)	Sander et al. (2003)*
G4202	TrGC	$C_2H_4 + OH \rightarrow HOCH_2CH_2O_2 + H_2O$	k_3rd(temp,cair,1.E-28,0.8,8.8E-12,0., 0.6)	Sander et al. (2003)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*EXP(700./temp)	Sander et al. (2003)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	2.6E-12*EXP(365./temp)	Sander et al. (2003)
G4205	TrGNC	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	2.3E-12	Atkinson et al. (1999)
G4206	TrGC	$C_2H_5O_2 \rightarrow .98\ CH_3CHO + .38\ HO_2 + .02\ HOCH_2CH_2O_2$	3.1E-13*RO2	Rickard and Pascoe (2009)*
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .43\ C_2H_5O_2 + .43\ H_2O + .57\ CH_3CHO + .57\ OH$	0.6*k_CH3OOH_OH + 8.01E-12	see note
G4208ea	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	4.4E-12*EXP(365./temp)*0.95	Atkinson et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G4208eb	TrGC	$CH_3CHO + OH \rightarrow .84\ HCOCH2O2 + .1\ HCHO + .1\ CO + .06\ GLYOX + .16\ OH + H_2O$	4.4E-12*EXP(365./temp)*0.05	Atkinson et al. (2006)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	KNO3AL	Sander et al. (2003)
G4210e	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2 + CO_2 + H_2O$	4.2E-14*exp(850./temp)	IUPAC (2013)
G4211et1	TrGC	$CH_3C(O)OO + HO_2 \rightarrow OH + CH_3O_2 + CO_2$	KAPHO2*0.70	Taraborrelli (2014)*
G4211et2	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	KAPHO2*0.12	Taraborrelli (2014)*
G4211et3	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	KAPHO2*0.18	Taraborrelli (2014)*
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + CO_2 + NO_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_CH3CO3_NO2	Tyndall et al. (2001)*
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2 + CO_2$	4.E-12	Canosa-Mas et al. (1996)
G4217	TrGC	$CH_3C(O)OO \rightarrow .7\ CH_3O_2 + .7\ CO_2 + .3\ CH_3COOH$	1.00E-11*RO2	Rickard and Pascoe (2009)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4220	TrGNC	$PAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	9.50E-13*EXP(-650./temp)	Rickard and Pascoe (2009)
G4221	TrGNC	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_PAN_M	Sander et al. (2003)*
G4223e	TrGC	$HOCH_2CHO + OH \rightarrow .84\ HOCH2CO + .16\ HOCHCHO + .2\ HO_2 + H_2O$	8.00E-12	Rickard and Pascoe (2009)
G4224e	TrGNC	$HOCH_2CHO + NO_3 \rightarrow HOCH2CO + HNO_3$	KNO3AL	Rickard and Pascoe (2009)
G4255et2	TrGC	$HOCH2CO \rightarrow HOCH_2CO_3$	KDEC*.97	Taraborrelli (2014)*
G4255et3	TrGC	$HOCH2CO \rightarrow OH + HCHO + CO$	KDEC*.03	Taraborrelli (2014)*
G4256et2	TrGC	$HOCHCHO \rightarrow GLYOX + HO_2$	KDEC	Taraborrelli (2014)
G4225	TrGC	$HOCH_2CO_3 \rightarrow .7\ HCHO + .7\ CO_2 + .7\ HO_2 + .3\ HOCH_2CO_2H$	1.00E-11*RO2	Rickard and Pascoe (2009)
G4226ea	TrGC	$HOCH_2CO_3 + HO_2 \rightarrow HCHO + HO_2 + OH + CO_2$	KAPHO2*rco3_oh	Taraborrelli (2014)*
G4226eb	TrGC	$HOCH_2CO_3 + HO_2 \rightarrow HOCH_2CO_3H$	KAPHO2*rco3_ooh	Taraborrelli (2014)*
G4226ec	TrGC	$HOCH_2CO_3 + HO_2 \rightarrow HOCH_2CO_2H + O_3$	KAPHO2*rco3_o3	Taraborrelli (2014)*
G4227	TrGNC	$HOCH_2CO_3 + NO \rightarrow NO_2 + HO_2 + HCHO + CO_2$	KAPNO	Rickard and Pascoe (2009)
G4228	TrGNC	$HOCH_2CO_3 + NO_2 \rightarrow PHAN$	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G4229	TrGNC	$HOCH_2CO_3 + NO_3 \rightarrow NO_2 + HO_2 + HCHO + CO_2$	KRO2NO3*1.60	Rickard and Pascoe (2009)
G4230e	TrGC	$HOCH_2CO_2H + OH \rightarrow .09\ HCHO + .09\ CO_2 + .91\ HCOCO_2H + HO_2 + H_2O$	kco2h+ks*fsoh*fco2h	Taraborrelli (2014)
G4231ea	TrGC	$HOCH_2CO_3H + OH \rightarrow HOCH_2CO_3 + H_2O$	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4231eb	TrGC	$HOCH_2CO_3H + OH \rightarrow HCOCO_3H + HO_2$	ks*fsoh*fco2h	Taraborrelli (2014)
G4232	TrGNC	$PHAN \rightarrow HOCH_2CO_3 + NO_2$	k_PAN_M	Rickard and Pascoe (2009)
G4233	TrGNC	$PHAN + OH \rightarrow HCHO + CO + NO_2 + H_2O$	1.12E-12	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4234e	TrGC	GLYOX + OH → 1.2 CO + .6 HO_2 + .4 HCOCO3A + H_2O	3.1E-12*EXP(340./temp)	IUPAC (2013)
G4235e	TrGNC	GLYOX + NO_3 → 1.2 CO + .6 HO_2 + .4 HCOCO3A + HNO_3	KNO3AL	Rickard and Pascoe (2009)
G4235et2	TrGNC	HCOCO3A → 1.5 CO + .5 HO_2 + .5 OH + .5 CO_2	KDEC	Taraborrelli (2014)
G4236	TrGC	$HCOCO_3$ → .7 CO + .7 HO_2 + .7 CO_2 + .3 $HCOCO_2H$	1.00E-11*RO2	Rickard and Pascoe (2009)
G4237e	TrGC	$HCOCO_3$ + HO_2 → HO_2 + CO + CO_2 + OH	KAPHO2	Feierabend et al. (2008),Taraborrelli (2014)
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	KRO2NO3*1.60	Rickard and Pascoe (2009)
G4239t2	TrGNC	$HCOCO_3$ + NO_2 → HO_2 + CO + NO_3 + CO_2	k_CH3CO3_NO2	Orlando and Tyndall (2001),Taraborrelli (2014)*
G4240	TrGC	$HCOCO_2H$ + OH → CO + HO_2 + CO_2 + H_2O	kco2h+kt*fo*fco2h	Taraborrelli (2014)
G4241	TrGC	$HCOCO_3H$ + OH → .2 $HCOCO_3$ + .8 CO + .8 OH + .8 CO_2 + H_2O	0.6*k_CH3OOH_OH+kt*fo*fco2h	Taraborrelli (2014)
G4242	TrGC	$HOCH_2CH_2O_2$ → .6 $HOCH_2CH_2O$ + .2 $HOCH_2CHO$ + .2 ETHGLY	2.00E-12*RO2	Rickard and Pascoe (2009)
G4244	TrGC	$HOCH_2CH_2O_2$ + HO_2 → HYETHO2H	2.00E-13*EXP(1250./temp)	Rickard and Pascoe (2009)
G4243	TrGNC	$HOCH_2CH_2O_2$ + NO → .24875 HO_2 + .4975 HCHO + .74625 $HOCH_2CH_2O$ + .995 NO_2 + .005 ETHOHNO3	KRO2NO	Orlando et al. (1998b)*
G4245	TrGNC	ETHOHNO3 + OH → .93 NO3CH2CHO + .93 HO_2 + .07 $HOCH_2CHO$ + .07 NO_2 + H_2O	ks*(fsoh*fch2ono2+fono2*fpch2oh) +krohro	Taraborrelli (2014)
G4246a	TrGC	HYETHO2H + OH → $HOCH_2CH_2O_2$ + H_2O	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G4246b	TrGC	HYETHO2H + OH → $HOCH_2CHO$ + OH + H_2O	ks*fsooh*fpch2oh	Taraborrelli (2014)
G4246c	TrGC	HYETHO2H + OH → HOOCH2CHO + HO_2 + H_2O	ks*fsoh*fpch2oh+krohro	Taraborrelli (2014)
G4247a	TrGC	$HOCH_2CH_2O$ → HO_2 + $HOCH_2CHO$	6.00E-14*EXP(-550./temp)*C(ind_O2)	Orlando et al. (1998b)
G4247b	TrGC	$HOCH_2CH_2O$ → HO_2 + HCHO + HCHO	9.50E+13*EXP(-5988./temp)	Orlando et al. (1998b)
G4248	TrGC	ETHGLY + OH → $HOCH_2CHO$ + HO_2 + H_2O	2*ks*fsoh*fpch2oh+2*krohro	Taraborrelli (2014)
G4249e	TrGC	HCOCH2O2 → 0.6 HCHO + 0.6 CO + 0.6 HO_2 + 0.2 GLYOX + 0.2 $HOCH_2CHO$	2.00E-12*RO2	Taraborrelli (2014)
G4250e	TrGC	HCOCH2O2 + HO_2 → 0.85 HOOCH2CHO + 0.15 HCHO + 0.15 CO + 0.15 HO_2 + 0.15 OH	KRO2HO2*0.387	Taraborrelli (2014)
G4251e	TrGC	HCOCH2O2 + NO → NO_2 + HCHO + CO + HO_2	KRO2NO	Taraborrelli (2014)
G4252e	TrGC	HCOCH2O2 + NO_3 → HCHO + CO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4253e	TrGC	HOOCH2CHO + OH → .71 OH + .31 HCHO + .31 CO + .40 GLYOX + .29 HCOCH2O2	0.6*k_CH3OOH_OH+ks*fsooh*fcho+.8*8.E-12	Taraborrelli (2014)
G4254e	TrGNC	HOOCH2CHO + NO_3 → OH + HCHO + CO + HNO_3	KNO3AL	Rickard and Pascoe (2009)
G4257e	TrGC	NO3CH2CHO + OH → HCHO + CO_2 + NO_2 + H_2O	1.E-11	Paulot et al. (2009a),Taraborrelli (2014)
G4258e	TrGNC	HOOCH2CO3 + NO → NO_2 + OH + HCHO + CO_2	KAPNO	Taraborrelli (2014)
G4259e	TrGNC	HOOCH2CO3 + NO_3 → NO_2 + OH + HCHO + CO_2	KRO2NO3*1.60	Taraborrelli (2014)
G4260e	TrGC	HOOCH2CO3 + HO_2 → 2 OH + HCHO + CO_2	KAPHO2*rco3_oh	Taraborrelli (2014)
G4260et2	TrGC	HOOCH2CO3 + HO_2 → HOOCH2CO3H	KAPHO2*rco3_ooh	Taraborrelli (2014)*
G4260et3	TrGC	HOOCH2CO3 + HO_2 → HOOCH2CO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2014)*
G4261e	TrGC	HOOCH2CO3 → .7 OH + .7 HCHO + .7 CO_2 + .3 HOOCH2CO2H	1.00E-11*RO2	Taraborrelli (2014)
G4262e	TrGC	HOOCH2CO3H + OH → HOOCH2CO3 + H_2O	2.*0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4263e	TrGC	HOOCH2CO3H + OH → $HCOCO_3H$ + OH + H_2O	ks*fsooh*fco2h	Taraborrelli (2014)
G4265e	TrGC	HOOCH2CO2H + OH → $HCOCO_2H$ + OH + H_2O	ks*fsooh*fco2h+kco2h	Taraborrelli (2014)
G4266e	TrGC	CH2CO + OH → .6 HCHO + .6 HO_2 + .6 CO + .4 HOOCH2CO2H	2.8E-12*exp(510./temp)	Baulch et al. (2005),Taraborrelli (2014)*
G4267e	TrGC	CH3CHOHOOH + OH → CH_3COOH + OH	kt*ftooh*ftoh + krohro	Taraborrelli (2014)
G4268e	TrGC	CH3CHOHOOH + OH → CH3CHOHO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4269e	TrGC	CH3CHOHO2 → CH_3CHO + HO_2	3.46E12*EXP(-12500./(1.98*temp))	Hermans et al. (2005),Taraborrelli (2014)
G4270e	TrGC	CH_3CHO + HO_2 → CH3CHOHO2	3.46E12*EXP(-12500./(1.98*temp)) /(6.34E26*EXP(-14700./(1.98*temp)))	Hermans et al. (2005),Taraborrelli (2014)
G4271e	TrGC	CH3CHOHO2 + HO_2 → .5 CH3CHOHOOH + .3 CH_3COOH + .2 CH_3O_2 + .2 HCOOH + .2 OH	5.6E-15*EXP(2300./temp)	Taraborrelli (2014)
G4272e	TrGC	CH3CHOHO2 → CH_3O_2 + HCOOH + OH	1.4E-12*RO2	Taraborrelli (2014)
G4273e	TrGC	CH3CHOHO2 + NO → CH_3O_2 + HCOOH + OH + NO_2	KRO2NO	Taraborrelli (2014)
G4300	TrGC	C_3H_8 + OH → .736 $iC_3H_7O_2$ + .264 $C_2H_5O_2$ + .264 CO_2 + .264 HO_2 + H_2O	1.55E-17*temp*temp*EXP(-61./temp)	Rickard and Pascoe (2009)*
G4301et2	TrGC	C_3H_6 + O_3 → .0855 CH3CHOHOOH + .4389 CH_3CHO + .4389 H_2O_2 + .0456 CH_3COOH + .285 HCOCH2O2 + .0855 CH_4 + .0855 CO_2 + .0342 CH2CO + .0513 CH_3OH + .0228 $CH_3C(O)OO$ + .57 HCHO + .2709 CO + .0688 HO_2 + .1591 HOCH2OOH + .43 CH_3CHO + .3766 OH	6.5E-15*EXP(-1900./temp)	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4302	TrGC	C_3H_6 + OH → HYPROPO2	k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)	Atkinson et al. (1999)
G4303	TrGNC	C_3H_6 + NO_3 → PRONO3BO2	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	$iC_3H_7O_2$ + HO_2 → iC_3H_7OOH	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G4305	TrGNC	$iC_3H_7O_2$ + NO → .96 CH_3COCH_3 + .96 HO_2 + .96 NO_2 + .04 $iC_3H_7ONO_2$	2.7E-12*EXP(360./temp)	Atkinson et al. (1999)
G4306	TrGC	$iC_3H_7O_2$ → CH_3COCH_3 + .8 HO_2	4.E-14*RO2	Rickard and Pascoe (2009)*
G4307	TrGC	iC_3H_7OOH + OH → .27 $iC_3H_7O_2$ + .73 CH_3COCH_3 + .73 OH + H_2O	1.66E-11 + 0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4311	TrGC	CH_3COCH_3 + OH → $CH_3COCH_2O_2$ + H_2O	1.33E-13+3.82E-11*EXP(-2000./temp)	Sander et al. (2003)
G4312e	TrGC	$CH_3COCH_2O_2$ + HO_2 → .15 OH + .15 $CH_3C(O)OO$ + .15 HCHO + .85 $CH_3COCH_2O_2H$	8.6E-13*EXP(700./temp)	Taraborrelli (2014)
G4313	TrGNC	$CH_3COCH_2O_2$ + NO → $CH_3C(O)OO$ + HCHO + NO_2	2.9E-12*EXP(300./temp)	Sander et al. (2003)
G4314	TrGC	$CH_3COCH_2O_2$ → .6 $CH_3C(O)OO$ + .6 HCHO + .2 MGLYOX + .2 CH_3COCH_2OH	7.5E-13*EXP(500./temp)*2.*RO2	Tyndall et al. (2001)
G4321	TrGNC	$CH_3COCH_2O_2$ + NO_3 → $CH_3C(O)OO$ + HCHO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4315a	TrGC	$CH_3COCH_2O_2H$ + OH → $CH_3COCH_2O_2$ + H_2O	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4315b	TrGC	$CH_3COCH_2O_2H$ + OH → MGLYOX + OH + H_2O	ks*fsooh*fco	Taraborrelli (2014)
G4316e	TrGC	CH_3COCH_2OH + OH → CH3COCHOH + H_2O	1.60E-12*EXP(305./temp)	Taraborrelli (2014)
G4336ea	TrGC	CH3COCHOH → MGLYOX + HO_2	0.8485	Taraborrelli (2014)
G4317e	TrGC	MGLYOX + OH → .4 CH_3O_2 + .6 $CH_3C(O)OO$ + 1.4 CO	1.9E-12*EXP(575./temp)	Baeza-Romero et al. (2007),IUPAC (2013)
G4331	TrGNC	MGLYOX + NO_3 → $CH_3C(O)OO$ + CO + HNO_3	KNO3AL*2.4	Rickard and Pascoe (2009)
G4320	TrGNC	$iC_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	6.2E-13*EXP(-230./temp)	Atkinson et al. (1999)
G4322	TrGC	HYPROPO2 → CH_3CHO + HCHO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009)
G4323	TrGC	HYPROPO2 + HO_2 → HYPROPO2H	KRO2HO2*0.520	Rickard and Pascoe (2009)
G4324	TrGNC	HYPROPO2 + NO → CH_3CHO + HCHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4325	TrGNC	HYPROPO2 + NO_3 → CH_3CHO + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4326a	TrGC	HYPROPO2H + OH → HYPROPO2	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)
G4326b	TrGC	HYPROPO2H + OH → CH_3COCH_2OH + OH	ks*fsoh*fpch2oh+kt*ftooh*fpch2oh	Taraborrelli (2014)
G4327	TrGNC	PRONO3BO2 + HO_2 → PR2O2HNO3	KRO2HO2*0.520	Rickard and Pascoe (2009)
G4328	TrGNC	PRONO3BO2 + NO → NOA + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4329	TrGNC	PRONO3BO2 + NO_3 → NOA + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4330a	TrGNC	PR2O2HNO3 + OH → PRONO3BO2	1.90E-12*EXP(190./temp)	Rickard and Pascoe (2009)
G4330b	TrGNC	PR2O2HNO3 + OH → NOA + OH	kt*ftooh*fch2ono2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4332	TrGNC	NOA + OH → MGLYOX + NO_2	ks*fco*fono2+kp*fco	Taraborrelli (2014)
G4333e	TrGC	HOCH2COCHO + OH → .8609 HOCH2CO + .8609 CO + .1391 HCOCOCHO + .1391 HO_2	1.9E-12*EXP(575./temp)+ks*fsoh*fco	Taraborrelli (2014)
G4334e	TrGNC	HOCH2COCHO + NO_3 → HOCH2CO + CO + HNO_3	KNO3AL*2.4	Taraborrelli (2014)
G4337e	TrGC	CH3COCO2H + OH → $CH_3C(O)OO$ + H_2O + CO_2	4.9E-14*EXP(276./temp)	Mellouki and Mu (2003),Taraborrelli (2014)
G4338e	TrGC	HOCH2COCH2O2 → HCHO + HOCH2CO	RO2*2.0E-12	Taraborrelli (2014)
G4339e	TrGC	HOCH2COCH2O2 + HO_2 → .15 HCHO + .15 HOCH2CO + .15 OH + .85 HOCH2COCH2OOH	KRO2HO2*0.520	Taraborrelli (2014)
G4340e	TrGC	HOCH2COCH2O2 + NO → HCHO + HOCH2CO + NO_2	KRO2NO	Taraborrelli (2014)
G4341e	TrGC	HOCH2COCH2OOH + OH → HOCH2COCHO + OH	ks*fsooh*fco	Taraborrelli (2014)
G4342e	TrGC	HOCH2COCH2OOH + OH → HOCH2COCH2O2	.6*k_CH3OOH_OH	Taraborrelli (2014)
G4343e	TrGC	HOCH2COCH2OOH + OH → HCOCOCH2OOH + HO_2	0.9295*1.60E-12*EXP(305./temp)	Taraborrelli (2014)*
G4344e	TrGC	HCOCOCH2O2 → 0.6 HCOCO3A + 0.6 HCHO + 0.2 HCOCOCHO + 0.2 HOCH2COCHO	2.00E-12*RO2	Taraborrelli (2014)
G4345e	TrGC	HCOCOCH2O2 + NO → HCOCO3A + HCHO + NO_2	KRO2NO	Taraborrelli (2014)
G4346e	TrGC	HCOCOCH2O2 + HO_2 → 0.85 HCOCOCH2OOH + 0.15 HCOCO3A + 0.15 HCHO + 0.15 OH	KRO2HO2*0.520	Taraborrelli (2014)
G4347e	TrGC	HCOCOCH2O2 + NO_3 → HCOCO3A + HCHO + NO_2	KRO2NO3	Taraborrelli (2014)
G4348e	TrGC	HCOCOCH2OOH + OH → HOOCH2CO3 + CO + H_2O	kt*fo*fco	Taraborrelli (2014)
G4349e	TrGC	HCOCOCH2OOH + OH → HCOCOCHO + OH + H_2O	ks*fsooh*fco	Taraborrelli (2014)
G4350e	TrGC	HCOCOCH2OOH + OH → HCOCOCH2O2 + H_2O	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4351e	TrGC	HCOCOCH2OOH + NO_3 → HOOCH2CO3 + CO + HNO_3	KNO3AL*2.4	Taraborrelli (2014)
G4352e	TrGC	HCOCOCHO + OH → HCOCO3A + CO	2*kt*fco*fo	Taraborrelli (2014)
G4353e	TrGC	CH3CHCO + OH → .72 CO + .72 CH_3CHO + .72 HO_2 + .21 CH3COCO2H + .07 CH_3CHO + .07 HO_2 + .07 CO_2	7.6E-11	Hatakeyama et al. (1985),Taraborrelli (2014)*
G4354e	TrGC	HCOCCH3CO + OH → CO + CH3COCHOH	1E-10*acho	Hatakeyama et al. (1985),Taraborrelli (2014)*
G4355e	TrGC	CH3COCHCO + OH → CO + CH3COCHOH	7.6E-11*acoch3	Hatakeyama et al. (1985),Taraborrelli (2014)*
G4400	TrGC	nC_4H_{10} + OH → $LC_4H_9O_2$ + H_2O	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)*
G4401	TrGC	$LC_4H_9O_2$ → 0.254 CO_2 + 0.5552 MEK + 0.5552 HO_2 + 0.3178 CH_3CHO + 0.4448 $C_2H_5O_2$	2.5E-13*RO2	Rickard and Pascoe (2009)*
G4402	TrGC	$LC_4H_9O_2$ + HO_2 → LC_4H_9OOH	KRO2HO2*0.625	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4403	TrGNC	$LC_4H_9O_2$ + NO → 0.9172 NO_2 + 0.233 CO_2 + 0.5092 MEK + 0.5092 HO_2 + 0.2915 CH_3CHO + 0.408 $C_2H_5O_2$ + 0.0828 LC4H9NO3	KRO2NO	Rickard and Pascoe (2009)*
G4404	TrGC	LC_4H_9OOH + OH → 0.2285796 $LC_4H_9O_2$ + 0.7117253 MEK + 0.1193902 CO_2 + 0.0596951 $C_2H_5O_2$ + 0.7714204 OH + H_2O	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 $CH_3C(O)OO$ + .026 CH_3CHO + .026 CO_2 + .026 HCHO + .026 HO_2 + 0.02402 MGLYOX + 0.02402 H_2O_2 + 0.007176 CH3COCO2H	8.5E-16*EXP(-1520./temp)	Taraborrelli (2014)
G4406e	TrGC	MVK + OH → LHMVKABO2	2.6E-12*EXP(610./temp)	Taraborrelli (2014)*
G4413	TrGC	MEK + OH → LMEKO2 + H_2O	3.24E-18*temp*temp*EXP(414./temp)	Rickard and Pascoe (2009)*
G4414ea	TrGC	LMEKO2 + HO_2 → LMEKOOH	KRO2HO2*0.625*rcoch2o2_ooh	Taraborrelli (2014)
G4414eb	TrGC	LMEKO2 + HO_2 → 0.538 HCHO + 0.538 CO_2 + 0.459 $HOCH_2CH_2O_2$ + 0.079 $C_2H_5O_2$ + 0.462 $CH_3C(O)OO$ + 0.462 CH_3CHO + OH	KRO2HO2*0.625*rcoch2o2_oh	Taraborrelli (2014)
G4415	TrGNC	LMEKO2 + NO → 0.538 HCHO + 0.538 CO_2 + 0.459 $HOCH_2CH_2O_2$ + 0.079 $C_2H_5O_2$ + 0.462 $CH_3C(O)OO$ + 0.462 CH_3CHO + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G4416	TrGC	LMEKOOH + OH → 0.40851 $CH_3COCH_2O_2$ + 0.350196 BIACET + 0.807212 OH + 0.048506 $C_2H_5O_2$ + 0.505522 CO_2 + 0.192788 LMEKO2 + H_2O	3.786E-11	Rickard and Pascoe (2009)*
