The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs5`

MECCA version: 3.6

Date: February 9, 2014.

Selected reactions:

"(((Tr && (G || Het) && !I) || St) && !Hg)"

Number of species in selected mechanism:

Gas phase:	155
Aqueous phase:	0
All species:	155

Number of aerosol phases: 0

Number of reactions in selected mechanism:

Gas phase (Gnnn):	224
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	74
Aqueous phase photolysis (PHnnn):	0
Heterogeneous (HETnnn):	12
Equilibria (EQnn):	0
Isotope exchange (DGnnn):	0
Dummy (Dnn):	0
All equations:	310

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.3E-11*EXP(55./temp)`	Sander et al. (2011)
G1001	UpStTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2011)
G1002a	UpStG	$O_3 + O(^1D) \rightarrow 2.0\ LossO3O + 2.\ LossO3 + 2\ O_2$	`1.2E-10`	Sander et al. (2011)[*]
G1003	UpStG	$O_3 + O(^3P) \rightarrow 2.0\ LossO3O + 2.\ LossO3 + 2\ O_2$	`8.E-12*EXP(-2060./temp)`	Sander et al. (2011)
G2100	UpStTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,4.4E-32,1.3,7.5E-11,` `-0.2,0.6)`	Sander et al. (2011)
G2101	UpStG	$H + O_3 \rightarrow LossO3H + 1.\ LossO3 + OH + O_2$	`1.4E-10*EXP(-470./temp)`	Sander et al. (2011)
G2102	UpStG	$H_2 + O(^1D) \rightarrow LossO3H + 1.\ LossO3 + H + OH$	`1.2E-10`	Sander et al. (2011)
G2103	UpStG	$OH + O(^3P) \rightarrow LossO3H + 1.\ LossO3 + H + O_2$	`1.8E-11*EXP(180./temp)`	Sander et al. (2011)
G2104	UpStTrG	$OH + O_3 \rightarrow 1.0\ LossG2104 + LossO3H + LossOH + 1.\ LossO3 + HO_2 + O_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2011)
G2105	UpStTrG	$OH + H_2 \rightarrow H_2O + H$	`2.8E-12*EXP(-1800./temp)`	Sander et al. (2011)
G2106	UpStG	$HO_2 + O(^3P) \rightarrow 1.0\ LossG2106 + LossO3H + 1.\ LossO3 + OH + O_2$	`3.E-11*EXP(200./temp)`	Sander et al. (2011)
G2107	UpStTrG	$HO_2 + O_3 \rightarrow 1.0\ LossG2107 + LossO3H + LossHO2 + 1.\ LossO3 + OH + 2\ O_2$	`1.E-14*EXP(-490./temp)`	Sander et al. (2011)
G2108a	UpStG	$HO_2 + H \rightarrow 2\ OH$	`7.2E-11`	Sander et al. (2011)
G2108b	UpStG	$HO_2 + H \rightarrow H_2 + O_2$	`6.9E-12`	Sander et al. (2011)
G2108c	UpStG	$HO_2 + H \rightarrow LossO3Hn + 1.\ ProdO3 + O(^3P) + H_2O$	`1.6E-12`	Sander et al. (2011)
G2109	UpStTrG	$HO_2 + OH \rightarrow H_2O + O_2$	`4.8E-11*EXP(250./temp)`	Sander et al. (2011)
G2110	UpStTrG	$HO_2 + HO_2 \rightarrow 1.0\ LossG2110 + H_2O_2 + O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)[*]
G2111	UpStTrG	$H_2O + O(^1D) \rightarrow LossO3O + LossO1D + 1.\ LossO3 + 2\ OH$	`1.63E-10*EXP(60./temp)`	Sander et al. (2011)
G2112	UpStTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`1.8E-12`	Sander et al. (2011)
G3100	UpStGN	$N + O_2 \rightarrow LossO3Nn + 1.\ ProdO3 + NO + O(^3P)$	`1.5E-11*EXP(-3600./temp)`	Sander et al. (2011)
G3101	UpStTrGN	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`2.15E-11*EXP(110./temp)`	Sander et al. (2011)
G3102a	UpStGN	$N_2O + O(^1D) \rightarrow LossO3O + 1.\ LossO3 + 2\ NO$	`7.25E-11*EXP(20./temp)`	Sander et al. (2011)
G3102b	StGN	$N_2O + O(^1D) \rightarrow LossO3O + 1.\ LossO3 + N_2 + O_2$	`4.63E-11*EXP(20./temp)`	Sander et al. (2011)
G3103	UpStTrGN	$NO + O_3 \rightarrow 1.0\ LossG3103 + NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`	Sander et al. (2011)
G3104	UpStGN	$NO + N \rightarrow LossO3Nn + 1.\ ProdO3 + O(^3P) + N_2$	`2.1E-11*EXP(100./temp)`	Sander et al. (2011)
G3105	UpStGN	$NO_2 + O(^3P) \rightarrow 1.0\ LossG3105 + 2.0\ LossO3N2 + 2.0\ LossO3N + 2.\ LossO3 + NO + O_2$	`5.1E-12*EXP(210./temp)`	Sander et al. (2011)
G3106	StTrGN	$NO_2 + O_3 \rightarrow 1.0\ LossG3106 + NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Sander et al. (2011)

