Supplemental Material:

The Chemical Mechanism of MECCA

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The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs3

MECCA version: 2.5

Date: February 2, 2010.

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

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	99
Aqueous phase:	0
All species:	99

Number of reactions in selected mechanism:

Gas phase (Gnnn):	406
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	100
Heterogeneous (HETnnn):	0
Equilibria (EQnn):	0
Isotope exchange (IEXann):	7
Dummy (Dnn):	2
All equations:	515

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	$OH + O_3 \rightarrow HO_2 + O_2$ O isotope transfer: $OH \rightarrow 0.5\ HO_2$ O isotope transfer: $O_3 \rightarrow 0.5\ HO_2 + O_2$	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	$HO_2 + O(^3P) \rightarrow OH + O_2$ O isotope transfer: $HO_2 \rightarrow OH + 0.5\ O_2$ O isotope transfer: $O(^3P) \rightarrow 0.5\ O_2$	3.E-11*EXP(200./temp)	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2\ O_2$ O isotope transfer: $HO_2 \rightarrow OH + 0.25\ O_2$ O isotope transfer: $O_3 \rightarrow 0.75\ O_2$	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	$HO_2 + OH \rightarrow H_2O + O_2$ O isotope transfer: $OH \rightarrow H_2O$ O isotope transfer: $HO_2 \rightarrow O_2$	4.8E-11*EXP(250./temp)	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	1.63E-10*EXP(60./temp)	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$ O isotope transfer: $OH \rightarrow H_2O$ O isotope transfer: $H_2O_2 \rightarrow HO_2$	1.8E-12	Sander et al. (2006)

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

#	labels	reaction	rate coefficient	reference
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)
		O isotope transfer: $O_3 \rightarrow O_2 + 0.5\ NO_2$		
		O isotope transfer: $NO \rightarrow 0.5\ NO_2$		
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)
		O isotope transfer: $NO_2 \rightarrow NO + 0.5\ O_2$		
		O isotope transfer: $O(^3P) \rightarrow 0.5\ O_2$		
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2006)
		O isotope transfer: $NO_2 \rightarrow 0.667\ NO_3$		
		O isotope transfer: $O_3 \rightarrow 0.333\ NO_3 + O_2$		
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)*
G3200	TrGN	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.0E-31,2.6,3.6E-11,0.1, 0.6)	Sander et al. (2006)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2006)
		O isotope transfer: $NO \rightarrow 0.5\ NO_2$		
		O isotope transfer: $HO_2 \rightarrow 0.5\ NO_2 + OH$		
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0.,0.6)	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2006)
		O isotope transfer: $NO_3 \rightarrow NO_2 + OH$		
		O isotope transfer: $HO_2 \rightarrow O_2$		
G3205	TrGN	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2006)
		O isotope transfer: $HONO \rightarrow NO_2$		
		O isotope transfer: $OH \rightarrow H_2O$		

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

#	labels	reaction	rate coefficient	reference
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2006)*
		O isotope transfer: $HNO_3 \rightarrow NO_3$		
		O isotope transfer: $OH \rightarrow H_2O$		
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./temp))	Sander et al. (2006)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2006)
		O isotope transfer: $HNO_4 \rightarrow NO_2 + O_2$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4100	StG	$CH_4 + O(^1D) \rightarrow 0.75\ CH_3O_2 + 0.75\ OH + 0.25\ HCHO + 0.4\ H + 0.05\ H_2$	1.5E-10	Sander et al. (2006)
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
		O isotope transfer: $O(^1D) \rightarrow OH + HCHO$		
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	1.85E-20*EXP(2.82*log(temp)-987./temp)	Atkinson (2003)*
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	2.9E-12*EXP(-345./temp)	Sander et al. (2006)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	4.1E-13*EXP(750./temp)	Sander et al. (2006)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2006)
		O isotope transfer: $CH_3O_2 \rightarrow 0.5\ NO_2 + HCHO$		
		O isotope transfer: $NO \rightarrow 0.5\ NO_2$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
		O isotope transfer: $CH_3O_2 \rightarrow 0.5\ NO_2 + HCHO$		
		O isotope transfer: $NO_3 \rightarrow 0.5\ NO_2 + HO_2$		
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	$CH_3OOH + OH \rightarrow 0.7\ CH_3O_2 + 0.3\ HCHO + 0.3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2006)*
		O isotope transfer: $CH_3OOH \rightarrow CH_3O_2 + HCHO + OH$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	9.52E-18*EXP(2.03*log(temp)+636./temp)	Sivakumaran et al. (2003)