G4417	TrGNC	LC4H9NO3 + OH → 0.91423 MEK + 0.08577 $C_2H_5O_2$ + 0.17154 CO_2 + NO_2 + H_2O	9.598E-13	Rickard and Pascoe (2009)*
G4418	TrGNC	MPAN + OH → CH_3COCH_2OH + CO + NO_2	3.2E-11	Orlando et al. (2002)
G4419	TrGNC	MPAN → MACO3 + NO_2	k_PAN_M	see note
G4420	TrGC	LMEKO2 → 0.538 HCHO + 0.538 CO_2 + 0.459 $HOCH_2CH_2O_2$ + 0.079 $C_2H_5O_2$ + 0.462 $CH_3C(O)OO$ + 0.462 CH_3CHO	1.483E-12*RO2	Rickard and Pascoe (2009)*
G4421e	TrGC	MACR + OH → .45 MACO3 + .55 MACRO2	8.E-12*EXP(380./temp)	Orlando et al. (1999b),Taraborrelli (2014)
G4422e	TrGC	MACR + O_3 → 0.5481 CO + 0.1392 HO_2 + 0.1392 OH + 0.3219 HOCH2OOH + .87 MGLYOX + .13 HCHO + .13 OH + .065 HCOCOCH2O2 + .065 CO + .065 $CH_3C(O)OO$	1.36E-15*EXP(-2112./temp)	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4423	TrGNC	MACR + NO_3 → MACO3 + HNO_3	KNO3AL*2.0	Rickard and Pascoe (2009)
G4424e	TrGC	MACO3 → .7 MACO2 + .3 MACO2H	1.00E-11*RO2	Taraborrelli (2014)
G4425e	TrGC	MACO3 + HO_2 → MACO2 + OH	KAPHO2*rco3_oh	Taraborrelli (2014)
G4425et2	TrGC	MACO3 + HO_2 → MACO3H	KAPHO2*rco3_ooh	Taraborrelli (2014)
G4425et3	TrGC	MACO3 + HO_2 → MACO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2014)
G4426e	TrGNC	MACO3 + NO → MACO2 + NO_2	8.70E-12*EXP(290./temp)	Taraborrelli (2014)
G4427	TrGNC	MACO3 + NO_2 → MPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G4428e	TrGNC	MACO3 + NO_3 → MACO2 + NO_2	KRO2NO3*1.60	Taraborrelli (2014)
G4429e	TrGC	MACRO2 → .7 CH_3COCH_2OH + .7 HCHO + .7 HO_2 + .3 MACROH	9.20E-14*RO2	Taraborrelli (2014)
G4430e	TrGC	MACRO2 + HO_2 → MACRO + OH	KRO2HO2*0.625*rcoch2o2_oh	Taraborrelli (2014)
G4430et2	TrGC	MACRO2 + HO_2 → MACROOH	KRO2HO2*0.625*rcoch2o2_ooh	Taraborrelli (2014)
G4431e	TrGNC	MACRO2 + NO → .85 MACRO + .85 NO_2 + .15 MACRN	KRO2NO	Taraborrelli (2014)
G4432e	TrGNC	MACRO2 + NO_3 → MACRO + NO_2	KRO2NO3	Taraborrelli (2014)
G4433ea	TrGC	MACROOH + OH → MACRO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4433eb	TrGC	MACROOH + OH → CO + OH + CH_3COCH_2OH	kt*fo*ftch2oh*falk	Taraborrelli (2014)
G4433ec	TrGC	MACROOH + OH → CO + MGLYOX + HO_2	ks*fsoh*fpch2oh + krohro	Taraborrelli (2014)
G4434e	TrGC	MACROH + OH → CH_3COCH_2OH + CO + HO_2	kt*fo*ftch2oh*falk	Taraborrelli (2014)
G4434et2	TrGC	MACRO → .885 CH_3COCH_2OH + .885 CO + .115 MGLYOX + .115 HCHO + HO_2	KDEC	Taraborrelli (2014)
G4435e	TrGC	MACO2H + OH → CH_3COCH_2OH + HO_2 + CO_2	(kadt+kadp)*aco2h+kco2h	Taraborrelli (2014)
G4436e	TrGC	MACO3H + OH → CH_3COCH_2OH + CO_2 + OH	0.6*k_CH3OOH_OH+(kadt+kadp)*aco2h	Taraborrelli (2014)
G4437e	TrGC	LHMVKABO2 → .024 CO2H3CHO + .072 CH3COCHOH + .072 HCHO + .5280 $CH_3C(O)OO$ + .5280 $HOCH_2CHO$ + .176 BIACETOH + .2 HO12CO3C4	1.014E-12*RO2	Taraborrelli (2014)*
G4438e	TrGC	LHMVKABO2 + HO_2 → OH + $HOCH_2CHO$ + $CH_3C(O)OO$	KRO2HO2*0.625*.88*rcoch2o2_oh	Taraborrelli (2014)
G4438et2	TrGC	LHMVKABO2 + HO_2 → LHMVKABOOH	KRO2HO2*0.625*(.12+.88*rcoch2o2_ooh)	Taraborrelli (2014)
G4439ea	TrGNC	LHMVKABO2 + NO → .12 CH3COCHOH + .88 $HOCH_2CHO$ + .88 $CH_3C(O)OO$ + .12 HCHO + NO_2	KRO2NO*(1.-0.11)	Taraborrelli (2014)*
G4439eb	TrGNC	LHMVKABO2 + NO → HMVKNO3	KRO2NO*0.11	Taraborrelli (2014)
G4440e	TrGNC	LHMVKABO2 + NO_3 → .12 MGLYOX + .88 $HOCH_2CHO$ + .88 $CH_3C(O)OO$ + .12 HCHO + .12 HO_2 + NO_2	KRO2NO3	Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G4441e	TrGC	LHMVKABOOH + OH → .12 CO2H3CHO + .88 BIACETOH + OH	0.6*k_CH3OOH_OH+.12*ks*fsooh*fpch2oh+ .88*kt*ftooh*fpch2oh*fco	Taraborrelli (2014)*
G4449e	TrGC	CO2H3CHO + OH → CO2H3CO3	kt*fo*falk	Taraborrelli (2014)
G4449et2	TrGC	CO2H3CHO + OH → CH3COCOCHO + HO_2 + H_2O	kt*fco*ftoh*fcho	Taraborrelli (2014)
G4450	TrGNC	CO2H3CHO + NO_3 → CO2H3CO3 + HNO_3	KNO3AL*4.0	Rickard and Pascoe (2009)
G4451e	TrGC	CO2H3CO3 → CH3COCHOH + CO_2	1.00E-11*RO2	Taraborrelli (2014)
G4452e	TrGC	CO2H3CO3 + HO_2 → OH + CH3COCHOH + CO_2	KAPHO2*rco3_oh	Taraborrelli (2014)
G4452et2	TrGC	CO2H3CO3 + HO_2 → CO2H3CO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2014)
G4452et3	TrGC	CO2H3CO3 + HO_2 → CO2H3CO3H	KAPHO2*rco3_ooh	Taraborrelli (2014)
G4453e	TrGNC	CO2H3CO3 + NO → CH3COCHOH + NO_2 + CO_2	KAPNO	Taraborrelli (2014)
G4454e	TrGNC	CO2H3CO3 + NO_3 → CH3COCHOH + NO_2 + CO_2	KRO2NO3*1.60	Taraborrelli (2014)
G4455	TrGC	CO2H3CO3H + OH → 0.5127 CO2H3CO3 + 0.4873 $CH_3C(O)OO$ + 0.4873 CO + 0.4873 CO_2 + 0.4873 OH	kt*fco2h*fco*ftoh+0.6*k_CH3OOH_OH	Taraborrelli (2014)*
G4455t2	TrGC	CO2H3CO2H + OH → CH3COCOCO2H + HO_2	kt*fco2h*fco*ftoh+kco2h	Taraborrelli (2014)
G4456a	TrGC	HO12CO3C4 + OH → BIACETOH + HO_2	kt*ftoh*falk*fco	Taraborrelli (2014)
G4456b	TrGC	HO12CO3C4 + OH → CO2H3CHO + HO_2	ks*fsoh*falk	Taraborrelli (2014)
G4457e	TrGC	MACO2 → .65 CH_3O_2 + .65 CO + .65 HCHO + .35 OH + .35 $CH_3COCH_2O_2$ + CO_2	KDEC	Taraborrelli (2014)
G4458e	TrGC	LHMVKABO2 → .88 MGLYOX + .88 HCHO + .12 HOOCH2CHO + .12 $CH_3C(O)OO$ + OH	KHSD	Taraborrelli (2014)
G4459e	TrGNC	MACRO2 → MGLYOX + HCHO + OH	KHSB	Taraborrelli (2014)
G4460e	TrGNC	HMVKNO3 + OH → .7 MGLYOX + .7 HCOOH + .7 NO_3 + .3 CO2H3CHO + .3 NO_2 + H_2O	5.6E-12	Taraborrelli (2014)
G4461e	TrGC	MACRN + OH → .08 CH_3COOH + .08 HCHO + .15 NO_3 + .07 HCOOH + .07 MGLYOX + .85 CH_3COCH_2OH + .85 NO_3 + .93 CO_2 + H_2O	5.E-11	Taraborrelli (2014)
G4462e	TrGC	EZCH3CO2CHCHO → .9 CH3COCHCO + .1 $CH_3C(O)OO$ + .01 GLYOX + .18 CO + .09 HO_2 + OH	k16HS	Taraborrelli (2014)*
G4463e	TrGC	EZCHOCCH3CHO2 → HCOCCH3CO + OH	K16HS	Taraborrelli (2014)*
G4500e	TrGC	C_5H_8 + O_3 → .3508 MACR + 0.01518 MACO2H + .2440 MVK + .7085 HCHO + .11 HOCH2OOH + .1275 C_3H_6 + .1575 $CH_3C(O)OO$ + .0510 CH_3O_2 + 0.2625 HO_2 + .27 OH + .09482 H_2O_2 + .255 CO_2 + .522 CO + 0.07182 HCHO + .03618 HCOCH2O2 + .01782 CO	1.03E-14*EXP(-1995./temp)	Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G4501e	TrGC	C_5H_8 + OH → .63 ISOPAB + .30 ISOPCD + .07 LISOPEFO2	2.7E-11*EXP(390./temp)*(1.-iseg)	Taraborrelli (2014)*
G4502	TrGNC	C_5H_8 + NO_3 → NISOPO2	3.15E-12*EXP(-450./temp)	Rickard and Pascoe (2009)
G4503e	TrGC	ISOPAB + O_2 → LISOPACO2	5.530E-13	Taraborrelli (2014)*
G4504e	TrGC	ISOPAB + O_2 → ISOPBO2	3.E-12	Taraborrelli (2014)*
G4505e	TrGC	ISOPCD + O_2 → DLISOPACO2	6.780E-13	Taraborrelli (2014)*
G4506e	TrGC	ISOPCD + O_2 → ISOPDO2	3.E-12	Taraborrelli (2014)*
G4507e	TrGC	LISOPACO2 → ISOPAB + O_2	3.1E12*exp(-7900./temp)*.6+ 7.8E13*exp(-8600./temp)*.4	Taraborrelli (2014)*
G4508e	TrGC	ISOPBO2 → ISOPAB + O_2	3.7E14*exp(-9570./temp) +4.2E14*exp(-9970./temp)	Taraborrelli (2014)*
G4509e	TrGC	DLISOPACO2 → ISOPCD + O_2	5.65E12*exp(-8410./temp)*.42+ 1.4E14*exp(-9110./temp)*.58	Taraborrelli (2014)*
G4510e	TrGC	ISOPDO2 → ISOPCD + O_2	5.0E14*exp(-10120./temp) +8.25E14*exp(-10220/temp)	Taraborrelli (2014)*
G4511e	TrGC	LISOPACO2 → ZCODC23DBCOOH + HO_2	K16HS	Taraborrelli (2014)*
G4512e	TrGC	DLISOPACO2 → ZCODC23DBCOOH + HO_2	K16HS	Taraborrelli (2014)*
G4513et3	TrGC	LISOPACO2 → .9 LHC4ACCHO + .8 HO_2 + .1 ISOPAOH	2.4E-12*RO2	Rickard and Pascoe (2009)
G4514t2	TrGC	LISOPACO2 + HO_2 → LISOPACOOH	.706*KRO2HO2	Rickard and Pascoe (2009)
G4515et2	TrGNC	LISOPACO2 + NO → 0.95 LHC4ACCHO + 0.95 HO_2 + 0.95 NO_2 + .05 LISOPACNO3	KRO2NO	Lockwood et al. (2010),Taraborrelli (2014)
G4506et3	TrGNC	LISOPACO2 + NO_3 → LHC4ACCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4507et3	TrGC	DLISOPACO2 → .9 LHC4ACCHO + .8 HO_2 + .1 ISOPAOH	2.4E-12*RO2	Rickard and Pascoe (2009)
G4511et3	TrGC	DLISOPACO2 + HO_2 → LISOPACOOH	.706*KRO2HO2	Rickard and Pascoe (2009)
G4512et3	TrGNC	DLISOPACO2 + NO → 0.95 LHC4ACCHO + 0.95 HO_2 + 0.95 NO_2 + .05 LISOPACNO3	KRO2NO	Lockwood et al. (2010),Taraborrelli (2014)
G4513et4	TrGNC	DLISOPACO2 + NO_3 → LHC4ACCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4514e	TrGC	LISOPACOOH + OH → LISOPACO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4514et2	TrGC	LISOPACOOH + OH → ZCODC23DBCOOH + HO_2	ks*fallyl*fsoh	Taraborrelli (2014)
G4514et3	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH	ks*fsooh*fallyl+ krohro	Taraborrelli (2014)
G4514et4	TrGC	LISOPACOOH + OH → IEPOX + OH	(kadt+kads)*ach2oh*ach2ooh	Taraborrelli (2014)
G4515	TrGC	ISOPAOH + OH → LHC4ACCHO + HO_2	(kadt+kads)*ach2oh*ach2oh+ ks*fsoh*fallyl+krohro	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4516e	TrGNC	LISOPACNO3 + OH → LISOPACNO3O2	9.5E-11	Paulot et al. (2009a),Taraborrelli (2014)
G4517e	TrGC	ISOPBO2 → .8 MVK + .8 HCHO + .8 HO_2 + .2 ISOPBOH	8.E-13*RO2	Rickard and Pascoe (2009)
G4518	TrGC	ISOPBO2 + HO_2 → ISOPBOOH	.706*KRO2HO2	Rickard and Pascoe (2009)
G4519e	TrGNC	ISOPBO2 + NO → .947 MVK + .947 HCHO + .947 HO_2 + .947 NO_2 + .053 ISOPBNO3	KRO2NO	Lockwood et al. (2010),Taraborrelli (2014)
G4520e	TrGNC	ISOPBO2 + NO_3 → MVK + .75 HCHO + .75 HO_2 + .25 CH_3O_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4521ea	TrGC	ISOPBOOH + OH → IEPOX + OH	(kads+kadp)*ach2ooh	Paulot et al. (2009b),Taraborrelli (2014)
G4521eb	TrGC	ISOPBOOH + OH → ISOPBO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4521ec	TrGC	ISOPBOOH + O_3 → 0.1368 MACROOH + 0.1368 H_2O_2 + 0.2280 HO_2 + 0.4332 CH_3COCH_2OH + 0.2280 CO_2 + 0.6384 OH + 0.2052 CO + .57 HCHO + .43 MACROOH + 0.06880 HO_2 + 0.06880 OH + 0.2709 CO + 0.1591 HOCH2OOH	1.E-17	Taraborrelli (2014)*
G41911	TrGC	ISOPBOOH + OH → MGLYOX + $HOCH_2CHO$	krohro+ks*falk*fsoh	Taraborrelli (2014)
G4522e	TrGC	ISOPBOH + OH → MVK + .75 HCHO + .75 HO_2 + .25 CH_3O_2	ks*falk*fsoh+(kadp+kads)*ach2oh	Taraborrelli (2014)
G4523e	TrGNC	ISOPBNO3 + OH → ISOPBDNO3O2	1.3E-11	Paulot et al. (2009a),Taraborrelli (2014)
G4524	TrGC	ISOPDO2 → .8 MACR + .8 HCHO + .8 HO_2 + .1 HCOC5 + .1 ISOPDOH	2.9E-12*RO2	Rickard and Pascoe (2009)
G4525	TrGC	ISOPDO2 + HO_2 → ISOPDOOH	.706*KRO2HO2	Rickard and Pascoe (2009)
G4526e	TrGNC	ISOPDO2 + NO → .85 MACR + .85 HCHO + .85 HO_2 + .85 NO_2 + .15 ISOPDNO3	KRO2NO	Lockwood et al. (2010),Taraborrelli (2014)
G4527	TrGNC	ISOPDO2 + NO_3 → MACR + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4528ea	TrGC	ISOPDOOH + OH → IEPOX + OH	(kadt+kadp)*ach2ooh	Paulot et al. (2009b),Taraborrelli (2014)
G4528eb	TrGC	ISOPDOOH + OH → ISOPDO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4528ec	TrGC	ISOPDOOH + OH → HCOC5 + OH	kt*ftooh*fallyl*fpch2oh	Taraborrelli (2014)
G4528ed	TrGC	ISOPDOOH + OH → CH_3COCH_2OH + GLYOX + OH	ks*fpch2oh*fsoh	Taraborrelli (2014)
G45222	TrGC	ISOPDOOH + O_3 → 1.393 OH + BIACETOH + .67 HCHO + 0.05280 HO_2 + 0.2079 CO + 0.1221 HOCH2OOH	1.E-17	Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G4529e	TrGC	ISOPDOH + OH → HCOC5 + HO_2	2.*krohro+(kt*ftoh*fallyl+ks*fsoh) *fpch2oh+(kadt+kadp)*ach2oh	Taraborrelli (2014)
G4530e	TrGNC	ISOPDNO3 + OH → ISOPBDNO3O2	1.3E-11	Paulot et al. (2009a),Taraborrelli (2014)
G4531	TrGNC	NISOPO2 → .8 NC4CHO + .6 HO_2 + .2 LISOPACNO3	1.3E-12*RO2	Rickard and Pascoe (2009)
G4532	TrGNC	NISOPO2 + HO_2 → NISOPOOH	.706*KRO2HO2	Rickard and Pascoe (2009)
G4533	TrGNC	NISOPO2 + NO → NC4CHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4534	TrGNC	NISOPO2 + NO_3 → NC4CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4535	TrGNC	NISOPOOH + OH → NC4CHO + OH	1.03E-10	Rickard and Pascoe (2009)
G4536	TrGNC	NC4CHO + OH → LNISO3	4.16E-11	Rickard and Pascoe (2009)
G4537e	TrGNC	NC4CHO + O_3 → .27 NOA + .027 $HCOCO_2H$ + .0162 GLYOX + .0162 H_2O_2 + .1458 HCOCO3A + .0405 HCOOH + .0405 CO + .8758 OH + .365 MGLYOX + .73 NO_2 + 0.7705 HCHO + .4055 CO_2 + .73 GLYOX	2.40E-17	Taraborrelli (2014)*
G4538	TrGNC	NC4CHO + NO_3 → LNISO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
G4539	TrGNC	LNISO3 + HO_2 → LNISOOH	.5*.706*KRO2HO2 + .5*KAPHO2	Rickard and Pascoe (2009)
G4540e	TrGNC	LNISO3 + NO → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	.5*KAPNO +.5*KRO2NO	Rickard and Pascoe (2009)
G4541e	TrGNC	LNISO3 + NO_3 → NOA + .5 HOCHCHO + .5 CO + .5 HO_2 + NO_2 + .5 CO_2	1.3*KRO2NO3	Rickard and Pascoe (2009)
G4542	TrGNC	LNISOOH + OH → LNISO3	2.65E-11	Rickard and Pascoe (2009)
G4543e	TrGC	LHC4ACCHO + OH → LC578O2	(kadtertprim+kads)*acho*ach2oh	Taraborrelli (2014)
G4543et2	TrGC	LHC4ACCHO + OH → LHC4ACCO3	kcho	Taraborrelli (2014)
G4543et3	TrGC	LHC4ACCHO + OH → ZCODC23DBCOD + HO_2	ks*fsoh*fallyl	Taraborrelli (2014)
G4544	TrGC	LHC4ACCHO + O_3 → .2225 $CH_3C(O)OO$ + .89 CO + .0171875 $HOCH_2CO_2H$ + .075625 H_2O_2 + .0171875 $HCOCO_2H$ + .2775 CH_3COCH_2OH + .6675 HO_2 + .2603125 GLYOX + .2225 HCHO + .89 OH + .2603125 $HOCH_2CHO$ + .5 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
G4545	TrGNC	LHC4ACCHO + NO_3 → LHC4ACCO3 + HNO_3	KNO3AL*4.25	Rickard and Pascoe (2009)
G4546e	TrGC	LC578O2 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2	9.20E-14*RO2	Rickard and Pascoe (2009)
G4547e	TrGC	LC578O2 + HO_2 → MGLYOX + $HOCH_2CHO$ + OH	KRO2HO2*0.706*rcoch2o2_oh	Rickard and Pascoe (2009)
G4547et2	TrGC	LC578O2 + HO_2 → LC578OOH	KRO2HO2*0.706*rcoch2o2_ooh	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4548e	TrGNC	LC578O2 + NO → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4549e	TrGNC	LC578O2 + NO_3 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4586e	TrGC	LC578O2 → .25 CH_3COCH_2OH + .75 MGLYOX + .25 $HOCH_2CHO$ + .75 $HOCH_2CHO$ + HO_2 + OH	KHSB	Taraborrelli (2014)
G4550e	TrGC	LC578OOH + OH → LC578O2	0.6*k_CH3OOH_OH	Taraborrelli (2014)*
G4550et2	TrGC	LC578OOH + OH → C1ODC2OOHC4OD + HO_2	kt*fo*ftch2oh*falk+ kt*ftoh*fpch2oh*fpch2oh+ ks*fsoh*fpch2oh	Taraborrelli (2014)*
G4551e	TrGC	LHC4ACCO3 → .3 LHC4ACCO2H + .7 OH + .35 MACRO2 + .35 LHMVKABO2 + .7 CO_2	1.00E-11*RO2	Taraborrelli (2014)*
G4552e	TrGC	LHC4ACCO3 + HO_2 → 2 OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	KAPHO2*rco3_oh	Taraborrelli (2014)*
G4552et2	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO3H	KAPHO2*rco3_ooh	Taraborrelli (2014)
G4552et3	TrGC	LHC4ACCO3 + HO_2 → LHC4ACCO2H + O_3	KAPHO2*rco3_o3	Taraborrelli (2014)
G4553e	TrGNC	LHC4ACCO3 + NO → .5 MACRO2 + .5 LHMVKABO2 + NO_2 + CO_2	KAPNO	Taraborrelli (2014)*
G4554	TrGNC	LHC4ACCO3 + NO_2 → LC5PAN1719	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G4555e	TrGNC	LHC4ACCO3 + NO_3 → .5 MACRO2 + .5 LHMVKABO2 + NO_2 + CO_2	1.6*KRO2NO3	Taraborrelli (2014)*
G4556e	TrGC	LHC4ACCO2H + OH → OH + .5 MACRO2 + .5 LHMVKABO2 + CO_2	2.52E-11	Taraborrelli (2014)
G4557	TrGC	LHC4ACCO3H + OH → LHC4ACCO3	2.88E-11	Rickard and Pascoe (2009)
G4558	TrGNC	LC5PAN1719 → LHC4ACCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009)
G4559	TrGNC	LC5PAN1719 + OH → .5 MACROH + .5 HO12CO3C4 + CO + NO_2	2.52E-11	Rickard and Pascoe (2009)
G4560a	TrGC	HCOC5 + OH → C59O2	3.81E-11	Rickard and Pascoe (2009)
G4560eb	TrGC	HCOC5 + O_3 → BIACETOH + .335 H_2O_2 + 0.67 HCHO + 0.2079 CO + 0.1221 HOCH2OOH + 0.05280 OH	7.51E-16*EXP(-1521./temp)	Taraborrelli (2014)
G4561	TrGC	C59O2 → CH_3COCH_2OH + HOCH2CO	9.20E-14*RO2	Taraborrelli (2014)
G4562e	TrGC	C59O2 + HO_2 → OH + CH_3COCH_2OH + HOCH2CO	KRO2HO2*0.706*rcoch2o2_oh	Taraborrelli (2014)
G4562et2	TrGC	C59O2 + HO_2 → C59OOH	KRO2HO2*0.706*rcoch2o2_ooh	Taraborrelli (2014)
G4563	TrGNC	C59O2 + NO → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO	Taraborrelli (2014)
G4564	TrGNC	C59O2 + NO_3 → CH_3COCH_2OH + HOCH2CO + NO_2	KRO2NO3	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4565	TrGC	C59OOH + OH → C59O2	9.7E-12	Taraborrelli (2014)
G4566e	TrGC	IEPOX + OH → LC578O2 + H_2O	5.78E-11*EXP(-400/temp)	Paulot et al. (2009b),Taraborrelli (2014)
G4567e	TrGC	ISOPBO2 → MVK + HCHO + OH	KHSB	Taraborrelli (2014)
G4568e	TrGC	ISOPDO2 → MACR + HCHO + OH	KHSD	Taraborrelli (2014)
G4577ea	TrGC	ZCODC23DBCOOH + OH → .6 C1ODC2O2C4OOH + .4 C1OOHC2O2C4OD	kadt*acho*ach2ooh	Taraborrelli (2014)
G4577eb	TrGC	ZCODC23DBCOOH + OH → .6 C1ODC3O2C4OOH + .4 C1OOHC3O2C4OD	kads*acho*ach2ooh	Taraborrelli (2014)
G4577e	TrGC	ZCODC23DBCOOH + OH → ZCO3HC23DBCOD	kt*fo*falk+0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4577et2	TrGC	ZCODC23DBCOOH + OH → OH + ZCODC23DBCOD	ks*fsooh*fallyl	Taraborrelli (2014)
