The Chemical Mechanism of MECCA

KPP version: `2.2.1_rs3`

MECCA version: `2.5i`

Date: July 8, 2009.

Selected reactions:
"`((Tr && (G || Het) && !I) || St)`"

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	134
Aqueous phase:	0
All species:	134

Number of reactions in selected mechanism:

Gas phase (Gnnn):	229
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	70
Heterogeneous (HETnnn):	22
Equilibria (EQnn):	0
Dummy (Dnn):	0
All equations:	321

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)
G1002	StG	$O_3 + O(^1D) \rightarrow 2\ O_2$	1.2E-10	Sander et al. (2006)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2\ O_2$	8.E-12*EXP(-2060./temp)	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)
G2101	StG	$H + O_3 \rightarrow OH + O_2$	1.4E-10*EXP(-470./temp)	Sander et al. (2006)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	1.1E-10	Sander et al. (2006)
G2103	StG	$OH + O(^3P) \rightarrow H + O_2$	2.2E-11*EXP(120./temp)	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow LossOH + HO_2 + O_2$	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)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH + O_2$	3.E-11*EXP(200./temp)	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow LossHO2 + OH + 2\ O_2$	1.E-14*EXP(-490./temp)	Sander et al. (2006)
G2108a	StG	$HO_2 + H \rightarrow 2\ OH$	7.2E-11	Sander et al. (2006)
G2108b	StG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Sander et al. (2006)
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	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	$H_2O + O(^1D) \rightarrow LossO1D + 2\ OH$	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)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	1.5E-11*EXP(-3600./temp)	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)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2\ NO$	6.7E-11*EXP(20./temp)	Sander et al. (2006)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.7E-11*EXP(20./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)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Sander et al. (2006)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.1E-12*EXP(210./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)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./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)*

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

#	labels	reaction	rate coefficient	reference
G3200	TrGN	NO + OH → 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 → ProdHO2 + NO_2 + OH	3.5E-12*EXP(250./temp)	Sander et al. (2006)
G3202	StTrGN	NO_2 + OH → 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 → HNO_4	k_NO2_HO2	Sander et al. (2006)*
G3204	TrGN	NO_3 + HO_2 → NO_2 + OH + O_2	3.5E-12	Sander et al. (2006)
G3205	TrGN	HONO + OH → NO_2 + H_2O	1.8E-11*EXP(-390./temp)	Sander et al. (2006)
G3206	StTrGN	HNO_3 + OH → H_2O + NO_3	k_HNO3_OH	Sander et al. (2006)*
G3207	StTrGN	HNO_4 → NO_2 + HO_2	k_NO2_HO2/(2.1E-27*EXP(10900./temp))	Sander et al. (2006)*
G3208	StTrGN	HNO_4 + OH → NO_2 + H_2O	1.3E-12*EXP(380./temp)	Sander et al. (2006)
G3209	TrGN	NH_3 + OH → NH_2 + H_2O	1.7E-12*EXP(-710./temp)	Kohlmann and Poppe (1999)
G3210	TrGN	NH_2 + O_3 → NH_2O + O_2	4.3E-12*EXP(-930./temp)	Kohlmann and Poppe (1999)
G3211	TrGN	NH_2 + HO_2 → NH_2O + OH	4.8E-07*EXP(-628./temp)*temp**(-1.32)	Kohlmann and Poppe (1999)
G3212	TrGN	NH_2 + HO_2 → HNO + H_2O	9.4E-09*EXP(-356./temp)*temp**(-1.12)	Kohlmann and Poppe (1999)
G3213	TrGN	NH_2 + NO → HO_2 + OH + N_2	1.92E-12*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3214	TrGN	NH_2 + NO → N_2 + H_2O	1.41E-11*((temp/298.)**(-1.5))	Kohlmann and Poppe (1999)
G3215	TrGN	NH_2 + NO_2 → N_2O + H_2O	1.2E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3216	TrGN	NH_2 + NO_2 → NH_2O + NO	0.8E-11*((temp/298.)**(-2.0))	Kohlmann and Poppe (1999)
G3217	TrGN	NH_2O + O_3 → NH_2 + O_2	1.2E-14	Kohlmann and Poppe (1999)
G3218	TrGN	NH_2O → NHOH	1.3E+3	Kohlmann and Poppe (1999)
G3219	TrGN	HNO + OH → NO + H_2O	8.0E-11*EXP(-500./temp)	Kohlmann and Poppe (1999)
G3220	TrGN	HNO + NHOH → NH_2OH + NO	1.66E-12*EXP(-1500./temp)	Kohlmann and Poppe (1999)
G3221	TrGN	HNO + NO_2 → HONO + NO	1.0E-12*EXP(-1000./temp)	Kohlmann and Poppe (1999)
G3222	TrGN	NHOH + OH → HNO + H_2O	1.66E-12	Kohlmann and Poppe (1999)
G3223	TrGN	NH_2OH + OH → NHOH + H_2O	4.13E-11*EXP(-2138./temp)	Kohlmann and Poppe (1999)
G3224	TrGN	HNO + O_2 → HO_2 + NO	3.65E-14*EXP(-4600./temp)	Kohlmann and Poppe (1999)
G4100	StG	CH_4 + $O(^1D)$ → .75 CH_3O_2 + .75 OH + .25 HCHO + .4 H + .05 H_2	1.5E-10	Sander et al. (2006)
G4101	StTrG	CH_4 + OH → CH_3O_2 + H_2O	1.85E-20*EXP(2.82*log(temp)-987./temp)	Atkinson (2003)*
G4102	TrG	CH_3OH + OH → HCHO + HO_2	2.9E-12*EXP(-345./temp)	Sander et al. (2006)
G4103	StTrG	CH_3O_2 + HO_2 → CH_3OOH + O_2	4.1E-13*EXP(750./temp)	Sander et al. (2006)*
G4104	StTrGN	CH_3O_2 + NO → ProdMeO2 + HCHO + NO_2 + HO_2	2.8E-12*EXP(300./temp)	Sander et al. (2006)
G4105	TrGN	CH_3O_2 + NO_3 → HCHO + HO_2 + NO_2	1.3E-12	Atkinson et al. (1999)

