

# The Chemical Mechanism of MECCA

## used for the MINATROC box model calculations in the accompanying paper

Table 1: Gas phase reactions

#	labels	reaction	rate constant	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	$3.2E-11*EXP(70./temp)$	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	$6.E-34*((temp/300.)**(-2.4))*cair$	Sander et al. (2003)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	$k\_3rd(temp, cair, 5.7E-32, 1.6, 7.5E-11, 0., 0.6)$	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2$	$1.7E-12*EXP(-940./temp)$	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	$5.5E-12*EXP(-2000./temp)$	Sander et al. (2003)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	$1.E-14*EXP(-490./temp)$	Sander et al. (2003)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	$4.8E-11*EXP(250./temp)$	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	$k\_HO2\_HO2$	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2 OH$	$2.2E-10$	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$2.9E-12*EXP(-160./temp)$	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	$1.8E-11*EXP(110./temp)$	Sander et al. (2003)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	$3.E-12*EXP(-1500./temp)$	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.2E-13*EXP(-2450./temp)$	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2 NO_2$	$1.5E-11*EXP(170./temp)$	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	$k\_NO3\_NO2$	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	$k\_NO3\_NO2/(3.E-27*EXP(10990./temp))$	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO$	$k\_3rd(temp, cair, 7.E-31, 2.6, 3.6E-11, 0.1, 0.6)$	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	$3.5E-12*EXP(250./temp)$	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	$k\_3rd(temp, cair, 2.E-30, 3., 2.5E-11, 0., 0.6)$	Sander et al. (2003)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	$k\_NO2\_HO2$	Sander et al. (2003)
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	$3.5E-12$	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	$1.8E-11*EXP(-390./temp)$	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	$k\_HNO3\_OH$	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	$k\_NO2\_HO2/(2.1E-27*EXP(10900./temp))$	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	$1.3E-12*EXP(380./temp)$	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	$1.85E-20*EXP(2.82*log(temp)-987./temp)$	Atkinson (2003)*

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

#	labels	reaction	rate constant	reference
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$7.3\text{E}-12*\text{EXP}(-620./\text{temp})$	Sander et al. (2003)
G4103a	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH}$	$4.1\text{E}-13*\text{EXP}(750./\text{temp})/(1.+1./497.7*\text{EXP}(1160./\text{temp}))$	Sander et al. (2003)*
G4103b	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$4.1\text{E}-13*\text{EXP}(750./\text{temp})/(1.+497.7*\text{EXP}(-1160./\text{temp}))$	Sander et al. (2003)*
G4104	StTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E}-12*\text{EXP}(300./\text{temp})$	Sander et al. (2003)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E}-12$	Atkinson et al. (1999)
G4106a	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$	$9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+1./26.2*\text{EXP}(1130./\text{temp}))$	Sander et al. (2003)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH}$	$9.5\text{E}-14*\text{EXP}(390./\text{temp})/(1.+26.2*\text{EXP}(-1130./\text{temp}))$	Sander et al. (2003)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH	Sander et al. (2003)*
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18*\text{EXP}(2.03*\log(\text{temp})+636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13*\text{EXP}(-1900./\text{temp})$	Sander et al. (2003)*
G4110	StTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$1.57\text{E}-13+\text{cair}*3.54\text{E}-33$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{HO}_2$	$4.\text{E}-13$	Sander et al. (2003)
G4200	TrGC	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(-499./\text{temp})$	Atkinson (2003)
G4201	TrGC	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + .22 \text{HO}_2 + .12 \text{OH} + .23 \text{CO} + .54 \text{HCOOH} + .1 \text{H}_2$	$1.2\text{E}-14*\text{EXP}(-2630./\text{temp})$	Sander et al. (2003)*
G4202	TrGC	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow .6666667 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 1.E-28, 0.8, 8.8E-12, 0., 0.6)	Sander et al. (2003)
G4203	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E}-13*\text{EXP}(700./\text{temp})$	Sander et al. (2003)
G4204	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E}-12*\text{EXP}(365./\text{temp})$	Sander et al. (2003)
G4205	TrGNC	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.3\text{E}-12$	Atkinson et al. (1999)
G4206	TrGC	$\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{HCHO} + \text{HO}_2 + .75 \text{CH}_3\text{CHO} + .25 \text{CH}_3\text{OH}$	$1.6\text{E}-13*\text{EXP}(195./\text{temp})$	see note
G4207	TrGC	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .3 \text{C}_2\text{H}_5\text{O}_2 + .7 \text{CH}_3\text{CHO} + .7 \text{OH}$	k_CH300H_OH	see note
G4208	TrGC	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$5.6\text{E}-12*\text{EXP}(270./\text{temp})$	Sander et al. (2003)
G4209	TrGNC	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E}-12*\text{EXP}(-1900./\text{temp})$	Sander et al. (2003)
G4210	TrGC	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2$	$4.\text{E}-13*\text{EXP}(200./\text{temp})$	Sander et al. (2003)
G4211a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+1./37.*\text{EXP}(660./\text{temp}))$	Tyndall et al. (2001)
G4211b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E}-13*\text{EXP}(1040./\text{temp})/(1.+37.*\text{EXP}(-660./\text{temp}))$	Tyndall et al. (2001)
G4212	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$8.1\text{E}-12*\text{EXP}(270./\text{temp})$	Tyndall et al. (2001)