G4577et3	TrGC	ZCODC23DBCOOH + O_3 → .4672 OH + .2336 HCOCOCH2O2 + .2336 CO + .2336 $CH_3C(O)OO$ + .4672 HOOCH2CHO + .1728 MGLYOX + .1901 OH + .0864 GLYOX + .02765 HOOCH2CHO + .02765 H_2O_2 + .02592 CH_3OOH + .02592 CO_2 + .01037 HCOCO3A + .01555 HOCH2OOH + .01555 CO + .006912 HOOCH2CO3 + .2628 OH + .1314 MGLYOX + .1314 OH + .1314 HCOCOCH2OOH + 0.2628 GLYOX + .0972 $CH_3COCH_2O_2H$ + .00972 $HCOCO_2H$ + .005832 GLYOX + .005832 H_2O_2 + .05249 OH + .05249 HCOCO3A + .01458 HCHO + .01458 CO_2 + .01458 HCOOH + .01458 CO	2.4E-17	Taraborrelli (2014)*
G4578e	TrGC	C1OOHC2O2C4OD → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH	8.00E-13*RO2	Taraborrelli (2014)
G4579e	TrGC	C1OOHC2O2C4OD + NO → .78 $CH_3COCH_2O_2H$ + .78 HOCHCHO + .22 CO2H3CHO + .22 HCHO + .22 OH + NO_2	KRO2NO	Taraborrelli (2014)
G4580e	TrGC	C1OOHC2O2C4OD + HO_2 → C1OOHC2OOHC4OD	KRO2HO2*0.706	Taraborrelli (2014)
G4580ea	TrGC	C1OOHC2O2C4OD → $CH_3COCH_2O_2H$ + GLYOX + OH	KHSB	Taraborrelli (2014)
G4581e	TrGC	C1ODC2O2C4OOH → OH + C1ODC2OOHC4OD	K15HSDHB	Taraborrelli (2014)
G4581et2	TrGC	C1OOHC2OOHC4OD + OH → C1ODC2OOHC4OD + OH	ks*fsooh*fpch2oh	Taraborrelli (2014)
G4581et3	TrGC	C1OOHC2OOHC4OD + OH → $CH_3COCH_2O_2H$ + OH + 2 CO + 2 HO_2	kt*ftoh*fpch2oh*fpch2oh	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4581et4	TrGC	C1OOHC2OOHC4OD + OH → C1OOHC2O2C4OD	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G4581et6	TrGC	C1ODC3O2C4OOH → MGLYOX + HOOCH2CHO + HO_2	2.90E-12*RO2	Taraborrelli (2014)
G4581et7	TrGC	C1ODC3O2C4OOH + NO → MGLYOX + HOOCH2CHO + HO_2 + NO_2	KRO2NO	Taraborrelli (2014)
G4581et8	TrGC	C1ODC3O2C4OOH + HO_2 → .5 $CH_3C(O)OO$ + .5 CO + .5 MGLYOX + .5 HO_2 + HOOCH2CO3	KRO2HO2*0.706	Taraborrelli (2014)*
G4581et9	TrGC	C1ODC3O2C4OOH → MGLYOX + OH + HOOCH2CHO	KHSD	Taraborrelli (2014)
G4581et10	TrGC	C1OOHC3O2C4OD → .625 MGLYOX + 2 CO + 1.625 HO_2 + .375 $CH_3C(O)OO$ + .375 CO_2 + OH	K15HSDHB	Taraborrelli (2014)*
G4582e	TrGC	LHC4ACCO3 → ZCO3HC23DBCOD + HO_2	K16HS	Taraborrelli (2014)*
G4583e	TrGC	ZCODC23DBCOD + OH → C1ODC2O2C4OD	2*kt*fo*falk+(kadt+kads)*acho*acho	Taraborrelli (2014)
G4584e	TrGC	C1ODC2O2C4OD + HO_2 → OH + MGLYOX + HOCHCHO	KRO2HO2*0.706*rcoch2o2_oh	Taraborrelli (2014)
G4584et2	TrGC	C1ODC2O2C4OD + HO_2 → C1ODC2OOHC4OD	KRO2HO2*0.706*rcoch2o2_ooh	Taraborrelli (2014)
G4585e	TrGC	C1ODC2O2C4OD + NO → NO_2 + MGLYOX + HOCHCHO	KRO2NO	Taraborrelli (2014)
G4585et2	TrGC	C1ODC2O2C4OD → MGLYOX + HOCHCHO	8.00E-13*RO2	Taraborrelli (2014)
G4585et3	TrGC	C1ODC2OOHC4OD + OH → MGLYOX + 2 CO + .5 OH	2.*kt*fo*ftch2oh*falk+kt*ftoh*fcho*fpch2oh	Taraborrelli (2014)*
G4587e	TrGC	LISOPACNO3O2 + NO → .21 NOA + .21 $HOCH_2CHO$ + .21 HO_2 + .49 HO12CO3C4 + .49 HCHO + .49 NO_2 + .045 HMVKNO3 + .045 HCHO + .255 CH_3COCH_2OH + .255 NO3CH2CHO + .225 H_2O_2 + NO_2	KRO2NO	Taraborrelli (2014)
G4587et2	TrGC	LISOPACNO3O2 → .21 NOA + .21 $HOCH_2CHO$ + .21 HO_2 + .49 HO12CO3C4 + .49 HCHO + .49 NO_2 + .045 HMVKNO3 + .045 HCHO + .255 CH_3COCH_2OH + .255 NO3CH2CHO + .225 H_2O_2	8.00E-13*RO2+KRO2HO2*0.706*c(ind_HO2)	Taraborrelli (2014)
G4587et3	TrGC	ISOPBDNO3O2 + NO → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRN + .14 HMVKNO3 + .4 HCHO + .4 HO_2 + 1.6 NO_2	KRO2NO	Taraborrelli (2014)
G4587et4	TrGC	ISOPBDNO3O2 → .6 CH_3COCH_2OH + .6 $HOCH_2CHO$ + .26 MACRN + .14 HMVKNO3 + .4 HCHO + .4 HO_2 + .6 NO_2	2.9E-12*RO2+KRO2HO2*0.706*c(ind_HO2)	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G4588e	TrGNC	LISOPACNO3 + O_3 → .8704 OH + .365 HO_2 + .73 MGLYOX + .4325 NO3CH2CHO + .135 CH_3COCH_2OH + .0675 GLYOX + .4325 NO_2 + .0891 H_2O_2 + .135 NOA + .0675 HOCHCHO + .3866 $HOCH_2CHO$ + .0405 CH_3OH + .0405 CO + .0054 HOCH2CO	4.E-16	Taraborrelli (2014)
G4599e	TrGC	LISOPACOOH + O_3 → 1.3272 OH + 0.36986 HO_2 + .0432 H_2O_2 + 0.23002 CO + .2025 CH_3OOH + .01215 HOCH2OOH + 0.3704 HCHO + .00405 CH_3OH + .0405 CO_2 + .1825 HOCH2COCH2O2 + .365 MGLYOX + .3866 HOOCH2CHO + .135 CH_3COCH_2OH + .0675 GLYOX + .00324 HCOCO3A + .3866 $HOCH_2CHO$ + .135 $CH_3COCH_2O_2H$ + .0675 HOCHCHO + .0054 HOCH2CO	4.829E-16	Taraborrelli (2014)
G4598et3	TrGC	ZCO3HC23DBCOD + OH → .62 CO2H3CHO + .62 OH + .62 CO_2 + .38 MGLYOX + .38 $HCOCO_3H$ + .38 HO_2	kadt*acho*aco2h	Taraborrelli (2014)*
G4598et4	TrGC	ZCO3HC23DBCOD + OH → .62 CH3COCO3H + 1.24 CO + 1.24 HO_2 + .38 CH3COCHOH + .38 CO + .38 HO_2 + .38 OH + .38 CO_2	kads*acho*aco2h	Taraborrelli (2014)*
G41311	TrGC	LISOPEFO2 → .7143 MACR + .2857 MVK + HCHO + HO_2	2.40E-12*RO2	Taraborrelli (2014)
G41341	TrGC	LISOPEFO2 + NO → .7143 MACR + .2857 MVK + HCHO + HO_2 + NO_2	KRO2NO	Taraborrelli (2014)
G41351t2	TrGC	LISOPEFO2 + HO_2 → .7143 MACR + .2857 MVK + HCHO + HO_2	KRO2HO2*0.706	Taraborrelli (2014)
G41361	TrGC	LISOPEFO2 + NO_3 → .7143 MACR + .2857 MVK + HCHO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2014)
G41378	TrGC	LISOPEFO2 → PEROXYRINGC2O2	9.39E9*EXP(-7322/temp)	Taraborrelli (2014)
G41341t2	TrGC	LISOPEFO2 → .7143 MACR + .2857 MVK + HCHO + OH	.7143*KHSD+.2857*KHSB	Taraborrelli (2014)
G413112	TrGC	PEROXYRINGC2O2 → CH3COCH2OOCH2CHO + HO_2	8.00E-13*RO2	Taraborrelli (2014)
G413416	TrGC	PEROXYRINGC2O2 + NO → CH3COCH2OOCH2CHO + HO_2 + NO_2	KRO2NO	Taraborrelli (2014)*
G413519	TrGC	PEROXYRINGC2O2 + HO_2 → PEROXYRINGC2OOH	KRO2HO2*0.706	Taraborrelli (2014)
G413618	TrGC	PEROXYRINGC2O2 + NO_3 → CH3COCH2OOCH2CHO + HO_2 + NO_2	KRO2NO3	Taraborrelli (2014)
G413417	TrGC	PEROXYRINGC2O2 → CH3COCH2OOCH2CHO + OH	KHSB	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G413619	TrGC	PEROXYRINGC2OOH + OH → PEROXYRINGC2O2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G413621	TrGC	PEROXYRINGC2OOH + OH → MGLYOX + 2 CO + 2 HO_2	kt*ftoh*falk*fpch2oh	Taraborrelli (2014)*
G413622	TrGC	PEROXYRINGC2OOH + OH → .8405 HCHO + .8405 OH + .8405 CO2H3CHO + .1595 C1ODC2OOHC4OD + .1595 HO_2	ks*fsoh*falk+ks*fsooh*falk	Taraborrelli (2014)
G4136	TrGC	CH3COCH2OOCH2CHO + OH → $CH_3C(O)OO$ + CO_2 + 2 HCHO	kt*fo*ftch2oh	Taraborrelli (2014)*
G413610	TrGC	CH3COCH2OOCH2CHO + OH → GLYOX + $CH_3C(O)OO$ + HCHO	ks*fcho*fsooh	Taraborrelli (2014)
G41361t2	TrGC	CH3COCH2OOCH2CHO + OH → MGLYOX + GLYOX + HO_2	ks*fco*fsooh	Taraborrelli (2014)
G45mbo1	TrGC	MBO + OH → LMBOABO2	8.1E-12*EXP(610/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo2	TrGC	MBO + O_3 → HCHO + .16 CH_3COCH_3 + .16 HO_2 + .16 CO + .16 OH + .84 MBOOO	1.0E-17*0.57	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo3	TrGC	MBO + O_3 → IBUTALOH + .63 CO + .37 HOCH2OOH + .16 OH + .16 HO_2	1.0E-17*0.43	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo4	TrGC	MBO + NO_3 → LNMBOABO2	4.6E-14*EXP(-400/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo5	TrGC	LMBOABO2 + HO_2 → LMBOABOOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo6	TrGC	LMBOABO2 + NO → LMBOABNO3	KRO2NO*(0.064+0.026)/2.	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo7	TrGC	LMBOABO2 + NO → $HOCH_2CHO$ + CH_3COCH_3 + HO_2 + NO_2	KRO2NO*(0.936+0.974)/2.*.67	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo8	TrGC	LMBOABO2 + NO → IBUTALOH + HCHO + HO_2 + NO_2	KRO2NO*(0.936+0.974)/2.*.33	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo9	TrGC	LMBOABO2 → $HOCH_2CHO$ + CH_3COCH_3 + HO_2	8.8E-13*RO2*.67	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo10	TrGC	LMBOABO2 → IBUTALOH + HCHO + HO_2	8.8E-13*RO2*.33	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo11	TrGC	LMBOABOOH + OH → MBOACO + OH	.67*2.93E-11+.33*2.05E-12	Rickard and Pascoe (2009), Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G45mbo12	TrGC	LMBOABOOH + OH → LMBOABO2	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo13	TrGC	LMBOABOOH + hν → $HOCH_2CHO$ + CH_3COCH_3 + HO_2 + OH	1.14*jx(ip_CH3OOH)*.67	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo14	TrGC	LMBOABOOH + hν → IBUTALOH + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)*.33	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo15	TrGC	LMBOABNO3 + OH → MBOACO + NO_2	.67*1.75E-12+.33*2.69E-12	Rickard and Pascoe (2009), Taraborrelli (2014)*
G45mbo16	TrGC	MBOACO + OH → MBOCOCO + HO_2	3.79E-12	Rickard and Pascoe (2009)
G45mbo17	TrGC	MBOACO + hν → HCHO + HO_2 + IPRHOCO3	J_ACETOL	Rickard and Pascoe (2009)
G45mbo18	TrGC	MBOCOCO + OH → CO + IPRHOCO3	1.38E-11	Rickard and Pascoe (2009)
G45mbo19	TrGC	MBOCOCO + hν → CO + HO_2 + IPRHOCO3	jx(ip_MGLYOX)	Rickard and Pascoe (2009)
G45mbo20	TrGC	IBUTALOH + OH → IPRHOCO3	1.4E-11	Rickard and Pascoe (2009)
G45mbo21	TrGC	IBUTALOH + hν → CH_3COCH_3 + HO_2 + HO_2 + CO	J_ACETOL	Rickard and Pascoe (2009)
G45mbo22	TrGC	IPRHOCO3 + HO_2 → CH_3COCH_3 + HO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo23	TrGC	IPRHOCO3 + HO_2 → IPRHOCO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo24	TrGC	IPRHOCO3 + HO_2 → IPRHOCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo25	TrGC	IPRHOCO3 + NO → CH_3COCH_3 + HO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G45mbo26	TrGC	IPRHOCO3 + NO_2 → C4PAN5	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45mbo27	TrGC	IPRHOCO3 + NO_3 → CH_3COCH_3 + HO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45mbo28	TrGC	IPRHOCO3 → CH_3COCH_3 + HO_2	1.00E-11*RO2*0.7	Rickard and Pascoe (2009)
G45mbo29	TrGC	IPRHOCO3 → IPRHOCO2H	1.00E-11*RO2*0.3	Rickard and Pascoe (2009)
G45mbo30	TrGC	IPRHOCO2H + OH → CH_3COCH_3 + HO_2	1.72E-12	Rickard and Pascoe (2009)
G45mbo31	TrGC	IPRHOCO3H + hν → CH_3COCH_3 + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)
G45mbo32	TrGC	OH + IPRHOCO3H → IPRHOCO3	4.80E-12	Rickard and Pascoe (2009)
G45mbo33	TrGC	C4PAN5 → IPRHOCO3 + NO_2	K_PAN_M	Rickard and Pascoe (2009)
G45mbo34	TrGC	C4PAN5 + OH → CH_3COCH_3 + CO + NO_2	4.75E-13	Rickard and Pascoe (2009)
G45mbo35	TrGC	LNMBOABO2 + HO_2 → LNMBOABOOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo36	TrGC	LNMBOABO2 + NO → .65 NO3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G45mbo37	TrGC	LNMBOABO2 + NO_3 → .65 NO3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo38	TrGC	LNMBOABO2 → .65 NO3CH2CHO + .65 CH_3COCH_3 + .65 HO_2 + .35 IBUTALOH + .35 HCHO + .35 NO_2	8.8E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo39	TrGC	LNMBOABOOH + OH → .65 C4MCONO3OH + .35 NMBOBCO + OH	.65*4.89E-12+.35*2.52E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo40	TrGC	LNMBOABOOH + OH → LNMBOABO2	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo41	TrGC	LNMBOABOOH + hν → NO3CH2CHO + CH_3COCH_3 + HO_2 + OH	1.14*jx(ip_CH3OOH)*.65	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo42	TrGC	LNMBOABOOH + hν → IBUTALOH + HCHO + NO_2 + OH	1.14*jx(ip_CH3OOH)*.35	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo43	TrGC	C4MCONO3OH + OH → CH_3COCH_3 + HCHO + CO_2 + NO_2	1.23E-12	Rickard and Pascoe (2009), Taraborrelli (2014)*
G45mbo44	TrGC	NMBOBCO + OH → NC4OHCO3	4.26E-12	Rickard and Pascoe (2009)
G45mbo45	TrGC	NC4OHCO3 + HO_2 → IBUTALOH + NO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo46	TrGC	NC4OHCO3 + HO_2 → NC4OHCO3H	KAPHO2*(rco3_o3+rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo47	TrGC	NC4OHCO3 + NO → IBUTALOH + NO_2 + NO_2	KAPNO	Rickard and Pascoe (2009)
G45mbo48	TrGC	NC4OHCO3 + NO_2 → NC4OHCPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G45mbo49	TrGC	NC4OHCO3 + NO_3 → IBUTALOH + NO_2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009)
G45mbo50	TrGC	NC4OHCO3 → IBUTALOH + NO_2	1.00E-11*RO2	Rickard and Pascoe (2009)
G45mbo51	TrGC	NC4OHCO3H + OH → NC4OHCO3	4.50E-12	Rickard and Pascoe (2009)
G45mbo52	TrGC	NC4OHCO3H → IBUTALOH + NO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)
G45mbo53	TrGC	NC4OHCPAN + OH → IBUTALOH + CO + NO_2 + NO_2	1.27E-12	Rickard and Pascoe (2009)
G45mbo54	TrGC	NC4OHCPAN → NC4OHCO3 + NO_2	K_PAN_M	Rickard and Pascoe (2009)
G45mbo55	TrGC	MBOOO → IPRHOCO2H	1.60E-17*C(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo56	TrGC	MBOOO → IBUTALOH + H_2O_2	1.60E-17*C(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2014)
G45mbo57	TrGC	MBOOO + CO → IBUTALOH	1.20E-15	Rickard and Pascoe (2009)
G45mbo58	TrGC	MBOOO + NO → IBUTALOH + NO_2	1.00E-14	Rickard and Pascoe (2009)
G45mbo59	TrGC	MBOOO + NO_2 → IBUTALOH + NO_3	1.00E-15	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G45mbo60	TrGC	MBOOO + SO_2 → IBUTALOH + H_2SO_4	7.00E-14	Rickard and Pascoe (2009)
G410apin1	TrGC	APINENE + OH → LAPINABO2	1.47E-11*EXP(467/TEMP)*(.50+.25)	Vereecken et al. (2007), Taraborrelli (2014)*
G410apin2	TrGC	APINENE + OH → MENTHEN6ONE + HO_2	1.47E-11*EXP(467/TEMP)*.25*.60	Vereecken et al. (2007), Taraborrelli (2014)*
G410apin3	TrGC	APINENE + OH → LVROO6R1O2	1.47E-11*EXP(467/TEMP)*.25*.40	Vereecken et al. (2007), Taraborrelli (2014)*
G410apin4	TrGC	LAPINABO2 + NO → PINAL + HO_2 + NO_2	KRO2NO*0.770	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin5	TrGC	LAPINABO2 + NO → LAPINABNO3	KRO2NO*0.230	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin6	TrGC	LAPINABO2 + HO_2 → LAPINABOOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin7	TrGC	LAPINABO2 → PINAL + HO_2	RO2*(.33*9.20E-14+.67*8.80E-13)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin9	TrGC	LAPINABOOH + OH → .33 LAPINABO2 + .67 C96CO3	.33*1.83E-11+.67*3.28E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin10	TrGC	LAPINABOOH + hν → PINAL + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin11	TrGC	LAPINABNO3 + OH → .33 PINAL + .67 C96CO3 + NO_2	.33*5.50E-12+.67*3.64E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin12	TrGC	MENTHEN6ONE + OH → OHMENTHEN6ONEO2	(kads+kadt)*acoch3	Vereecken et al. (2007), Taraborrelli (2014)
G410apin13	TrGC	MENTHEN6ONE + hν → LVRO6R1O2 + OH	1.14*jx(ip_CH3OOH)	Vereecken et al. (2007), Taraborrelli (2014)
G410apin14	TrGC	OHMENTHEN6ONEO2 + NO → LV2OHMENTHEN6ONE + HO_2 + NO_2	KRO2NO	Vereecken et al. (2007), Taraborrelli (2014)
G410apin15	TrGC	OHMENTHEN6ONEO2 + HO_2 → LV2OHMENTHEN6ONE	KRO2HO2*0.914	Vereecken et al. (2007), Taraborrelli (2014)
G410apin16	TrGC	OHMENTHEN6ONEO2 → LV2OHMENTHEN6ONE + HO_2	RO2*9.20E-14	Vereecken et al. (2007), Taraborrelli (2014)
G410apin17	TrGC	LV2OHMENTHEN6ONE + OH → LCARBON	1E-11	Vereecken et al. (2007), Taraborrelli (2014)
