The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs3`

MECCA version: `2.5d`

Date: April 19, 2012.

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

Number of aerosol phases: 1

Number of species in selected mechanism:

Gas phase:	97
Aqueous phase:	31
All species:	128

Number of reactions in selected mechanism:

Gas phase (Gnnn):	173
Aqueous phase (Annn):	14
Henry (Hnnn):	37
Photolysis (Jnnn):	53
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	28
Dummy (Dnn):	1
All equations:	306

The following describes the full chemical mechanism and relevant parameters as used for the simulations reported in this publication. Reactions labeled with "a01" correspond to a specific aerosol size bin. Since the reaction mechanisms were identical for each size bin, the chemical mechanism for only one of the eight bins is described here. Further information can be found in the article "Technical Note: The new comprehensive atmospheric chemistry module MECCA" by R. Sander et al. (Atmos. Chem. Phys. **5**, 445-450, 2005), available at `http://www.atmos-chem-phys.net/5/445`.

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)
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	TrG	$NO + OH \rightarrow HONO$	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	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	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)*

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

#	labels	reaction	rate coefficient	reference
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2006)
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. (1999)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	9.5E-14*EXP(390./temp)/(1.+1./ 26.2*EXP(1130./temp))	Sander et al. (2006)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	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	$HCOOH + OH \rightarrow HO_2$	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	$C_2H_4 + O_3 \rightarrow HCHO + .22\ HO_2 + .12\ OH + .23\ CO + .54\ HCOOH + .1\ H_2$	1.2E-14*EXP(-2630./temp)	Sander et al. (2006)*
G4202	TrGC	$C_2H_4 + OH \rightarrow .6666667\ CH_3CH(O_2)CH_2OH$	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	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	1.6E-13*EXP(195./temp)	see note

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

#	labels	reaction	rate coefficient	reference
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	k_CH3OOH_OH	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	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	1.4E-12*EXP(-1900./temp)	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	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_PA_NO2	Sander et al. (2006)
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2$	4.E-12	Canosa-Mas et al. (1996)
G4215a	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	0.9*2.E-12*EXP(500./temp)	Sander et al. (2006)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO$	0.1*2.E-12*EXP(500./temp)	Sander et al. (2006)
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	4.9E-12*EXP(211./temp)	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	2.5E-12*EXP(500./temp)	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	k_CH3OOH_OH	see note
G4219	TrGNC	$NACA + OH \rightarrow NO_2 + HCHO + CO$	5.6E-12*EXP(270./temp)	see note
G4220	TrGNC	$PAN + OH \rightarrow HCHO + NO_2$	2.E-14	see note
G4221	TrGNC	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_PAN_M	Sander et al. (2006)*
G4222	TrGC	$C_2H_2 + OH \rightarrow CH_3O_2$	k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,-2.,0.6)	Sander et al. (2006)
G4300	TrGC	$C_3H_8 + OH \rightarrow .82\ C_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	1.65E-17*temp*temp*EXP(-87./temp)	Atkinson (2003)

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

#	labels	reaction	rate coefficient	reference
G4301	TrGC	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ CH_3COCHO + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	6.5E-15*EXP(-1900./temp)	Sander et al. (2006)*
G4302	TrGC	$C_3H_6 + OH \rightarrow CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,8.E-27,3.5, 3.E-11,0.,0.5)	Atkinson et al. (1999)
G4303	TrGNC	$C_3H_6 + NO_3 \rightarrow ONIT$	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	k_PrO2_HO2	Atkinson (1997)*
G4305	TrGNC	$C_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	k_PrO2_NO	Atkinson et al. (1999)*
G4306	TrGC	$C_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	k_PrO2_CH3O2	Kirchner and Stockwell (1996)
G4307	TrGC	$C_3H_7OOH + OH \rightarrow .3\ C_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	k_CH3OOH_OH	see note
G4308	TrGC	$CH_3CH(O_2)CH_2OH + HO_2 \rightarrow CH_3CH(OOH)CH_2OH$	6.5E-13*EXP(650./temp)	Müller and Brasseur (1995)
G4309	TrGNC	$CH_3CH(O_2)CH_2OH + NO \rightarrow .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ ONIT$	4.2E-12*EXP(180./temp)	Müller and Brasseur (1995)*
G4310	TrGC	$CH_3CH(OOH)CH_2OH + OH \rightarrow .5\ CH_3CH(O_2)CH_2OH + .5\ CH_3COCH_2OH + .5\ OH + H_2O$	3.8E-12*EXP(200./temp)	Müller and Brasseur (1995)
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	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	2.9E-12*EXP(300./temp)	Sander et al. (2006)
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ CH_3COCHO + .5\ CH_3OH + .3\ CH_3C(O)OO + .8\ HCHO + .3\ HO_2 + .2\ CH_3COCH_2OH$	7.5E-13*EXP(500./temp)	Tyndall et al. (2001)

