The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs5`

MECCA version: `3.0`

Date: March 3, 2014.

Selected reactions:
"`Tr && (G || (Aa && Mbl)) && !I && !Hg`"

Number of aerosol phases: 2

Number of species in selected mechanism:

Gas phase:	161
Aqueous phase:	62
All species:	223

Number of reactions in selected mechanism:

Gas phase (Gnnn):	313
Aqueous phase (Annn):	28
Henry (Hnnn):	74
Photolysis (Jnnn):	90
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	56
Isotope exchange (DGnnn):	0
Dummy (Dnn):	2
All equations:	563

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

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.3E-11*EXP(55./temp)`	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2006)
G1004	StTrG	$O_3 \rightarrow O_2$	`1.3E-5`	see note
G2100	StTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,4.4E-32,1.3,4.7E-11, 0.2,0.6)`	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	`2.8E-12*EXP(-1800./temp)`	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$	`1.E-14*EXP(-490./temp)`	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	`4.8E-11*EXP(250./temp)`	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`1.63E-10*EXP(60./temp)`	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`1.8E-12`	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`2.15E-11*EXP(110./temp)`	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Sander et al. (2006)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Sander et al. (2006)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(2.7E-27*EXP(11000./temp))`	Sander et al. (2006)*
G3200	TrGN	$NO + OH \rightarrow HONO$	`k_3rd(temp,cair,7.0E-31,2.6,3.6E-11, 0.1,0.6)`	Sander et al. (2006)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	`3.5E-12*EXP(250./temp)`	Sander et al. (2006)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	`k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0., 0.6)`	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	`3.5E-12`	Sander et al. (2006)
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	`1.8E-11*EXP(-390./temp)`	Sander et al. (2006)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	`k_HNO3_OH`	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Sander et al. (2006)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`	Sander et al. (2006)
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	`1.7E-12*EXP(-710./temp)`	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow NH_2O + O_2$	`4.3E-12*EXP(-930./temp)`	Kohlmann and Poppe (1999)
G3211	TrGN	$NH_2 + HO_2 \rightarrow NH_2O + OH$	`4.8E-07*EXP(-628./temp)*temp**(-1.32)`	Kohlmann and Poppe (1999)
G3212	TrGN	$NH_2 + HO_2 \rightarrow HNO + H_2O$	`9.4E-09*EXP(-356./temp)*temp**(-1.12)`	Kohlmann and Poppe (1999)

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

#	labels	reaction	rate coefficient	reference
G3213	TrGN	$NH_2 + NO \rightarrow HO_2 + OH + N_2$	1.92E-12*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3214	TrGN	$NH_2 + NO \rightarrow N_2 + H_2O$	1.41E-11*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3215	TrGN	$NH_2 + NO_2 \rightarrow N_2O + H_2O$	1.2E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3216	TrGN	$NH_2 + NO_2 \rightarrow NH_2O + NO$	0.8E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3217	TrGN	$NH_2O + O_3 \rightarrow NH_2 + O_2$	1.2E-14	Kohlmann and Poppe (1999)
G3218	TrGN	$NH_2O \rightarrow NHOH$	1.3E3	Kohlmann and Poppe (1999)
G3219	TrGN	$HNO + OH \rightarrow NO + H_2O$	8.0E-11*EXP(-500./temp)	Kohlmann and Poppe (1999)
G3220	TrGN	$HNO + NHOH \rightarrow NH_2OH + NO$	1.66E-12*EXP(-1500./temp)	Kohlmann and Poppe (1999)
G3221	TrGN	$HNO + NO_2 \rightarrow HONO + NO$	1.0E-12*EXP(-1000./temp)	Kohlmann and Poppe (1999)
G3222	TrGN	$NHOH + OH \rightarrow HNO + H_2O$	1.66E-12	Kohlmann and Poppe (1999)
G3223	TrGN	$NH_2OH + OH \rightarrow NHOH + H_2O$	4.13E-11*EXP(-2138./temp)	Kohlmann and Poppe (1999)
G3224	TrGN	$HNO + O_2 \rightarrow HO_2 + NO$	3.65E-14*EXP(-4600./temp)	Kohlmann and Poppe (1999)
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	$CH_3OH + OH \rightarrow HCHO + HO_2$	2.9E-12*EXP(-345./temp)	Sander et al. (2006)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	4.1E-13*EXP(750./temp)	Sander et al. (2006)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2006)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (2006)
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. (2006)
G4106b	StTrG	$CH_3O_2 \rightarrow .5\ HCHO + .5\ CH_3OH + .5\ O_2$	2.*RO2*9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2006)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2006)*
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. (2006)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	(1.57E-13+cair*3.54E-33)	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow CO_2 + HO_2 + H_2O$	4.0E-13	Sander et al. (2006)
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	1.49E-17*temp*temp*EXP(-499./temp)	Atkinson (2003)
G4201	TrGC	$C_2H_4 + O_3 \rightarrow HCHO + .63\ CO + .13\ HO_2 + 0.23125\ HCOOH + 0.13875\ HCHO + 0.13875\ H_2O_2 + .13\ OH$	1.2E-14*EXP(-2630./temp)	Sander et al. (2006)*
G4202	TrGC	$C_2H_4 + OH \rightarrow HOCH_2CH_2O_2$	k_3rd(temp,cair,1.0E-28,4.5,8.8E-12, 0.85,0.6)	Sander et al. (2006)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*EXP(700./temp)	Sander et al. (2006)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	2.6E-12*EXP(365./temp)	Sander et al. (2006)
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)*