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

#	labels	reaction	rate coefficient	reference
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	$C_2H_5O_2 + NO \rightarrow ProdRO2 + CH_3CHO + HO_2 + NO_2$	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
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	$CH_3C(O)OO + NO \rightarrow ProdRO2 + CH_3O_2 + NO_2$	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)

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

#	labels	reaction	rate coefficient	reference
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)*
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)
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	$C_3H_7O_2 + NO \rightarrow 0.96\ ProdRO2 + .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	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	$CH_3CH(O_2)CH_2OH + NO \rightarrow 0.98\ ProdRO2 + .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ ONIT$	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	$CH_3COCH_2O_2 + NO \rightarrow ProdRO2 + NO_2 + CH_3C(O)OO + HCHO$	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)
G4315	TrGC	$CH_3COCH_2O_2H + OH \rightarrow .3\ CH_3COCH_2O_2 + .7\ CH_3COCHO + .7\ OH$	k_CH3OOH_OH	see note
G4316	TrGC	$CH_3COCH_2OH + OH \rightarrow CH_3COCHO + HO_2$	2.15E-12*EXP(305./temp)	Dillon et al. (2006)
G4317	TrGC	$CH_3COCHO + OH \rightarrow CH_3C(O)OO + CO$	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)

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

#	labels	reaction	rate coefficient	reference
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 → ProdRO2 + .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 → ProdRO2 + 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)*
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 → 0.985 ProdRO2 + .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)