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

#	labels	reaction	rate coefficient	reference
G3107	UpStGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	`5.8E-12*EXP(220./temp)`	Sander et al. (2011)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Sander et al. (2011)
G3109	UpStTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Sander et al. (2011)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(2.7E-27*EXP(11000./temp))`	Sander et al. (2011)*
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. (2011)
G3201	UpStTrGN	$NO + HO_2 \rightarrow 1.0\ LossG3201 + ProdHO2 + 1.\ ProdO3 + NO_2 + OH$	`3.3E-12*EXP(270./temp)`	Sander et al. (2011)
G3202	UpStTrGN	$NO_2 + OH \rightarrow 1.0\ LossG3202 + HNO_3$	`k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0.,` `0.6)`	Sander et al. (2011)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Sander et al. (2011)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow LossO3N + 1.\ LossO3 + NO_2 + OH + O_2$	`3.5E-12`	Sander et al. (2011)
G3205	TrGN	$HONO + OH \rightarrow LossO3Nn + 1.\ ProdO3 + NO_2 + H_2O$	`1.8E-11*EXP(-390./temp)`	Sander et al. (2011)
G3206	StTrGN	$HNO_3 + OH \rightarrow LossO3Nn + 1.\ ProdO3 + H_2O + NO_3$	`k_HNO3_OH`	Sander et al. (2011)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Sander et al. (2011)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`	Sander et al. (2011)
G3209	TrGN	$NH_3 + OH \rightarrow NH_2 + H_2O$	`1.7E-12*EXP(-710./temp)`	Kohlmann and Poppe (1999)
G3210	TrGN	$NH_2 + O_3 \rightarrow 1.\ LossO3 + NH_2O + O_2$	`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)
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	$NH_2 + NO_2 \rightarrow 1.\ LossO3 + N_2O + H_2O$	`1.2E-11*((temp/298.)**(-2.0))`	Kohlmann and Poppe (1999)
G3216	TrGN	$NH_2 + NO_2 \rightarrow 1.\ LossO3 + NH_2O + NO$	`0.8E-11*((temp/298.)**(-2.0))`	Kohlmann and Poppe (1999)
G3217	TrGN	$NH_2O + O_3 \rightarrow 1.\ LossO3 + NH_2 + O_2$	`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	$HNO + NO_2 \rightarrow 1.\ LossO3 + HONO + NO$	`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)
G4100	UpStG	$CH_4 + O(^1D) \rightarrow 1.\ LossO3 + .75\ CH_3O_2 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	`1.75E-10`	Sander et al. (2011)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	`1.85E-20*EXP(2.82*log(temp)-987./temp)`	Atkinson (2003)

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

#	labels	reaction	rate coefficient	reference
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	`2.9E-12*EXP(-345./temp)`	Sander et al. (2011)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	`4.1E-13*EXP(750./temp)`	Sander et al. (2011)[*]
G4104	UpStTrGN	$CH_3O_2 + NO \rightarrow ProdMeO2 + 1.\ ProdO3 + HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`	Sander et al. (2011)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow LossO3N + 1.\ LossO3 + HCHO + HO_2 + NO_2$	`1.3E-12`	Atkinson et al. (2006)
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. (2011)
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. (2011)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`k_CH3OOH_OH`	Sander et al. (2011)[*]
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	$HCHO + NO_3 \rightarrow LossO3N + 1.\ LossO3 + HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2011)[*]
G4110	UpStTrG	$CO + OH \rightarrow 1.0\ LossG4110 + H + CO_2$	`(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. (2011)
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	$C_2H_4 + O_3 \rightarrow LossO3R + 1.\ LossO3 + HCHO + .63\ CO + .13\ HO_2 + 0.23125\ HCOOH + 0.13875\ HCHO + 0.13875\ H_2O_2 + .13\ OH$	`1.2E-14*EXP(-2630./temp)`	Sander et al. (2011)[*]
G4202	TrGC	$C_2H_4 + OH \rightarrow .6666667\ CH_3CH(O_2)CH_2OH$	`k_3rd(temp,cair,1.0E-28,4.5,7.5E-12,0.85,0.6)`	Sander et al. (2011)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	`7.5E-13*EXP(700./temp)`	Sander et al. (2011)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow ProdRO2 + 1.\ ProdO3 + CH_3CHO + HO_2 + NO_2$	`2.6E-12*EXP(365./temp)`	Sander et al. (2011)
G4205	TrGNC	$C_2H_5O_2 + NO_3 \rightarrow 1.\ LossO3 + CH_3CHO + HO_2 + NO_2$	`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
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	$CH_3CHO + NO_3 \rightarrow LossO3N + 1.\ LossO3 + CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2011)
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)