G410apin18	TrGC	LV2OHMENTHEN6ONE + hν → LCARBON + OH	1.14*jx(ip_CH3OOH)	Vereecken et al. (2007), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apin18t2	TrGC	PINAL + OH → C96CO3	4.20E-11*0.772	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin19	TrGC	PINAL + OH → PINALO2	4.20E-11*0.228	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin20	TrGC	PINAL → C96O2 + CO + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin21	TrGC	PINAL + NO_3 → C96CO3 + HNO_3	3.80E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apin	TrGC	C96CO3 → 0.3 PINONIC + 0.7 C96O2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint2	TrGC	C96CO3 + HO_2 → PERPINONIC	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint3	TrGC	C96CO3 + HO_2 → PINONIC + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint4	TrGC	C96CO3 + HO_2 → C96O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint5	TrGC	C96CO3 + NO_2 → C10PAN2	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint6	TrGC	C96CO3 + NO → C96O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint7	TrGC	C96CO3 + NO_3 → C96O2 + NO_2	KRO2NO3*1.60	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint8	TrGC	C10PAN2 → C96CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint9	TrGC	C10PAN2 + OH → NORPINAL + CO + NO_2	3.66E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint10	TrGC	C96O2 → C97O2	1.30E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint11	TrGC	C96O2 + NO → C96NO3	KRO2NO*0.157	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint12	TrGC	C96O2 + HO_2 → C96OOH	KRO2HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint13	TrGC	C96O2 + NO → C97O2 + NO_2	KRO2NO*0.843	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint14	TrGC	C96NO3 + hν → C97O2 + NO_2	J_IC3H7NO3+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint15	TrGC	C96NO3 + OH → NORPINAL + NO_2	2.88E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint16	TrGC	C96OOH + hν → C97O2 + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint17	TrGC	C96OOH + OH → C96O2	1.90E-12*EXP(190/TEMP)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint18	TrGC	C96OOH + OH → NORPINAL + OH	1.30E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint19	TrGC	C97O2 → C98O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint20	TrGC	C97O2 + NO → C98O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint21	TrGC	C97O2 + HO_2 → C97OOH	KRO2HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint22	TrGC	C97OOH + hν → C98O2 + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint23	TrGC	C97OOH + OH → C97O2	1.05E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint24	TrGC	C98O2 → C614O2 + CH_3COCH_3	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint25	TrGC	C98O2 + NO → C98NO3	KRO2NO*0.118	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint26	TrGC	C98O2 + NO → C614O2 + CH_3COCH_3 + NO_2	KRO2NO*0.882	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint27	TrGC	C98O2 + HO_2 → C98OOH	KRO2HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint28	TrGC	C98OOH + hν → C614O2 + CH_3COCH_3 + OH	1.14*jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint29	TrGC	C98OOH + OH → C98O2	2.05E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint30	TrGC	PINONIC + OH → C96O2	6.65E-12	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint31	TrGC	PINONIC + hν → C96O2 + HO_2	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint32	TrGC	NORPINAL + OH → C85CO3	2.64E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint33	TrGC	NORPINAL + hν → C85O2 + CO + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint34	TrGC	NORPINAL + NO_3 → C85CO3 + HNO_3	KNO3AL*8.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint35	TrGC	PERPINONIC + hν → C96O2 + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint36	TrGC	PERPINONIC + OH → C96CO3	9.73E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint37	TrGC	C85CO3 → C85O2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint38	TrGC	C85CO3 + NO → C85O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint39	TrGC	C85CO3 + NO_2 → C9PAN2	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint40	TrGC	C85CO3 + HO_2 → C85CO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint41	TrGC	C85CO3 + HO_2 → C85O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint42	TrGC	C85O2 → C86O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint43	TrGC	C85O2 + HO_2 → C85OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint44	TrGC	C85O2 + NO → C86O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint45	TrGC	C9PAN2 → C85CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint46	TrGC	C9PAN2 + OH → C85OOH + CO + NO_2	6.60E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint47	TrGC	C85CO3H → C85O2 + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint48	TrGC	C85CO3H + OH → C85CO3	1.02E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint49	TrGC	C85OOH + hν → C86O2 + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint50	TrGC	C85OOH + OH → C85O2	1.29E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint51	TrGC	C86O2 → C511O2 + CH_3COCH_3	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint52	TrGC	C86O2 + NO → C511O2 + CH_3COCH_3 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint53	TrGC	C86O2 + HO_2 → C86OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint54	TrGC	C86OOH + hν → C511O2 + CH_3COCH_3 + OH	1.14*jx(ip_CH3OOH)+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint55	TrGC	C86OOH + OH → C86O2	3.45E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint56	TrGC	PINALO2 + HO_2 → PINALOOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint57	TrGC	PINALO2 + NO → PINALNO3	KRO2NO*0.050	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint58	TrGC	PINALO2 + NO → C106O2 + NO_2	KRO2NO*0.950	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint59	TrGC	PINALO2 → C106O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint60	TrGC	PINALOOH + OH → PINALO2	2.75E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint61	TrGC	PINALOOH + hν → C106O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint62	TrGC	PINALNO3 + OH → CO235C6CHO + CH_3COCH_3 + NO_2	2.25E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint63	TrGC	PINALNO3 + hν → C106O2 + NO_2	J_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint64	TrGC	C106O2 + HO_2 → C106OOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint65	TrGC	C106O2 + NO → C106NO3	KRO2NO*0.125	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint66	TrGC	C106O2 + NO → C716O2 + CH_3COCH_3 + NO_2	KRO2NO*0.875	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint67	TrGC	C106O2 → C716O2 + CH_3COCH_3	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint68	TrGC	C106OOH + OH → C106O2	8.01E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint69	TrGC	C106OOH + hν → C716O2 + CH_3COCH_3 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint70	TrGC	C106NO3 + OH → CO235C6CHO + CH_3COCH_3 + NO_2	7.03E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint71	TrGC	C106NO3 + hν → C716O2 + CH_3COCH_3 + NO_2	J_IC3H7NO3+ jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint72	TrGC	CO235C6CHO + NO_3 → CO235C6CO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint73	TrGC	CO235C6CHO + OH → CO235C6CO3	6.70E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint74	TrGC	CO235C6CHO + hν → CHOC3COCO3 + $CH_3C(O)OO$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint75	TrGC	CO235C6CO3 + HO_2 → C235C6CO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint76	TrGC	CO235C6CO3 + HO_2 → CO235C6O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint77	TrGC	CO235C6CO3 + NO → CO235C6O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint78	TrGC	CO235C6CO3 + NO_2 → C7PAN3	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint79	TrGC	CO235C6CO3 → CO235C6O2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint80	TrGC	C235C6CO3H + OH → CO235C6CO3	4.75E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint81	TrGC	C235C6CO3H + hν → CO235C6O2 + OH	1.14*jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint82	TrGC	CO235C6O2 + HO_2 → CO235C6OOH	KRO2HO2*0.770	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint83	TrGC	CO235C6O2 + NO → CO23C4CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint84	TrGC	CO235C6O2 → CO23C4CO3 + HCHO	2.00E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint85	TrGC	C7PAN3 + OH → CO235C5CHO + CO + NO_2	8.83E-13	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint86	TrGC	C7PAN3 → CO235C6CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint87	TrGC	CO235C6OOH + OH → CO235C6O2	1.01E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint88	TrGC	CO235C6OOH + hν → CO23C4CO3 + HCHO + OH	1.14*jx(ip_CH3OOH)+ 2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint89	TrGC	C716O2 + HO_2 → C716OOH	KRO2HO2*0.820	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint90	TrGC	C716O2 + NO → CO13C4CHO + $CH_3C(O)OO$ + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint91	TrGC	C716O2 → CO13C4CHO + $CH_3C(O)OO$	8.80E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint92	TrGC	C716OOH + OH → CO235C6CHO + OH	1.20E-10	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint93	TrGC	C716OOH + hν → CO13C4CHO + $CH_3C(O)OO$ + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint94	TrGC	C511O2 → $CH_3C(O)OO$ + HCOCH2CHO	8.80E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint95	TrGC	C511O2 + NO → $CH_3C(O)OO$ + HCOCH2CHO + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint96	TrGC	C511O2 + HO_2 → C511OOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint97	TrGC	C511OOH + hν → $CH_3C(O)OO$ + HCOCH2CHO + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint98	TrGC	C511OOH + OH → C511O2	7.49E-11	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint99	TrGC	HCOCH2CHO + OH → HCOCH2CO3	4.29E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint100	TrGC	HCOCH2CHO + hν → HCOCH2O2 + HO_2 + CO	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint101	TrGC	HCOCH2CHO + NO_3 → HCOCH2CO3 + HNO_3	2*KNO3AL*2.4	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint102	TrGC	C614O2 → CO23C4CHO + HCHO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint103	TrGC	C614O2 + NO → C614NO3	KRO2NO*0.098	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint104	TrGC	C614O2 + NO → CO23C4CHO + HCHO + HO_2 + NO_2	KRO2NO*0.902	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint105	TrGC	C614O2 + HO_2 → C614OOH	KRO2HO2*0.770	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint106	TrGC	C614NO3 + hν → CO23C4CHO + HCHO + HO_2 + NO_2	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint107	TrGC	C614NO3 + OH → C614CO + NO_2	7.11E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint108	TrGC	C614OOH + hν → CO23C4CHO + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint109	TrGC	C614OOH + OH → C614CO + OH	8.69E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint110	TrGC	C614CO + hν → CH3COCOCH2O2 + $HOCH_2CO_3$	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint111	TrGC	C614CO + OH → CO235C5CHO + HO_2	3.22E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint112	TrGC	CH3COCOCH2O2 → $CH_3C(O)OO$ + HCHO + CO	2.00E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint113	TrGC	CH3COCOCH2O2 + HO_2 → CH3COCOCH2OOH	KRO2HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint114	TrGC	CH3COCOCH2O2 + NO → $CH_3C(O)OO$ + HCHO + CO + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint115	TrGC	CH3COCOCH2OOH + OH → CH3COCOCHO + OH	ks*fco*fsooh	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint116	TrGC	CH3COCOCH2OOH + OH → CH3COCOCH2O2	.6*k_CH3OOH_OH	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint117	TrGC	CH3COCOCH2OOH + hν → CH3COCOCHO + OH + HO_2	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint118	TrGC	CH3COCOCH2OOH + hν → $CH_3C(O)OO$ + CO + OH + HCHO	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint119	TrGC	CH3COCOCH2OOH + hν → $CH_3C(O)OO$ + $HCOCO_3$	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint120	TrGC	CO235C5CHO + OH → CO23C4CO3 + CO	1.33E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint121	TrGC	CO235C5CHO + hν → CO23C4CO3 + CO + HO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint122	TrGC	CO235C5CHO + NO_3 → CO23C4CO3 + CO + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint123	TrGC	CO23C4CHO + OH → CO23C4CO3	6.65E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint124	TrGC	CO23C4CHO + hν → CH3COCOCH2O2 + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint125	TrGC	CO23C4CHO + hν → $CH_3C(O)OO$ + HCOCH2CO3	2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint126	TrGC	CO23C4CHO + NO_3 → CO23C4CO3 + HNO_3	KNO3AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint127	TrGC	CO23C4CO3 → CH3COCOCH2O2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint128	TrGC	CO23C4CO3 + NO → CH3COCOCH2O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint129	TrGC	CO23C4CO3 + NO_2 → C5PAN9	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint130	TrGC	CO23C4CO3 + HO_2 → CO23C4CO3H	KAPHO2*(rco3_ooh+rco3_o3)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint131	TrGC	CO23C4CO3 + HO_2 → CH3COCOCH2O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint132	TrGC	CO23C4CO3H + hν → CH3COCOCH2O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint133	TrGC	CO23C4CO3H + hν → CO23C4CO3	4.23E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint134	TrGC	C5PAN9 → CO23C4CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint135	TrGC	C5PAN9 + OH → CO23C3CHO + CO + NO_2	3.12E-13	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint136	TrGC	HCOCH2CO3 → 0.7 HCOCH2O2 + 0.3 HCOCH2CO2H	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint137	TrGC	HCOCH2CO3 + NO → HCOCH2O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint138	TrGC	HCOCH2CO3 + NO_2 → C3PAN2	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint139	TrGC	HCOCH2CO3 + HO_2 → HCOCH2CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint140	TrGC	HCOCH2CO3 + HO_2 → HCOCH2CO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint141	TrGC	HCOCH2CO3 + HO_2 → HCOCH2O2 + CO_2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint142	TrGC	C3PAN2 → HCOCH2CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint143	TrGC	C3PAN2 + OH → GLYOX + CO + NO_2	2.10E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint144	TrGC	HCOCH2CO2H + OH → HCOCH2O2	2.14E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint145	TrGC	HCOCH2CO2H + hν → HCOCH2O2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint146	TrGC	APINENE + O_3 → APINBOO	1.01E-15*EXP(-732/TEMP)*.50*.18	Capouet et al. (2008)
G410apint147	TrGC	APINENE + O_3 → PINONIC	1.01E-15*EXP(-732/TEMP)*.50*.16	Capouet et al. (2008)
G410apint148	TrGC	APINENE + O_3 → OH + NORPINAL + CO + HO_2	1.01E-15*EXP(-732/TEMP)*.50*.66	Capouet et al. (2008)
G410apint149	TrGC	APINENE + O_3 → APINAOO	1.01E-15*EXP(-732/TEMP)*.50*.12	Capouet et al. (2008)
G410apint150	TrGC	APINENE + O_3 → OH + C109O2	1.01E-15*EXP(-732/TEMP)*.50*(.22+.66)	Capouet et al. (2008)*