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

#	labels	reaction	rate coefficient	reference
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)*
G4504a	TrGNC	ISO2 + NO → 0.956 ProdRO2 + .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 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)
G6101	StGCl	ClO + $O(^3P)$ → Cl + O_2	2.5E-11*EXP(110./temp)	Atkinson et al. (2007)
G6102a	StTrGCl	ClO + ClO → Cl_2 + O_2	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	ClO + ClO → 2 Cl + O_2	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	ClO + ClO → Cl + OClO	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	ClO + ClO → Cl_2O_2	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6200	StGCl	Cl + H_2 → HCl + H	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	Cl + HO_2 → HCl + O_2	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	Cl + HO_2 → ClO + OH	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	Cl + H_2O_2 → HCl + HO_2	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	ClO + OH → .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 → HOCl	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)
G6205	StTrGCl	HCl + OH → Cl + H_2O	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	HOCl+ OH → ClO + H_2O	3.0E-12*EXP(-500./temp)	Sander et al. (2006)
G6300	StTrGNCl	ClO + NO → NO_2 + Cl	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGNCl	ClO + NO_2 → $ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31,3.4, 7.E-11,0.,0.4)	Atkinson et al. (2007)
G6302	TrGCl	$ClNO_3$ → ClO + NO_2	6.918E-7*exp(-10909./temp)*cair	Anderson and Fahey (1990)
G6303	StGNCl	$ClNO_3$ + $O(^3P)$ → ClO + NO_3	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGNCl	$ClNO_3$ + Cl → Cl_2 + NO_3	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	Cl + CH_4 → HCl + CH_3O_2	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO_2	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	Cl + CH_3OOH → HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)	Sander et al. (2006)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow ClO + 3\ Cl$	3.3E-10	Sander et al. (2006)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow OH + Cl$	1.65E-10	see note
G6406	StGCl	$CH_3Cl + OH \rightarrow H_2O + Cl$	2.4E-12*EXP(-1250./temp)	Sander et al. (2006)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow OH + 3\ Cl$	3.E-10	see note
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)*
G6412	TrGCCl	$C_2H_6 + Cl \rightarrow CH_3O_2 + HCl$	8.3E-11*EXP(-100./temp)	Atkinson et al. (2006)
G6500	StGFCl	$CF_2Cl_2 + O(^1D) \rightarrow ClO + Cl$	1.4E-10	Sander et al. (2006)
G6501	StGFCl	$CFCl_3 + O(^1D) \rightarrow ClO + 2\ Cl$	2.3E-10	Sander et al. (2006)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	$BrO + O(^3P) \rightarrow RG7101 + Br + O_2$	1.9E-11*EXP(230./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)
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7300	TrGBr	$Br + BrNO_3 \rightarrow Br_2 + NO_3$	4.9E-11	Orlando and Tyndall (1996)
G7301	StTrGNBr	$BrO + NO \rightarrow RG7301 + Br + NO_2$	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_02))	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)
G7407	TrGBr	$CHBr_3 + OH \rightarrow H_2O + 3\ Br$	1.35E-12*EXP(-600./temp)	Sander et al. (2006)*

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

#	labels	reaction	rate coefficient	reference
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)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	1.E-10	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	1.9E13*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)
G9600	TrGSCl	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	3.3E-10	Atkinson et al. (2004)
G9700	TrGSBr	$DMS + Br \rightarrow CH_3SO_2 + HBr + HCHO$	9.E-11*EXP(-2386./temp)	Jefferson et al. (1994)
G9701	TrGSBr	$DMS + BrO \rightarrow DMSO + Br$	2.54E-14*EXP(850./temp)	Ingham et al. (1999)
G10600	TrGHgCl	$Hg + Cl \rightarrow HgCl$	1.0E-11	Ariya et al. (2002)
G10601	TrGHgCl	$Hg + Cl_2 \rightarrow HgCl_2$	2.6E-18	Ariya et al. (2002)
G10700	TrGHgBr	$Hg + Br \rightarrow HgBr$	3.0E-13	Donohoue et al. (2006)
G10701	TrGHgBr	$HgBr + Br \rightarrow HgBr_2$	3.0E-12	Calvert and Lindberg (2003)
G10702	TrGHgBr	$Hg + Br_2 \rightarrow HgBr_2$	9.0E-17	Ariya et al. (2002)
G10703	TrGHgBr	$Hg + BrO \rightarrow HgO + Br$	1.0E-15	Raofie and Ariya (2003)
G10704	TrGHgBr	$HgBr + BrO \rightarrow BrHgOBr$	3.0E-12	Calvert and Lindberg (2003)
G10705	TrGHgClBr	$HgCl + BrO \rightarrow ClHgOBr$	3.0E-12	Calvert and Lindberg (2003)
G10706	TrGHgClBr	$HgBr + Cl \rightarrow ClHgBr$	3.0E-12	Calvert and Lindberg (2003)
G10707	TrGHgClBr	$HgCl + Br \rightarrow ClHgBr$	3.0E-12	Calvert and Lindberg (2003)
G01Diag	StTrG	$O_3(s) \rightarrow LO_3(s)$	k_O3s	?*

*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:

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

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

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

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

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

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 $CH_3CHO+NO_3$.

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.

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).