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: HCHO → CO		
		O isotope transfer: OH → H_2O		
		O isotope transfer: O_2 → HO_2		
G4109	TrGN	HCHO + NO_3 → HNO_3 + CO + HO_2	3.4E-13*EXP(-1900./temp)	Sander et al. (2006)*
G4110	StTrG	CO + OH → H + CO_2	1.57E-13 + cair*3.54E-33	McCabe et al. (2001)
G4111	TrG	HCOOH + OH → HO_2	4.0E-13	Sander et al. (2006)
G4200	TrGC	C_2H_6 + OH → $C_2H_5O_2$ + H_2O	1.49E-17*temp*temp*EXP(-499./temp)	Atkinson (2003)
		O isotope transfer: OH → H_2O		
		O isotope transfer: O_2 → $C_2H_5O_2$		
G4201	TrGC	C_2H_4 + O_3 → HCHO + 0.22 HO_2 + 0.12 OH + 0.23 CO + 0.54 HCOOH + 0.1 H_2	1.2E-14*EXP(-2630./temp)	Sander et al. (2006)*
		O isotope transfer: O_3 → HCHO + OH + CO + 0.5 HCOOH + CO_2 + 0.5 H_2O_2		
		O isotope transfer: O_2 → HO_2		
		O isotope transfer: H_2O → 0.5 HCOOH + 0.5 H_2O_2		
G4202	TrGC	C_2H_4 + OH → 0.6666667 $CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,1.0E-28,4.5,8.8E-12,0.85, 0.6)	Sander et al. (2006)
		O isotope transfer: O_2 → $CH_3CH(O_2)CH_2OH$		
G4203	TrGC	$C_2H_5O_2$ + HO_2 → C_2H_5OOH	7.5E-13*EXP(700./temp)	Sander et al. (2006)
		O isotope transfer: $C_2H_5O_2$ → C_2H_5OOH		
		O isotope transfer: HO_2 → O_2		
G4204	TrGNC	$C_2H_5O_2$ + NO → CH_3CHO + HO_2 + NO_2	2.6E-12*EXP(365./temp)	Sander et al. (2006)
		O isotope transfer: $C_2H_5O_2$ → 0.5 NO_2 + CH_3CHO		
		O isotope transfer: NO → 0.5 NO_2		
		O isotope transfer: O_2 → HO_2		
G4205	TrGNC	$C_2H_5O_2$ + NO_3 → CH_3CHO + HO_2 + NO_2	2.3E-12	Atkinson et al. (1999)
		O isotope transfer: $C_2H_5O_2$ → CH_3CHO + 0.5 O_2		
		O isotope transfer: NO_3 → NO_2 + 0.5 O_2		
		O isotope transfer: O_2 → HO_2		
G4206	TrGC	$C_2H_5O_2$ + CH_3O_2 → 0.75 HCHO + HO_2 + 0.75 CH_3CHO + 0.25 CH_3OH	1.6E-13*EXP(195./temp)	see note

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: $C_2H_5O_2 \rightarrow CH_3CHO + 0.5\ O_2$		
		O isotope transfer: $CH_3O_2 \rightarrow HCHO + CH_3OH + 0.5\ O_2$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
		C isotope transfer: $C_2H_5O_2 \rightarrow CH_3CHO$		
		C isotope transfer: $CH_3O_2 \rightarrow HCHO + CH_3OH$		
G4207	TrGC	$C_2H_5OOH + OH \rightarrow 0.3\ C_2H_5O_2 + 0.7\ CH_3CHO + 0.7\ OH$	k_CH3OOH_OH	see note
		O isotope transfer: $C_2H_5OOH \rightarrow C_2H_5O_2 + CH_3CHO + OH$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	4.4E-12*EXP(365./temp)	Atkinson et al. (2006)
		O isotope transfer: $OH \rightarrow H_2O$		
		O isotope transfer: $CH_3CHO \rightarrow 0.333\ CH_3C(O)OO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO$		
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	1.4E-12*EXP(-1900./temp)	Sander et al. (2006)
		O isotope transfer: $NO_3 \rightarrow HNO_3$		
		O isotope transfer: $CH_3CHO \rightarrow 0.333\ CH_3C(O)OO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO$		
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2 + CO_2 + H_2O$	4.2E-14*EXP(855./temp)	Atkinson et al. (2006)
		O isotope transfer: $CH_3COOH \rightarrow CO_2$		
		O isotope transfer: $OH \rightarrow H_2O$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
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)
		O isotope transfer: $CH_3C(O)OO \rightarrow CH_3C(O)OOH$		
		O isotope transfer: $HO_2 \rightarrow O_2$		
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)
		O isotope transfer: $HO_2 \rightarrow 0.667\ O_3$		
		O isotope transfer: $CH_3C(O)OO \rightarrow 0.333\ O_3 + CH_3COOH$		
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	8.1E-12*EXP(270./temp)	Tyndall et al. (2001)
		O isotope transfer: $CH_3C(O)OO \rightarrow 0.5\ NO_2 + CO_2$		
		O isotope transfer: $NO \rightarrow 0.5\ NO_2$		

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
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)
		O isotope transfer: $CH_3C(O)OO \rightarrow CO_2 + 0.5\ O_2$		
		O isotope transfer: $NO_3 \rightarrow NO_2 + 0.5\ O_2$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
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)
		O isotope transfer: $CH_3C(O)OO \rightarrow CO_2$		
		O isotope transfer: $CH_3O_2 \rightarrow HCHO$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2 + HO_2$		
		C isotope transfer: $CH_3C(O)OO \rightarrow CH_3O_2 + CO_2$		
		C isotope transfer: $CH_3O_2 \rightarrow HCHO$		
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)
		O isotope transfer: $CH_3C(O)OO \rightarrow CH_3COOH$		
		O isotope transfer: $CH_3O_2 \rightarrow HCHO$		
		C isotope transfer: $CH_3C(O)OO \rightarrow CH_3COOH$		
		C isotope transfer: $CH_3O_2 \rightarrow HCHO$		
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow 0.82\ CH_3O_2 + CH_3CHO + 0.82\ HO_2 + 0.18\ CH_3COOH$	4.9E-12*EXP(211./temp)	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
		O isotope transfer: $CH_3C(O)OO \rightarrow CH_3COOH + CH_3O_2 + 0.5\ CO_2$		
		O isotope transfer: $C_2H_5O_2 \rightarrow CH_3CHO + 0.5\ CO_2$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
		C isotope transfer: $CH_3C(O)OO \rightarrow CH_3COOH + CH_3O_2 + CO_2$		
		C isotope transfer: $C_2H_5O_2 \rightarrow CH_3CHO$		
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	2.5E-12*EXP(500./temp)	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	k_CH3OOH_OH	see note
		O isotope transfer: $CH_3C(O)OOH \rightarrow CH_3C(O)OO$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4219	TrGNC	$NACA + OH \rightarrow NO_2 + HCHO + CO$	5.6E-12*EXP(270./temp)	see note