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

#	labels	reaction	rate coefficient	reference
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow 1.\ ProdO3 + CH_3COOH + O_3$	4.3E-13*EXP(1040./temp)/(1.+ 37.*EXP(-660./temp))	Tyndall et al. (2001)
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow ProdRO2 + 1.\ ProdO3 + CH_3O_2 + CO_2 + NO_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_PA_NO2	Sander et al. (2011)
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow LossO3N + 1.\ LossO3 + CH_3O_2 + NO_2 + CO_2$	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*2.0E-12*EXP(500./temp)	Sander et al. (2011)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO$	0.1*2.0E-12*EXP(500./temp)	Sander et al. (2011)
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	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO + H_2O$	0.6*k_CH3OOH_OH	Rickard and Pascoe (2009)*
G4219	TrGNC	$NACA + OH \rightarrow NO_2 + HCHO + CO$	5.6E-12*EXP(270./temp)	see note
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. (2011)*
G4300	TrGC	$C_3H_8 + OH \rightarrow .82\ iC_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	1.65E-17*temp*temp*EXP(-87./temp)	Atkinson (2003)
G4301	TrGC	$C_3H_6 + O_3 \rightarrow LossO3R + 1.\ LossO3 + .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ MGLYOX + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	6.5E-15*EXP(-1900./temp)	Sander et al. (2011)*
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	$C_3H_6 + NO_3 \rightarrow 1.\ LossO3 + LC4H9NO3$	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	$iC_3H_7O_2 + HO_2 \rightarrow iC_3H_7OOH$	k_PrO2_HO2	Atkinson (1997)*
G4305	TrGNC	$iC_3H_7O_2 + NO \rightarrow ProdRO2 + 1.\ ProdO3 + .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ iC_3H_7ONO_2$	k_PrO2_NO	Atkinson et al. (1999)*
G4306	TrGC	$iC_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	k_PrO2_CH3O2	Kirchner and Stockwell (1996)
G4307	TrGC	$iC_3H_7OOH + OH \rightarrow .3\ iC_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	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	$CH_3CH(O_2)CH_2OH + NO \rightarrow ProdRO2 + 1.\ ProdO3 + .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ LC4H9NO3$	4.2E-12*EXP(180./temp)	Müller and Brasseur (1995)*