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

#	labels	reaction	rate coefficient	reference
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
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	4.4E-12*EXP(365./temp)	Atkinson et al. (2006)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	KNO3AL	Sander et al. (2006)
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2 + CO_2 + H_2O$	4.2E-14*EXP(855./temp)	Atkinson et al. (2006)
G4211a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))	Tyndall et al. (2001)
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))	Tyndall et al. (2001)
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	Sander et al. (2006)
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. (2006)*
G4222	TrGC	$C_2H_2 + OH \rightarrow 0.636\ GLYOX + 0.636\ OH + 0.364\ HCOOH + 0.364\ CO + 0.364\ HO_2$	k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,-2.,0.6)	Sander et al. (2006)
G4223	TrGC	$HOCH_2CHO + OH \rightarrow .8\ HOCH_2CO_3 + .2\ GLYOX + .2\ HO_2 + H_2O$	1.00E-11	Rickard and Pascoe (2009)
G4224	TrGNC	$HOCH_2CHO + NO_3 \rightarrow HOCH_2CO_3 + HNO_3$	KNO3AL	Rickard and Pascoe (2009)
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)
G4226	TrGC	$HOCH_2CO_3 + HO_2 \rightarrow .71\ HOCH_2CO_3H + .29\ HOCH_2CO_2H + .29\ O_3$	KAPHO2	Rickard and Pascoe (2009)
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)
G4230	TrGC	$HOCH_2CO_2H + OH \rightarrow HCHO + HO_2 + CO_2 + H_2O$	2.73E-12	Rickard and Pascoe (2009)
G4231	TrGC	$HOCH_2CO_3H + OH \rightarrow HOCH_2CO_3 + H_2O$	6.19E-12	Rickard and Pascoe (2009)
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)
G4234	TrGC	$GLYOX + OH \rightarrow 1.2\ CO + .6\ HO_2 + .4\ HCOCO_3 + H_2O$	1.14E-11	Rickard and Pascoe (2009)
G4235	TrGNC	$GLYOX + NO_3 \rightarrow 1.2\ CO + .6\ HO_2 + .4\ HCOCO_3 + HNO_3$	KNO3AL	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4236	TrGC	$HCOCO_3 \rightarrow .7\ CO + .7\ HO_2 + .7\ CO_2 + .3\ HCOCO_2H$	1.00E-11*RO2	Rickard and Pascoe (2009)
G4237	TrGC	$HCOCO_3 + HO_2 \rightarrow .71\ HCOCO_3H + .29\ HCOCO_2H + .29\ O_3$	KAPHO2	Rickard and Pascoe (2009)
G4238	TrGNC	$HCOCO_3 + NO \rightarrow HO_2 + CO + NO_2 + CO_2$	KAPNO	Rickard and Pascoe (2009)
G4239	TrGNC	$HCOCO_3 + NO_3 \rightarrow HO_2 + CO + NO_2 + CO_2$	KRO2NO3*1.60	Rickard and Pascoe (2009)
G4240	TrGC	$HCOCO_2H + OH \rightarrow CO + HO_2 + CO_2 + H_2O$	1.23E-11	Rickard and Pascoe (2009)
G4241	TrGC	$HCOCO_3H + OH \rightarrow HCOCO_3 + H_2O$	1.58E-11	Rickard and Pascoe (2009)
G4242	TrGC	$HOCH_2CH_2O_2 \rightarrow .6\ HOCH_2CH_2O + .2\ HOCH_2CHO + .2$ ETHGLY	2.00E-12*RO2	Rickard and Pascoe (2009)
G4243	TrGNC	$HOCH_2CH_2O_2 + NO \rightarrow .24875\ HO_2 + .4975\ HCHO + .74625\ HOCH_2CH_2O + .995\ NO_2 + .005$ ETHOHNO3	KRO2NO	Rickard and Pascoe (2009)*
G4244	TrGC	$HOCH_2CH_2O_2 + HO_2 \rightarrow$ HYETHO2H	2.00E-13*EXP(1250./temp)	Rickard and Pascoe (2009)
G4245	TrGNC	ETHOHNO3 + OH $\rightarrow HOCH_2CHO + NO_2 + H_2O$	8.40E-13	Rickard and Pascoe (2009)
G4246a	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CH_2O_2 + H_2O$	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4246b	TrGC	HYETHO2H + OH $\rightarrow HOCH_2CHO + OH + H_2O$	1.38E-11	Rickard and Pascoe (2009)
G4247a	TrGC	$HOCH_2CH_2O \rightarrow HO_2 + HOCH_2CHO$	6.00E-14*EXP(-550./temp)*C(ind_O2)	Rickard and Pascoe (2009)
G4247b	TrGC	$HOCH_2CH_2O \rightarrow HO_2 + HCHO + HCHO$	9.50E13*EXP(-5988./temp)	Rickard and Pascoe (2009)
G4248	TrGC	ETHGLY + OH $\rightarrow HOCH_2CHO + HO_2 + H_2O$	7.70E-12	Rickard and Pascoe (2009)
G4300	TrGC	$C_3H_8 + OH \rightarrow .736\ iC_3H_7O_2 + .264\ C_2H_5O_2 + .264\ CO_2 + .264\ HO_2 + H_2O$	1.55E-17*temp*temp*EXP(-61./temp)	Rickard and Pascoe (2009)*
G4301	TrGC	$C_3H_6 + O_3 \rightarrow .28\ CH_3O_2 + .1\ CH_4 + .075\ CH_3COOH + .56\ CO + .075\ HCOOH + .09\ H_2O_2 + .28\ HO_2 + .2\ CO_2 + .545\ CH_3CHO + .545\ HCHO + .36\ OH$	6.5E-15*EXP(-1900./temp)	Sander et al. (2006)*
G4302	TrGC	$C_3H_6 + OH \rightarrow$ HYPROPO2	k_3rd(temp,cair,8.E-27,3.5,3.E-11,0., 0.5)	Atkinson et al. (1999)
G4303	TrGNC	$C_3H_6 + NO_3 \rightarrow$ PRONO3BO2	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	1.9E-13*EXP(1300./temp)	Atkinson (1997)*
G4305	TrGNC	$iC_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ iC_3H_7ONO_2$	2.7E-12*EXP(360./temp)	Atkinson et al. (1999)
G4306	TrGC	$iC_3H_7O_2 \rightarrow CH_3COCH_3 + .8\ HO_2$	4.E-14*RO2	Rickard and Pascoe (2009)*
G4307	TrGC	$iC_3H_7OOH + OH \rightarrow .27\ iC_3H_7O_2 + .73\ CH_3COCH_3 + .73\ OH + H_2O$	1.66E-11 + 0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4311	TrGC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	(1.33E-13+3.82E-11*EXP(-2000./temp))	Sander et al. (2006)
G4312	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	8.6E-13*EXP(700./temp)	Tyndall et al. (2001)
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow CH_3C(O)OO + HCHO + NO_2$	2.9E-12*EXP(300./temp)	Sander et al. (2006)

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

#	labels	reaction	rate coefficient	reference
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)
G4315a	TrGC	$CH_3COCH_2O_2H$ + OH → $CH_3COCH_2O_2$ + H_2O	0.6*k_CH3OOH_OH	see note
G4315b	TrGC	$CH_3COCH_2O_2H$ + OH → MGLYOX + OH + H_2O	8.39E-12	Rickard and Pascoe (2009)
G4316	TrGC	CH_3COCH_2OH + OH → MGLYOX + HO_2 + H_2O	3.E-12	Atkinson et al. (1999)
G4317	TrGC	MGLYOX + OH → $CH_3C(O)OO$ + CO	8.4E-13*EXP(830./temp)	Tyndall et al. (1995)
G4320	TrGNC	$iC_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	6.2E-13*EXP(-230./temp)	Atkinson et al. (1999)
G4321	TrGNC	$CH_3COCH_2O_2$ + NO_3 → $CH_3C(O)OO$ + HCHO + NO_2	KRO2NO3	Rickard and Pascoe (2009)
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	1.90E-12*EXP(190./temp)	Rickard and Pascoe (2009)
G4326b	TrGC	HYPROPO2H + OH → CH_3COCH_2OH + OH	2.44E-11	Rickard and Pascoe (2009)
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	3.47E-12	Rickard and Pascoe (2009)
G4331	TrGNC	MGLYOX + NO_3 → $CH_3C(O)OO$ + CO + HNO_3	KNO3AL*2.4	Rickard and Pascoe (2009)
G4332	TrGNC	NOA + OH → MGLYOX + NO_2	1.30E-13	Rickard and Pascoe (2009)
G4333	TrGC	HOCH2COCHO + OH → $HOCH_2CO_3$ + CO	1.44E-11	Rickard and Pascoe (2009)
G4334	TrGNC	HOCH2COCHO + NO_3 → $HOCH_2CO_3$ + CO + HNO_3	KNO3AL*2.4	Rickard and Pascoe (2009)
G4335	TrGC	HOCH2COCO2H + OH → $HOCH_2CO_3$ + CO_2	2.89E-12	Rickard and Pascoe (2009)
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)
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)*