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: NACA → NO_2 + HCHO + CO		
		O isotope transfer: OH → H_2O		
G4220	TrGNC	PAN + OH → HCHO + NO_2	2.E-14	see note
		O isotope transfer: PAN → HCHO + NO_2 + CO		
		O isotope transfer: OH → H_2O		
G4221	TrGNC	PAN → $CH_3C(O)OO$ + NO_2	k_PAN_M	Sander et al. (2006)*
G4300	TrGC	C_3H_8 + OH → 0.82 $C_3H_7O_2$ + 0.18 $C_2H_5O_2$ + H_2O	1.65E-17*temp*temp*EXP(-87./temp)	Atkinson (2003)
		O isotope transfer: OH → H_2O		
		O isotope transfer: O_2 → $C_3H_7O_2$ + $C_2H_5O_2$		
G4301	TrGC	C_3H_6 + O_3 → 0.57 HCHO + 0.47 CH_3CHO + 0.33 OH + 0.26 HO_2 + 0.07 CH_3O_2 + 0.06 $C_2H_5O_2$ + 0.23 $CH_3C(O)OO$ + 0.04 CH_3COCHO + 0.06 CH_4 + 0.31 CO + 0.22 HCOOH + 0.03 CH_3OH	6.5E-15*EXP(-1900./temp)	Sander et al. (2006)*
		O isotope transfer: O_3 → HCHO + CH_3CHO + OH + 0.5 $C_2H_5O_2$ + 0.333 $CH_3C(O)OO$ + 0.5 CH_3COCHO + CO + 0.5 HCOOH		
		O isotope transfer: O_2 → HO_2 + 0.5 $C_2H_5O_2$ + 0.667 $CH_3C(O)OO$ + 0.5 CH_3COCHO + CH_3O_2 + CH_3OH		
		O isotope transfer: H_2O → 0.5 HCOOH		
G4302	TrGC	C_3H_6 + OH → $CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)	Atkinson et al. (1999)
		O isotope transfer: O_2 → $CH_3CH(O_2)CH_2OH$		
G4303	TrGNC	C_3H_6 + NO_3 → ONIT	4.6E-13*EXP(-1155./temp)	Atkinson et al. (1999)
G4304	TrGC	$C_3H_7O_2$ + HO_2 → C_3H_7OOH	k_PrO2_HO2	Atkinson (1997)*
		O isotope transfer: $C_3H_7O_2$ → C_3H_7OOH		
		O isotope transfer: HO_2 → O_2		
G4305	TrGNC	$C_3H_7O_2$ + NO → 0.96 CH_3COCH_3 + 0.96 HO_2 + 0.96 NO_2 + 0.04 $C_3H_7ONO_2$	k_PrO2_NO	Atkinson et al. (1999)*
		O isotope transfer: $C_3H_7O_2$ → 0.5 NO_2 + $C_3H_7ONO_2$ + CH_3COCH_3		
		O isotope transfer: NO → 0.5 NO_2		
		O isotope transfer: O_2 → HO_2		

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

#	labels	reaction	rate coefficient	reference
G4306	TrGC	$C_3H_7O_2$ + CH_3O_2 → CH_3COCH_3 + 0.8 HCHO + 0.8 HO_2 + 0.2 CH_3OH O isotope transfer: $C_3H_7O_2$ → CH_3COCH_3 O isotope transfer: CH_3O_2 → HCHO + CH_3OH O isotope transfer: O_2 → HO_2 C isotope transfer: $C_3H_7O_2$ → CH_3COCH_3 C isotope transfer: CH_3O_2 → HCHO + CH_3OH	k_PrO2_CH3O2	Kirchner and Stockwell (1996)
G4307	TrGC	C_3H_7OOH + OH → 0.3 $C_3H_7O_2$ + 0.7 CH_3COCH_3 + 0.7 OH O isotope transfer: C_3H_7OOH → $C_3H_7O_2$ + CH_3COCH_3 + OH O isotope transfer: OH → H_2O	k_CH3OOH_OH	see note
G4308	TrGC	$CH_3CH(O_2)CH_2OH$ + HO_2 → $CH_3CH(OOH)CH_2OH$ O isotope transfer: $CH_3CH(O_2)CH_2OH$ → $CH_3CH(OOH)CH_2OH$ O isotope transfer: HO_2 → O_2	6.5E-13*EXP(650./temp)	Müller and Brasseur (1995)
G4309	TrGNC	$CH_3CH(O_2)CH_2OH$ + NO → 0.98 CH_3CHO + 0.98 HCHO + 0.98 HO_2 + 0.98 NO_2 + 0.02 ONIT O isotope transfer: $CH_3CH(O_2)CH_2OH$ → 0.5 NO_2 + CH_3CHO + HCHO + ONIT O isotope transfer: NO → 0.5 NO_2 O isotope transfer: O_2 → HO_2	4.2E-12*EXP(180./temp)	Müller and Brasseur (1995)*
G4310	TrGC	$CH_3CH(OOH)CH_2OH$ + OH → 0.5 $CH_3CH(O_2)CH_2OH$ + 0.5 CH_3COCH_2OH + 0.5 OH + H_2O O isotope transfer: $CH_3CH(OOH)CH_2OH$ → $CH_3CH(O_2)CH_2OH$ + CH_3COCH_2OH + OH O isotope transfer: OH → H_2O	3.8E-12*EXP(200./temp)	Müller and Brasseur (1995)
G4311	TrGC	CH_3COCH_3 + OH → $CH_3COCH_2O_2$ + H_2O O isotope transfer: CH_3COCH_3 → 0.333 $CH_3COCH_2O_2$ O isotope transfer: O_2 → 0.667 $CH_3COCH_2O_2$ O isotope transfer: OH → H_2O	1.33E-13+3.82E-11*EXP(-2000./temp)	Sander et al. (2006)
G4312	TrGC	$CH_3COCH_2O_2$ + HO_2 → $CH_3COCH_2O_2H$ O isotope transfer: $CH_3COCH_2O_2$ → $CH_3COCH_2O_2H$	8.6E-13*EXP(700./temp)	Tyndall et al. (2001)