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

#	labels	reaction	rate coefficient	reference
G4315	TrGC	$CH_3COCH_2O_2H$ + OH → .3 $CH_3COCH_2O_2$ + .7 CH_3COCHO + .7 OH	k_CH3OOH_OH	see note
G4316	TrGC	CH_3COCH_2OH + OH → CH_3COCHO + HO_2	2.15E-12*EXP(305./temp)	Dillon et al. (2006)
G4317	TrGC	CH_3COCHO + OH → $CH_3C(O)OO$ + CO	8.4E-13*EXP(830./temp)	Tyndall et al. (1995)
G4318	TrGNC	MPAN + OH → CH_3COCH_2OH + NO_2	3.2E-11	Orlando et al. (2002)
G4319	TrGNC	MPAN → MVKO2 + NO_2	k_PAN_M	see note
G4320	TrGNC	$C_3H_7ONO_2$ + OH → CH_3COCH_3 + NO_2	6.2E-13*EXP(-230./temp)	Atkinson et al. (1999)
G4400	TrGC	C_4H_{10} + OH → $C_4H_9O_2$ + H_2O	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)
G4401	TrGC	$C_4H_9O_2$ + CH_3O_2 → .88 $CH_3COC_2H_5$ + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	k_PrO2_CH3O2	see note
G4402	TrGC	$C_4H_9O_2$ + HO_2 → C_4H_9OOH	k_PrO2_HO2	see note
G4403	TrGNC	$C_4H_9O_2$ + NO → .84 NO_2 + .56 $CH_3COC_2H_5$ + .56 HO_2 + .28 $C_2H_5O_2$ + .84 CH_3CHO + .16 ONIT	k_PrO2_NO	see note
G4404	TrGC	C_4H_9OOH + OH → .15 $C_4H_9O_2$ + .85 $CH_3COC_2H_5$ + .85 OH + .85 H_2O	k_CH3OOH_OH	see note
G4405	TrGC	MVK + O_3 → .45 HCOOH + .9 CH_3COCHO + .1 $CH_3C(O)OO$ + .19 OH + .22 CO + .32 HO_2	.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))	Pöschl et al. (2000)
G4406	TrGC	MVK + OH → MVKO2	.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))	Pöschl et al. (2000)
G4407	TrGC	MVKO2 + HO_2 → MVKOOH	1.82E-13*EXP(1300./temp)	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO → NO_2 + .25 $CH_3C(O)OO$ + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 CH_3COCHO	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO_2 → MPAN	.25*k_3rd(temp,cair,9.7E-29,5.6, 9.3E-12,1.5,0.6)	Pöschl et al. (2000)*

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

#	labels	reaction	rate coefficient	reference
G4410	TrGC	MVKO2 + CH_3O_2 → .5 CH_3COCHO + .375 CH_3COCH_2OH + .125 $CH_3C(O)OO$ + 1.125 HCHO + .875 HO_2 + .125 CO + .25 CH_3OH	2.E-12	von Kuhlmann (2001)
G4411	TrGC	MVKO2 + MVKO2 → CH_3COCH_2OH + CH_3COCHO + .5 CO + .5 HCHO + HO_2	2.E-12	Pöschl et al. (2000)
G4412	TrGC	MVKOOH + OH → MVKO2	3.E-11	Pöschl et al. (2000)
G4413	TrGC	$CH_3COC_2H_5$ + OH → MEKO2	1.3E-12*EXP(-25./temp)	Atkinson et al. (1999)
G4414	TrGC	MEKO2 + HO_2 → MEKOOH	k_PrO2_HO2	see note
G4415	TrGNC	MEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 ONIT	k_PrO2_NO	see note
G4416	TrGC	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	k_CH3OOH_OH	see note
G4417	TrGNC	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	ISOP + O_3 → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 $CH_3C(O)OO$ + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)
G4501	TrGC	ISOP + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO_3 → ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO_2 → ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)*
G4504	TrGNC	ISO2 + NO → .88 NO_2 + .88 MVK + .88 HCHO + .88 HO_2 + .12 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)*
G4505	TrGC	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .25 CH_3COCH_2OH + .25 CH_3OH	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	2.E-12	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH	1.E-10	Pöschl et al. (2000)
G4508	TrGNC	ISON + OH → CH_3COCH_2OH + NACA	1.3E-11	Pöschl et al. (2000)
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)