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

#	labels	reaction	rate coefficient	reference
G4405	TrGC	MVK + O_3 → 0.28 $CH_3C(O)OO$ + 0.56 CO + 0.225 LCARBON + 0.075 HCOOH + 0.09 H_2O_2 + 0.28 HO_2 + 0.1 CO_2 + 0.1 CH_3CHO + 0.645 HCHO + 0.36 OH + 0.545 MGLYOX	`7.51E-16*EXP(-1521./temp)`	Rickard and Pascoe (2009)
G4406	TrGC	MVK + OH → LHMVKABO2	`4.13E-12*EXP(452./temp)`	Rickard and Pascoe (2009)
G4413	TrGC	MEK + OH → LMEKO2 + H_2O	`3.24E-18*temp*temp*EXP(414./temp)`	Rickard and Pascoe (2009)*
G4414	TrGC	LMEKO2 + HO_2 → LMEKOOH	`KRO2HO2*0.625`	Rickard and Pascoe (2009)
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)*
G4421	TrGC	MACR + OH → .57 MACO3 + .43 MACRO2	`1.86E-11*EXP(175./temp)`	Rickard and Pascoe (2009)
G4422	TrGC	MACR + O_3 → .59 MGLYOX + .41 $CH_3C(O)OO$ + .03375 HCOOH + .55625 HCHO + .82 CO + .12375 H_2O_2 + .41 HO_2 + .82 OH	`1.36E-15*EXP(-2112./temp)`	Rickard and Pascoe (2009)
G4423	TrGNC	MACR + NO_3 → MACO3 + HNO_3	`KNO3AL*2.0`	Rickard and Pascoe (2009)
G4424	TrGC	MACO3 → .7 $CH_3C(O)OO$ + .7 HCHO + .7 CO_2 + .3 MACO2H	`1.00E-11*RO2`	Rickard and Pascoe (2009)
G4425	TrGC	MACO3 + HO_2 → .71 MACO3H + .29 MACO2H + .29 O_3	`KAPHO2`	Rickard and Pascoe (2009)
G4426	TrGNC	MACO3 + NO → $CH_3C(O)OO$ + HCHO + NO_2 + CO_2	`8.70E-12*EXP(290./temp)`	Rickard and Pascoe (2009)
G4427	TrGNC	MACO3 + NO_2 → MPAN	`k_CH3CO3_NO2`	Rickard and Pascoe (2009)
G4428	TrGNC	MACO3 + NO_3 → $CH_3C(O)OO$ + HCHO + NO_2 + CO_2	`KRO2NO3*1.60`	Rickard and Pascoe (2009)
G4429	TrGC	MACRO2 → .7 CH_3COCH_2OH + .7 HCHO + .7 HO_2 + .3 MACROH	`9.20E-14*RO2`	Rickard and Pascoe (2009)
G4430	TrGC	MACRO2 + HO_2 → MACROOH	`KRO2HO2*0.625`	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4431	TrGNC	MACRO2 + NO → CH_3COCH_2OH + HCHO + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4432	TrGNC	MACRO2 + NO_3 → CH_3COCH_2OH + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4433	TrGC	MACROOH + OH → MACRO2	2.82E-11	Rickard and Pascoe (2009)
G4434	TrGC	MACROH + OH → CH_3COCH_2OH + HCHO + HO_2	2.46E-11	Rickard and Pascoe (2009)
G4435	TrGC	MACO2H + OH → $CH_3C(O)OO$ + HCHO + CO_2	1.51E-11	Rickard and Pascoe (2009)
G4436	TrGC	MACO3H + OH → MACO3	1.87E-11	Rickard and Pascoe (2009)
G4437	TrGC	LHMVKABO2 → 0.06 CO2H3CHO + 0.18 HO_2 + 0.18 HCHO + 0.18 MGLYOX + 0.42 $CH_3C(O)OO$ + .42 $HOCH_2CHO$+ .2 HO12CO3C4 + .14 BIACETOH	(.3*2.00E-12 + .7*8.80E-13)*RO2	Rickard and Pascoe (2009)*
G4438	TrGC	LHMVKABO2 + HO_2 → LHMVKABOOH	KRO2HO2*0.625	Rickard and Pascoe (2009)
G4439	TrGNC	LHMVKABO2 + NO → .3 MGLYOX + .7 $HOCH_2CHO$ + .7 $CH_3C(O)OO$ + .3 HCHO + .3 HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G4440	TrGNC	LHMVKABO2 + NO_3 → .3 MGLYOX + .7 $HOCH_2CHO$ + .7 $CH_3C(O)OO$ + .3 HCHO + .3 HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G4441	TrGC	LHMVKABOOH + OH → .3 CO2H3CHO + .7 BIACETOH + OH	4.496E-11	Rickard and Pascoe (2009)*
G4442	TrGC	MVKOH + OH → LMVKOHABO2	4.60E-12*EXP(452./temp)	Rickard and Pascoe (2009)
G4443	TrGC	MVKOH + O_3 → 0.56 CO + 0.545 HOCH2COCHO + 0.075 HOCH2COCO2H + 0.075 HCOOH + 0.09 H_2O_2 + 0.28 $HOCH_2CO_3$ + 0.28 HO_2 + 0.2 CO_2 + 0.545 HCHO + 0.36 OH + 0.1 $HOCH_2CHO$	7.51E-16*EXP(-1521./temp)	Rickard and Pascoe (2009)
G4444	TrGC	LMVKOHABO2 → .7 $HOCH_2CHO$ + .7 $HOCH_2CO_3$ + .3 HOCH2COCHO + .3 HCHO + .3 HO_2	(0.3*2.00E-12+0.7*8.80E-13)*RO2	Rickard and Pascoe (2009)*
G4445	TrGC	LMVKOHABO2 + HO_2 → LMVKOHABOOH	KRO2HO2*0.625	Rickard and Pascoe (2009)
G4446	TrGNC	LMVKOHABO2 + NO → .3 HOCH2COCHO + .3 HCHO + .3 HO_2 + .7 $HOCH_2CHO$ + .7 $HOCH_2CO_3$ + NO_2	KRO2NO	Rickard and Pascoe (2009)*
G4447	TrGNC	LMVKOHABO2 + NO_3 → .3 HOCH2COCHO + .3 HCHO + .3 HO_2 + .7 $HOCH_2CHO$ + .7 $HOCH_2CO_3$ + NO_2	KRO2NO3	Rickard and Pascoe (2009)*
G4448	TrGC	LMVKOHABOOH + OH → .7 HO12CO3C4 + .3 CO2H3CHO + OH	5.98E-11	Rickard and Pascoe (2009)*
G4449	TrGC	CO2H3CHO + OH → CO2H3CO3	2.45E-11	Rickard and Pascoe (2009)
G4450	TrGNC	CO2H3CHO + NO_3 → CO2H3CO3 + HNO_3	KNO3AL*4.0	Rickard and Pascoe (2009)
G4451	TrGC	CO2H3CO3 → MGLYOX + HO_2 + CO_2	1.00E-11*RO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4452	TrGC	CO2H3CO3 + HO_2 → CO2H3CO3H	KAPHO2	Rickard and Pascoe (2009)
G4453	TrGNC	CO2H3CO3 + NO → MGLYOX + HO_2 + NO_2 + CO_2	KAPNO	Rickard and Pascoe (2009)
G4454	TrGNC	CO2H3CO3 + NO_3 → MGLYOX + HO_2 + NO_2 + CO_2	KRO2NO3*1.60	Rickard and Pascoe (2009)
G4455	TrGC	CO2H3CO3H + OH → CO2H3CO3	7.34E-12	Rickard and Pascoe (2009)
G4456	TrGC	HO12CO3C4 + OH → BIACETOH + HO_2	1.88E-11	Rickard and Pascoe (2009)
G4500	TrGC	C_5H_8 + O_3 → .051 CH_3O_2 + .1575 $CH_3C(O)OO$ + .054 LHMVKABO2 + .522 CO + .06875 HCOOH + .11 H_2O_2 + .32475 MACR + .1275 C_3H_6 + .2625 HO_2 + .255 CO_2 + .74975 HCHO + .04125 MACO2H + .27 OH + .244 MVK	7.86E-15*EXP(-1913./temp)	Rickard and Pascoe (2009)
G4501	TrGC	C_5H_8 + OH → .25 LISOPACO2 + .491 ISOPBO2 + .259 ISOPDO2	2.54E-11*EXP(410./temp)	Atkinson (1997)
G4509	TrGNC	C_5H_8 + NO_3 → NISOPO2	3.03E-12*EXP(-446./temp)	Rickard and Pascoe (2009)
G4510	TrGC	LISOPACO2 → .9 LHC4ACCHO + .8 HO_2 + .1 ISOPAOH	2.4E-12*RO2	Rickard and Pascoe (2009)
G4511	TrGC	LISOPACO2 + HO_2 → LISOPACOOH	0.706*KRO2HO2	Rickard and Pascoe (2009)
G4512	TrGNC	LISOPACO2 + NO → .892 LHC4ACCHO + .892 HO_2 + .892 NO_2 + .108 LISOPACNO3	KRO2NO	Rickard and Pascoe (2009)
G4513	TrGNC	LISOPACO2 + NO_3 → LHC4ACCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4514	TrGC	LISOPACOOH + OH → LHC4ACCHO + OH	1.07E-10	Rickard and Pascoe (2009)
G4515	TrGC	ISOPAOH + OH → LHC4ACCHO + HO_2	9.30E-11	Rickard and Pascoe (2009)
G4516	TrGNC	LISOPACNO3 + OH → LHC4ACCHO + NO_2	8.91E-11	Rickard and Pascoe (2009)
G4517	TrGC	ISOPBO2 → .6 MVK + .2 MVKOH + .6 HCHO + .6 HO_2 + .2 CH_3O_2 + .2 ISOPBOH	8.E-13*RO2	Rickard and Pascoe (2009)
G4518	TrGC	ISOPBO2 + HO_2 → ISOPBOOH	0.706*KRO2HO2	Rickard and Pascoe (2009)
G4519	TrGNC	ISOPBO2 + NO → .696 MVK + .232 MVKOH + .696 HCHO + .696 HO_2 + .232 CH_3O_2 + .928 NO_2 + .072 ISOPBNO3	KRO2NO	Rickard and Pascoe (2009)
G4520	TrGNC	ISOPBO2 + NO_3 → .75 MVK + .25 MVKOH + .75 HCHO + .75 HO_2 + .25 CH_3O_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4521	TrGC	ISOPBOOH + OH → ISOPBO2	4.2E-11	Rickard and Pascoe (2009)
G4522	TrGC	ISOPBOH + OH → .75 MVK + .25 MVKOH + .75 HCHO + .75 HO_2 + .25 CH_3O_2	3.85E-11	Rickard and Pascoe (2009)
G4523	TrGNC	ISOPBNO3 + OH → MVK + HCHO + NO_2	3.55E-11	Rickard and Pascoe (2009)
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	0.706*KRO2HO2	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4526	TrGNC	ISOPDO2 + NO → .855 MACR + .855 HCHO + .855 HO_2 + .855 NO_2 + .145 ISOPDNO3	KRO2NO	Rickard and Pascoe (2009)
G4527	TrGNC	ISOPDO2 + NO_3 → MACR + HCHO + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4528	TrGC	ISOPDOOH + OH → HCOC5 + OH	1.07E-10	Rickard and Pascoe (2009)
G4529	TrGC	ISOPDOH + OH → HCOC5 + HO_2	7.38E-11	Rickard and Pascoe (2009)
G4530	TrGNC	ISOPDNO3 + OH → HCOC5 + NO_2	6.1E-11	Rickard and Pascoe (2009)
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)
G4537	TrGNC	NC4CHO + O_3 → .445 NO_2 + .89 CO + .075625 H_2O_2 + .034375 $HCOCO_2H$ + .555 NOA + .445 HO_2 + .520625 GLYOX + .89 OH + .445 MGLYOX	2.40E-17	Rickard and Pascoe (2009)
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)
G4540	TrGNC	LNISO3 + NO → NOA + .5 GLYOX + .5 CO + HO_2 + NO_2 + .5 CO_2	.5*KAPNO +.5*KRO2NO	Rickard and Pascoe (2009)
G4541	TrGNC	LNISO3 + NO_3 → NOA + .5 GLYOX + .5 CO + 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)
G4543	TrGC	LHC4ACCHO + OH → .52 LC578O2 + .48 LHC4ACCO3	4.52E-11	Rickard and Pascoe (2009)
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)
G4546	TrGC	LC578O2 → .5 CH_3COCH_2OH + .5 MGLYOX + .5 GLYOX + .5 $HOCH_2CHO$ + HO_2	9.20E-14*RO2	Rickard and Pascoe (2009)
G4547	TrGC	LC578O2 + HO_2 → LC578OOH	KRO2HO2*0.706	Rickard and Pascoe (2009)
G4548	TrGNC	LC578O2 + NO → .5 CH_3COCH_2OH + .5 MGLYOX + .5 GLYOX + .5 $HOCH_2CHO$ + HO_2 + NO_2	KRO2NO	Rickard and Pascoe (2009)