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: $HO_2 \rightarrow O_2$		
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	2.9E-12*EXP(300./temp)	Sander et al. (2006)
		O isotope transfer: $CH_3COCH_2O_2 \rightarrow 0.5\ NO_2 + HCHO + 0.333\ CH_3C(O)OO$		
		O isotope transfer: $NO \rightarrow 0.5\ NO_2$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO$		
G4314	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow 0.5\ CH_3COCHO + 0.5\ CH_3OH + 0.3\ CH_3C(O)OO + 0.8\ HCHO + 0.3\ HO_2 + 0.2\ CH_3COCH_2OH$	7.5E-13*EXP(500./temp)	Tyndall et al. (2001)
		O isotope transfer: $CH_3COCH_2O_2 \rightarrow CH_3COCHO + 0.333\ CH_3C(O)OO + 0.3\ HCHO + CH_3COCH_2OH$		
		O isotope transfer: $CH_3O_2 \rightarrow CH_3OH + 0.5\ HCHO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO + HO_2$		
		C isotope transfer: $CH_3COCH_2O_2 \rightarrow CH_3COCHO + CH_3C(O)OO + HCHO + CH_3COCH_2OH$		
		C isotope transfer: $CH_3O_2 \rightarrow CH_3OH$		
G4315	TrGC	$CH_3COCH_2O_2H + OH \rightarrow 0.3\ CH_3COCH_2O_2 + 0.7\ CH_3COCHO + 0.7\ OH$	k_CH3OOH_OH	see note
		O isotope transfer: $CH_3COCH_2O_2H \rightarrow CH_3COCH_2O_2 + CH_3COCHO + OH$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4316	TrGC	$CH_3COCH_2OH + OH \rightarrow CH_3COCHO + HO_2$	2.15E-12*EXP(305./temp)	Dillon et al. (2006)
		O isotope transfer: $CH_3COCH_2OH \rightarrow CH_3COCHO$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4317	TrGC	$CH_3COCHO + OH \rightarrow CH_3C(O)OO + CO$	8.4E-13*EXP(830./temp)	Tyndall et al. (1995)
		O isotope transfer: $CH_3COCHO \rightarrow 0.333\ CH_3C(O)OO + CO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO$		
		O isotope transfer: $OH \rightarrow H_2O$		
G4318	TrGNC	$MPAN + OH \rightarrow CH_3COCH_2OH + NO_2$	3.2E-11	Orlando et al. (2002)
		O isotope transfer: $MPAN \rightarrow CH_3COCH_2OH + NO_2$		
		O isotope transfer: $OH \rightarrow H_2O$		

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 O isotope transfer: $C_3H_7ONO_2$ → CH_3COCH_3 + NO_2 O isotope transfer: OH → H_2O	6.2E-13*EXP(-230./temp)	Atkinson et al. (1999)
G4400	TrGC	C_4H_{10} + OH → $C_4H_9O_2$ + H_2O O isotope transfer: O_2 → $C_4H_9O_2$ O isotope transfer: OH → H_2O	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)
G4401	TrGC	$C_4H_9O_2$ + CH_3O_2 → 0.88 $CH_3COC_2H_5$ + 0.68 HCHO + 1.23 HO_2 + 0.12 CH_3CHO + 0.12 $C_2H_5O_2$ + 0.18 CH_3OH O isotope transfer: $C_4H_9O_2$ → $CH_3COC_2H_5$ + CH_3CHO + $C_2H_5O_2$ O isotope transfer: CH_3O_2 → HCHO + CH_3OH O isotope transfer: O_2 → HO_2 C isotope transfer: $C_4H_9O_2$ → $CH_3COC_2H_5$ + CH_3CHO + $C_2H_5O_2$ C isotope transfer: CH_3O_2 → HCHO + CH_3OH	k_PrO2_CH3O2	see note
G4402	TrGC	$C_4H_9O_2$ + HO_2 → C_4H_9OOH O isotope transfer: $C_4H_9O_2$ → C_4H_9OOH O isotope transfer: HO_2 → O_2	k_PrO2_HO2	see note
G4403	TrGNC	$C_4H_9O_2$ + NO → 0.84 NO_2 + 0.56 $CH_3COC_2H_5$ + 0.56 HO_2 + 0.28 $C_2H_5O_2$ + 0.84 CH_3CHO + 0.16 ONIT O isotope transfer: $C_4H_9O_2$ → 0.5 NO_2 + $CH_3COC_2H_5$ + CH_3CHO + 0.667 ONIT O isotope transfer: NO → 0.5 NO_2 + 0.333 ONIT O isotope transfer: O_2 → HO_2 + $C_2H_5O_2$	k_PrO2_NO	see note
G4404	TrGC	C_4H_9OOH + OH → 0.15 $C_4H_9O_2$ + 0.85 $CH_3COC_2H_5$ + 0.85 OH + 0.85 H_2O O isotope transfer: C_4H_9OOH → $C_4H_9O_2$ + $CH_3COC_2H_5$ + OH O isotope transfer: OH → H_2O	k_CH3OOH_OH	see note

