The Chemical Mechanism of MECCA

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Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.2E-11*EXP(70./temp)	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4))*cair	Sander et al. (2003)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	k_3rd(temp,cair,5.7E-32,1.6,7.5E-11,0.,0.6)	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2$	1.7E-12*EXP(-940./temp)	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	5.5E-12*EXP(-2000./temp)	Sander et al. (2003)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	1.E-14*EXP(-490./temp)	Sander et al. (2003)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	4.8E-11*EXP(250./temp)	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	2.2E-10	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	2.9E-12*EXP(-160./temp)	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	1.8E-11*EXP(110./temp)	Sander et al. (2003)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(3.E-27*EXP(10990./temp))	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.E-31,2.6,3.6E-11,0.1,0.6)	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,2.E-30,3.,2.5E-11,0.,0.6)	Sander et al. (2003)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2003)
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./temp))	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*log(temp)-987./temp)	Atkinson (2003)*
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	7.3E-12*EXP(-620./temp)	Sander et al. (2003)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	4.1E-13*EXP(750./temp)/(1.+1./ 497.7*EXP(1160./temp))	Sander et al. (2003)*
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	4.1E-13*EXP(750./temp)/(1.+ 497.7*EXP(-1160./temp))	Sander et al. (2003)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2003)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	9.5E-14*EXP(390./temp)/(1.+1./ 26.2*EXP(1130./temp))	Sander et al. (2003)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH$	9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2003)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2003)*
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	9.52E-18*EXP(2.03*log(temp)+636./temp)	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	3.4E-13*EXP(-1900./temp)	Sander et al. (2003)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	1.57E-13 + cair*3.54E-33	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	4.E-13	Sander et al. (2003)
G9200	TrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	k_3rd(temp,cair,3.E-31,3.3,1.5E-12,0., 0.6)	Sander et al. (2003)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2003)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2003)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2003)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	1.9E13*EXP(-8661./temp)	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	3.E-13	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	5.E-11	Barone et al. (1995)

*Notes:

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

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

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

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

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

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:

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

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

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

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

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

G1002: path leading to 2 O(^{3}P) + O$_2$ neglected

G01Diag: `k_O3s = (1.7E-12*EXP(-940./temp)) * C(KPP_OH) + (1.E-14*EXP(-490./temp)) * C(KPP_HO2) + J_O1D * 2.2E-10 * C(KPP_H2O) / ( 3.2E-11*EXP(70./temp)*C(KPP_O2) + 1.8E-11*EXP(110./temp)*C(KPP_N2) + 2.2E-10*C(KPP_H2O) )`

G2108: branching ratio from Hack et al., see note B5 of Sander et al. (2003)

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(KPP_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: product distribution is from Elrod et al. (2001)

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

G4109: same temperature dependence assumed as for CH$_3$CHO+NO$_3$

G4201: product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))

G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH$_3$OO and C$_2$H$_5$OO 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$_3$OOH+OH assumed

G4213: The rate coefficient is: `k_PA_NO2 = k_3rd(temp,cair,8.5E-29,6.5,1.1E-11,1.,0.6)`.

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

G4218: same value as for G4107: CH$_3$OOH+OH assumed

G4219: according to Pöschl et al. (2000), the same value as for CH$_3$CHO+OH can be assumed

G4220: 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: 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)`

G4306: The rate coefficient is: `k_PrO2_CH3O2 = 9.46E-14*EXP(431./temp)`. The product distribution is from von Kuhlmann (2001).

G4307: same value as for G4107: CH$_3$OOH+OH assumed

G4309: 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).

G6102: The rate coefficient is: k_ClO_ClO = k_3rd_iupac(temp,cair,2.E-32,4.,1.E-11,0.,0.45).

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

G6204: At low temperatures, there may be a minor reaction channel leading to O_3+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.

G6405: average of reactions with CH_3Br and CH_3F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

G6407: extrapolated from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

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 (Sander et al., 2003) divided by equilibrium constant (Orlando and Tyndall, 1996).

G8101: This value was assumed by Jimenez et al. (2003).