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

#	labels	reaction	rate coefficient	reference
G4549	TrGNC	LC578O2 + NO_3 → .5 CH_3COCH_2OH + .5 MGLYOX + .5 GLYOX + .5 $HOCH_2CHO$ + HO_2 + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4550	TrGC	LC578OOH + OH → LC578O2	3.16E-11	Rickard and Pascoe (2009)
G4551	TrGC	LHC4ACCO3 → .3 LHC4ACCO2H + .35 CH_3COCH_2OH + .35 $HOCH_2CHO$ + .35 $CH_3C(O)OO$ + .35 CO + .35 HO_2 + .7 CO_2	1.00E-11*RO2	Rickard and Pascoe (2009)
G4552	TrGC	LHC4ACCO3 + HO_2 → .71 LHC4ACCO3H + .29 LHC4ACCO2H + .29 O_3	KAPHO2	Rickard and Pascoe (2009)
G4553	TrGNC	LHC4ACCO3 + NO → .5 CH_3COCH_2OH + .5 $HOCH_2CHO$ + .5 $CH_3C(O)OO$ + .5 CO + .5 HO_2 + NO_2 + CO_2	KAPNO	Rickard and Pascoe (2009)
G4554	TrGNC	LHC4ACCO3 + NO_2 → LC5PAN1719	k_CH3CO3_NO2	Rickard and Pascoe (2009)
G4555	TrGNC	LHC4ACCO3 + NO_3 → .5 CH_3COCH_2OH + .5 $HOCH_2CHO$ + .5 $CH_3C(O)OO$ + .5 CO + .5 HO_2 + NO_2 + CO_2	1.6*KRO2NO3	Rickard and Pascoe (2009)
G4556	TrGC	LHC4ACCO2H + OH → .5 CH_3COCH_2OH + .5 $HOCH_2CHO$ + .5 $CH_3C(O)OO$ + .5 CO + .5 HO_2 + CO_2	2.52E-11	Rickard and Pascoe (2009)
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)
G4560	TrGC	HCOC5 + OH → C59O2	3.81E-11	Rickard and Pascoe (2009)
G4561	TrGC	C59O2 → CH_3COCH_2OH + $HOCH_2CO_3$	9.20E-14*RO2	Rickard and Pascoe (2009)
G4562	TrGC	C59O2 + HO_2 → C59OOH	KRO2HO2*0.706	Rickard and Pascoe (2009)
G4563	TrGNC	C59O2 + NO → CH_3COCH_2OH + $HOCH_2CO_3$ + NO_2	KRO2NO	Rickard and Pascoe (2009)
G4564	TrGNC	C59O2 + NO_3 → CH_3COCH_2OH + $HOCH_2CO_3$ + NO_2	KRO2NO3	Rickard and Pascoe (2009)
G4565	TrGC	C59OOH + OH → C59O2	9.7E-12	Rickard and Pascoe (2009)
G6100	StTrGCl	Cl + O_3 → ClO + O_2	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl + O_2$	`2.2E-12*EXP(340./temp)`	Atkinson et al. (2007)
G6205	StTrGCl	$HCl + OH \rightarrow Cl + H_2O$	`1.7E-12*EXP(-230./temp)`	Atkinson et al. (2007)
G6209	TrGCl	$HOCl \rightarrow Cl + OH$	`0.020391678`	[redacted]
G6210	TrGBr	$HOBr \rightarrow Br + OH$	`0.12034`	[redacted]
G6300	StTrGNCl	$ClO + NO \rightarrow NO_2 + Cl$	`6.2E-12*EXP(295./temp)`	Atkinson et al. (2007)
G6301	StTrGNCl	$ClO + NO_2 \rightarrow ClNO_3$	`k_3rd_iupac(temp,cair,1.6E-31,3.4, 7.E-11,0.,0.4)`	Atkinson et al. (2007)
G6302	TrGCl	$ClNO_3 \rightarrow ClO + NO_2$	`6.918E-7*exp(-10909./temp)*cair`	Anderson and Fahey (1990)
G6304	StTrGNCl	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	`6.2E-12*EXP(145./temp)`	Atkinson et al. (2007)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	`6.6E-12*EXP(-1240./temp)`	Atkinson et al. (2006)
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	`8.1E-11*EXP(-34./temp)`	Atkinson et al. (2006)
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	`5.9E-11`	Atkinson et al. (2006)*
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	`3.3E-12*EXP(-115./temp)`	Sander et al. (2006)
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow H_2O + 3\ Cl$	`1.64E-12*EXP(-1520./temp)`	Sander et al. (2006)
G6409	TrGCCl	$Cl + C_2H_4 \rightarrow HOCH_2CH_2O_2 + HCl$	`k_3rd_iupac(temp,cair,1.85E-29,3.3, 6.0E-10,0.0,0.4)`	Atkinson et al. (2006)*
G6410	TrGCCl	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)OO$	`8.0e-11`	Atkinson et al. (2006)
G6411	TrGCCl	$C_2H_2 + Cl \rightarrow CH_3O_2 + HCl$	`k_3rd_iupac(temp,cair,6.1e-30,3.0, 2.0e-10,0.,0.6)`	Atkinson et al. (2006)
G6412	TrGCCl	$C_2H_6 + Cl \rightarrow CH_3O_2 + HCl$	`8.3E-11*EXP(-100./temp)`	Atkinson et al. (2006)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	`1.7E-11*EXP(-800./temp)`	Atkinson et al. (2007)
G7102a	StTrGBr	$BrO + BrO \rightarrow 2\ Br + O_2$	`2.7E-12`	Atkinson et al. (2007)
G7102b	StTrGBr	$BrO + BrO \rightarrow Br_2 + O_2$	`2.9E-14*EXP(840./temp)`	Atkinson et al. (2007)
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr + O_2$	`7.7E-12*EXP(-450./temp)`	Atkinson et al. (2007)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr + O_2$	`4.5E-12*EXP(500./temp)`	Atkinson et al. (2007)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	`6.7E-12*EXP(155./temp)`	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	`2.0E-11*EXP(240./temp)`	Atkinson et al. (2007)
G7300	TrGBr	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	`4.9E-11`	Orlando and Tyndall (1996)
G7301	StTrGNBr	$BrO + NO \rightarrow Br + NO_2$	`8.7E-12*EXP(260./temp)`	Atkinson et al. (2007)
G7302	StTrGNBr	$BrO + NO_2 \rightarrow BrNO_3$	`k_BrO_NO2`	Atkinson et al. (2007)*
G7303	TrGBr	$BrNO_3 \rightarrow BrO + NO_2$	`k_BrO_NO2/(5.44E-9*exp(14192./temp) *1.E6*R_gas*temp/(atm2Pa*N_A))`	Orlando and Tyndall (1996), Atkinson et al. (2007)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	`7.7E-12*EXP(-580./temp)`	Atkinson et al. (2006)
G7401	TrGBr	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	`2.6E-12*EXP(-1600./temp)`	Kondo and Benson (1984)
G7402a	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + HCHO$	`G7402a_yield*5.7E-12`	Aranda et al. (1997)