G410apint151	TrGC	APINAOO → PINAL + H_2O_2	1.00E-17*c(ind_H2O)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint152	TrGC	APINAOO + CO → PINAL	1.20E-15	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint153	TrGC	APINAOO + NO → PINAL + NO_2	1.00E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint154	TrGC	APINAOO + NO_2 → PINAL + NO_3	1.00E-15	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint155	TrGC	APINAOO + SO_2 → PINAL + H_2SO_4	7.00E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint156	TrGC	APINBOO → PINONIC	1.00E-17*c(ind_H2O)*(0.08+0.15)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint157	TrGC	APINBOO → PINAL + H_2O_2	1.00E-17*c(ind_H2O)*0.77	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint158	TrGC	APINBOO + CO → PINAL	1.20E-15	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint159	TrGC	APINBOO + NO → PINAL + NO_2	1.00E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint160	TrGC	APINBOO + NO_2 → PINAL + NO_3	1.00E-15	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint161	TrGC	APINBOO + SO_2 → PINAL + H_2SO_4	7.00E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint162	TrGC	C109O2 → C89CO3 + HCHO	2.00E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint163	TrGC	C109O2 + NO → C89CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint164	TrGC	C109O2 + HO_2 → C109OOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint165	TrGC	C109OOH → C89CO3 + HCHO + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint166	TrGC	C109OOH + OH → C109CO + OH	5.47E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint167	TrGC	C109OOH + hν → C89CO3 + HCHO + OH	J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint168	TrGC	C109CO + OH → C89CO3 + CO	5.47E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint169	TrGC	C109CO + hν → C89CO3 + CO + HO_2	jx(ip_MGLYOX)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint170	TrGC	C89CO3 → .56 C811CO3 + .14 C89O2 + 0.3 C89CO2H	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint171	TrGC	C89CO3 + HO_2 → C89CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint172	TrGC	C89CO3 + HO_2 → C89CO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint173	TrGC	C89CO3 + HO_2 → .80 C811CO3 + 0.20 C89O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint174	TrGC	C89CO3 + NO_2 → C89PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint175	TrGC	C89CO3 + NO → 0.80 C811CO3 + 0.20 C89O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint176	TrGC	C89CO2H + OH → 0.80 C811CO3 + 0.20 C89O2	2.69E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint177	TrGC	C89CO2H + hν → 0.80 C811CO3 + 0.20 C89O2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint178	TrGC	C89CO3H → 0.80 C811CO3 + 0.20 C89O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint179	TrGC	C89CO3H + OH → C89CO3	3.00E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint180	TrGC	C89PAN → C89CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint181	TrGC	C89PAN + OH → CH_3COCH_3 + CO13C4CHO + CO + NO_2	2.52E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint182	TrGC	C811CO3 → 0.7 C811O2 + 0.3 PINIC	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint183	TrGC	C811CO3 + HO_2 → C811CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint184	TrGC	C811CO3 + HO_2 → PINIC + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint185	TrGC	C811CO3 + HO_2 → C811O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint186	TrGC	C811CO3 + NO → C811O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint187	TrGC	C811CO3 + NO_2 → C811PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint188	TrGC	PINIC + OH → C811O2	7.29E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf1	TrGC	C89O2 + HO_2 → C89OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf2	TrGC	C89O2 + NO → C89NO3	KRO2NO*0.104	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf3	TrGNC	C89O2 + NO → C810O2 + NO_2	KRO2NO*0.896	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf4	TrGNC	C89O2 + NO_3 → C810O2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf5	TrGC	C89O2 → C810O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf6	TrGC	C89OOH + OH → C89O2	3.61E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf7	TrGJC	C89OOH + hν → C810O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf8	TrGC	C89NO3 + OH → CH_3COCH_3 + CO13C4CHO + NO_2	2.56E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf9	TrGJNC	C89NO3 + hν → C810O2 + NO_2	J_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf10	TrGC	C810O2 + HO_2 → C810OOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf11	TrGNC	C810O2 + NO → C810NO3	KRO2NO*0.104	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf12	TrGNC	C810O2 + NO → CH_3COCH_3 + C514O2 + NO_2	KRO2NO*0.896	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf13	TrGNC	C810O2 + NO_3 → CH_3COCH_3 + C514O2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf14	TrGC	C810O2 → CH_3COCH_3 + C514O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf15	TrGC	C810OOH + OH → C810O2	8.35E-11	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410ap188bf16	TrGJC	C810OOH + hν → CH_3COCH_3 + C514O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf17	TrGNC	C810NO3 + OH → CH_3COCH_3 + CO13C4CHO + NO_2	4.96E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf18	TrGJC	C810NO3 + hν → CH_3COCH_3 + C514O2 + NO_2	2.84*J_IC3H7NO3+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf19	TrGC	C514O2 + HO_2 → C514OOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf20	TrGNC	C514O2 + NO → C514NO3	KRO2NO*0.129	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf21	TrGNC	C514O2 + NO → CO13C4CHO + HO_2 + NO_2	KRO2NO*0.871	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf22	TrGNC	C514O2 + NO_3 → CO13C4CHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf23	TrGC	C514O2 → CO13C4CHO + HO_2	2.50E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf24	TrGC	C514OOH + OH → CO13C4CHO + OH	1.10E-10	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf25	TrGJC	C514OOH + hν → CO13C4CHO + HO_2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO) *2.0	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf26	TrGC	C514NO3 + OH → CO13C4CHO + NO_2	4.33E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410ap188bf27	TrGJC	C514NO3 + hν → CO13C4CHO + HO_2 + NO_2	J_IC3H7NO3+jx(ip_HOCH2CHO)*2.0	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint189	TrGC	C811O2 → C812O2	1.30E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint190	TrGC	C811O2 + HO_2 → C811OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint191	TrGC	C811O2 + NO → C812O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint192	TrGC	C811CO3H + hν → C811O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint193	TrGC	C811CO3H + OH → C811CO3	1.04E-11	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint194	TrGC	C811PAN → C811CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint195	TrGC	C811PAN + OH → C721CHO + CO + NO_2	6.77E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint196	TrGC	C812O2 → C813O2	9.20E-14*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint197	TrGC	C812O2 + NO → C813O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint198	TrGC	C812O2 + HO_2 → C812OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint199	TrGC	C812OOH + hν → C813O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint200	TrGC	C812OOH + OH → C812O2	1.09E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint201	TrGC	C813O2 → CH_3COCH_3 + C512O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint202	TrGC	C813O2 + NO → CH_3COCH_3 + C512O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint203	TrGC	C813O2 + HO_2 → C813OOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint204	TrGC	C813OOH + hν → CH_3COCH_3 + C512O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint205	TrGC	C813OOH + OH → C813O2	1.86E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint206	TrGC	C721CHO + NO_3 → C721CO3 + HNO_3	KNO3AL*8.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint207	TrGC	C721CHO + OH → C721CO3	2.63E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint208	TrGC	C721CHO → C721O2 + CO + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint209	TrGC	C721CO3 + HO_2 → C721CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint210	TrGC	C721CO3 + HO_2 → C721O2 + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint211	TrGC	C721CO3 + HO_2 → NORPINIC + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint212	TrGC	C721CO3 + NO → C721O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint213	TrGC	C721CO3 + NO_2 → C721PAN	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint214	TrGC	C721CO3 + NO_3 → C721O2 + NO_2	KRO2NO3*1.74	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint215	TrGC	C721CO3 → C721O2	1.00E-11*RO2*0.7	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint216	TrGC	C721CO3 → NORPINIC	1.00E-11*RO2*0.3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint217	TrGC	C721O2 + HO_2 → C721OOH	KRO2HO2*0.820	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint218	TrGC	C721O2 + NO → C722O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint219	TrGC	C721O2 → C722O2	1.30E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint220	TrGC	C721CO3H + OH → C721CO3	9.65E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint221	TrGC	C721CO3H + hν → C721O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint222	TrGC	NORPINIC + OH → C721O2	6.57E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint223	TrGC	C721PAN + OH → C721OOH + CO + NO_2	2.96E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint224	TrGC	C721PAN → C721CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint225	TrGC	C721OOH + OH → C721O2	1.27E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint226	TrGC	C721OOH + hν → C722O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint227	TrGC	C722O2 + HO_2 → C722OOH	KRO2HO2*0.820	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint228	TrGC	C722O2 + NO → CH_3COCH_3 + C44O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint229	TrGC	C722O2 → CH_3COCH_3 + C44O2	6.70E-15*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint230	TrGC	C722OOH + OH → C722O2	3.31E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint231	TrGC	C722OOH + hν → CH_3COCH_3 + C44O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint232	TrGC	C44O2 + HO_2 → C44OOH	KRO2HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint233	TrGC	C44O2 + NO → HCOCH2CHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint234	TrGC	C44O2 → HCOCH2CHO + HO_2	8.80E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint235	TrGC	C44OOH + OH → C44O2	7.46E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint236	TrGC	C44OOH + hν → HCOCH2CHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint237	TrGC	C512O2 → C513O2	1.30E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint238	TrGC	C512O2 + HO_2 → C512OOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint239	TrGC	C512O2 + NO → C513O2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint240	TrGC	C512OOH + hν → C513O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint241	TrGC	C512OOH + OH → CO13C4CHO + OH	1.01E-10	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint242	TrGC	C513O2 → GLYOX + HOC2H4CO3	8.80E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint243	TrGC	C513O2 + NO → GLYOX + HOC2H4CO3 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint244	TrGC	C513O2 + HO_2 → C513OOH	KRO2HO2*0.706	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint245	TrGC	CO13C4CHO + OH → CHOC3COCO3	1.33E-10	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint246	TrGC	CO13C4CHO + hν → CHOC3COO2 + CO + HO_2	jx(ip_HOCH2CHO)*2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint247	TrGC	CO13C4CHO + NO_3 → CHOC3COCO3 + HNO_3	2*KNO3AL*5.5	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint248	TrGC	C513OOH + hν → GLYOX + HOC2H4CO3 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint249	TrGC	C513OOH + OH → C513CO + OH	9.23E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint250	TrGC	CHOC3COCO3 → CHOC3COO2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint251	TrGC	CHOC3COCO3 + HO_2 → CHOC3COOOH	KAPHO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint252	TrGC	CHOC3COCO3 + NO_2 → CHOC3COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint253	TrGC	CHOC3COCO3 + NO → CHOC3COO2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint254	TrGC	CHOC3COO2 → HCOCH2CO3 + HCHO	2.00E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint255	TrGC	CHOC3COO2 + HO_2 → C413COOOH	KRO2HO2*0.625	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint256	TrGC	CHOC3COO2 + NO → HCOCH2CO3 + HCHO + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint257	TrGC	C513CO + OH → HOC2H4CO3 + CO + CO	2.64E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint258	TrGC	C513CO + hν → HOC2H4CO3 + HO_2 + CO + CO	jx(ip_MGLYOX)+2.15*jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint259	TrGC	C413COOOH + OH → CHOC3COO2	8.33E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint260	TrGC	C413COOOH + hν → HCOCH2CO3 + HCHO + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint261	TrGC	CHOC3COOOH + OH → CHOC3COCO3	7.55E-11	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint262	TrGC	CHOC3COOOH + hν → CHOC3COO2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO) +J_ACETOL	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint263	TrGC	CHOC3COPAN → CHOC3COCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint264	TrGC	CHOC3COPAN + OH → C4CODIAL + CO + NO_2	7.19E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint265	TrGC	C4CODIAL + OH → C312COCO3	3.39E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint266	TrGC	C4CODIAL + hν → HCOCOCH2O2 + HO_2 + CO	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint267	TrGC	C4CODIAL + hν → HCOCH2CO3 + HO_2 + CO	jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint268	TrGC	C4CODIAL + NO_3 → C312COCO3 + HNO_3	2*KNO3AL*4.0	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint269	TrGC	C312COCO3 → HCOCOCH2O2	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint270	TrGC	C312COCO3 + HO_2 → C312COCO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint271	TrGC	C312COCO3 + HO_2 → HCOCOCH2O2 + OH	KAPHO2*(1-rco3_ooh)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint272	TrGC	C312COCO3 + NO_2 → C312COPAN	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint273	TrGC	C312COCO3 + NO → HCOCOCH2O2 + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint274	TrGC	C312COCO3H + OH → C312COCO3	1.63E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint275	TrGC	C312COCO3H + hν → HCOCOCH2O2 + OH	1.14*jx(ip_CH3OOH)+jx(ip_MGLYOX)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint276	TrGC	C312COPAN → C312COCO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint277	TrGC	C312COPAN + OH → HCOCOCHO + CO + NO_2	1.27E-11	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410apint278	TrGC	HOC2H4CO3 → 0.7 $HOCH_2CH_2O_2$ + 0.3 HOC2H4CO2H	1.00E-11*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint279	TrGC	HOC2H4CO3 + NO → $HOCH_2CH_2O_2$ + NO_2	KAPNO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint280	TrGC	HOC2H4CO3 + HO_2 → HOC2H4CO3H	KAPHO2*rco3_ooh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint281	TrGC	HOC2H4CO3 + HO_2 → $HOCH_2CH_2O_2$ + OH	KAPHO2*rco3_oh	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint282	TrGC	HOC2H4CO3 + HO_2 → HOC2H4CO2H + O_3	KAPHO2*rco3_o3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint283	TrGC	HOC2H4CO3 + NO_2 → C3PAN1	k_CH3CO3_NO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint284	TrGC	HOC2H4CO2H + OH → $HOCH_2CH_2O_2$	1.39E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint285	TrGC	HOC2H4CO3H + OH → HOC2H4CO3	1.73E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint286	TrGC	HOC2H4CO3H + hν → $HOCH_2CH_2O_2$ + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint287	TrGC	C3PAN1 → HOC2H4CO3 + NO_2	k_PAN_M	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint288	TrGC	C3PAN1 + OH → $HOCH_2CHO$ + CO + NO_2	4.51E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint289	TrGC	APINENE + NO_3 → LNAPINABO2	1.2E-12*EXP(490./temp)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint290	TrGC	LNAPINABO2 → PINAL + NO_2	(.65*6.70E-15+.35*2.50E-13)*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint291	TrGC	LNAPINABO2 + NO → PINAL + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint292	TrGC	LNAPINABO2 + HO_2 → LNAPINABOOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint293	TrGC	LNAPINABO2 + NO_3 → PINAL + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint294	TrGC	LNAPINABOOH + hν → PINAL + NO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint295	TrGC	LNAPINABOOH + OH → C96CO3	.65*6.87E-12+.35*1.23E-11	Rickard and Pascoe (2009), Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G410bpin	TrGC	BPINENE + OH → BPINAO2	1.47E-11*EXP(467/TEMP)*(0.8326*0.3+0.068)/(0.8326+0.068)	Vereecken and Peeters (2012)*
G410bpint2	TrGC	BPINENE + OH → LVROO6R1O2	1.47E-11*EXP(467/TEMP)*0.8326*0.7/(0.8326+0.068)	Vereecken and Peeters (2012)*
G410bpint3	TrGC	BPINAO2 + HO_2 → BPINAOOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint4	TrGC	BPINAO2 + NO → BPINANO3	KRO2NO*0.240	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint5	TrGC	BPINAO2 + NO → NOPINONE + HCHO + HO_2 + NO_2	KRO2NO*0.760	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint6	TrGC	BPINAO2 → NOPINONE + HCHO + HO_2	9.20E-14*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint7	TrGC	BPINAOOH + OH → BPINAO2	1.33E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint8	TrGC	BPINAOOH + hν → NOPINONE + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint9	TrGC	BPINANO3 + OH → NOPINONE + HCHO + NO_2	4.70E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint10	TrGC	LVROO6R1O2 + NO → LVROO6R3O2 + CH_3COCH_3 + NO_2	KRO2NO*0.892	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint11	TrGC	LVROO6R1O2 + NO → LVROO6R1NO3	KRO2NO*0.108	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint12	TrGC	LVROO6R1O2 + HO_2 → LVROO6R1OOH	KRO2HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint13	TrGC	LVROO6R1O2 → LVROO6R3O2 + CH_3COCH_3	1.60E-13*RO2	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint14	TrGC	LVROO6R3O2 → LVROO6R5O2	5.68E10*exp(-8745/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2014)*