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

#	labels	reaction	rate coefficient	reference
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. (2011)
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	$CH_3COCH_2O_2 + NO \rightarrow ProdRO2 +$ 1. $ProdO3 + CH_3C(O)OO + HCHO + NO_2$	`2.9E-12*EXP(300./temp)`	Sander et al. (2011)
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow$ .5 $MGLYOX +$ .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)
G4315	TrGC	$CH_3COCH_2O_2H + OH \rightarrow$ .3 $CH_3COCH_2O_2 +$ .7 $MGLYOX +$ .7 OH	`k_CH3OOH_OH`	see note
G4316	TrGC	$CH_3COCH_2OH + OH \rightarrow MGLYOX + HO_2$	`2.15E-12*EXP(305./temp)`	Dillon et al. (2006)
G4317	TrGC	$MGLYOX + OH \rightarrow CH_3C(O)OO + CO$	`8.4E-13*EXP(830./temp)`	Tyndall et al. (1995)
G4318	TrGNC	$MPAN + OH \rightarrow CH_3COCH_2OH + NO_2$	`3.2E-11`	Orlando et al. (2002)
G4319	TrGNC	$MPAN \rightarrow MVKO2 + NO_2$	`k_PAN_M`	see note
G4320	TrGNC	$iC_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	`6.2E-13*EXP(-230./temp)`	Atkinson et al. (1999)
G4400	TrGC	$nC_4H_{10} + OH \rightarrow LC_4H_9O_2 + H_2O$	`1.81E-17*temp*temp*EXP(114./temp)`	Atkinson (2003)
G4401	TrGC	$LC_4H_9O_2 + CH_3O_2 \rightarrow$ .88 $MEK +$ .68 $HCHO +$ 1.23 $HO_2 +$ .12 $CH_3CHO +$ .12 $C_2H_5O_2 +$ .18 CH_3OH	`k_PrO2_CH3O2`	see note
G4402	TrGC	$LC_4H_9O_2 + HO_2 \rightarrow LC_4H_9OOH$	`k_PrO2_HO2`	see note
G4403	TrGNC	$LC_4H_9O_2 + NO \rightarrow ProdRO2 +$ 1. $ProdO3 +$ .84 $NO_2 +$ .56 $MEK +$ .56 $HO_2 +$ .28 $C_2H_5O_2 +$ .28 $CH_3CHO +$ .16 $LC4H9NO3$	`k_PrO2_NO`	see note
G4404	TrGC	$LC_4H_9OOH + OH \rightarrow$ .15 $LC_4H_9O_2 +$ .85 $MEK +$ .85 $OH +$ .85 H_2O	`k_CH3OOH_OH`	see note
G4405	TrGC	$MVK + O_3 \rightarrow LossO3R +$ 1. $LossO3 +$ .45 $HCOOH +$ .9 $MGLYOX +$ .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	$MVK + OH \rightarrow MVKO2$	`.5*(4.1E-12*EXP(452./temp)` `+1.9E-11*EXP(175./temp))`	Pöschl et al. (2000)
G4407	TrGC	$MVKO2 + HO_2 \rightarrow MVKOOH$	`1.82E-13*EXP(1300./temp)`	Pöschl et al. (2000)
G4408	TrGNC	$MVKO2 + NO \rightarrow ProdRO2 +$ 1. $ProdO3 + NO_2 +$ .25 $CH_3C(O)OO +$ .25 $CH_3COCH_2OH +$ .75 $HCHO +$ .25 $CO +$ .75 $HO_2 +$ .5 $MGLYOX$	`2.54E-12*EXP(360./temp)`	Pöschl et al. (2000)
G4409	TrGNC	$MVKO2 + NO_2 \rightarrow MPAN$	`.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 MGLYOX + .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 + MGLYOX + .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	MEK + OH → LMEKO2	1.3E-12*EXP(-25./temp)	Atkinson et al. (1999)
G4414	TrGC	LMEKO2 + HO_2 → LMEKOOH	k_PrO2_HO2	see note
G4415	TrGNC	LMEKO2 + NO → ProdRO2 + 1. ProdO3 + .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 LC4H9NO3	k_PrO2_NO	see note
G4416	TrGC	LMEKOOH + OH → .8 BIACET + .8 OH + .2 LMEKO2	k_CH3OOH_OH	see note
G4417	TrGNC	LC4H9NO3 + OH → MEK + NO_2 + H_2O	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	C_5H_8 + O_3 → LossO3R + 1. LossO3 + .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	C_5H_8 + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	C_5H_8 + NO_3 → 1. LossO3 + 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)*
G4504a	TrGNC	ISO2 + NO → ProdRO2 + 1. ProdO3 + .956 NO_2 + .956 MVK + .956 HCHO + .956 HO_2 + .044 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 MGLYOX + .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	UpStTrGCl	Cl + O_3 → ClO + O_2	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	UpStGCl	ClO + $O(^3P)$ → 2.0 LossO3Cl + 2. LossO3 + Cl + O_2	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → 2. LossO3 + Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2. LossO3 + 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → 1. LossO3 + 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/(1.72E-27*EXP(8649./temp))	Atkinson et al. (2007), Sander et al. (2011)*
G6200	StGCl	Cl + H_2 → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)