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

#	labels	reaction	rate constant	reference
G4213	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_PA_NO2	Tyndall et al. (2001)
G4214	TrGNC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	4.E-12	Canosa-Mas et al. (1996)
G4215a	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9 \cdot 2.E-12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2003)
G4215b	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO} + \text{CO}_2$	$0.1 \cdot 2.E-12 \cdot \text{EXP}(500./\text{temp})$	Sander et al. (2003)
G4216	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{HO}_2 + .18 \text{CH}_3\text{COOH}$	$4.9E-12 \cdot \text{EXP}(211./\text{temp})$	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow 2 \text{CH}_3\text{O}_2 + 2 \text{CO}_2 + \text{O}_2$	$2.5E-12 \cdot \text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4218	TrGC	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	k_CH300H_OH	see note
G4219	TrGNC	$\text{NACA} + \text{OH} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6E-12 \cdot \text{EXP}(270./\text{temp})$	see note
G4220	TrGNC	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2$	2.E-14	see note
G4221	TrGNC	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M	Sander et al. (2003)*
G4300	TrGC	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .82 \text{C}_3\text{H}_7\text{O}_2 + .18 \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65E-17 \cdot \text{temp} \cdot \text{temp} \cdot \text{EXP}(-87./\text{temp})$	Atkinson (2003)
G4301	TrGC	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .04 \text{CH}_3\text{COCHO} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5E-15 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2003)*
G4302	TrGC	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 8.E-27, 3.5, 3.E-11, 0., 0.5)	Atkinson et al. (1999)
G4303	TrGNC	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{ONIT}$	$4.6E-13 \cdot \text{EXP}(-1155./\text{temp})$	Atkinson et al. (1999)
G4304	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	k_Pr02_HO2	Atkinson (1997)*
G4305	TrGNC	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow .96 \text{CH}_3\text{COCH}_3 + .96 \text{HO}_2 + .96 \text{NO}_2 + .04 \text{C}_3\text{H}_7\text{ONO}_2$	k_Pr02_NO	Atkinson et al. (1999)*
G4306	TrGC	$\text{C}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{HCHO} + .8 \text{HO}_2 + .2 \text{CH}_3\text{OH}$	k_Pr02_CH3O2	Kirchner and Stockwell (1996)
G4307	TrGC	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .3 \text{C}_3\text{H}_7\text{O}_2 + .7 \text{CH}_3\text{COCH}_3 + .7 \text{OH}$	k_CH300H_OH	see note
G4308	TrGC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HO}_2 \rightarrow \text{C}_3\text{H}_6\text{OOH}$	$6.5E-13 \cdot \text{EXP}(650./\text{temp})$	Müller and Brasseur (1995)
G4309	TrGNC	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow .98 \text{CH}_3\text{CHO} + .98 \text{HCHO} + .98 \text{HO}_2 + .98 \text{NO}_2 + .02 \text{ONIT}$	$4.2E-12 \cdot \text{EXP}(180./\text{temp})$	Müller and Brasseur (1995)*
G4310	TrGC	$\text{C}_3\text{H}_6\text{OOH} + \text{OH} \rightarrow .5 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{OH} + \text{H}_2\text{O}$	$3.8E-12 \cdot \text{EXP}(200./\text{temp})$	Müller and Brasseur (1995)
G4311	TrGC	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$1.33E-13 + 3.82E-11 \cdot \text{EXP}(-2000./\text{temp})$	Sander et al. (2003)
G4312	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6E-13 \cdot \text{EXP}(700./\text{temp})$	Tyndall et al. (2001)
G4313	TrGNC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO}$	$2.9E-12 \cdot \text{EXP}(300./\text{temp})$	Sander et al. (2003)