G410bpint15	TrGC	LVROO6R3O2 + NO → LVROO6R3O + NO_2	KRO2NO*0.890	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint16	TrGC	LVROO6R3O2 + NO → LVROO6R3NO3	KRO2NO*0.110	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint17	TrGC	LVROO6R3O2 + HO_2 → LVROO6R3OOH	KRO2HO2*0.820	Vereecken and Peeters (2012), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410bpint18	TrGC	LVROO6R3O2 → LVROO6R3O	2.50E-13*RO2	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint19	TrGC	LVROO6R3O → LVROO6R4P + HO_2	5.7E10*exp(-2949/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2014)*
G410bpint20	TrGC	LVROO6R5O2 → LVROO6R5P + OH	9.17E10*exp(-8706/TEMP)	Vereecken and Peeters (2012), Taraborrelli (2014)*
G410bpint21	TrGC	LVRO6R1O2 + NO → LVRO6R3O2 + NO_2	KRO2NO*0.747	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint22	TrGC	LVRO6R1O2 + NO → LVRO6R1NO3	KRO2NO*0.253	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint23	TrGC	LVRO6R1O2 + HO_2 → LVRO6R1OOH	KRO2HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint24	TrGC	LVRO6R1O2 → LVRO6R3O2	8.80E-13*RO2	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint25	TrGC	LVRO6R3O2 + NO → LVRO6R3P + NO_2	KRO2NO*0.893	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint26	TrGC	LVRO6R3O2 + NO → LVRO6R3NO3	KRO2NO*0.107	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint27	TrGC	LVRO6R3O2 + HO_2 → LVRO6R3OOH	KRO2HO2*0.914	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint28	TrGC	LVRO6R3O2 → LVRO6R3P	5.00E-12*RO2	Vereecken and Peeters (2012), Taraborrelli (2014)
G410bpint29	TrGC	NOPINONE + OH → NOPINDO2	1.55E-11	Lewis et al. (2005), Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint30	TrGC	NOPINDO2 + HO_2 → NOPINDOOH	KRO2HO2*0.890	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint31	TrGC	NOPINDO2 + NO → C89CO3 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint32	TrGC	NOPINDO2 → C89CO3	2.00E-12*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint33	TrGC	NOPINDOOH + OH → NOPINDCO + OH	2.63E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint34	TrGC	NOPINDOOH + hν → C89CO3 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410bpint35	TrGC	NOPINDCO + OH → C89CO3	3.07E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint36	TrGC	BPINENE + O_3 → NOPINONE + .63 CO + .37 HOCH2OOH + .16 OH + .16 HO_2	1.5E-17*.051/(1-.027)	Nguyen et al. (2009), Taraborrelli (2014)
G410bpint37	TrGC	BPINENE + O_3 → NOPINOO	1.5E-17*.368/(1-.027)	Nguyen et al. (2009), Taraborrelli (2014)
G410bpint38	TrGC	BPINENE + O_3 → NOPINDO2 + OH	1.5E-17*.283/(1-.027)	Nguyen et al. (2009), Taraborrelli (2014)
G410bpint40	TrGC	BPINENE + O_3 → C8BC + CO_2	1.5E-17*(.104+.167)/(1-.027)	Nguyen et al. (2009), Taraborrelli (2014)*
G410bpint41	TrGC	C8BC + OH → C8BCO2	3.04E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint42	TrGC	C8BCO2 + HO_2 → C8BCOOH	KRO2HO2*0.859	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint43	TrGC	C8BCO2 + NO → C8BCNO3	KRO2NO*0.138	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint44	TrGC	C8BCO2 + NO → C89O2 + NO_2	KRO2NO*0.862	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint45	TrGC	C8BCO2 → C89O2	2.50E-13*RO2	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint46	TrGC	C8BCOOH + OH → C8BCCO + OH	1.62E-11	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint47	TrGC	C8BCOOH + hν → C89O2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint48	TrGC	C8BCNO3 + OH → C8BCCO + NO_2	1.84E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint49	TrGC	C8BCNO3 → C89O2 + NO_2	J_IC3H7NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint50	TrGC	C8BCCO + OH → C89O2	3.94E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint51	TrGC	NOPINOO → NOPINONE + H_2O_2	6.00E-18*c(ind_H2O)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint52	TrGC	NOPINOO + CO → NOPINONE	1.2E-15	Rickard and Pascoe (2009), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410bpint53	TrGC	NOPINOO + NO → NOPINONE + NO_2	1.E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint54	TrGC	NOPINOO + NO_2 → NOPINONE + NO_3	1.E-15	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint55	TrGC	NOPINOO + SO_2 → NOPINONE + H_2SO_4	7.E-14	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint56	TrGC	BPINENE + NO_3 → LNBPINABO2	2.51E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint57	TrGC	LNBPINABO2 + HO_2 → LNBPINABOOH	KRO2HO2*0.914	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint58	TrGC	LNBPINABO2 + NO → NOPINONE + HCHO + NO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint59	TrGC	LNBPINABO2 + NO_3 → NOPINONE + HCHO + NO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint60	TrGC	LNBPINABO2 → NOPINONE + HCHO + NO_2	9.20E-14*RO2*0.7	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint61	TrGC	LNBPINABO2 → BPINANO3	9.20E-14*RO2*0.3	Rickard and Pascoe (2009), Taraborrelli (2014)*
G410bpint62	TrGC	LNBPINABOOH + OH → LNBPINABO2	9.58E-12	Rickard and Pascoe (2009), Taraborrelli (2014)
G410bpint63	TrGC	LNBPINABOOH + hν → NOPINONE + HCHO + NO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009), Taraborrelli (2014)
G410apint296	TrGC	CARENE + OH → LAPINABO2	8.7E-11*(.50+.25)	Wolfe et al. (2011), Taraborrelli (2014)*
G410apint297	TrGC	CARENE + OH → MENTHEN6ONE + HO_2	8.7E-11*.25*.60	Wolfe et al. (2011), Taraborrelli (2014)
G410apint298	TrGC	CARENE + OH → LVROO6R1O2	8.7E-11*.25*.40	Wolfe et al. (2011), Taraborrelli (2014)
G410apint299	TrGC	CARENE + O_3 → APINBOO	2.E-16*.50*.18	Wolfe et al. (2011), Taraborrelli (2014)
G410apint300	TrGC	CARENE + O_3 → PINONIC	2.E-16*.50*.16	Wolfe et al. (2011), Taraborrelli (2014)
G410apint301	TrGC	CARENE + O_3 → OH + NORPINAL + CO + HO_2	2.E-16*.50*.66	Wolfe et al. (2011), Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410apint302	TrGC	CARENE + O_3 → APINAOO	2.E-16*.50*.12	Wolfe et al. (2011), Taraborrelli (2014)
G410apint303	TrGC	CARENE + O_3 → OH + C109O2	2.E-16*.50*(.22+.66)	Wolfe et al. (2011), Taraborrelli (2014)*
G410apint304	TrGC	CARENE + NO_3 → LNAPINABO2	9.5E-12	Wolfe et al. (2011), Taraborrelli (2014)
G410myrc	TrGC	BMYRCENE + OH → MYRCISOPO2	9.19E-12*exp(1071./temp)*0.64	Hites and Turner (2009), Orlando et al. (2000), Taraborrelli (2014)
G410myrct2	TrGC	BMYRCENE + OH → MYRCO2	9.19E-12*exp(1071./temp)*0.36	Hites and Turner (2009), Orlando et al. (2000), Taraborrelli (2014)
G410myrct3	TrGC	BMYRCENE + O_3 → .25 CH_3COCH_3 + .75 OH + .75 $CH_3COCH_2O_2$ + MYRCCHO	4.7E-16	Atkinson and Arey (2003), Taraborrelli (2014)
G410myrct4	TrGNC	BMYRCENE + NO_3 → MYRCNO3	1.1E-11	Atkinson and Arey (2003), Taraborrelli (2014)
G410myrct5	TrGC	MYRCO2 → CH_3COCH_3 + HO_2 + MYRCCHO	8.E-13*RO2	Taraborrelli (2014)
G410myrct6	TrGC	MYRCO2 + HO_2 → MYRCOOH	KRO2HO2	Taraborrelli (2014)
G410myrct7	TrGCN	MYRCO2 + NO → .80 CH_3COCH_3 + .80 HO_2 + .80 MYRCCHO + .80 NO_2 + .20 MYRCNO3	KRO2NO	Taraborrelli (2014)*
G410myrct8	TrGCJ	MYRCOOH + hν → CH_3COCH_3 + OH + HO_2 + MYRCCHO	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410myrct9	TrGC	MYRCOOH + OH → MYRCOOHISOPO2	1.55E-10	Baker et al. (2004), Taraborrelli (2014)
G410myrct10	TrGC	MYRCOOH + NO_3 → CH_3COCH_3 + SURCH3CHO + NISOPO2	4.7E-13	Baker et al. (2004), Taraborrelli (2014)
G410myrct11	TrGC	MYRCNO3 + OH → $iC_3H_7ONO_2$ + MYRCCHOISOPO2	1.55E-10	see note
G410myrct12	TrGC	MYRCISOPO2 → MYRCISOPO	1.E-12*RO2	Taraborrelli (2014)
G410myrct13	TrGC	MYRCISOPO2 + HO_2 → MYRCISOPOOH	KRO2HO2	Taraborrelli (2014)
G410myrct14	TrGC	MYRCISOPO2 + NO → .8 MYRCISOPO + .8 NO_2 + .2 MYRCISOPNO3	KRO2NO	Taraborrelli (2014)
G410myrct15	TrGC	MYRCISOPO2 → MYRCHPALD + HO_2	K16HS	Taraborrelli (2014)*
G410myrct16	TrGC	MYRCISOPO → CH_3COCH_3 + SURCH3CHO + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO_2	KDEC	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410myrct17	TrGC	MYRCISOPNO3 + OH → CH_3COCH_3 + HO_2 + SURCH3CHO + ISOPBNO3	kadt+kads	Taraborrelli (2014)
G410myrct18	TrGC	MYRCISOPOOH + hν → MYRCISOPO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410myrct19	TrGC	MYRCISOPOOH + OH → SURCH3CHO + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH + CH_3COCH_3 + HO_2	kadt+kads	Taraborrelli (2014)
G410myrct20	TrGCJ	MYRCHPALD + hν → OH + ZCODC23DBCOOH + HO_2	J_HPALD	Taraborrelli (2014)
G410myrct21	TrGC	MYRCHPALD + OH → MYRCCHOHPALD + HO_2 + CH_3COCH_3	kadt+kads	Taraborrelli (2014)
G410myrct22	TrGC	MYRCHPALD + OH → SURCH3CO3 + SURCH3CHO + HCHO + GLYOX + HO_2	(kadt+kads)*acho*ach2ooh	Taraborrelli (2014)
G410myrct23	TrGC	MYRCHPALD + O_3 → MYRCCHOHPALD + .25 CH_3COCH_3 + .75 OH + .75 $CH_3COCH_2O_2$	4.7E-16	Taraborrelli (2014)
G410myrct24	TrGC	MYRCCHO + OH → SURCH3CHO + MYRCCHOISOPO2	1.55E-10	Baker et al. (2004), Taraborrelli (2014)
G410myrct25	TrGC	MYRCCHO + NO_3 → SURCH3CHO + NISOPO2	4.7E-13	Baker et al. (2004), Taraborrelli (2014)
G410myrct26	TrGC	MYRCCHOISOPO2 → MYRCCHOISOPO	1.E-12*RO2	Taraborrelli (2014)
G410myrct27	TrGC	MYRCCHOISOPO2 + HO_2 → SURCH3CHO + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH	KRO2HO2	Taraborrelli (2014)
G410myrct28	TrGC	MYRCCHOISOPO2 + NO → .8 MYRCCHOISOPO + .8 NO_2 + .2 SURCH3CHO + .2 ISOPBNO3	KRO2NO	Taraborrelli (2014)
G410myrct29	TrGC	MYRCCHOISOPO2 → MYRCCHOHPALD + HO_2	K16HS	Taraborrelli (2014)*
G410myrct30	TrGC	MYRCCHOISOPO → SURCH3CHO + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO_2	KDEC	Taraborrelli (2014)
G410myrct31	TrGCJ	MYRCCHOHPALD + hν → SURCH3CHO + OH + ZCODC23DBCOOH + HO_2	J_HPALD	Taraborrelli (2014)
G410myrct32	TrGC	MYRCCHOHPALD + OH → SURCH3CHO + .3 C1ODC2O2C4OOH + .2 C1OOHC2O2C4OD + .3 C1ODC3O2C4OOH + .2 C1OOHC3O2C4OD	(kadt+kads)*acho*ach2ooh	Taraborrelli (2014)
G410myrct33	TrGC	MYRCOOHISOPO2 → MYRCOOHISOPO	1.E-12*RO2	Taraborrelli (2014)
G410myrct34	TrGC	MYRCOOHISOPO2 + HO_2 → MYRCOOHISOPOOH	KRO2HO2	Taraborrelli (2014)
G410myrct35	TrGC	MYRCOOHISOPO2 + NO → .8 MYRCOOHISOPO + .8 NO_2 + .2 CH_3COCH_3 + .2 SURCH3CHO + .2 ISOPBNO3	KRO2NO	Taraborrelli (2014)
G410myrct36	TrGC	MYRCOOHISOPO2 → MYRCOOHHPALD + HO_2	K16HS	Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G410myrct37	TrGC	MYRCOOHISOPO → CH_3COCH_3 + SURCH3CHO + .43 MVK + .27 MACR + .7 HCHO + .29 LHC4ACCHO + HO_2 + OH	KDEC	Taraborrelli (2014)
G410myrct38	TrGCJ	MYRCOOHISOPOOH + hν → MYRCOOHISOPO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410myrct39	TrGCJ	MYRCOOHISOPOOH + hν → CH_3COCH_3 + HO_2 + SURCH3CHO + .43 ISOPBOOH + .27 ISOPDOOH + .29 LISOPACOOH + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410myrct40	TrGCJ	MYRCOOHHPALD + hν → CH_3COCH_3 + OH + SURCH3CHO + OH + ZCODC23DBCOOH + HO_2	J_HPALD	Taraborrelli (2014)
G410myrct41	TrGC	MYRCOOHHPALD + OH → CH_3COCH_3 + OH + SURCH3CHO + .3 C1ODC2O2C4OOH + .2 C1OOHC2O2C4OD + .3 C1ODC3O2C4OOH + .2 C1OOHC3O2C4OD	(kadt+kads)*acho*ach2ooh	Taraborrelli (2014)
G410myrct42	TrGC	SURCH3CHO + OH → SURCH3CO3 + H_2O	4.4E-12*EXP(365./temp)	Taraborrelli (2014)*
G410myrct43	TrGC	SURCH3CHO + hν → HCHO + HO_2 + HO_2 + CO	jx(ip_CH3CHO)	Taraborrelli (2014)
G410myrct44	TrGC	SURCH3CHO + NO_3 → HNO_3 + SURCH3CO3	KNO3AL	Taraborrelli (2014)
G410myrct45	TrGC	SURCH3CO3 → HCHO + HO_2 + CO_2	1.00E-11*0.7*RO2	Taraborrelli (2014)
G410myrct46	TrGC	SURCH3CO3 → SURCH3CO2H	1.00E-11*0.3*RO2	Taraborrelli (2014)
G410myrct47	TrGC	SURCH3CO3 + HO_2 → OH + HCHO + HO_2 + CO_2	KAPHO2*0.44	Taraborrelli (2014)
G410myrct48	TrGC	SURCH3CO3 + HO_2 → SURCH3CO3H	KAPHO2*0.41	Taraborrelli (2014)
G410myrct49	TrGC	SURCH3CO3 + HO_2 → SURCH3CO2H + O_3	KAPHO2*0.15	Taraborrelli (2014)
G410myrct50	TrGC	SURCH3CO3 + NO_2 → SURPAN	k_CH3CO3_NO2	Taraborrelli (2014)
G410myrct51	TrGC	SURCH3CO3 + NO → NO_2 + HCHO + HO_2 + CO_2	KAPNO	Taraborrelli (2014)
G410myrct52	TrGC	SURCH3CO3 + NO_3 → NO_2 + HCHO + HO_2 + CO_2	KRO2NO3*1.60	Taraborrelli (2014)
G410myrct53	TrGC	SURCH3CO2H + OH → HCHO + HO_2 + CO_2	4.2E-14*exp(850./temp)	Taraborrelli (2014)*
G410myrct54	TrGC	SURCH3CO3H + hν → HCHO + HO_2 + OH + CO_2	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410myrct55	TrGC	SURCH3CO3H + OH → SURCH3CO3 + H_2O	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G410myrct56	TrGC	SURPAN → SURCH3CO3 + NO_2	k_PAN_M	Taraborrelli (2014)
G410myrct57	TrGC	SURPAN + OH → HCHO + CO + NO_2	9.50E-13*EXP(-650./temp)	Taraborrelli (2014)
G410afarn	TrGC	FARNESENE + OH → LFARNISOPO2	2.7E-11*EXP(390./temp)	Taraborrelli (2014)*
G410afarnt2	TrGC	FARNESENE + OH → LFARNO2	2.*1.9E-11*exp(450./temp)	Taraborrelli (2014)*
G410afarnt3	TrGC	FARNESENE + O_3 → FARNCHO + .25 CH_3COCH_3 + .75 OH + .75 $CH_3COCH_2O_2$	6.51E-15*exp(-829./temp)	Taraborrelli (2014)*
G410afarnt4	TrGC	FARNESENE + O_3 → MHO + MYRCCHO + .75 OH	6.51E-15*exp(-829./temp)	Taraborrelli (2014)*
G410afarnt5	TrGNC	FARNESENE + NO_3 → LFARNO2	2E-12+2*9.37E-12	Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G410afarnt6	TrGC	LFARNO2 → LFARNO	8.E-13*RO2	Taraborrelli (2014)
G410afarnt7	TrGC	LFARNO2 + HO_2 → LFARNOOH	KRO2HO2	Taraborrelli (2014)
G410afarnt8	TrGC	LFARNO2 + NO → .75 LFARNO + .75 NO_2 + .25 LFARNONO2	KRO2NO	Taraborrelli (2014)
G410afarnt9	TrGCJ	LFARNOOH + hν → LFARNO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410afarnt10	TrGC	LFARNOOH + OH → MHOOOH + MYRCCHOISOPO2	2.7E-11*EXP(390./temp)	Taraborrelli (2014)
G410afarnt11	TrGC	LFARNONO2 + OH → .5 MHO + .5 FARNCHO + MYRCISOPNO3	2.*1.9E-11*exp(450./temp)	Taraborrelli (2014)
G410afarnt12	TrGC	LFARNO → .5 MHO + .5 MYRCCHO + .5 FARNCHO + .5 CH_3COCH_3 + HO_2	KDEC	Taraborrelli (2014)
G410afarnt13	TrGC	LFARNISOPO2 → LFARNISOPO	1.E-12*RO2	Taraborrelli (2014)
G410afarnt14	TrGC	LFARNISOPO2 + HO_2 → LFARNISOPOOH	KRO2HO2	Taraborrelli (2014)
G410afarnt15	TrGC	LFARNISOPO2 + NO → .75 LFARNISOPO + .75 NO_2 + .25 LFARNISOPNO3	KRO2NO	Taraborrelli (2014)
G410afarnt16	TrGC	LFARNISOPO2 → MYRCCHOHPALD + HO_2 + MHO	K16HS	Taraborrelli (2014)*
G410afarnt17	TrGC	LFARNISOPO → MHO + MYRCCHOISOPO	KDEC	Taraborrelli (2014)
G410afarnt18	TrGC	LFARNISOPNO3 + OH → MHO + HO_2 + ISOPBNO3	kadt+kads	Taraborrelli (2014)
G410afarnt19	TrGC	LFARNISOPOOH + hν → LFARNISOPO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410afarnt20	TrGC	LFARNISOPOOH + OH → MHO + MYRCCHOISOPO2	kadt+kads	Taraborrelli (2014)
G410afarnt21	TrGC	LFARNISOPOOH + O_3 → MHO + MYRCCHOISOPO2 + .75 OH	2.*6.51E-15*exp(-829./temp)	Taraborrelli (2014)*
G410afarnt22	TrGC	FARNCHO + OH → FARNCHOO2	1.9E-11*exp(450./temp)	Taraborrelli (2014)*
G410afarnt23	TrGC	FARNCHO + OH → FARNCHOISOPO2	2.7E-11*EXP(390./temp)	Taraborrelli (2014)*
G410afarnt24	TrGC	FARNCHO + O_3 → OPA + MYRCCHO + .75 OH	6.51E-15*exp(-829./temp)	Taraborrelli (2014)*
G410afarnt25	TrGNC	FARNCHO + NO_3 → FARNCHOISOPO2	2E-12	Taraborrelli (2014)*
G410afarnt26	TrGNC	FARNCHO + NO_3 → FARNCHOO2	9.37E-12	Taraborrelli (2014)*
G410afarnt27	TrGC	FARNCHOO2 → FARNCHOO	8.E-13*RO2	Taraborrelli (2014)
G410afarnt28	TrGC	FARNCHOO2 + HO_2 → FARNCHOOOH	KRO2HO2	Taraborrelli (2014)
G410afarnt29	TrGC	FARNCHOO2 + NO → .75 FARNCHOO + .75 NO_2 + .25 FARNCHONO3	KRO2NO	Taraborrelli (2014)
G410afarnt30	TrGCJ	FARNCHOOOH + hν → FARNCHOO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410afarnt31	TrGC	FARNCHOOOH + OH → OPA + HO_2 + MYRCCHOISOPO2	2.7E-11*EXP(390./temp)	Taraborrelli (2014)*
G410afarnt32	TrGC	FARNCHONO3 + OH → OPA + MYRCISOPNO3	1.9E-11*exp(450./temp)	Taraborrelli (2014)*
G410afarnt33	TrGC	FARNCHOO → OPA + MYRCCHO + HO_2	KDEC	Taraborrelli (2014)