#	labels	reaction	rate coefficient	reference
G6201a	StGCl	$Cl + HO_2 \rightarrow HCl + O_2$	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	$Cl + HO_2 \rightarrow LossO3Cln + 1. ProdO3 + ClO + OH$	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	$ClO + OH \rightarrow LossO3Cl + 1. LossO3 + .94 Cl + .94 HO_2 + .06 HCl + .06 O_2$	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
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)
G6206	StGCl	$HOCl + OH \rightarrow ClO + H_2O$	3.0E-12*EXP(-500./temp)	Sander et al. (2011)
G6300	UpStTrGNCl	$ClO + NO \rightarrow 1.0 LossO3Cl + LossO3Nn + NO_2 + Cl$	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	TrGNCl	$ClNO_3 \rightarrow ClO + NO_2$	6.918E-7*exp(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGNCl	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
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	$ClO + CH_3O_2 \rightarrow LossO3Cl + 1. LossO3 + HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)	Sander et al. (2011)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow 3.0 ProdLCl + ClO + 3 Cl$	3.3E-10	Sander et al. (2011)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow 1.0 ProdLCl + LossO3Cl + 1. LossO3 + OH + Cl$	1.65E-10	see note
G6406	StGCl	$CH_3Cl + OH \rightarrow 1.0 ProdLCl + H_2O + Cl$	2.4E-12*EXP(-1250./temp)	Sander et al. (2011)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow 3.0 ProdLCl + LossO3Cl + 1. LossO3 + OH + 3 Cl$	3.E-10	see note
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow 3.0 ProdLCl + H_2O + 3 Cl$	1.64E-12*EXP(-1520./temp)	Sander et al. (2011)
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	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)OO$	8.0e-11	Atkinson et al. (2006)
G6500	StGFCl	$CF_2Cl_2 + O(^1D) \rightarrow 1.0 ProdLCl + ClO + Cl$	1.4E-10	Sander et al. (2011)
G6501	StGFCl	$CFCl_3 + O(^1D) \rightarrow 2.0 ProdLCl + ClO + 2 Cl$	2.3E-10	Sander et al. (2011)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	$BrO + O(^3P) \rightarrow 2.0 LossO3Br + 2. LossO3 + Br + O_2$	1.9E-11*EXP(230./temp)	Atkinson et al. (2007)
G7102a	StTrGBr	$BrO + BrO \rightarrow 2.0 LossO3Br + 2. LossO3 + 2 Br + O_2$	2.7E-12	Atkinson et al. (2007)
G7102b	StTrGBr	$BrO + BrO \rightarrow 2.0 LossO3Br + 2. LossO3 + Br_2 + O_2$	2.9E-14*EXP(840./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
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)
G7203	StGBr	$HOBr + O(^3P) \rightarrow LossO3Br + 1. LossO3 + OH + BrO$	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow 1. ProdO3 + HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGNBr	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGNBr	$BrO + NO \rightarrow LossO3Br + LossO3Nn + Br + NO_2$	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	TrGNBr	$BrNO_3 \rightarrow BrO + NO_2$	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)
G7402b	TrGBr	$BrO + CH_3O_2 \rightarrow LossO3Br + 1. LossO3 + Br + HCHO + HO_2$	(1.-G7402a_yield)*5.7E-12	Aranda et al. (1997)
G7403	StTrGBr	$CH_3Br + OH \rightarrow 1.0 ProdLBr + H_2O + Br$	2.35E-12*EXP(-1300./temp)	Sander et al. (2011)
G7404	TrGCBr	$Br + C_2H_4 \rightarrow .6666667 CH_3CH(O_2)CH_2OH + HBr$	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)
G7407	TrGBr	$CHBr_3 + OH \rightarrow 3.0 ProdSBr + H_2O + 3 Br$	1.35E-12*EXP(-600./temp)	Sander et al. (2011)*
G7408	TrGBr	$CH_2Br_2 + OH \rightarrow 2.0 ProdSBr + H_2O + 2 Br$	2.0E-12*EXP(-840./temp)	Sander et al. (2011)*
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	$BrO + ClO \rightarrow 1. LossO3 + Br + OClO$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGClBr	$BrO + ClO \rightarrow LossO3Br + LossO3Cl + 2. LossO3 + Br + Cl + O_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGClBr	$BrO + ClO \rightarrow LossO3Br + LossO3Cl + 2. LossO3 + BrCl + O_2$	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	$CHCl_2Br + OH \rightarrow 1.0 ProdSBr + H_2O + Br$	2.0E-12*EXP(-840./temp)	see note
G7606	TrGClBr	$CHClBr_2 + OH \rightarrow 2.0 ProdSBr + H_2O + 2 Br$	2.0E-12*EXP(-840./temp)	see note
G7607	TrGClBr	$CH_2ClBr + OH \rightarrow 1.0 ProdSBr + H_2O + Br$	2.4E-12*EXP(-920./temp)	Sander et al. (2011)*
G9200	StTrGS	$SO_2 + OH \rightarrow 1. LossO3 + H_2SO_4 + HO_2$	k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0., 0.6)	Sander et al. (2011)

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

#	labels	reaction	rate coefficient	reference
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	$DMS + NO_3 \rightarrow 1.\ LossO3 + CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2004)
G9402	TrGS	$DMSO + OH \rightarrow 0.6\ ProdO3 + .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow 1.\ ProdO3 + SO_2 + CH_3O_2$	`1.8E13*EXP(-8661./temp)`	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow 1.\ LossO3 + CH_3SO_3$	`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	$DMS + BrO \rightarrow 1.\ LossO3 + DMSO + Br$	`4.4E-13`	Ingham et al. (1999)
G01Diag	StTrG	$O_3(s) \rightarrow LO_3(s)$	`k_O3s`	?*
G10G6501	StGFCl	$(CFCl_3)_c + O(^1D) \rightarrow O(^1D)$	`2.3E-10`	Sander et al. (2011)
G12G6500	StGFCl	$(CF_2Cl_2)_c + O(^1D) \rightarrow O(^1D)$	`1.4E-10`	Sander et al. (2011)
G14G3102a	UpStGN	$(N_2O)_c + O(^1D) \rightarrow O(^1D)$	`7.25E-11*EXP(20./temp)`	Sander et al. (2011)
G15G3102b	StGN	$(N_2O)_c + O(^1D) \rightarrow O(^1D) + \ldots$	`4.63E-11*EXP(20./temp)`	Sander et al. (2011)
G17G6407	StGCCl	$(CH_3CCl_3)_c + O(^1D) \rightarrow O(^1D)$	`3.E-10`	see note
G18G6408	StTrGCCl	$(CH_3CCl_3)_c + OH \rightarrow OH$	`1.64E-12*EXP(-1520./temp)`	Sander et al. (2011)

*Notes:

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

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

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

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

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

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:

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

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

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

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

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

G1002: The path leading to 2 O(^{3}P) + O$_2$ results in a null cycle regarding odd oxygen and is neglected.