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

#	labels	reaction	rate coefficient	reference
G4405	TrGC	MVK + O_3 → 0.45 HCOOH + 0.9 CH_3COCHO + 0.1 $CH_3C(O)OO$ + 0.19 OH + 0.22 CO + 0.32 HO_2 O isotope transfer: MVK → 0.5 CH_3COCHO + 0.333 $CH_3C(O)OO$ O isotope transfer: O_3 → 0.5 CH_3COCHO + 0.5 HCOOH + OH + CO O isotope transfer: O_2 → HO_2 + 0.667 $CH_3C(O)OO$ O isotope transfer: H_2O → 0.5 HCOOH	.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))	Pöschl et al. (2000)
G4406	TrGC	MVK + OH → MVKO2 O isotope transfer: MVK → 0.25 MVKO2 O isotope transfer: OH → 0.25 MVKO2 O isotope transfer: O_2 → 0.5 MVKO2	.5*(4.1E-12*EXP(452./temp)+1.9E-11*EXP(175./ temp))	Pöschl et al. (2000)
G4407	TrGC	MVKO2 + HO_2 → MVKOOH O isotope transfer: MVKO2 → MVKOOH O isotope transfer: HO_2 → O_2	1.82E-13*EXP(1300./temp)	Pöschl et al. (2000)
G4408	TrGNC	MVKO2 + NO → NO_2 + 0.25 $CH_3C(O)OO$ + 0.25 CH_3COCH_2OH + 0.75 HCHO + 0.25 CO + 0.75 HO_2 + 0.5 CH_3COCHO O isotope transfer: MVKO2 → 0.5 NO_2 + 0.333 $CH_3C(O)OO$ + CH_3COCH_2OH + HCHO + CO + CH_3COCHO O isotope transfer: NO → 0.5 NO_2 O isotope transfer: O_2 → HO_2 + 0.667 $CH_3C(O)OO$	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)
G4409	TrGNC	MVKO2 + NO_2 → MPAN O isotope transfer: MVKO2 → 0.8 MPAN O isotope transfer: NO_2 → 0.2 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 → 0.5 CH_3COCHO + 0.375 CH_3COCH_2OH + 0.125 $CH_3C(O)OO$ + 1.125 HCHO + 0.875 HO_2 + 0.125 CO + 0.25 CH_3OH	2.E-12	von Kuhlmann (2001)

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: MVKO2 → CH_3COCHO + CH_3COCH_2OH		
		+ 0.333 $CH_3C(O)OO$ + 0.778 HCHO + CO		
		O isotope transfer: CH_3O_2 → 0.222 HCHO + CH_3OH		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$ + HO_2		
		C isotope transfer: MVKO2 → CH_3COCHO + CH_3COCH_2OH		
		+ $CH_3C(O)OO$ + 0.778 HCHO + CO		
		C isotope transfer: CH_3O_2 → 0.222 HCHO + CH_3OH		
G4411	TrGC	MVKO2 + MVKO2 → CH_3COCH_2OH + CH_3COCHO + 0.5	2.E-12	Pöschl et al. (2000)
		CO + 0.5 HCHO + HO_2		
G4412	TrGC	MVKOOH + OH → MVKO2	3.E-11	Pöschl et al. (2000)
		O isotope transfer: MVKOOH → MVKO2		
		O isotope transfer: OH → H_2O		
G4413	TrGC	$CH_3COC_2H_5$ + OH → MEKO2	1.3E-12*EXP(-25./temp)	Atkinson et al. (1999)
		O isotope transfer: $CH_3COC_2H_5$ → 0.333 MEKO2		
		O isotope transfer: OH → H_2O		
		O isotope transfer: O_2 → 0.667 MEKO2		
G4414	TrGC	MEKO2 + HO_2 → MEKOOH	k_PrO2_HO2	see note
		O isotope transfer: MEKO2 → MEKOOH		
		O isotope transfer: HO_2 → O_2		
G4415	TrGNC	MEKO2 + NO → 0.985 CH_3CHO + 0.985 $CH_3C(O)OO$ + 0.985	k_PrO2_NO	see note
		NO_2 + 0.015 ONIT		
		O isotope transfer: MEKO2 → 0.5 NO_2 + CH_3CHO + 0.333		
		$CH_3C(O)OO$ + 0.75 ONIT		
		O isotope transfer: NO → 0.5 NO_2 + 0.25 ONIT		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$		
G4416	TrGC	MEKOOH + OH → 0.8 MeCOCO + 0.8 OH + 0.2 MEKO2	k_CH3OOH_OH	see note
		O isotope transfer: MEKOOH → MeCOCO + MEKO2 + OH		
		O isotope transfer: OH → H_2O		
G4417	TrGNC	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	1.7E-12	Atkinson et al. (1999)*
		O isotope transfer: ONIT → $CH_3COC_2H_5$ + NO_2		
		O isotope transfer: OH → H_2O		