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

#	labels	reaction	rate coefficient	reference
G410afarnt34	TrGC	FARNCHOISOPO2 → FARNCHOISOPO	1.E-12*RO2	Taraborrelli (2014)
G410afarnt35	TrGC	FARNCHOISOPO2 + HO_2 → FARNCHOISOPOOH	KRO2HO2	Taraborrelli (2014)
G410afarnt36	TrGC	FARNCHOISOPO2 + NO → .75 FARNCHOISOPO + .75 NO_2 + .25 FARNCHOISOPNO3	KRO2NO	Taraborrelli (2014)
G410afarnt37	TrGC	FARNCHOISOPO2 → OPA + MYRCCHOHPALD + HO_2 + MHO	K16HS	Taraborrelli (2014)*
G410afarnt38	TrGC	FARNCHOISOPO → OPA + MYRCCHOISOPO	KDEC	Taraborrelli (2014)
G410afarnt39	TrGC	FARNCHOISOPNO3 + OH → OPA + HO_2 + ISOPBNO3	kadt+kads	Taraborrelli (2014)
G410afarnt40	TrGC	FARNCHOISOPOOH + hν → FARNCHOISOPO + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410afarnt41	TrGC	FARNCHOISOPOOH + OH → OPA + MYRCCHOISOPO2	kadt+kads	Taraborrelli (2014)
G410afarnt42	TrGC	FARNCHOISOPOOH + O_3 → OPA + MYRCCHOISOPO2 + .75 OH	6.51E-15*exp(-829./temp)	Taraborrelli (2014)
G410afarnt43	TrGC	MHO + OH → MHOO2	1.37E-10	Smith et al. (1996), Taraborrelli (2014)*
G410afarnt44	TrGC	MHO + O_3 → .25 CH_3COCH_3 + .125 OPA + .25 GLYOX + .25 $CH_3COCH_2O_2$ + .125 H_2O_2 + .75 OH + .75 $CH_3COCH_2O_2$ + .75 OPA	3.9E-16	Grosjean et al. (1996), Taraborrelli (2014)*
G410afarnt45	TrGC	MHO + NO_3 → MHOO2	7E-12	Smith et al. (1996), Taraborrelli (2014)
G410afarnt46	TrGC	MHOO2 → CH_3COCH_3 + OPA + HO_2	8.E-13*RO2	Taraborrelli (2014)
G410afarnt47	TrGC	MHOO2 + HO_2 → MHOOOH	KRO2HO2	Taraborrelli (2014)
G410afarnt48	TrGC	MHOO2 + NO → .25 MHONO3 + .75 CH_3COCH_3 + .75 OPA + .75 HO_2 + .75 NO_2	KRO2NO	Taraborrelli (2014)
G410afarnt49	TrGC	MHOOOH + OH → MHOO2	0.6*k_CH3OOH_OH	Taraborrelli (2014)
G410afarnt50	TrGC	MHOOOH + OH → MHOCODOOH + HO_2	kt*ftoh*falk*falk	Taraborrelli (2014)
G410afarnt51	TrGCJ	MHOOOH + hν → CH_3COCH_3 + OPA + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
G410afarnt52	TrGCJ	MHOCODOOH + hν → CH_3COCH_3 + $CH_3COCH_2O_2$ + SURCH3CO3 + OH	1.14*jx(ip_CH3OOH)+2.77*jx(ip_HOCH2CHO)	Taraborrelli (2014)*
G410afarnt53	TrGC	MHONO3 + OH → MHOCODNO3 + HO_2	kt*ftoh*falk*fch2ono2	Taraborrelli (2014)
G410afarnt54	TrGC	MHOCODNO3 + hν → CH_3COCH_3 + NO_2 + $CH_3COCH_2O_2$ + SURCH3CO3	2.84*J_IC3H7NO3	Taraborrelli (2014)
G410afarnt55	TrGC	OPA + OH → $CH_3COCH_2O_2$ + SURCH3CO3	2.E-11	Fruekilde et al. (1997), Taraborrelli (2014)*

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

#	labels	reaction	rate coefficient	reference
G410afarnt56	TrGCJ	OPA + hν $\rightarrow$ $CH_3COCH_2O_2$ + SURCH3CO3 + HO_2	jx(ip_CH3CHO)+jx(ip_CH3COCH3)	Taraborrelli (2014)

*Notes:

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

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

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

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

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

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:

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

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

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

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

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

Structure Activity Relationship (SAR) for estimation of rate constants as developed by Taraborrelli (2010).

SAR for H-abstraction:

base rate constants

$$ks = 8.42E-13 \quad (10)$$
$$kt = 1.75E-12 \quad (11)$$
$$kp = 1.24E-13 \quad (12)$$
$$kcho = 5.55E-12 \times EXP(311/T) * .95 \quad (13)$$
$$krohro = 1.6E-13 \quad (14)$$
$$kco2h = .66 \times 4.2E-14 \times exp(850/T) \quad (15)$$

activation factors (parameter names starting with f)

$$fsoh = 3.44 \quad (16)$$
$$ftoh = 2.68 \quad (17)$$
$$fsooh = 7. \quad (18)$$
$$ftooh = 7. \quad (19)$$
$$fono2 = 0.04 \quad (20)$$
$$fch2ono2 = 0.2 \quad (21)$$
$$fcpan = .25 \quad (22)$$
$$fallyl = 3.6 \quad (23)$$
$$falk = 1.23 \quad (24)$$
$$fcho = 0.55 \quad (25)$$
$$fco2h = 1.67 \quad (26)$$
$$fco = 0.73 \quad (27)$$
$$fo = 8.15 \quad (28)$$
$$fpch2oh = 1.29 \quad (29)$$
$$ftch2oh = 0.53 \quad (30)$$

SAR for H-addition do C-C double bonds:

base rate constants

$$kadp = 0.45E-11 \quad (31)$$
$$kads = 3.0E-11 \quad (32)$$
$$kadt = 5.5E-11 \quad (33)$$
$$kadsecprim = 3.0E-11 \quad (34)$$
$$kadtertprim = 5.7E-11 \quad (35)$$

activation factors (parameter names starting with a)

$$apan = 0.56 \quad (36)$$
$$acho = 0.31 \quad (37)$$
$$acoch3 = 0.76 \quad (38)$$
$$ach2ono2 = 0.47 \quad (39)$$
$$ach2oh = 1.7 \quad (40)$$
$$ach2ooh = 0.21 \quad (41)$$
$$acoh = 2.2 \quad (42)$$
$$acooh = 2.2 \quad (43)$$
$$aco2h = 0.25 \quad (44)$$

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.

G3203: The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.

G3206: The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./`

`(6.5E-34 * EXP(1335./temp)*cair) + 1./ (2.7E-17 * EXP(2199./temp)) )`

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

G4103a: Sander et al. (2006) recommend a zero product yield for HCHO. G4103b: Sander et al. (2006) recommend a zero product yield for HCHO.

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.

G4201e: The product distribution is from Rickard and Pascoe (2009), after substitution of the Criegee intermediate by its decomposition products.

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.

G4211et1: personal communication C. Gross (MPICH)
G4211et2: personal communication C. Gross (MPICH)
G4211et3: personal communication C. Gross (MPICH)

G4213: The rate coefficient is: `k_CH3CO3_NO2 = k_3rd(temp,cair,9.7E-29,5.6,9.3E-12,1.5,0.6)`.

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_CH3CO3_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

G4226ea: personal communication C. Gross (MPICH)
G4226eb: personal communication C. Gross (MPICH)
G4226ec: personal communication C. Gross (MPICH)

G4243: Orlando et al. (1998a) estimated that about 25% of the $HOCH_2CH_2O$ in this reaction is produced with sufficient excess energy that it decomposes promptly. The decomposition products are 2 HCHO + HO_2.

G4255et2: personal communication C. Gross (MPICH)
G4255et3: personal communication C. Gross (MPICH)

G4260et2: personal communication C. Gross (MPICH)
G4260et3: personal communication C. Gross (MPICH)

G4266e: 0.4 CO2HCH2O2 approximated to HOOCH2CO2H

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 IPROPOL + 0.2 CH_3COCH_3 + 0.6 IC3H7O. IPROPOL and IC3H7O are substituted with their degradation products. We assume IPROPOL 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.

G4315a: The same value as for G4107 (CH_3OOH + OH) is used, multiplied by the branching ratio of the CH_3O_2 channel.

G4343e: k for the major channel of ACETOL + OH

G4353e: .28 CH3CHO2CO2H yield approximated by .14 CH3COCO2H + .14 CH3CHO

G4354e: k for (CH3)2CCO adjusted

G4355e: k for (CH3)2CCO adjusted

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 + $C_2H_5O_2$, repectively. 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.

G4406e: Lumped products from Taraborrelli et al. (2009).

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 HCHO + CO_2 + $HOCH_2CH_2O_2$ and HCHO + CO_2 + $C_2H_5O_2$.

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 + H_2O. CO2C3CHO is substituted with $CH_3COCH_2O_2$ + CO_2 and the products become 0.89 $CH_3COCH_2O_2$ + 0.89 CO_2 + 0.89 OH + 0.11 MEKAO2 + H_2O. MEKBOOH + OH gives 0.758 BIACET + 0.758 OH + 0.242 MEKBO2 + H_2O. MEKCOOH + OH gives 0.614 EGLYOX + 0.614 OH + 0.386 MEKCO2 + H_2O. EGLYOX is substituted with $C_2H_5O_2$ + 2 CO_2 and the products become 0.614 $C_2H_5O_2$ + 1.228 CO_2 + 0.614 OH + 0.386 MEKCO2 + H_2O.

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 + NO_2 + H_2O with C3H7CHO being substituted with 2 CO_2 + $C_2H_5O_2$. After substitution is obtained 2 CO_2 + $C_2H_5O_2$ + NO_2 + H_2O. SC4H9NO3 + OH gives MEK + NO_2 + H_2O 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.

G4437e: LHMVKABO2 is a lumped species of virtual composition 0.3 HMVKAO2 + 0.7 HMVKBO2. The products are the weighted average for the permutation reactions of each single RO2 in the MCM (Rickard and Pascoe, 2009).

G4439ea: products are the weighted average for the decomposition of 0.3 HMVKAO + 0.7 HMVKBO.

G4440e: as for G4439ea

G4441e: The rate coefficient and products are 30% for HMVKAOOH and 70% for HMVKBOOH.

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

G4462e: EZCH3CO2CHCHO 90:10 mixture of the Z- and E-isomer, CH3COCHO2CHO → .1 CH3CO3 + .1 GLYOX + .9 CH3COCHOOHCHO → .1 CH3CO3 + .1 GLYOX + .9 CH3COCOCHO → CH3CO3 + .1 GLYOX + 1.8 CO + .9 HO2;$k^{1,6}_{H-shift}$

G4463e: $k^{1,6}_{H-shift}$

G4500e: MVKO2 substituted with HCHO + ACO3 = 1.33 HCHO + .67 HCOCH2O2 + .33 CO

G4501e: coefficients from Paulot et al(2009)ACP

G4503e: k=.3E-12*.77+1.4E-12*.23

G4504e: k=1.5E-12*2.

G4505e: k=.3E-12*.46+1.E-12*.54

G4506e: k=1.5E-12*2.

G4507e: eisopao2 60percent zisopao2 40percent, MIME species

G4508e: as for G4507e

G4509e: eisopco2 42percent and zisopao2 58percent

G4510e: as for G4509e

G4511e: $k^{1,6}_{H-shift}$

G4512e: $k^{1,6}_{H-shift}$

G4521ec: k parent alkene, branching from Rickard et al(1999)

G45222: HYBIACETOOA approximated to yield BIACETOH only, CH3COCHOOHCH2OH's main reaction with OH yields BIACETOH recycling OH → substitution with BIACETOH

G4537e: O2NOCH2COCH2O2 = NO2 + 2 HCHO + CO2

G4550e: LC578OOH = .6 C57OOH + .4 C58OOH

G4550et2: LC578OOH = .6 C57OOH + .4 C58OOH

G4551e: Peroxy vinyl radical chemistry neglected G4552e: Peroxy vinyl radical chemistry neglected G4553e: Peroxy vinyl radical chemistry neglected G4555e: Peroxy vinyl radical chemistry neglected

G4577et3: from MIME ZCODC23DBCOOH = 0.64 ZC1ODC23DBC4OOH + 0.36 ZC1OOHC23DBC4OD, HOOCH2COCH2O2 substituted with HCOCOCH2OOH

G4581et8: C1ODC3OOHC4OOH → C1ODC3ODC4OOH → .5 CH3CO3 + .5 CO + .5 MGLYOX + .5 HO2 + HOOCH2CO3

G4581et10: C1ODC3OOHC4OD + OH → .25 C1ODC3ODC4OD + .375 CO + .375 CH3COCOCHO + .375 CO2 + .375 HCOCOHCH3CHO → .25(MGLYOX + 2 CO + 2 HO2) + .375 CO + .375(CH3CO3 + 2 CO + HO2) + .375 CO2 + .375(MGLYOX + CO + 2 HO2)

G4582e: $k^{1,6}_{H-shift}$

G4585et3: approximation H-abstraction only at C1

G4598et3: ZC1O3HC23DBC4OD 62percent G4598et4: HCOCOHCH3CHO substituted with CH3COCHOH + CO + HO2

G4136: CH3COCH2OOCH2CO3 → CH3CO3 + CO2 + 2 HCHO

G45mbo11: approximated to yield only MBOACO

G45mbo15: approx. not as in MCM!!!

G45mbo43: NO3CH2CO3 = HCHO + CO2 + NO2 following to Paulot et al(2009)

G410apin1: H-abstraction channels neglected, branching ratios re-scaled. G410apin2: H-abstraction channels neglected, branching ratios re-scaled. G410apin3: H-abstraction channels neglected, branching ratios re-scaled.

G410apint150: endo-cyclic vinyl ROOH assumed not be formed

G410apint162: C920CO3, C109CO, C109OH neglected

G410apint191: C811NO3 neglected

G410apint196: C812OH neglected

G410apint201: C813OH neglected

G410apint202: C813NO3 neglected

G410apint237: C512OH and CO13C4CHO neglected

G410apint239: C512NO3 neglected

G410apint242: C513OH + C513CO neglected

G410apint277: C33CO is called HCOCOCHO here

G410apint295: NC101CO substituted with C96CO3

G410bpin: BPINBO2 minor and similar to BPINAO2, peroxy ring closure of BPINCO2 is 0.6/s fast and traditional chemistry is neglected BPINCO2=LVROO6R1O2. G410bpint2: BPINBO2 minor and similar to BPINAO2, peroxy ring closure of BPINCO2 is 0.6/s fast and traditional chemistry is neglected BPINCO2=LVROO6R1O2.