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

#	labels	reaction	rate coefficient	reference
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	(1.-G7402a_yield)*5.7E-12	Aranda et al. (1997)
G7403	StTrGBr	$CH_3Br + OH \rightarrow H_2O + Br$	2.35E-12*EXP(-1300./temp)	Sander et al. (2006)
G7404	TrGCBr	$Br + C_2H_4 \rightarrow HOCH_2CH_2O_2 + HBr$	2.8E-13*EXP(224./temp)/(1.+ 1.13E24*EXP(-3200./temp)/C(ind_O2))	Atkinson et al. (2006)*
G7405	TrGCBr	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)OO$	1.8e-11*EXP(-460./temp)	Atkinson et al. (2006)
G7406	TrGCBr	$Br + C_2H_2 \rightarrow CH_3O_2 + HBr$	6.35e-15*EXP(440./temp)	Atkinson et al. (2006)
G7407	TrGBr	$CHBr_3 + OH \rightarrow H_2O + 3\ Br$	1.35E-12*EXP(-600./temp)	Sander et al. (2006)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	Sander et al. (2006)*
G7600	TrGClBr	$Br + BrCl \rightarrow Br_2 + Cl$	3.32E-15	Manion et al. (2010)
G7601	TrGClBr	$Br + Cl_2 \rightarrow BrCl + Cl$	1.10E-15	Dolson and Leone (1987)
G7602	TrGClBr	$Br_2 + Cl \rightarrow BrCl + Br$	2.3E-10*EXP(135./temp)	Bedjanian et al. (1998)
G7603a	StTrGClBr	$BrO + ClO \rightarrow Br + OClO$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGClBr	$BrO + ClO \rightarrow Br + Cl + O_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGClBr	$BrO + ClO \rightarrow BrCl + O_2$	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G7604	TrGClBr	$BrCl + Cl \rightarrow Br + Cl_2$	1.45E-11	Clyne and Cruse (1972)
G7605	TrGClBr	$CHCl_2Br + OH \rightarrow H_2O + Br$	2.0E-12*EXP(-840./temp)	see note
G7606	TrGClBr	$CHClBr_2 + OH \rightarrow H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	see note
G7607	TrGClBr	$CH_2ClBr + OH \rightarrow H_2O + Br$	2.4E-12*EXP(-920./temp)	Sander et al. (2006)*
G9200	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0., 0.6)	Sander et al. (2006)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2004)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	1.8E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	5.E-11	Barone et al. (1995)
G9600	TrGSCl	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	$DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	$DMS + BrO \rightarrow DMSO + Br$	4.4E-13	Ingham et al. (1999)

*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:

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

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

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

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

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:

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

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

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

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

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

G2110: The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984).

G3109: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)`.

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

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.

G4103: 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.

G4201: 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 ≈ 0.1 $HOCH_2CH_2O_2$ + 0.9 CH_3CHO + 0.9 HO_2.

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

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

G4221: The rate coefficient is`k_PAN_M = k_CH3CO3_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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

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

G4301: The product distribution is for terminal olefin carbons from Zaveri and Peters (1999).

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.

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.

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.

G4437: 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).

G4439: products are the weighted average for the decomposition of 0.3 HMVKAO + 0.7 HMVKBO.

G4440: as for G4439

G4441: The rate coefficient and products are 30% for HMVKAOOH and 70% for HMVKBOOH.

G4444: LMVKOHABO2 is a lumped species of virtual composition 0.3 MVKOHAO2 + 0.7 MVKOHBO2. The products are the weighted average for the permutation reactions of each single RO2 in the MCM (Rickard and Pascoe, 2009).

G4446: products are the weighted average for the decomposition of 0.3 MVKOHAO + 0.7 MVKOHBO.

G4447: as for G4446

G4448: The rate coefficient and products are 30% for MVKOHAOOH and 70% for MVKOHBOOH.

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

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

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

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

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

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

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

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

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

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

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

G9400: Addition path. The rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

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
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	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
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)*
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH + CO_2$	jx(ip_CH3CO3H)	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	see note
J4205	TrGCJ	$HOCH_2CHO + h\nu \rightarrow HO_2 + HCHO + HO_2 + CO$	jx(ip_HOCH2CHO)	see note
J4206	TrGCJ	$HOCH_2CO_3H + h\nu \rightarrow HCHO + HO_2 + OH + CO_2$	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)*
J4210	TrGNCJ	$HCOCO_3H + h\nu \rightarrow HO_2 + CO + OH + CO_2$	(jx(ip_CH3OOH)+jx(ip_HOCH2CHO))	Rickard and Pascoe (2009)*
J4211	TrGCJ	$HYETHO2H + h\nu \rightarrow HOCH_2CH_2O + OH$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4212	TrGCJ	$ETHOHNO3 + h\nu \rightarrow HO_2 + 2\ HCHO + NO_2$	J_IC3H7NO3	see note
J4300	TrGCJ	$iC_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH3OOH)	von Kuhlmann (2001)*
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	see note
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	J_ACETOL	see note
J4303	TrGCJ	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4304	TrGCJ	$CH_3COCH_2O_2H$ + hν $\rightarrow$ $CH_3C(O)OO$ + HCHO + OH	jx(ip_CH3OOH)+J_ACETOL	Rickard and Pascoe (2009)*
J4306	TrGNCJ	$iC_3H_7ONO_2$ + hν $\rightarrow$ CH_3COCH_3 + NO_2 + HO_2	J_IC3H7NO3	von Kuhlmann et al. (2003)*
J4307	TrGCJ	NOA + hν $\rightarrow$ $CH_3C(O)OO$ + HCHO + NO_2	J_IC3H7NO3+jx(ip_CH3COCH3)	see note
J4308	TrGCJ	HOCH2COCO2H + hν $\rightarrow$ $HOCH_2CO_3$ + HO_2 + CO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)*
J4309	TrGCJ	HYPROPO2H + hν $\rightarrow$ CH_3CHO + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4310	TrGNCJ	PR2O2HNO3 + hν $\rightarrow$ NOA + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4311	TrGCJ	HOCH2COCHO + hν $\rightarrow$ $HOCH_2CO_3$ + CO + HO_2	jx(ip_MGLYOX)	Rickard and Pascoe (2009)*
J4400	TrGCJ	LC_4H_9OOH + hν $\rightarrow$ OH + 0.254 CO_2 + 0.5552 MEK + 0.5552 HO_2 + 0.3178 CH_3CHO + 0.4448 $C_2H_5O_2$	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4401	TrGCJ	MVK + hν $\rightarrow$ .5 C_3H_6 + .5 $CH_3C(O)OO$ + .5 HCHO + CO + .5 HO_2	jx(ip_MVK)	see note
J4403	TrGCJ	MEK + hν $\rightarrow$ $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*jx(ip_CHOH)	von Kuhlmann et al. (2003)*
J4404	TrGCJ	LMEKOOH + hν $\rightarrow$ 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	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4405	TrGCJ	BIACET + hν $\rightarrow$ 2 $CH_3C(O)OO$	2.15*jx(ip_MGLYOX)	see note
J4406	TrGNCJ	LC4H9NO3 + hν $\rightarrow$ 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
J4407	TrGNCJ	MPAN + hν $\rightarrow$ MACO3 + NO_2	jx(ip_PAN)	see note
J4408	TrGCJ	LMVKOHABOOH + hν $\rightarrow$ .3 HOCH2COCHO + .3 HCHO + .3 HO_2 + .7 $HOCH_2CHO$ + .7 $HOCH_2CO_3$ + OH	J_ACETOL+jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4409	TrGCJ	CO2H3CO3H + hν $\rightarrow$ MGLYOX + HO_2 + OH + CO_2	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4410	TrGCJ	CO2H3CO3H + hν $\rightarrow$ $CH_3C(O)OO$ + HO_2 + $HCOCO_3H$	J_ACETOL	Rickard and Pascoe (2009)*
J4411	TrGCJ	MACR + hν $\rightarrow$ .5 MACO3 + .5 $CH_3C(O)OO$ + .5 HCHO + .5 CO + HO_2	jx(ip_MACR)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4412	TrGCJ	MACROOH + hν $\rightarrow$ CH_3COCH_2OH + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4413	TrGCJ	MACROOH + hν $\rightarrow$ CH_3COCH_2OH + CO + HO_2 + OH	2.77*jx(ip_HOCH2CHO)	see note
J4414	TrGCJ	MACROH + hν $\rightarrow$ CH_3COCH_2OH + CO + HO_2 + HO_2	2.77*jx(ip_HOCH2CHO)	see note
J4415	TrGCJ	MACO3H + hν $\rightarrow$ $CH_3C(O)OO$ + HCHO + OH + CO_2	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4416	TrGCJ	LHMVKABOOH + hν $\rightarrow$ .3 MGLYOX + .7 $CH_3C(O)OO$ + .7 $HOCH_2CHO$ + .3 HCHO + .3 HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4417	TrGCJ	MVKOH + hν $\rightarrow$ .5 HCHO + .5 HO_2 + .5 $HOCH_2CO_3$ + CO + 1.5 LCARBON	jx(ip_MVK)	Rickard and Pascoe (2009)*
J4418	TrGCJ	CO2H3CHO + hν $\rightarrow$ MGLYOX + CO + HO_2 + HO_2	jx(ip_HOCH2CHO)	Rickard and Pascoe (2009)*
J4419	TrGCJ	HO12CO3C4 + hν $\rightarrow$ $CH_3C(O)OO$ + $HOCH_2CHO$ + HO_2	J_ACETOL	Rickard and Pascoe (2009)*
J4420	TrGCJ	BIACETOH + hν $\rightarrow$ $CH_3C(O)OO$ + $HOCH_2CO_3$	2.15*jx(ip_MGLYOX)	see note
J4502	TrGCJ	LISOPACOOH + hν $\rightarrow$ LHC4ACCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4503	TrGNCJ	LISOPACNO3 + hν $\rightarrow$ LHC4ACCHO + HO_2 + NO_2	0.59*J_IC3H7NO3	see note
J4504	TrGCJ	ISOPBOOH + hν $\rightarrow$ .75 MVK + .25 MVKOH + .75 HCHO + .75 HO_2 + .25 CH_3O_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4505	TrGNCJ	ISOPBNO3 + hν $\rightarrow$ .75 MVK + .25 MVKOH + .75 HCHO + .75 HO_2 + .25 CH_3O_2 + NO_2	2.84*J_IC3H7NO3	see note
J4506	TrGCJ	ISOPDOOH + hν $\rightarrow$ MACR + HCHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4507	TrGNCJ	ISOPDNO3 + hν $\rightarrow$ MACR + HCHO + HO_2 + NO_2	J_IC3H7NO3	see note
J4508	TrGNCJ	NISOPOOH + hν $\rightarrow$ NC4CHO + HO_2 + OH	jx(ip_CH3OOH)	Rickard and Pascoe (2009)*
J4509	TrGNCJ	NC4CHO + hν $\rightarrow$ NOA + 2 CO + 2 HO_2	jx(ip_MACR)	see note
J4510	TrGNCJ	LNISOOH + hν $\rightarrow$ NOA + OH + .5 GLYOX + .5 CO + HO_2 + .5 CO_2	jx(ip_CH3OOH)	Taraborrelli et al. (2009)*
J4511	TrGCJ	LHC4ACCHO + hν $\rightarrow$ .5 LHC4ACCO3 + .25 CH_3COCH_2OH + .25 $HOCH_2CHO$ + .25 $CH_3C(O)OO$ + .75 CO + 1.25 HO_2	jx(ip_MACR)	Rickard and Pascoe (2009)*
J4512	TrGCJ	LC578OOH + hν $\rightarrow$ .5 CH_3COCH_2OH + .5 MGLYOX + .5 GLYOX + .5 $HOCH_2CHO$ + HO_2 + OH	jx(ip_CH3OOH)	Taraborrelli et al. (2009)*