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
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	jx(ip_H2O)	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	jx(ip_H2O2)	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	jx(ip_N2O)	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	jx(ip_NO2)	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	jx(ip_NO)	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
J3104b	StGNJ	$N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$	jx(ip_NO3NOO)	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
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	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)	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

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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
J4401	TrGCJ	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	0.019*jx(ip_COH2)+.015*jx(ip_CH3COCHO)	see note
J4402	TrGCJ	$MVKOOH + h\nu \rightarrow OH + .5\ CH_3COCHO + .25\ CH_3COCH_2OH + .75\ HCHO + .75\ HO_2 + .25\ CH_3C(O)OO + .25\ CO$	jx(ip_CH3OOH)	see note
J4403	TrGCJ	$CH_3COC_2H_5 + h\nu \rightarrow CH_3C(O)OO + C_2H_5O_2$	0.42*jx(ip_CHOH)	see note
J4404	TrGCJ	$MEKOOH + h\nu \rightarrow CH_3C(O)OO + CH_3CHO + OH$	jx(ip_CH3OOH)	see note
J4405	TrGCJ	$MeCOCO + h\nu \rightarrow 2\ CH_3C(O)OO$	2.15*jx(ip_CH3COCHO)	see note
J4406	TrGNCJ	$ONIT + h\nu \rightarrow NO_2 + .67\ CH_3COC_2H_5 + .67\ HO_2 + .33\ C_2H_5O_2 + .33\ CH_3CHO$	3.7*jx(ip_PAN)	see note
J4500	TrGCJ	$ISOOH + h\nu \rightarrow MVK + HCHO + HO_2 + OH$	jx(ip_CH3OOH)	see note
J4501	TrGNCJ	$ISON + h\nu \rightarrow MVK + HCHO + NO_2 + HO_2$	3.7*jx(ip_PAN)	see note
J6000	StTrGClJ	$Cl_2 + h\nu \rightarrow Cl + Cl$	jx(ip_Cl2)	see note
J6100	StTrGClJ	$Cl_2O_2 + h\nu \rightarrow 2\ Cl$	1.4*jx(ip_Cl2O2)	see note
J6101	StTrGClJ	$OClO + h\nu \rightarrow ClO + O(^3P)$	jx(ip_OClO)	see note
J6200	StGClJ	$HCl + h\nu \rightarrow Cl + H$	jx(ip_HCl)	see note
J6201	StTrGClJ	$HOCl + h\nu \rightarrow OH + Cl$	jx(ip_HOCl)	see note
J6300	TrGNClJ	$ClNO_2 + h\nu \rightarrow Cl + NO_2$	jx(ip_ClNO2)	see note
J6301a	StTrGNClJ	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	jx(ip_ClNO3)	see note
J6301b	StTrGNClJ	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	jx(ip_ClONO2)	see note
J6400	StGClJ	$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$	jx(ip_CH3Cl)	see note
J6401	StGClJ	$CCl_4 + h\nu \rightarrow 4\ Cl$	jx(ip_CCl4)	see note
J6402	StGCClJ	$CH_3CCl_3 + h\nu \rightarrow 3\ Cl$	jx(ip_CH3CCl3)	see note
J6500	StGFClJ	$CFCl_3 + h\nu \rightarrow 3\ Cl$	jx(ip_CFCl3)	see note
J6501	StGFClJ	$CF_2Cl_2 + h\nu \rightarrow 2\ Cl$	jx(ip_CF2Cl2)	see note
J7000	StTrGBrJ	$Br_2 + h\nu \rightarrow Br + Br$	jx(ip_Br2)	see note
J7100	TrGBrJ	$BrO + h\nu \rightarrow RJ7100 + Br + O(^3P)$	jx(ip_BrO)	see note
J7200	StTrGBrJ	$HOBr + h\nu \rightarrow Br + OH$	jx(ip_HOBr)	see note
J7300	TrGNBrJ	$BrNO_2 + h\nu \rightarrow Br + NO_2$	jx(ip_BrNO2)	see note
J7301	StTrGNBrJ	$BrNO_3 + h\nu \rightarrow 0.29\ Br + 0.29\ NO_3 + 0.71\ BrO + 0.71\ NO_2$	jx(ip_BrNO3)	see note
J7400	StGBrJ	$CH_3Br + h\nu \rightarrow Br + CH_3O_2$	jx(ip_CH3Br)	see note
J7401	TrGBrJ	$CH_2Br_2 + h\nu \rightarrow 2\ Br$	jx(ip_CH2Br2)	see note
J7402	TrGBrJ	$CHBr_3 + h\nu \rightarrow 3\ Br$	jx(ip_CHBr3)	see note
J7500	StGFBrJ	$CF_3Br + h\nu \rightarrow Br$	jx(ip_CF3Br)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J7600	StTrGClBrJ	$BrCl + h\nu \rightarrow Br + Cl$	jx(ip_BrCl)	see note
J7601	StGFBrJ	$CF_2ClBr + h\nu \rightarrow Br + Cl$	jx(ip_CF2ClBr)	see note
J7602	TrGClBrJ	$CH_2ClBr + h\nu \rightarrow Br + Cl$	jx(ip_CH2ClBr)	see note
J7603	TrGClBrJ	$CHCl_2Br + h\nu \rightarrow Br + 2\ Cl$	jx(ip_CHCl2Br)	see note
J7604	TrGClBrJ	$CHClBr_2 + h\nu \rightarrow 2\ Br + Cl$	jx(ip_CHClBr2)	see note
J8401a	TrGJ	$CH_3I + h\nu \rightarrow CH_3O_2$	JX(ip_CH3I)	see note
J9002	StGSJ	$SF_6 + h\nu \rightarrow$ products	JX(ip_SF6)	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)*
Hg	0.13	0.	Schroeder and Munthe (1998)
HgO	3.2×10^{6}	0.	Shon et al. (2005)
$HgCl_2$	2.4×10^{7}	0.	Shon et al. (2005)
$HgBr_2$	2.4×10^{7}	0.	see note
ClHgBr	2.4×10^{7}	0.	see note
BrHgOBr	2.4×10^{7}	0.	see note