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

#	labels	reaction	rate coefficient	reference
G6102b	StTrGCl	$ClO + ClO \rightarrow 2\ Cl + O_2$	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	$ClO + ClO \rightarrow Cl + OClO$	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	$ClO + ClO \rightarrow Cl_2O_2$	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	$Cl_2O_2 \rightarrow ClO + ClO$	k_ClO_ClO/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6202	StTrGCl	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl$	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)
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	$Cl + C_2H_4 \rightarrow .6666667\ CH_3CH(O_2)CH_2OH + HCl$	k_3rd_iupac(temp,cair,1.85E-29,3.3,6.0E-10,0.0,0.4)	Atkinson et al. (2006)
G6410	TrGCCl	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)OO$	7.9e-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)
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)

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

#	labels	reaction	rate coefficient	reference
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	$Br + CH_3OOH \rightarrow CH_3O_2 + HBr$	2.66E-12*EXP(-1610./temp)	Mallard et al. (1993)
G7402a	TrGBr	$BrO + CH_3O_2 \rightarrow HOBr + HCHO$	0.8/1.1*5.7E-12	Aranda et al. (1997)
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow Br + HCHO + HO_2$	0.3/1.1*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	$Br + C_2H_4 \rightarrow .6666667\ CH_3CH(O_2)CH_2OH + HBr$	2.8E-13*EXP(224./temp)/(1.+1.13E+24*EXP(-3200./temp)/C(ind_O2))	Atkinson et al. (2006)
G7405	TrGCCl	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)OO$	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	TrGBrCl	$Br + BrCl \rightarrow Br_2 + Cl$	3.3E-15	Mallard et al. (1993)
G7601	TrGClBr	$Br + Cl_2 \rightarrow BrCl + Cl$	1.1E-15	Mallard et al. (1993)
G7602	TrGClBr	$Br_2 + Cl \rightarrow BrCl + Br$	1.2E-10	Mallard et al. (1993)
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	$BrCl + Cl \rightarrow Br + Cl_2$	1.5E-11	Mallard et al. (1993)
G7605	TrGBr	$CHCl_2Br + OH \rightarrow H_2O + Br$	2.0E-12*EXP(-840./temp)	see note
G7606	TrGBr	$CHClBr_2 + OH \rightarrow H_2O + 2\ Br$	2.0E-12*EXP(-840./temp)	see note
G7607	TrGBr	$CH_2ClBr + OH \rightarrow H_2O + Br$	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)*

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

#	labels	reaction	rate coefficient	reference
G9400b	TrGS	DMS + OH → DMSO + HO_2	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	DMS + NO_3 → CH_3SO_2 + HNO_3 + HCHO	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
G9402	TrGS	DMSO + OH → .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 → SO_2 + CH_3O_2	1.9E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	CH_3SO_2 + O_3 → CH_3SO_3	3.E-13	Barone et al. (1995)
G9405	TrGS	CH_3SO_3 + HO_2 → CH_3SO_3H	5.E-11	Barone et al. (1995)
G9600	TrGSCl	DMS + Cl → CH_3SO_2 + HCl + HCHO	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	DMS + Br → CH_3SO_2 + HBr + HCHO	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	DMS + BrO → DMSO + Br	2.54E-14*EXP(850./temp)	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:

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

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

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

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

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:

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

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

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

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

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

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 von Kuhlmann (2001) (see also Neeb et al. (1998)).

G4206: The rate coefficient was calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH_3OO and C_2H_5OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: Same value as for G4107: $CH_3OOH+OH$ assumed.

G4216: The value `1.0E-11` is from Atkinson et al. (1999), the temperature dependence from Kirchner and Stockwell (1996).

G4218: Same value as for G4107: $CH_3OOH+OH$ assumed.

G4219: According to Pöschl et al. (2000), the same value as for $CH_3CHO+OH$ can be assumed.

G4220: This is 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001).

G4221: The rate coefficient is: `k_PAN_M = k_PA_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.

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

G4304: The rate coefficient is: `k_PrO2_HO2 = 1.9E-13*EXP(1300./temp)`. Value for generic RO_2 + HO_2 reaction from Atkinson (1997) is used.

G4305: The rate coefficient is: `k_PrO2_NO = 2.7E-12*EXP(360./temp)`.

G4307: Same value as for G4107: CH_3OOH+OH assumed.