G410bpint14: 1,5-H-shift

G410bpint19: LVROO6R13OO formation neglected

G410bpint20: traditional reactions neglected because of complexity

G410bpint40: .167 is for the neglected lactone stemming from the dioxirane as C8BC

G410bpint61: BPINBNO3 produced but approximated by BPINANO3

G410apint296: 2- and 3-CARENE together treated as the more emitted 3-CARENE, being similar to APINENE and assumed to yield the same products.

G410apint303: endo-cyclic vinyl ROOH assumed not be formed

G410myrct7: 20percent alkylnitrate yield like for APINENE

G410myrct15: $k^{1,6}_{H-shift}$

G410myrct29: $k^{1,6}_{H-shift}$

G410myrct36: $k^{1,6}_{H-shift}$

G410myrct53: k acetic acid + OH

G410myrct42: Surrogate acetaldehyde.

G410afarn: k for addition to the isoprene unit

G410afarnt2: k for 2-methyl-2-butene

G410afarnt3: O3 + outer double bond k for 2-methyl-2-butene, OH-yield might be much lower

G410afarnt4: O3 + inner double bond, k for 2-methyl-2-butene, MYRCCHO approximation, OH-yield might be much lower

G410afarnt5: k sum of 4-methylhexa-3,5-dienal (Baker et al., 2004) and twice 2-methyl-2-butene.

G410afarnt16: $k^{1,6}_{H-shift}$

G410afarnt21: k for 2-methyl-2-butene

G410afarnt22: k for 2-methyl-2-butene

G410afarnt23: k for addition to the isoprene unit

G410afarnt24: k for 2-methyl-2-butene

G410afarnt25: k of 4-methylhexa-3,5-dienal (Baker et al., 2004).

G410afarnt26: k of 2-methyl-2-butene

G410afarnt31: k for addition to the isoprene unit

G410afarnt32: k of 2-methyl-2-butene

G410afarnt37: $k^{1,6}_{H-shift}$

G410afarnt43: 1.57E-10 for k was relative to k(trans-2-butene), with the new k=5.662E-11(IUPAC), k(MHO+OH) is 13percent lower

G410afarnt44: .25 GLYOX + .25 CH3COCH2O2 maor products of CH3OCCH2CHO2CHO ox.

G410afarnt52: CO2H3CO3 approximation

G410afarnt55: Approximation: OPACO3 is CH3COCH2O2 + SURCH3CO3.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	jx(ip_O2)	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	jx(ip_O1D)	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	jx(ip_O3P)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2$ OH	JX(ip_H2O2)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	jx(ip_NO2O)	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow$ NO	jx(ip_NOO2)	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N2O5)	see note
J3200	TrGJ	HONO + $h\nu \rightarrow$ NO + OH	JX(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2$ + OH	JX(ip_HNO3)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333$ OH	JX(ip_HNO4)	see note
J4100e	StTrGJ	$CH_3OOH + h\nu \rightarrow$ HCHO + OH + HO_2	1.14*jx(ip_CH3OOH)	see note
J4101a	StTrGJ	HCHO + $h\nu \rightarrow H_2$ + CO	jx(ip_COH2)	see note
J4101b	StTrGJ	HCHO + $h\nu \rightarrow$ H + CO + HO_2	jx(ip_CHOH)	see note
J4104e	StTrGJ	HOCH2OOH + $h\nu \rightarrow$ OH + HO_2 + HCOOH	1.14*jx(ip_CH3OOH)	see note
J4200e	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2$ + OH	1.14*jx(ip_CH3OOH)	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2$ + CO	jx(ip_CH3CHO)	see note
J4202e	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2$ + OH + CO_2	1.14*jx(ip_CH3CO3H)	see note
J4204e	TrGNCJ	PAN + $h\nu \rightarrow .6\ CH_3C(O)OO + .6\ NO_2 + .4\ CH_3O_2 + .4\ CO_2$ + .4 NO_3	jx(ip_PAN)	see note
J4205ae	TrGCJ	$HOCH_2CHO + h\nu \rightarrow$ HCHO + 2 HO_2 + CO	jx(ip_HOCH2CHO)*0.70	Taraborrelli (2014)
J4205be	TrGCJ	$HOCH_2CHO + h\nu \rightarrow 1.16$ OH + .84 HCOCH2O2 + .1 HCHO + .1 CO + .06 GLYOX	jx(ip_HOCH2CHO)*0.15	Taraborrelli (2014)
J4205ce	TrGCJ	$HOCH_2CHO + h\nu \rightarrow CH_3OH$ + CO	jx(ip_HOCH2CHO)*0.15	Taraborrelli (2014)
J4206e	TrGCJ	HOOCH2CHO + $h\nu \rightarrow$ OH + HCHO + CO + HO_2	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Taraborrelli (2014)
J4206et2	TrGCJ	$HOCH_2CO_3H + h\nu \rightarrow$ HCHO + HO_2 + OH + CO_2	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4207	TrGCJ	PHAN + $h\nu \rightarrow HOCH_2CO_3 + NO_2$	jx(ip_PAN)	see note
J4208	TrGCJ	GLYOX + $h\nu \rightarrow$ 2 CO + 2 HO_2	jx(ip_GLYOX)	see note
J4209	TrGNCJ	$HCOCO_2H + h\nu \rightarrow 2\ HO_2$ + CO + CO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)*
J4210e	TrGNCJ	$HCOCO_3H + h\nu \rightarrow HO_2$ + CO + OH + CO_2	1.14*jx(ip_CH3OOH)+jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4211e	TrGCJ	HYETHO2H + hν → $HOCH_2CH_2O$ + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4212	TrGCJ	ETHOHNO3 + hν → HO_2 + 2 HCHO + NO_2	J_IC3H7NO3	see note
J4213e	TrGCJ	HOOCH2CO3H + hν → OH + HCHO + CO_2 + OH	2*1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4214e	TrGC	HOOCH2CO2H + hν → OH + HCHO + HO_2 + CO_2	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4215e	TrGC	CH2CO + hν → .4 CO_2 + .8 H + .34 CO + .34 OH + .34 HO_2 + .16 HCHO + .16 $O(^3P)$ + .1 HCOOH + CO	J_ketene* 0.36	Taraborrelli (2014)
J4216e	TrGC	CH3CHOHOOH + hν → CH_3O_2 + HCOOH + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4217e	TrGCJ	NO3CH2CHO + hν → HO_2 + CO + HCHO + NO_2	1.59*J_IC3H7NO3+jx(ip_CH3COCH3)	Taraborrelli (2014)
J4300e	TrGCJ	iC_3H_7OOH + hν → CH_3COCH_3 + HO_2 + OH	1.14*jx(ip_CH3OOH)	von Kuhlmann (2001)*
J4301	TrGCJ	CH_3COCH_3 + hν → $CH_3C(O)OO$ + CH_3O_2	jx(ip_CH3COCH3)	see note
J4302	TrGCJ	CH_3COCH_2OH + hν → $CH_3C(O)OO$ + HCHO + HO_2	J_ACETOL	see note
J4303	TrGCJ	MGLYOX + hν → $CH_3C(O)OO$ + CO + HO_2	jx(ip_MGLYOX)	see note
J4304e	TrGCJ	$CH_3COCH_2O_2H$ + hν → $CH_3C(O)OO$ + HCHO + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2014)
J4305e	TrGCJ	HOCH2COCH2OOH + hν → HOCH2CO + HCHO + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2014)
J4306	TrGNCJ	$iC_3H_7ONO_2$ + hν → CH_3COCH_3 + NO_2 + HO_2	J_IC3H7NO3	von Kuhlmann et al. (2003)*
J4307	TrGCJ	NOA + hν → $CH_3C(O)OO$ + HCHO + NO_2	J_IC3H7NO3+jx(ip_CH3COCH3)	see note
J4309e	TrGCJ	HYPROPO2H + hν → CH_3CHO + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4310e	TrGNCJ	PR2O2HNO3 + hν → NOA + HO_2 + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4311e	TrGCJ	HOCH2COCHO + hν → HOCH2CO + CO + HO_2	jx(ip_MGLYOX)	Taraborrelli (2014)
J4312e	TrGCJ	CH3COCO2H + hν → .5 CH_3CHO + .8 CO_2 + .4 $CH_3C(O)OO$ + .3 HO_2 + .1 CH_3COOH + .1 OH + .2 CO	JX(IP_MGLYOX)	Taraborrelli (2014)
J4313e	TrGCJ	HCOCOCH2OOH + hν → HCOCO3A + HCHO + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2014)
J4314e	TrGCJ	HCOCOCH2OOH + hν → HOOCH2CO3 + CO + HO_2	JX(IP_MGLYOX)	Taraborrelli (2014)
J4315e	TrGCJ	HCOCOCHO + hν → HCOCO3A + HO_2 + CO	2*JX(IP_MGLYOX)	Taraborrelli (2014)
J4316e	TrGC	CH3COCO3H + hν → $CH_3C(O)OO$ + OH + CO_2	JX(IP_MGLYOX)+1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4317e	TrGC	CH3CHCO + hν → C_2H_4 + CO	J_ketene*0.36*2.	Taraborrelli (2014)*
J4400e	TrGCJ	LC_4H_9OOH + hν → OH + 0.254 CO_2 + 0.5552 MEK + 0.5552 HO_2 + 0.3178 CH_3CHO + 0.4448 $C_2H_5O_2$	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4401	TrGCJ	MVK + hν → C_3H_6 + CO	jx(ip_MVK)	Taraborrelli (2014)*
J4403	TrGCJ	MEK + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*jx(ip_CHOH)	von Kuhlmann et al. (2003)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4404e	TrGCJ	LMEKOOH + hν → 0.538 HCHO + 0.538 CO_2 + 0.459 $HOCH_2CH_2O_2$ + 0.079 $C_2H_5O_2$ + 0.462 $CH_3C(O)OO$ + 0.462 CH_3CHO + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)*
J4405	TrGCJ	BIACET + hν → 2 $CH_3C(O)OO$	2.15*jx(ip_MGLYOX)	see note
J4406	TrGNCJ	LC4H9NO3 + hν → NO_2 + 0.254 CO_2 + 0.5552 MEK + 0.5552 HO_2 + 0.3178 CH_3CHO + 0.4448 $C_2H_5O_2$	J_IC3H7NO3	see note
J4407e	TrGNCJ	MPAN + hν → .6 MACO3 + .6 NO_2 + .4 MACO2 + .4 NO_3	jx(ip_PAN)	Taraborrelli (2014)*
J4409e	TrGCJ	CO2H3CO3H + hν → CH3COCHOH + OH + CO_2	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4410	TrGCJ	CO2H3CO3H + hν → $CH_3C(O)OO$ + HO_2 + $HCOCO_3H$	J_ACETOL	Rickard and Pascoe (2009)*
J4410t2	TrGCJ	CO2H3CO2H + hν → $CH_3C(O)OO$ + $HCOCO_2H$ + HO_2	J_ACETOL	Taraborrelli (2014)
J4411	TrGCJ	MACR + hν → .5 MACO3 + .5 MACO2 + .5 CO + HO_2	jx(ip_MACR)	see note
J4412e	TrGCJ	MACROOH + hν → MACRO + OH	1.14*jx(ip_CH3OOH)+ 2.77*jx(ip_HOCH2CHO)	see note
J4414	TrGCJ	MACROH + hν → CH_3COCH_2OH + CO + HO_2 + HO_2	2.77*jx(ip_HOCH2CHO)	see note
J4415e	TrGCJ	MACO3H + hν → MACO2 + OH	1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4416e	TrGCJ	LHMVKABOOH + hν → .12 CH3COCHOH + .88 $CH_3C(O)OO$ + .88 $HOCH_2CHO$ + .12 HCHO + OH	1.14*jx(ip_CH3OOH)+J_ACETOL	Taraborrelli (2014)
J4418e	TrGCJ	CO2H3CHO + hν → CH3COCHOH + CO + HO_2	jx(ip_HOCH2CHO)+J_ACETOL	Taraborrelli (2014)
J4419	TrGCJ	HO12CO3C4 + hν → $CH_3C(O)OO$ + $HOCH_2CHO$ + HO_2	J_ACETOL	Rickard and Pascoe (2009)*
J4420e	TrGCJ	BIACETOH + hν → $CH_3C(O)OO$ + HOCH2CO	2.15*jx(ip_MGLYOX)	Taraborrelli (2014)
J4421e	TrGC	HCOCCH3CO + hν → .5 OH + .25 HCOCOCH2O2 + .25 $CH_3C(O)OO$ + .5 CH3CHCO + .5 CO	J_KETENE	Taraborrelli (2014)
J4422e	TrGC	CH3COCHCO + hν → .0192 CH3COCO2H + .1848 H_2O_2 + .2208 MGLYOX + .36 OH + .36 CO + .56 $CH_3C(O)OO$ + .2 CH_3CHO + .2 CO_2 + .2 HCHO + .2 HO_2	J_KETENE*0.5	Taraborrelli (2014)
J4422et2	TrGC	CH3COCHCO + hν → CH3CHCO + CO	J_KETENE*0.5	Taraborrelli (2014)
J4423e	TrGCJ	CH3COCOCHO + hν → $CH_3C(O)OO$ + CO + CO + HO_2	jx(ip_MGLYOX)	Taraborrelli (2014)
J4424e	TrGCJ	CH3COCOCHO + hν → $CH_3C(O)OO$ + HCOCO3A	2.15*jx(ip_MGLYOX)	Taraborrelli (2014)
J4424et2	TrGC	CH3COCOCO2H + hν → $CH_3C(O)OO$ + CO + CO_2 + HO_2	3.15*jx(ip_MGLYOX)	Taraborrelli (2014)
J4502et2	TrGCJ	LISOPACOOH + hν → LHC4ACCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4503et2	TrGNCJ	LISOPACNO3 + hν → LHC4ACCHO + HO_2 + NO_2	0.59*J_IC3H7NO3	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4504e	TrGCJ	ISOPBOOH + hν → MVK + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4505e	TrGNCJ	ISOPBNO3 + hν → MVK + HCHO + HO_2 + NO_2	2.84*J_IC3H7NO3	see note
J4506e	TrGCJ	ISOPDOOH + hν → MACR + HCHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4507	TrGNCJ	ISOPDNO3 + hν → MACR + HCHO + HO_2 + NO_2	J_IC3H7NO3	see note
J4508e	TrGNCJ	NISOPOOH + hν → NC4CHO + HO_2 + OH	1.14*jx(ip_CH3OOH)	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 HOCHCHO + .5 CO + .5 HO_2 + .5 CO_2	1.14*jx(ip_CH3OOH)	Taraborrelli et al. (2009)*
J4511e	TrGCJ	LHC4ACCHO + hν → .5 LHC4ACCO3 + .5 HO_2 + .5 OH + .25 MACRO2 + .25 LHMVKABO2	jx(ip_MACR)	Taraborrelli (2014)*
J4512e	TrGCJ	LC578OOH + hν → .25 CH_3COCH_2OH + .75 MGLYOX + .25 HOCHCHO + .75 $HOCH_2CHO$ + .75 HO_2 + OH	1.14*jx(ip_CH3OOH)+ 2.77*jx(ip_HOCH2CHO)	Taraborrelli (2014)
J4513e	TrGCJ	LHC4ACCO3H + hν → OH + .5 MACRO2 + .5 LHMVKABO2 + OH + CO_2	J_HPALD	Taraborrelli (2014)*
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 → MACO2 + HOCH2CO	0.5*jx(ip_MVK)	Taraborrelli (2014)
J4516e	TrGCJ	C59OOH + hν → CH_3COCH_2OH + HOCH2CO + OH	J_ACETOL+1.14*jx(ip_CH3OOH)	Taraborrelli (2014)
J4517e	TrGCJ	ZCODC23DBCOOH + hν → LHC4ACCO3 + OH	J_HPALD	Taraborrelli (2014)
J4518e	TrGCJ	ZCO3HC23DBCOD + hν → .62 EZCH3CO2CHCHO + .38 EZCHOCCH3CHO2 + OH + CO_2	J_HPALD	Taraborrelli (2014)
J4519e	TrGCJ	C1OOHC2OOHC4OD + hν → $CH_3COCH_2O_2H$ + OH + 2 CO + HO_2	2.77*JX(IP_HOCH2CHO)	Taraborrelli (2014)
J4520e	TrGCJ	C1OOHC2OOHC4OD + hν → .5 $CH_3COCH_2O_2H$ + .5 HOCHCHO + .5 CO2H3CHO + .5 HCHO + 1.5 OH	2.*1.14*JX(IP_CH3OOH)	Taraborrelli (2014)
J4523e	TrGCJ	C1ODC2OOHC4OD + hν → MGLYOX + HOCHCHO + OH	1.14*JX(IP_CH3OOH)	Taraborrelli (2014)
J4524e	TrGCJ	C1ODC2OOHC4OD + hν → CO2H3CHO + CO + HO_2 + OH	2.*2.77*JX(IP_HOCH2CHO)	Taraborrelli (2014)*
J4525	TrGCJ	PEROXYRINGC2OOH + hν → CH3COCH2OOCH2CHO + HO_2 + OH	1.14*JX(IP_CH3OOH)	Taraborrelli (2014)
J4526	TrGCJ	PEROXYRINGC2OOH + hν → HCHO + OH + HO_2 + CO2H3CHO	1.14*JX(IP_CH3OOH)	Taraborrelli (2014)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4525e	TrGCJ	ZCODC23DBCOD + hν → .5 CH3COCHCO + .5 HCOCCH3CO + CO + HO_2 + OH	jx(ip_NO2)*0.1*0.5	Taraborrelli (2014)
J4526e	TrGCJ	CH3COCH2OOCH2CHO + hν → $CH_3C(O)OO$ + HCHO + GLYOX + HO_2	1.14*JX(IP_CH3OOH)+J_ACETOL	Taraborrelli (2014)
J4527e	TrGCJ	CH3COCH2OOCH2CHO + hν → $CH_3C(O)OO$ + HCHO + HCHO + CO + HO_2	jx(ip_HOCH2CHO)	Taraborrelli (2014)

*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($iC_3H_7ONO_2$)
J(54) → J($iC_3H_7ONO_2$)
J(55) → J($iC_3H_7ONO_2$)
J(56)+J(57) → jx(ip_NOA)

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

J4212: It is assumed that J(ETHOHNO3) is the same as J($iC_3H_7ONO_2$).

J4302: Following von Kuhlmann et al. (2003), we use J(CH_3COCH_2OH) = 0.11*jx(ip_CHOH). As an additional factor, the quantum yield of 0.65 is taken from Orlando et al. (1999a).

J4306: Following von Kuhlmann et al. (2003), we use J($iC_3H_7ONO_2$) = 3.7*jx(ip_PAN).

J4307: NOA contains the cromophores of both CH_3COCH_3 and a nitrate group. It is assumed here that the J values are additive, i.e.: J(NOA) = J(CH_3COCH_3) + J($iC_3H_7ONO_2$).

J4317e: products Chong and Kistiakowsky 1964, 0.36 quantum yield at 334nm Kelley and Hase1975, factor 2 because of bigger structure and fit to C2H4_LBA

J4401: Romero et al(2005)

J4406: It is assumed that J(LC4H9NO3) is the same as J($iC_3H_7ONO_2$).

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($HOCH_2CHO$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4505: It is assumed that J(ISOPBNO3) = 2.84 × J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

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

J4511e: Peroxy vinyl radical chemistry approximated

J4513e: Peroxy vinyl radical chemistry approximated

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

J4524e: the loss of C4OD is neglected

J4526: decomposition of a dialkoxy radical

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