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4513	TrGCJ	LHC4ACCO3H + hν → .5 CH_3COCH_2OH + .5 $HOCH_2CHO$ + .5 $CH_3C(O)OO$ + .5 CO + .5 HO_2 + OH + CO_2	`jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J4514	TrGNCJ	LC5PAN1719 + hν → .5 MACROH + .5 HO12CO3C4 + CO + NO_2	`jx(ip_PAN)`	see note
J4515	TrGCJ	HCOC5 + hν → $CH_3C(O)OO$ + HCHO + $HOCH_2CO_3$	`0.5*jx(ip_MVK)`	see note
J4516	TrGCJ	C59OOH + hν → CH_3COCH_2OH + $HOCH_2CO_3$ + OH	`J_ACETOL+jx(ip_CH3OOH)`	Rickard and Pascoe (2009)*
J6000	StTrGClJ	Cl_2 + hν → Cl + Cl	`jx(ip_Cl2)`	see note
J6100	StTrGClJ	Cl_2O_2 + hν → 2 Cl	`1.4*jx(ip_Cl2O2)`	see note
J6101	StTrGClJ	OClO + hν → ClO + $O(^3P)$	`jx(ip_OClO)`	see note
J6201	StTrGClJ	HOCl + hν → OH + Cl	`jx(ip_HOCl)`	see note
J6300	TrGNClJ	$ClNO_2$ + hν → Cl + NO_2	`jx(ip_ClNO2)`	see note
J6301a	StTrGNClJ	$ClNO_3$ + hν → Cl + NO_3	`jx(ip_ClNO3)`	see note
J6301b	StTrGNClJ	$ClNO_3$ + hν → ClO + NO_2	`jx(ip_ClONO2)`	see note
J7000	StTrGBrJ	Br_2 + hν → Br + Br	`jx(ip_Br2)`	see note
J7100	StTrGBrJ	BrO + hν → Br + $O(^3P)$	`jx(ip_BrO)`	see note
J7200	StTrGBrJ	HOBr + hν → Br + OH	`jx(ip_HOBr)`	see note
J7300	TrGNBrJ	$BrNO_2$ + hν → Br + NO_2	`jx(ip_BrNO2)`	see note
J7301	StTrGNBrJ	$BrNO_3$ + hν → 0.29 Br + 0.29 NO_3 + 0.71 BrO + 0.71 NO_2	`jx(ip_BrNO3)`	see note
J7401	TrGBrJ	CH_2Br_2 + hν → 2 Br	`jx(ip_CH2Br2)`	see note
J7402	TrGBrJ	$CHBr_3$ + hν → 3 Br	`jx(ip_CHBr3)`	see note
J7600	StTrGClBrJ	BrCl + hν → Br + Cl	`jx(ip_BrCl)`	see note
J7602	TrGClBrJ	CH_2ClBr + hν → Br + Cl	`jx(ip_CH2ClBr)`	see note
J7603	TrGClBrJ	$CHCl_2Br$ + hν → Br + 2 Cl	`jx(ip_CHCl2Br)`	see note
J7604	TrGClBrJ	$CHClBr_2$ + hν → 2 Br + Cl	`jx(ip_CHClBr2)`	see note

*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. (1999).

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($iC_3H_7ONO_2$).

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

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

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

J4413: It is assumed that J(MACROOH) is 2.77 times larger than J($HOCH_2CHO$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

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).

J4420: It is assumed that J(BIACETOH) is 2.15 times larger than J(MGLYOX), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4503: It is assumed that J(LISOPACNO3) = 0.59 $\times$ J($iC_3H_7ONO_2$), consistent with the photolysis rate coefficients used in the MCM (Rickard and Pascoe, 2009).

J4505: It is assumed that J(ISOPBNO3) = 2.84 $\times$ 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).

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

J4515: Consistent with the MCM (Rickard and Pascoe, 2009), we assume that J(HCOC5) is half as large as J(MVK).

J6100: Stimpfle et al. (2004) claim that the combination of absorption cross sections from Burkholder et al. (1990) and the Cl_2O_2 formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed Cl_2O_2/ClO ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the Cl_2O_2 formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

J7301: The quantum yields are from Sander et al. (2003).

Table 3: Henry's law coefficients

substance	$\frac{k_H^\ominus}{M/atm}$	$\frac{-\Delta_{soln}H/R}{K}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1.\times10^{5}$	6338.	Lind and Kok (1994)
NH_3	58.	4085.	Chameides (1984)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
N_2O_5	BIG	0.	see note
HONO	4.9×10^{1}	4780.	Schwartz and White (1981)
HNO_3	$2.45\times10^{6}/1.5\times10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CH_3COOH	4.1×10^{3}	6200.	Sander et al. (2006)
PAN	2.8	5730.	Sander et al. (2006)
$C_2H_5O_2$	6.	5600.	see note
CH_3CHO	1.29×10^{1}	5890.	Sander et al. (2006)
CH_3COCH_3	28.1	5050.	Sander et al. (2006)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^{2}	5862.	Huthwelker et al. (1995)
$ClNO_3$	BIG	0.	see note
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	9.3×10^{1}	5862.	Vogt et al. (1996)*
$BrNO_3$	BIG	0.	see note
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO_2	1.2	3120.	Chameides (1984)

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

substance	$\frac{k_H^\ominus}{\text{M/atm}}$	$\frac{-\Delta_{soln}H/R}{\text{K}}$	reference
H_2SO_4	$1.\times10^{11}$	0.	see note
CH_3SO_3H	BIG	0.	see note
DMS	5.4×10^{-1}	3500.	Staudinger and Roberts (2001)
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*

*Notes:

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

The temperature dependence of the Henry constants is:

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

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

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

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

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

$C_2H_5O_2$: Assumed to be the same as $K_H(CH_3O_2)$.

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

HOBr: This value was estimated by Vogt et al. (1996).