G8102: The product as well as the reaction were assumed by von Glasow et al. (2002). An alternative pathway is the formation of new particles. This reaction needs to be updated when laboratory measurements become available.

G8103: product distribution is from Bloss et al. (2001)

G8203: assumed (J. Crowley, pers. comm. 2004)

G8300: The rate coefficient is: k_I_NO2 = k_3rd(temp,cair,3.E-31,1.,6.6E-11,0.,0.6).

G8304: J. Moldanova and J. Plane, pers. comm.

G8305: The rate coefficient is defined as backward reaction (Sander et al., 2003) divided by equilibrium constant (van den Bergh and Troe, 1976).

G8306: Note that in an earlier study by Jenkin et al. (1985), a value of 5E-3 s^{-1} was assumed.

G8600: Turnipseed et al. (1997) found a branching ratio of 14% for the sum of channels which do not produce I atoms. We assume that OIO and Cl are produced in this case.

G8701: Gilles et al. (1997) found an upper limit of 35% for I atom production. We assume 35% I and 65% OIO as products. See also Rowley et al. (2001) for info about products.

G9400a: Abstraction path. The assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

$$
\begin{aligned}
DMS + OH &\rightarrow CH_3SCH_2 \\
CH_3SCH_2 + O_2 &\rightarrow CH_3SCH_2OO \\
CH_3SCH_2OO + NO &\rightarrow CH_3SCH_2O + NO_2 \\
CH_3SCH_2O &\rightarrow CH_3S + HCHO \\
CH_3S + O_3 &\rightarrow CH_3SO \\
CH_3SO + O_3 &\rightarrow CH_3SO_2 \\
\hline
DMS + OH + NO + 2O_3 &\rightarrow CH_3SO_2 + HCHO + NO_2
\end{aligned}
$$

Neglecting the effect on O_3 and NO_x, the remaining reaction is:

$$
DMS + OH + O_3 \rightarrow CH_3SO_2 + HCHO
$$

G9400b: Addition path. The rate coefficient is: k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(KPP_O2) / (1.+5.0E-30*EXP(6280./temp)*C(KPP_O2)).

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	J_O1D	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	J_O3P	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	J_H2O2	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	J_NO2	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	J_NO2O	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	J_NOO2	see note
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	J_N2O5	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	J_HONO	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	J_HNO3	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	J_HNO4	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	J_CH3OOH	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	J_COH2	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	J_CHOH	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.

Table 3: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca_mbl.f90` using the accommodation coefficients in subroutine `mecca_mbl_alpha` and Henry's law constants in subroutine `mecca_mbl_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 4: PSC reactions

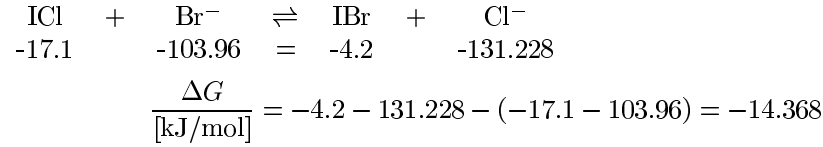| #	labels	reaction	rate coefficient	reference

*Notes: PSC reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see `http://www.messy-interface.org` for details)

Table 5: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference

*Notes:

EQ82 and EQ83: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):

ICl	+	Br^-	$\rightleftharpoons$	IBr	+	Cl^-
-17.1		-103.96	=	-4.2		-131.228

$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[\text{Cl}^-]/[\text{Br}^-]$ ratio equals 330.

Table 6: Aqueous phase reactions

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

A6102: Jacobi (1996) found an upper limit of 6E9 and cite an upper limit from another study of 2E9. Here, we set the rate coefficient to 1E9.

A6301: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A7400: assumed to be the same as for $Br_2^- + H_2O_2$.

A9106: see also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, we use SO_4^{2-} as a proxy. Note that this destroys the mass consistency for sulfur species.

A9205: D. Sedlak, pers. comm. (1993)

A9208: D. Sedlak, pers. comm. (1993)

A9105: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

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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