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

#	labels	reaction	rate coefficient	reference
G4500	TrGC	ISOP + O_3 → 0.28 HCOOH + 0.65 MVK + 0.1 MVKO2 + 0.1 $CH_3C(O)OO$ + 0.14 CO + 0.58 HCHO + 0.09 H_2O_2 + 0.08 CH_3O_2 + 0.25 OH + 0.25 HO_2 O isotope transfer: O_3 → 0.5 HCOOH + MVK + 0.333 MVKO2 + 0.333 $CH_3C(O)OO$ + CO + 0.081 HCHO + 0.5 H_2O_2 + OH O isotope transfer: O_2 → 0.667 MVKO2 + 0.667 $CH_3C(O)OO$ + 0.919 HCHO + CH_3O_2 + HO_2 O isotope transfer: H_2O → 0.5 HCOOH + 0.5 H_2O_2	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)
G4501	TrGC	ISOP + OH → ISO2 O isotope transfer: O_2 → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO_3 → ISON O isotope transfer: O_2 → 0.4 ISON O isotope transfer: NO_3 → 0.6 ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO_2 → ISOOH O isotope transfer: ISO2 → ISOOH O isotope transfer: HO_2 → O_2	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)*
G4504a	TrGNC	ISO2 + NO → 0.956 NO_2 + 0.956 MVK + 0.956 HCHO + 0.956 HO_2 + 0.044 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)*
G4505	TrGC	ISO2 + CH_3O_2 → 0.5 MVK + 1.25 HCHO + HO_2 + 0.25 CH_3COCHO + 0.25 CH_3COCH_2OH + 0.25 CH_3OH O isotope transfer: ISO2 → MVK + 0.8 HCHO + CH_3COCHO + CH_3COCH_2OH O isotope transfer: CH_3O_2 → 0.2 HCHO + CH_3OH O isotope transfer: O_2 → HO_2	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO_2 O isotope transfer: ISO2 → MVK + HCHO O isotope transfer: O_2 → HO_2	2.E-12	Pöschl et al. (2000)
G4507	TrGC	ISOOH + OH → MVK + OH O isotope transfer: ISOOH → OH + MVK O isotope transfer: O_2 → H_2O	1.E-10	Pöschl et al. (2000)
G4508	TrGNC	ISON + OH → CH_3COCH_2OH + NACA	1.3E-11	Pöschl et al. (2000)

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: ISON → CH_3COCH_2OH + NACA		
		O isotope transfer: OH → H_2O		
G6100	StTrGCl	Cl + O_3 → ClO + O_2	2.8E-11*EXP(-250./temp)	Atkinson et al. (2007)
G6101	StGCl	ClO + O(^{3}P) → 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 → 0.94 Cl + 0.94 HO_2 + 0.06 HCl + 0.06 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(^{3}P) → 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)
		O isotope transfer: O_2 → CH_3O_2		
G6401	StTrGCl	Cl + HCHO → HCl + CO + HO_2	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
		O isotope transfer: HCHO → CO		
		O isotope transfer: O_2 → HO_2		
G6402	StTrGCl	Cl + CH_3OOH → HCHO + HCl + OH	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	ClO + CH_3O_2 → HO_2 + Cl + HCHO	3.3E-12*EXP(-115./temp)	Sander et al. (2006)

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

#	labels	reaction	rate coefficient	reference
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	$Cl + C_2H_4 \rightarrow 0.6666667\ CH_3CH(O_2)CH_2OH + HCl$	k_3rd_iupac(temp,cair,1.85E-29,3.3,6.0E-10, 0.0,0.4)	Atkinson et al. (2006)
		O isotope transfer: $O_2 \rightarrow CH_3CH(O_2)CH_2OH$		
G6410	TrGCCl	$Cl + CH_3CHO \rightarrow HCl + CH_3C(O)OO$	7.9e-11	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)
G7405	TrGCCl	$Br + CH_3CHO \rightarrow HBr + CH_3C(O)OO$	1.8e-11*EXP(-460./temp)	Atkinson et al. (2006)
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO$		
		O isotope transfer: $CH_3CHO \rightarrow 0.333\ CH_3C(O)OO$		
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)
		O isotope transfer: $SO_2 \rightarrow 0.5\ H_2SO_4$		
		O isotope transfer: $OH \rightarrow 0.25\ H_2SO_4$		
		O isotope transfer: $H_2O \rightarrow 0.25\ H_2SO_4$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2004)*
		O isotope transfer: $O_2 \rightarrow CH_3SO_2 + HCHO$		
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
		O isotope transfer: $OH \rightarrow DMSO$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
		O isotope transfer: $NO_3 \rightarrow HNO_3$		
		O isotope transfer: $O_2 \rightarrow CH_3SO_2 + HCHO$		
G9402	TrGS	$DMSO + OH \rightarrow 0.6\ SO_2 + HCHO + 0.6\ CH_3O_2 + 0.4\ HO_2 + 0.4\ CH_3SO_3H$	1.E-10	Hynes and Wine (1996)
		O isotope transfer: $OH \rightarrow 0.5\ SO_2 + 0.333\ CH_3SO_3H$		
		O isotope transfer: $DMSO \rightarrow 0.5\ SO_2 + 0.333\ CH_3SO_3H$		