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

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	(default)	DeMore et al. (1997)*
OH	0.01	(default)	Takami et al. (1998)*
HO_2	0.5	(default)	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NH_3	0.06	(default)	DeMore et al. (1997)*
NO	5.0×10^{-5}	(default)	Saastad et al. (1993)*
NO_2	0.0015	(default)	Ponche et al. (1993)*
NO_3	0.04	(default)	Rudich et al. (1996)*
N_2O_5	(default)	(default)	DeMore et al. (1997)*
HONO	0.04	(default)	DeMore et al. (1997)*
HNO_3	0.5	(default)	Abbatt and Waschewsky (1998)*
HNO_4	(default)	(default)	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
CO_2	0.01	2000.	see note
HCHO	0.04	(default)	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CH_3COOH	2.0×10^{-2}	4079.	Davidovits et al. (1995)
PAN	(default)	(default)	see note
$C_2H_5O_2$	(default)	(default)	see note
CH_3CHO	3.0×10^{-2}	(default)	see note
CH_3COCH_3	3.72×10^{-3}	6395.	Davidovits et al. (1995)
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	(default)	see note
$ClNO_3$	0.108	(default)	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	(default)	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	(default)	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO_2	0.11	(default)	DeMore et al. (1997)
H_2SO_4	0.65	(default)	Pöschl et al. (1998)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{obs}H/R}{K}$	reference
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMS	(default)	(default)	see note
DMSO	0.048	2578.	De Bruyn et al. (1994)

*Notes:

If no data are available, the following default values are used:
$\alpha^{\ominus} = 0.1$
$-\Delta_{obs}H/R = 0$ K

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

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

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

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

and further:

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

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NH_3: Value measured at 295 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

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

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

HONO: Value measured between 247 and 297 K.

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

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

CO_2: Estimate.

HCHO: Value measured between 260 and 270 K.

PAN: Estimate.

$C_2H_5O_2$: Estimate.

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

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

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

$ClNO_3$: Value measured at 274.5 K.

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

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

$BrNO_3$: Value measured at 273 K.

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

H_2SO_4: Value measured at 303 K.

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

#	labels	reaction	rate coefficient	reference
H1001f_a01	TrAa01MblScScm	$O_3 \rightarrow O_3(aq)$	k_exf(01,ind_O3)	see note
H1001b_a01	TrAa01MblScScm	$O_3(aq) \rightarrow O_3$	k_exb(01,ind_O3)	see note
H2102f_a01	TrAa01MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	k_exf(01,ind_H2O2)	see note
H2102b_a01	TrAa01MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	k_exb(01,ind_H2O2)	see note
H3200f_a01	TrAa01NMblScScm	$NH_3 \rightarrow NH_3(aq)$	k_exf(01,ind_NH3)	see note
H3200b_a01	TrAa01NMblScScm	$NH_3(aq) \rightarrow NH_3$	k_exb(01,ind_NH3)	see note
H3201_a01	TrAa01MblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	k_exf_N2O5(01)*C(ind_H2O_a01)	Behnke et al. (1994), Behnke et al. (1997)*
H3203f_a01	TrAa01MblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	k_exf(01,ind_HNO3)	see note
H3203b_a01	TrAa01MblNScScm	$HNO_3(aq) \rightarrow HNO_3$	k_exb(01,ind_HNO3)	see note
H4100f_a01	TrAa01MblScScm	$CO_2 \rightarrow CO_2(aq)$	k_exf(01,ind_CO2)	see note
H4100b_a01	TrAa01MblScScm	$CO_2(aq) \rightarrow CO_2$	k_exb(01,ind_CO2)	see note
H6000f_a01	TrAa01ClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	k_exf(01,ind_Cl2)	see note
H6000b_a01	TrAa01ClMblSc	$Cl_2(aq) \rightarrow Cl_2$	k_exb(01,ind_Cl2)	see note
H6200f_a01	TrAa01ClMblScScm	$HCl \rightarrow HCl(aq)$	k_exf(01,ind_HCl)	see note
H6200b_a01	TrAa01ClMblScScm	$HCl(aq) \rightarrow HCl$	k_exb(01,ind_HCl)	see note
H6201f_a01	TrAa01ClMblSc	$HOCl \rightarrow HOCl(aq)$	k_exf(01,ind_HOCl)	see note
H6201b_a01	TrAa01ClMblSc	$HOCl(aq) \rightarrow HOCl$	k_exb(01,ind_HOCl)	see note
H6300_a01	TrAa01ClMblN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	k_exf_N2O5(01) * 5.E2	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a01	TrAa01ClMblN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	k_exf_ClNO3(01) * C(ind_H2O_a01)	see note
H6302_a01	TrAa01ClMblN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 5.E2	see note
H7000f_a01	TrAa01BrMblSc	$Br_2 \rightarrow Br_2(aq)$	k_exf(01,ind_Br2)	see note
H7000b_a01	TrAa01BrMblSc	$Br_2(aq) \rightarrow Br_2$	k_exb(01,ind_Br2)	see note
H7200f_a01	TrAa01BrMblScScm	$HBr \rightarrow HBr(aq)$	k_exf(01,ind_HBr)	see note
H7200b_a01	TrAa01BrMblScScm	$HBr(aq) \rightarrow HBr$	k_exb(01,ind_HBr)	see note
H7201f_a01	TrAa01BrMblSc	$HOBr \rightarrow HOBr(aq)$	k_exf(01,ind_HOBr)	see note
H7201b_a01	TrAa01BrMblSc	$HOBr(aq) \rightarrow HOBr$	k_exb(01,ind_HOBr)	see note
H7300_a01	TrAa01BrMblN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	k_exf_N2O5(01) * 3.E5	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a01	TrAa01BrMblN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	k_exf_BrNO3(01) * C(ind_H2O_a01)	see note
H7302_a01	TrAa01BrMblN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 3.E5	see note

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

#	labels	reaction	rate coefficient	reference
H7600f_a01	TrAa01ClBrMblSc	$BrCl \rightarrow BrCl(aq)$	k_exf(01,ind_BrCl)	see note
H7600b_a01	TrAa01ClBrMblSc	$BrCl(aq) \rightarrow BrCl$	k_exb(01,ind_BrCl)	see note
H7601_a01	TrAa01ClBrMblN	$ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_ClNO3(01) * 3.E5	see note
H7602_a01	TrAa01ClBrMblN	$BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_BrNO3(01) * 5.E2	see note
H9100f_a01	TrAa01SMblScScm	$SO_2 \rightarrow SO_2(aq)$	k_exf(01,ind_SO2)	see note
H9100b_a01	TrAa01SMblScScm	$SO_2(aq) \rightarrow SO_2$	k_exb(01,ind_SO2)	see note
H9200_a01	TrAa01SMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	xnom7sulf*k_exf(01,ind_H2SO4)	see note
H9401_a01	TrAa01SMbl	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	k_exf(01,ind_CH3SO3H)	see note
H1001f_a02	TrAa02MblScScm	$O_3 \rightarrow O_3(aq)$	k_exf(02,ind_O3)	see note
H1001b_a02	TrAa02MblScScm	$O_3(aq) \rightarrow O_3$	k_exb(02,ind_O3)	see note
H2102f_a02	TrAa02MblScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	k_exf(02,ind_H2O2)	see note
H2102b_a02	TrAa02MblScScm	$H_2O_2(aq) \rightarrow H_2O_2$	k_exb(02,ind_H2O2)	see note
H3200f_a02	TrAa02NMblScScm	$NH_3 \rightarrow NH_3(aq)$	k_exf(02,ind_NH3)	see note
H3200b_a02	TrAa02NMblScScm	$NH_3(aq) \rightarrow NH_3$	k_exb(02,ind_NH3)	see note
H3201_a02	TrAa02MblNScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	k_exf_N2O5(02)*C(ind_H2O_a02)	Behnke et al. (1994), Behnke et al. (1997)*
H3203f_a02	TrAa02MblNScScm	$HNO_3 \rightarrow HNO_3(aq)$	k_exf(02,ind_HNO3)	see note
H3203b_a02	TrAa02MblNScScm	$HNO_3(aq) \rightarrow HNO_3$	k_exb(02,ind_HNO3)	see note
H4100f_a02	TrAa02MblScScm	$CO_2 \rightarrow CO_2(aq)$	k_exf(02,ind_CO2)	see note
H4100b_a02	TrAa02MblScScm	$CO_2(aq) \rightarrow CO_2$	k_exb(02,ind_CO2)	see note
H6000f_a02	TrAa02ClMblSc	$Cl_2 \rightarrow Cl_2(aq)$	k_exf(02,ind_Cl2)	see note
H6000b_a02	TrAa02ClMblSc	$Cl_2(aq) \rightarrow Cl_2$	k_exb(02,ind_Cl2)	see note
H6200f_a02	TrAa02ClMblScScm	$HCl \rightarrow HCl(aq)$	k_exf(02,ind_HCl)	see note
H6200b_a02	TrAa02ClMblScScm	$HCl(aq) \rightarrow HCl$	k_exb(02,ind_HCl)	see note
H6201f_a02	TrAa02ClMblSc	$HOCl \rightarrow HOCl(aq)$	k_exf(02,ind_HOCl)	see note
H6201b_a02	TrAa02ClMblSc	$HOCl(aq) \rightarrow HOCl$	k_exb(02,ind_HOCl)	see note
H6300_a02	TrAa02ClMblN	$N_2O_5 + Cl^-(aq) \rightarrow ClNO_2 + NO_3^-(aq)$	k_exf_N2O5(02) * 5.E2	Behnke et al. (1994), Behnke et al. (1997)*
H6301_a02	TrAa02ClMblN	$ClNO_3 \rightarrow HOCl(aq) + HNO_3(aq)$	k_exf_ClNO3(02) * C(ind_H2O_a02)	see note
H6302_a02	TrAa02ClMblN	$ClNO_3 + Cl^-(aq) \rightarrow Cl_2(aq) + NO_3^-(aq)$	k_exf_ClNO3(02) * 5.E2	see note
H7000f_a02	TrAa02BrMblSc	$Br_2 \rightarrow Br_2(aq)$	k_exf(02,ind_Br2)	see note
H7000b_a02	TrAa02BrMblSc	$Br_2(aq) \rightarrow Br_2$	k_exb(02,ind_Br2)	see note