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$_3$CHO+NO$_3$. At 298 K, $k = 5.8 \times 10^{-16}$.

G4201: The product distribution is from Rickard and Pascoe (2009), after substitution of the Criegee intermediate by its decomposition products.

G4206: The product C$_2$H$_5$OH, which reacts only with OH, is substituted by its degradation products $\approx$ 0.1 HOCH$_2$CH$_2$O$_2$ + 0.9 CH$_3$CHO + 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$_2$H$_5$O$_2$ 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$_3$O$_2$ channel in G4107 (CH$_3$OOH+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.

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.

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

G4401: NC4H9O and SC4H9O are substituted with 2 CO$_2$ + C$_2$H$_5$O$_2$ and 0.636 MEK + HO$_2$ and 0.364 CH$_3$CHO + C$_2$H$_5$O$_2$, 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$_2$H$_5$O$_2$. Hence, 0.327 NC4H9O2 + 1.346 CO$_2$ + 0.673 C$_2$H$_5$O$_2$ + 0.673 OH. For SC4H9OOH the products are 0.219 SC4H9O2 + 0.781 MEK + 0.781 OH.

G4415: Alkyl nitrate formation is neglected. The products of MEKAO and MEKCO are substituted with HCHO + CO$_2$ + HOCH$_2$CH$_2$O$_2$ and HCHO + CO$_2$ + C$_2$H$_5$O$_2$.

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.

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.

G6405: Average of reactions with CH_3Br and CH_3F from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F from Sander et al. (2006).

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
J1000a	UpStTrGJ	$O_2 + h\nu \rightarrow$ 2. ProdO3 + $O(^3P)$ + $O(^3P)$	jx(ip_O2)	see note
J1001a	UpStTrGJ	$O_3 + h\nu \rightarrow O(^1D) + O_2$	jx(ip_O1D)	see note
J1001b	UpStTrGJ	$O_3 + h\nu \rightarrow O(^3P) + O_2$	jx(ip_O3P)	see note
J2100a	UpStGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H2O)	see note
J2101	UpStTrGJ	$H_2O_2 + h\nu \rightarrow$ 2 OH	jx(ip_H2O2)	see note
J3100	UpStGNJ	$N_2O + h\nu \rightarrow$ 1. ProdO3 + $O(^1D)$ + N_2	jx(ip_N2O)	see note
J3101	UpStTrGNJ	$NO_2 + h\nu \rightarrow$ 1.0 LossJ3101 + NO + $O(^3P)$	jx(ip_NO2)	see note
J3102a	UpStGNJ	$NO + h\nu \rightarrow$ 1. ProdO3 + N + $O(^3P)$	jx(ip_NO)	see note
J3103a	UpStTrGNJ	$NO_3 + h\nu \rightarrow$ 1.0 LossJ3103a + NO_2 + $O(^3P)$	jx(ip_NO2O)	see note
J3103b	UpStTrGNJ	$NO_3 + h\nu \rightarrow$ 2.0 LossO3N + 2. LossO3 + NO + O_2	jx(ip_NOO2)	see note
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	jx(ip_N2O5)	see note
J3200	TrGNJ	$HONO + h\nu \rightarrow NO + OH$	jx(ip_HONO)	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	jx(ip_HNO3)	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow$ 0.333 ProdO3 + .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
J4102	StGJ	$CO_2 + h\nu \rightarrow$ 1. ProdO3 + CO + $O(^3P)$	jx(ip_CO2)	see note
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31 H + 0.69 H_2 + 1.155 H_2O$	jx(ip_CH4)	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
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	jx(ip_PAN)	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	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note
J4303	TrGCJ	$MGLYOX + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_MGLYOX)	see note
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HCHO + OH$	jx(ip_CH3OOH)	see note
J4305	TrGNCJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	jx(ip_PAN)	see note
J4306	TrGNCJ	$iC_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*jx(ip_PAN)	see note
J4400	TrGCJ	$LC_4H_9OOH + h\nu \rightarrow OH + .67 MEK + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	jx(ip_CH3OOH)	see note