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

#	labels	reaction	rate coefficient	reference
		O isotope transfer: $O_2 \rightarrow CH_3O_2 + HCHO + HO_2 + 0.333\ CH_3SO_3H$		
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	1.9E13*EXP(-8661./temp)	Barone et al. (1995)
		O isotope transfer: $CH_3SO_2 \rightarrow SO_2$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	3.E-13	Barone et al. (1995)
		O isotope transfer: $CH_3SO_2 \rightarrow 0.667\ CH_3SO_3$		
		O isotope transfer: $O_3 \rightarrow 0.333\ CH_3SO_3$		
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	5.E-11	Barone et al. (1995)
		O isotope transfer: $CH_3SO_3 \rightarrow CH_3SO_3H$		
G9600	TrGSCl	$DMS + Cl \rightarrow CH_3SO_2 + HCl + HCHO$	3.3E-10	Atkinson et al. (2004)
		O isotope transfer: $O_2 \rightarrow CH_3SO_2 + HCHO$		

*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).

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	$HNO_4 + h\nu \rightarrow 0.667\ NO_2 + 0.667\ HO_2 + 0.333\ NO_3 + 0.333\ OH$	jx(ip_HNO4)	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	jx(ip_CH3OOH)	see note
		O isotope transfer: $CH_3OOH \rightarrow OH + HCHO$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
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
		O isotope transfer: $HCHO \rightarrow CO$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
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
		O isotope transfer: $O_2 \rightarrow CO + H_2O$		
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	jx(ip_CH3OOH)	see note
		O isotope transfer: $C_2H_5OOH \rightarrow CH_3CHO + OH$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	jx(ip_CH3CHO)	see note
		O isotope transfer: $CH_3CHO \rightarrow CO$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2 + HO_2$		

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	jx(ip_PAA)	see note
		O isotope transfer: $CH_3C(O)OOH \rightarrow OH$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*jx(ip_CHOH)	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow 0.6\ CH_3C(O)OO + 0.6\ NO_2 + 0.4\ CH_3O_2 + 0.4\ NO_3 + 0.4\ CO_2$	jx(ip_PAN)	see note
		O isotope transfer: $PAN \rightarrow CH_3C(O)OO + NO_2 + NO_3 + CO_2$		
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
J4300	TrGCJ	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	jx(ip_CH3OOH)	see note
		O isotope transfer: $C_3H_7OOH \rightarrow CH_3COCH_3 + OH$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	jx(ip_CH3COCH3)	see note
		O isotope transfer: $CH_3COCH_3 \rightarrow 0.333\ CH_3C(O)OO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO + CH_3O_2$		
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*jx(ip_CHOH)	see note
		O isotope transfer: $CH_3COCH_2OH \rightarrow 0.333\ CH_3C(O)OO + HCHO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO + HO_2$		
J4303	TrGCJ	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	jx(ip_CH3COCHO)	see note
		O isotope transfer: $CH_3COCHO \rightarrow 0.333\ CH_3C(O)OO + CO$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO + HO_2$		
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	jx(ip_CH3OOH)	see note
		O isotope transfer: $CH_3COCH_2O_2H \rightarrow 0.333\ CH_3C(O)OO + OH$		
		O isotope transfer: $O_2 \rightarrow 0.667\ CH_3C(O)OO + HO_2$		
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
		O isotope transfer: $C_3H_7ONO_2 \rightarrow CH_3COCH_3 + NO_2$		
		O isotope transfer: $O_2 \rightarrow HO_2$		
J4400	TrGCJ	$C_4H_9OOH + h\nu \rightarrow OH + 0.67\ CH_3COC_2H_5 + 0.67\ HO_2 + 0.33\ C_2H_5O_2 + 0.33\ CH_3CHO$	jx(ip_CH3OOH)	see note
		O isotope transfer: $C_4H_9OOH \rightarrow OH + CH_3COC_2H_5 + CH_3CHO$		
		O isotope transfer: $O_2 \rightarrow HO_2 + C_2H_5O_2$		