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

substance	$\frac{k_{\mathrm{H}}^{\ominus}}{\mathrm{M/atm}}$	$\frac{-\Delta_{\mathrm{soln}}H/R}{\mathrm{K}}$	reference
ClHgOBr	2.4×10^{7}	0.	see note

*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.

$HgBr_2$: Assumed to be the same as for $HgCl_2$

ClHgBr: Assumed to be the same as for $HgCl_2$

BrHgOBr: Assumed to be the same as for $HgCl_2$

ClHgOBr: Assumed to be the same as for $HgCl_2$

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)*
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)
Hg	0.1	0.	see note
HgO	0.1	0.	see note
$HgCl_2$	0.1	0.	see note

Table 4: Accommodation coefficients (... continued)

substance	$\alpha^{\ominus}$	$\frac{-\Delta_{\rm obs}H/R}{\rm K}$	reference
$HgBr_2$	0.1	0.	see note
ClHgBr	0.1	0.	see note
BrHgOBr	0.1	0.	see note
ClHgOBr	0.1	0.	see note

*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.

Hg: Estimate.

HgO: Estimate.

$HgCl_2$: Estimate.

$HgBr_2$: Estimate.

ClHgBr: Estimate.

BrHgOBr: Estimate.

ClHgOBr: Estimate.

Table 5: Henry's law equilibria

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

H6301, H6302, H7601: The total uptake is determined by $k_{\mathrm{mt}}(ClNO_3)$. 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 $k_{\mathrm{mt}}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	khet_St(ihs_N2O5_H2O)	see note
HET201	TrHetN	$N_2O_5 \rightarrow 2\ NO_3^-(aq) + 2\ H^+(aq)$	khet_Tr(iht_N2O5)	see note
HET202	TrHetN	$HNO_3 \rightarrow NO_3^-(aq) + H^+(aq)$	khet_Tr(iht_HNO3)	see note
HET410	StHetCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	khet_St(ihs_HOCl_HCl)	see note
HET420	StHetNCl	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	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	$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	khet_St(ihs_N2O5_HCl)	see note
HET510	StHetBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	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	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	khet_St(ihs_ClNO3_HBr)	see note
HET541	StHetNClBr	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	khet_St(ihs_BrNO3_HCl)	see note
HET542	StHetClBr	$HOCl + HBr \rightarrow BrCl + H_2O$	khet_St(ihs_HOCl_HBr)	see note
HET543	StHetClBr	$HOBr + HCl \rightarrow BrCl + H_2O$	khet_St(ihs_HOBr_HCl)	see note
HET1001	StTrHetHg	$Hg \rightarrow Hg(aq)$	khet_Tr(iht_Hg) + khet_St(ihs_Hg)	see note
HET1002	StTrHetHg	$HgO \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1003	StTrHetHg	$HgCl \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1004	StTrHetHg	$HgCl_2 \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1005	StTrHetHg	$HgBr \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1006	StTrHetHg	$HgBr_2 \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1007	StTrHetHg	$ClHgBr \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1008	StTrHetHg	$BrHgOBr \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	see note
HET1009	StTrHetHg	$ClHgOBr \rightarrow Hg(aq)$	khet_Tr(iht_RGM) + khet_St(ihs_RGM)	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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