#	labels	reaction	rate coefficient	reference
J4401	TrGCJ	MVK + hν → CH$_3$C(O)OO + HCHO + CO + HO$_2$	0.019*jx(ip_COH2)+.015*jx(ip_MGLYOX)	see note
J4402	TrGCJ	MVKOOH + hν → OH + .5 MGLYOX + .25 CH$_3$COCH$_2$OH + .75 HCHO + .75 HO$_2$ + .25 CH$_3$C(O)OO + .25 CO	jx(ip_CH3OOH)	see note
J4403	TrGCJ	MEK + hν → CH$_3$C(O)OO + C$_2$H$_5$O$_2$	0.42*jx(ip_CHOH)	see note
J4404	TrGCJ	LMEKOOH + hν → CH$_3$C(O)OO + CH$_3$CHO + OH	jx(ip_CH3OOH)	see note
J4405	TrGCJ	BIACET + hν → 2 CH$_3$C(O)OO	2.15*jx(ip_MGLYOX)	see note
J4406	TrGNCJ	LC4H9NO3 + hν → NO$_2$ + .67 MEK + .67 HO$_2$ + .33 C$_2$H$_5$O$_2$ + .33 CH$_3$CHO	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$_2$O$_2$ + hν → 2. LossO3 + 2 Cl	jx(ip_Cl2O2)	see note
J6101	StTrGClJ	OClO + hν → 1. ProdO3 + ClO + O(^{3}P)	jx(ip_OClO)	see note
J6200	StGClJ	HCl + hν → Cl + H	jx(ip_HCl)	see note
J6201	StTrGClJ	HOCl + hν → LossO3Cl + 1. LossO3 + OH + Cl	jx(ip_HOCl)	see note
J6300	TrGNClJ	ClNO$_2$ + hν → 1. ProdO3 + 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
J6400	StGClJ	CH$_3$Cl + hν → 1.0 ProdLCl + Cl + CH$_3$O$_2$	jx(ip_CH3Cl)	see note
J6401	StGClJ	CCl$_4$ + hν → 4.0 ProdLCl + 4 Cl	jx(ip_CCl4)	see note
J6402	StGCClJ	CH$_3$CCl$_3$ + hν → 3.0 ProdLCl + 3 Cl	jx(ip_CH3CCl3)	see note
J6500	StGFClJ	CFCl$_3$ + hν → 3.0 ProdLCl + 3 Cl	jx(ip_CFCl3)	see note
J6501	StGFClJ	CF$_2$Cl$_2$ + hν → 2.0 ProdLCl + 2 Cl	jx(ip_CF2Cl2)	see note
J7000	StTrGBrJ	Br$_2$ + hν → Br + Br	jx(ip_Br2)	see note
J7100	StTrGBrJ	BrO + hν → Br + O(^{3}P)	jx(ip_BrO)	see note
J7200	StTrGBrJ	HOBr + hν → LossO3Br + 1. LossO3 + Br + OH	jx(ip_HOBr)	see note
J7300	TrGNBrJ	BrNO$_2$ + hν → 1. ProdO3 + Br + NO$_2$	jx(ip_BrNO2)	see note
J7301	StTrGNBrJ	BrNO$_3$ + hν → 0.85 Br + 0.85 NO$_3$ + 0.15 BrO + 0.15 NO$_2$	jx(ip_BrNO3)	see note
J7400	StGBrJ	CH$_3$Br + hν → 1.0 ProdLBr + Br + CH$_3$O$_2$	jx(ip_CH3Br)	see note
J7401	TrGBrJ	CH$_2$Br$_2$ + hν → 2.0 ProdSBr + 2 Br	jx(ip_CH2Br2)	see note
J7402	TrGBrJ	CHBr$_3$ + hν → 3.0 ProdSBr + 3 Br	jx(ip_CHBr3)	see note
J7500	StGFBrJ	CF$_3$Br + hν → 1.0 ProdLBr + Br	jx(ip_CF3Br)	see note
J7600	StTrGClBrJ	BrCl + hν → Br + Cl	jx(ip_BrCl)	see note
J7601	StGFBrJ	CF$_2$ClBr + hν → 1.0 ProdLBr + 1.0 ProdLCl + Br + Cl	jx(ip_CF2ClBr)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7602	TrGClBrJ	$CH_2ClBr + h\nu \rightarrow 1.0\ ProdSBr + 1.0\ ProdSCl + Br + Cl$	`jx(ip_CH2ClBr)`	see note
J7603	TrGClBrJ	$CHCl_2Br + h\nu \rightarrow 1.0\ ProdSBr + 2.0\ ProdSCl + Br + 2\ Cl$	`jx(ip_CHCl2Br)`	see note
J7604	TrGClBrJ	$CHClBr_2 + h\nu \rightarrow 2.0\ ProdSBr + 1.0\ ProdSCl + 2\ Br + Cl$	`jx(ip_CHClBr2)`	see note
J8401a	TrGJ	$CH_3I + h\nu \rightarrow CH_3O_2$	`JX(ip_CH3I)`	see note
J11J6500	StGFClJ	$(CFCl_3)_c + h\nu \rightarrow \ldots$	`jx(ip_CFCl3)`	see note
J13J6501	StGFClJ	$(CF_2Cl_2)_c + h\nu \rightarrow \ldots$	`jx(ip_CF2Cl2)`	see note
J16J3100	UpStGNJ	$(N_2O)_c + h\nu \rightarrow \ldots$	`jx(ip_N2O)`	see note
J19J6402	StGCClJ	$(CH_3CCl_3)_c + h\nu \rightarrow \ldots$	`jx(ip_CH3CCl3)`	see note
J20J7601	StGFBrJ	$(CF_2ClBr)_c + h\nu \rightarrow \ldots$	`jx(ip_CF2ClBr)`	see note
J21J7500	StGFBrJ	$(CF_3Br)_c + h\nu \rightarrow \ldots$	`jx(ip_CF3Br)`	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(iC3H7ONO2)
J(54) → J(iC3H7ONO2)
J(55) → J(iC3H7ONO2)
J(56)+J(57) → jx(ip_NOA)