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J4401	TrGCJ	MVK + hν → $CH_3C(O)OO$ + HCHO + CO + HO_2	0.019*jx(ip_COH2)+.015*jx(ip_CH3COCHO)	see note
		O isotope transfer: MVK → 0.333 $CH_3C(O)OO$ + CO		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$ + HCHO + HO_2		
J4402	TrGCJ	MVKOOH + hν → OH + 0.5 CH_3COCHO + 0.25 CH_3COCH_2OH + 0.75 HCHO + 0.75 HO_2 + 0.25 $CH_3C(O)OO$ + 0.25 CO	jx(ip_CH3OOH)	see note
		O isotope transfer: MVKOOH → OH + CH_3COCHO + CH_3COCH_2OH + 0.5 HCHO + 0.333 $CH_3C(O)OO$ + CO		
		O isotope transfer: O_2 → HO_2 + 0.5 HCHO + 0.667 $CH_3C(O)OO$		
J4403	TrGCJ	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*jx(ip_CHOH)	see note
		O isotope transfer: $CH_3COC_2H_5$ → 0.333 $CH_3C(O)OO$		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$ + $C_2H_5O_2$		
J4404	TrGCJ	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	jx(ip_CH3OOH)	see note
		O isotope transfer: MEKOOH → 0.333 $CH_3C(O)OO$ + CH_3CHO + OH		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$		
J4405	TrGCJ	MeCOCO + hν → 2 $CH_3C(O)OO$	2.15*jx(ip_CH3COCHO)	see note
		O isotope transfer: MeCOCO → 0.333 $CH_3C(O)OO$		
		O isotope transfer: O_2 → 0.667 $CH_3C(O)OO$		
J4406	TrGNCJ	ONIT + hν → NO_2 + 0.67 $CH_3COC_2H_5$ + 0.67 HO_2 + 0.33 $C_2H_5O_2$ + 0.33 CH_3CHO	3.7*jx(ip_PAN)	see note
		O isotope transfer: ONIT → NO_2 + $CH_3COC_2H_5$ + CH_3CHO		
		O isotope transfer: O_2 → HO_2 + $C_2H_5O_2$		
J4500	TrGCJ	ISOOH + hν → MVK + HCHO + HO_2 + OH	jx(ip_CH3OOH)	see note
		O isotope transfer: ISOOH → MVK + HCHO + OH		
		O isotope transfer: O_2 → HO_2		
J4501	TrGNCJ	ISON + hν → MVK + HCHO + NO_2 + HO_2	3.7*jx(ip_PAN)	see note
		O isotope transfer: ISON → MVK + HCHO + NO_2		
		O isotope transfer: O_2 → HO_2		
J6000	StTrGClJ	Cl_2 + hν → Cl + Cl	jx(ip_Cl2)	see note
J6100	StTrGClJ	Cl_2O_2 + hν → 2 Cl	1.4*jx(ip_Cl2O2)	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
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
		O isotope transfer: $O_2 \rightarrow CH_3O_2$		
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
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.

Table 3: Isotope exchange reactions

#	labels	reaction	rate coefficient	reference
IEX001	StTrG	$OH + H_2O \rightleftharpoons H_2O + OH$	2.3E-13*exp(-2100./temp)	Dubey et al. (1997)
IEX002	StTrG	$OH + HO_2 \rightleftharpoons HO_2 + OH$	1.7E-11*exp(+400./temp)	Dransfeld and Wagner (1987)
IEX003	StTrG	$OH + NO \rightleftharpoons NO + OH$	1.8E-11	Greenblatt and Howard (1989)
IEX004	StTrG	$OH + NO_2 \rightleftharpoons NO_2 + OH$	1.0E-11	Greenblatt and Howard (1989)
IEX005	StTrG	$O(^3P) + O_2 \rightleftharpoons O_2 + O(^3P)$	2.9E-12	Anderson et al. (1985)*
IEX006	StTrG	$O(^3P) + NO \rightleftharpoons NO + O(^3P)$	3.7E-11	Anderson et al. (1985)
IEX007	StTrG	$NO + NO_2 \rightleftharpoons NO_2 + NO$	3.6E-14	Klein et al. (1963)

*Notes:

IEXO05: Fractionation values for exchange are assigned to those calculated by Johnston et al. (2000).

Table 4: Kinetic isotope effects

#	reaction	isotopologue	fractionation factor α	reference
G1001	$O_2 + O(^3P) \rightarrow O_3$	$^{18}O_2$	1.099	Johnston et al. (2000)*
		$^{17}O_2$	1.094	
J1001a	$O_3 + h\nu \rightarrow O(^1D)$	$^{18}O_3$	0.978	Johnston et al. (2000)
		$^{17}O_3$	0.976	
J1001b	$O_3 + h\nu \rightarrow O(^3P)$	$^{18}O_3$	0.978	Johnston et al. (2000)
		$^{17}O_3$	0.976	
G4100	$CH_4 + O(^1D) \rightarrow 0.75\ CH_3O_2 + 0.75\ OH + 0.25\ HCHO + 0.4\ H + 0.05\ H_2$	$^{13}CH_4$	1.013	Saueressig et al. (2001)*
		^{18}OH	0.9765	
		^{18}OH	0.9876	
G4101	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	$^{13}CH_4$	1.0039	Saueressig et al. (2001)*
		^{18}OH	0.9765	
		^{18}OH	0.9876	
G6400	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	$^{13}CH_4$	1.0658	Saueressig et al. (1995)*
G4110	$CO + OH \rightarrow H + CO_2$	^{13}CO	1.0065	Röckmann et al. (1998)*
	$CO + OH \rightarrow H + CO_2$	$C^{18}O$	1.0094	
	$CO + OH \rightarrow H + CO_2$	$C^{17}O$	1.0002	

*Notes:

G1001: Yields $\delta^{18}O(O_3) = 90.0‰$ and $\delta^{17}O(O_3) = 78.0‰$, respectively, when combined with J1001a, J1001b and IEXO05 reactions kinetic isotope effects.

G4100: Yields $\delta^{18}O = 0‰$ and $\delta^{18}O = 0‰$ in products from O_2.

G4101: Same as for G4100.

G4110: Pressure dependent; given is approximate value at 1 bar pressure.

G6400: Temperature dependent; given is approximate value at 298K.

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