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

#	labels	reaction	rate coefficient	reference
H7200f_a02	TrAa02BrMblScScm	$HBr \rightarrow HBr(aq)$	k_exf(02,ind_HBr)	see note
H7200b_a02	TrAa02BrMblScScm	$HBr(aq) \rightarrow HBr$	k_exb(02,ind_HBr)	see note
H7201f_a02	TrAa02BrMblSc	$HOBr \rightarrow HOBr(aq)$	k_exf(02,ind_HOBr)	see note
H7201b_a02	TrAa02BrMblSc	$HOBr(aq) \rightarrow HOBr$	k_exb(02,ind_HOBr)	see note
H7300_a02	TrAa02BrMblN	$N_2O_5 + Br^-(aq) \rightarrow BrNO_2 + NO_3^-(aq)$	k_exf_N2O5(02) * 3.E5	Behnke et al. (1994), Behnke et al. (1997)*
H7301_a02	TrAa02BrMblN	$BrNO_3 \rightarrow HOBr(aq) + HNO_3(aq)$	k_exf_BrNO3(02) * C(ind_ H2O_a02)	see note
H7302_a02	TrAa02BrMblN	$BrNO_3 + Br^-(aq) \rightarrow Br_2(aq) + NO_3^-(aq)$	k_exf_BrNO3(02) * 3.E5	see note
H7600f_a02	TrAa02ClBrMblSc	$BrCl \rightarrow BrCl(aq)$	k_exf(02,ind_BrCl)	see note
H7600b_a02	TrAa02ClBrMblSc	$BrCl(aq) \rightarrow BrCl$	k_exb(02,ind_BrCl)	see note
H7601_a02	TrAa02ClBrMblN	$ClNO_3 + Br^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_ClNO3(02) * 3.E5	see note
H7602_a02	TrAa02ClBrMblN	$BrNO_3 + Cl^-(aq) \rightarrow BrCl(aq) + NO_3^-(aq)$	k_exf_BrNO3(02) * 5.E2	see note
H9100f_a02	TrAa02SMblScScm	$SO_2 \rightarrow SO_2(aq)$	k_exf(02,ind_SO2)	see note
H9100b_a02	TrAa02SMblScScm	$SO_2(aq) \rightarrow SO_2$	k_exb(02,ind_SO2)	see note
H9200_a02	TrAa02SMblScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	xnom7sulf*k_exf(02,ind_ H2SO4)	see note
H9401_a02	TrAa02SMbl	$CH_3SO_3H \rightarrow CH_3SO_3^-(aq) + H^+(aq)$	k_exf(02,ind_CH3SO3H)	see note

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca_aero.f90` using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry's law constants in subroutine `mecca_aero_henry`.

k_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

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

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

The total uptake rate of X is only determined by k_{mt}. The factors only affect the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[Cl^-] > 0.1$ M (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[H_2O]/[Cl^-]$ is less than 5×10^2. The ratio $5\times10^2/3\times10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference

*Notes:

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

Table 7: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
EQ21_a01	TrAa01MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a01	TrAa01MblNScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ32_a01	TrAa01MblNScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ40_a01	TrAa01MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ61_a01	TrAa01ClMblScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ71_a01	TrAa01BrMblScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ73_a01	TrAa01ClBrMbl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a01	TrAa01ClBrMbl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a01	TrAa01ClBrMbl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ76_a01	TrAa01ClBrMbl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ90_a01	TrAa01SMblScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a01	TrAa01SMblScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a01	TrAa01SMblScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a01	TrAa01SMblScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)
EQ21_a02	TrAa02MblScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716	Chameides (1984)
EQ30_a02	TrAa02MblNScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391	Chameides (1984)
EQ32_a02	TrAa02MblNScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700	Davis and de Bruin (1964)
EQ40_a02	TrAa02MblScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913	Chameides (1984)*
EQ61_a02	TrAa02ClMblScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896	Marsh and McElroy (1985)
EQ71_a02	TrAa02BrMblScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9		Lax (1969)
EQ73_a02	TrAa02ClBrMbl	$BrCl + Cl^- \rightleftharpoons BrCl_2^-$	3.8	1191	Wang et al. (1994)
EQ74_a02	TrAa02ClBrMbl	$BrCl + Br^- \rightleftharpoons Br_2Cl^-$	1.8E4	7457	Wang et al. (1994)
EQ75_a02	TrAa02ClBrMbl	$Br_2 + Cl^- \rightleftharpoons Br_2Cl^-$	1.3	0	Wang et al. (1994)
EQ76_a02	TrAa02ClBrMbl	$Br^- + Cl_2 \rightleftharpoons BrCl_2^-$	4.2E6	14072	Wang et al. (1994)
EQ90_a02	TrAa02SMblScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090	Chameides (1984)
EQ91_a02	TrAa02SMblScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120	Chameides (1984)
EQ92_a02	TrAa02SMblScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720	Seinfeld and Pandis (1998)
EQ93_a02	TrAa02SMblScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3		Seinfeld and Pandis (1998)

*Notes:

EQ40: For $pK_a(CO_2)$, see also Dickson and Millero (1987).

Table 8: Aqueous phase reactions

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference
A6204_a01	TrAa01ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6208_a01	TrAa01ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A7202_a01	TrAa01BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7208_a01	TrAa01BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7602_a01	TrAa01ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a01	TrAa01ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604_a01	TrAa01ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A9101_a01	TrAa01SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206_a01	TrAa01SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9209_a01	TrAa01SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9601_a01	TrAa01SClMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9605_a01	TrAa01SClMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9702_a01	TrAa01SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9705_a01	TrAa01SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note
A6204_a02	TrAa02ClMbl	$Cl_2 \rightarrow Cl^- + HOCl + H^+$	21.8	-8012	Wang and Margerum (1994)
A6208_a02	TrAa02ClMbl	$HOCl + Cl^- + H^+ \rightarrow Cl_2$	2.2E4	-3508	Wang and Margerum (1994)
A7202_a02	TrAa02BrMbl	$Br_2 \rightarrow Br^- + HOBr + H^+$	9.7E1	-7457	Beckwith et al. (1996)
A7208_a02	TrAa02BrMbl	$HOBr + Br^- + H^+ \rightarrow Br_2$	1.6E10		Beckwith et al. (1996)
A7602_a02	TrAa02ClBrMbl	$Br^- + HOCl + H^+ \rightarrow BrCl$	1.32E6		Kumar and Margerum (1987)
A7603_a02	TrAa02ClBrMbl	$HOBr + Cl^- + H^+ \rightarrow BrCl$	2.3E10		see note
A7604_a02	TrAa02ClBrMbl	$BrCl \rightarrow Cl^- + HOBr + H^+$	3.0E6		Liu and Margerum (2001)
A9101_a02	TrAa02SMblScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300	Hoffmann (1986)
A9206_a02	TrAa02SMblScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500	Hoffmann (1986)
A9209_a02	TrAa02SMblScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650	Martin and Damschen (1981)
A9601_a02	TrAa02SClMbl	$SO_3^{2-} + HOCl \rightarrow Cl^- + HSO_4^-$	7.6E8		Fogelman et al. (1989)
A9605_a02	TrAa02SClMbl	$HSO_3^- + HOCl \rightarrow Cl^- + HSO_4^- + H^+$	7.6E8		see note
A9702_a02	TrAa02SBrMbl	$SO_3^{2-} + HOBr \rightarrow Br^- + HSO_4^-$	5.0E9		Troy and Margerum (1991)
A9705_a02	TrAa02SBrMbl	$HSO_3^- + HOBr \rightarrow Br^- + HSO_4^- + H^+$	5.0E9		see note

*Notes: A9605: assumed to be the same as for SO_3^{2-} + HOCl. A9705: assumed to be the same as for SO_3^{2-} + HOBr.

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