G4309: The products are from von Kuhlmann (2001).

G4315: Same value as for G4107: CH_3OOH+OH assumed.

G4319: Same value as for PAN assumed.

G4401: Same value as for propyl group assumed (`k_PrO2_CH3O2`).

G4402: Same value as for propyl group assumed (`k_PrO2_HO2`).

G4403: Same value as for propyl group assumed (`k_PrO2_NO`).

G4404: Same value as for G4107: CH_3OOH+OH assumed.

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

G4414: Same value as for propyl group assumed (`k_PrO2_HO2`).

G4415: Same value as for propyl group assumed (`k_PrO2_NO`).

G4416: Same value as for G4107: CH_3OOH+OH assumed.

G4417: Value for $C_4H_9ONO_2$ used here.

G4503: Same temperature dependence assumed as for other RO_2+HO_2 reactions.

G4504: Yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).

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.

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).

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)	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	jx(ip_PAA)	see note
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow .6\ CH_3C(O)OO + .6\ NO_2 + .4\ CH_3O_2 + .4\ NO_3 + .4\ CO_2$	jx(ip_PAN)	see note
J4300	TrGCJ	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH3OOH)	see note
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	see note
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note
J4303	TrGCJ	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_CH3COCHO)	see note
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	jx(ip_CH3OOH)	see note
J4305	TrGNCJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	jx(ip_PAN)	see note
J4306	TrGNCJ	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*jx(ip_PAN)	see note
J4400	TrGCJ	$C_4H_9OOH + h\nu \rightarrow OH + .67\ CH_3COC_2H_5 + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	jx(ip_CH3OOH)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4401	TrGCJ	MVK + hν → $CH_3C(O)OO$ + HCHO + CO + HO_2	0.019*jx(ip_COH2) +.015*jx(ip_CH3COCHO)	see note
J4402	TrGCJ	MVKOOH + hν → OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	jx(ip_CH3OOH)	see note
J4403	TrGCJ	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*jx(ip_CHOH)	see note
J4404	TrGCJ	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	jx(ip_CH3OOH)	see note
J4405	TrGCJ	MeCOCO + hν → 2 $CH_3C(O)OO$	2.15*jx(ip_CH3COCHO)	see note
J4406	TrGNCJ	ONIT + hν → NO_2 + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	3.7*jx(ip_PAN)	see note
J4500	TrGCJ	ISOOH + hν → MVK + HCHO + HO_2 + OH	jx(ip_CH3OOH)	see note
J4501	TrGNCJ	ISON + hν → MVK + HCHO + NO_2 + HO_2	3.7*jx(ip_PAN)	see note
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	TrGBrJ	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

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	$\frac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\frac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	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)
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)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
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)
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)*
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1.\times10^{11}$	0.	see note
DMSO	$5.\times10^{4}$	6425.	De Bruyn et al. (1994)*

*Notes:

The temperature dependence of the Henry constants is:

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

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

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).

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	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO_2	0.5	0.	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NH_3	0.06	0.	DeMore et al. (1997)*
NO	5.0×10^{-5}	0.	Saastad et al. (1993)*
NO_2	0.0015	0.	Ponche et al. (1993)*
NO_3	0.04	0.	Rudich et al. (1996)*
N_2O_5	0.1	0.	DeMore et al. (1997)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO_3	0.5	0.	Abbatt and Waschewsky (1998)*
HNO_4	0.1	0.	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO_2	0.01	2000.	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
$ClNO_3$	0.108	0.	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	0.	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO_2	0.11	0.	DeMore et al. (1997)
H_2SO_4	0.65	0.	Pöschl et al. (1998)*

Table 4: Accommodation coefficients (... continued)

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

*Notes:

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

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

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

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

and further:

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

If no data were available, a value of $\alpha = 0.01$, $\alpha = 0.1$, or $\alpha = 0.5$, and a temperature dependence of $-\Delta_{\rm obs}H/R = 2000$ K has been assumed.

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.

HCHO: Value measured between 260 and 270 K.

CO_2: Estimate.

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) transfer 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

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

#	labels	reaction	rate coefficient	reference
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
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

*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 (= N_2O_5, $ClNO_3$, $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^-, we define $k_{exf}(X) = k_{mt}(X) \times lwc/([H_2O] + 5.0E2[Cl^-] + 3.0E5[Br^-])$.

H6301, H6302, H7601: The total uptake is determined by $k_{mt}(ClNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by $k_{mt}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 6: 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)

*Notes:

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

Table 7: 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

*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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