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

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

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

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).

J7301: The quantum yields are recommended by Sander et al. (2011) for $\lambda > 300$nm and used here for the entire spectrum.

Table 3: Henry's law coefficients

substance	$\dfrac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\dfrac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	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)
H_2O	BIG	0.	see note
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_3OH	2.20×10^{2}	5200.	Snider and Dawson (1985)
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)
MGLYOX	3.70×10^{3}	7500.	???
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)*

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

substance	$\dfrac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\dfrac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	reference
$BrNO_3$	BIG	0.	see note
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
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:

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

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).

$C_2H_5O_2$: Assumed to be the same as $K_{\mathrm{H}}(CH_3O_2)$.

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	$\alpha^{\ominus}$	$\dfrac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	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)
H_2O	0.0	(default)	see note
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_3OH	(default)	(default)	see note
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)
MGLYOX	(default)	(default)	see note
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)*

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^{\ominus}$	$\dfrac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
BrCl	0.038	6546.	see note
SO_2	0.11	(default)	DeMore et al. (1997)
H_2SO_4	0.65	(default)	Pöschl et al. (1998)*
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:
$\alpha^{\ominus} = 0.1$
$-\Delta_{\mathrm{obs}}H/R = 0$ K

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

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

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

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

and further:

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

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 $\alpha(\text{HOBr})$.

$ClNO_3$: 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 $\alpha(\text{Cl}_2)$.

H_2SO_4: Value measured at 303 K.

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

#	labels	reaction	rate coefficient	reference

*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 $5 \times 10^2 / 3 \times 10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow$ LossO3N + 1. LossO3 + 2 HNO_3	`khet_St(ihs_N2O5_H2O)`	see note
HET201	TrHetN	$N_2O_5 \rightarrow$ 3. LossO3 + 2 NO_3^-(aq) + 2 H^+(aq)	`khet_Tr(iht_N2O5)`	see note
HET410	StHetCl	$HOCl + HCl \rightarrow$ LossO3Cl + 1. LossO3 + Cl_2 + H_2O	`khet_St(ihs_HOCl_HCl)`	see note
HET420	StHetNCl	$ClNO_3 + HCl \rightarrow$ LossO3Cl + 1. LossO3 + Cl_2 + HNO_3	`khet_St(ihs_ClNO3_HCl)`	see note
HET421	StHetNCl	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_St(ihs_ClNO3_H2O)`	see note
HET422	StHetNCl	$N_2O_5 + HCl \rightarrow$ 2. LossO3 + $ClNO_2$ + HNO_3	`khet_St(ihs_N2O5_HCl)`	see note
HET510	StHetBr	$HOBr + HBr \rightarrow$ LossO3Br + 1. LossO3 + Br_2 + H_2O	`khet_St(ihs_HOBr_HBr)`	see note
HET520	StHetNBr	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_St(ihs_BrNO3_H2O)`	see note
HET540	StHetNClBr	$ClNO_3 + HBr \rightarrow$ LossO3Cl + 1. LossO3 + BrCl + HNO_3	`khet_St(ihs_ClNO3_HBr)`	see note
HET541	StHetNClBr	$BrNO_3 + HCl \rightarrow$ LossO3Br + 1. LossO3 + BrCl + HNO_3	`khet_St(ihs_BrNO3_HCl)`	see note
HET542	StHetClBr	$HOCl + HBr \rightarrow$ LossO3Cl + 1. LossO3 + BrCl + H_2O	`khet_St(ihs_HOCl_HBr)`	see note
HET543	StHetClBr	$HOBr + HCl \rightarrow$ LossO3Br + 1. LossO3 + BrCl + H_2O	`khet_St(ihs_HOBr_HCl)`	see note

*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

*Notes:

Table 8: Aqueous phase reactions

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

*Notes:

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