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

#	labels	reaction	rate constant	reference
G4314	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{COCHO} + .5 \text{CH}_3\text{OH}$ + .3 $\text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2 + .2$ $\text{CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E}-13*\text{EXP}(500./\text{temp})$	Tyndall et al. (2001)
G4315	TrGC	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow .3 \text{CH}_3\text{COCH}_2\text{O}_2 + .7$ $\text{CH}_3\text{COCHO} + .7 \text{OH}$	k_CH300H_OH	see note
G4316	TrGC	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{CH}_3\text{COCHO} + \text{HO}_2$	3.E-12	Atkinson et al. (1999)
G4317	TrGC	$\text{CH}_3\text{COCHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}$	$8.4\text{E}-13*\text{EXP}(830./\text{temp})$	Tyndall et al. (1995)
G4318	TrGNC	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	3.2E-11	Orlando et al. (2002)
G4319	TrGNC	$\text{MPAN} \rightarrow \text{MVKO}_2 + \text{NO}_2$	k_PAN_M	see note
G4320	TrGNC	$\text{C}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E}-13*\text{EXP}(-230./\text{temp})$	Atkinson et al. (1999)
G4400	TrGC	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{C}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.81\text{E}-17*\text{temp}*\text{temp}*\text{EXP}(114./\text{temp})$	Atkinson (2003)
G4401	TrGC	$\text{C}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .88 \text{CH}_3\text{COC}_2\text{H}_5 + .68 \text{HCHO} +$ $1.23 \text{HO}_2 + .12 \text{CH}_3\text{CHO} + .12 \text{C}_2\text{H}_5\text{O}_2 + .18 \text{CH}_3\text{OH}$	k_Pr02_CH302	see note
G4402	TrGC	$\text{C}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_4\text{H}_9\text{OOH}$	k_Pr02_H02	see note
G4403	TrGNC	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO} \rightarrow .84 \text{NO}_2 + .56 \text{CH}_3\text{COC}_2\text{H}_5 + .56 \text{HO}_2$ + .28 $\text{C}_2\text{H}_5\text{O}_2 + .84 \text{CH}_3\text{CHO} + .16 \text{ONIT}$	k_Pr02_NO	see note
G4404	TrGC	$\text{C}_4\text{H}_9\text{OOH} + \text{OH} \rightarrow .15 \text{C}_4\text{H}_9\text{O}_2 + .85 \text{CH}_3\text{COC}_2\text{H}_5 + .85$ $\text{OH} + .85 \text{H}_2\text{O}$	k_CH300H_OH	see note
G4405	TrGC	$\text{MVK} + \text{O}_3 \rightarrow .45 \text{HCOOH} + .9 \text{CH}_3\text{COCHO} + .1$ $\text{CH}_3\text{C}(\text{O})\text{OO} + .19 \text{OH} + .22 \text{CO} + .32 \text{HO}_2$	$.5*(1.36\text{E}-15*\text{EXP}(-2112./\text{temp})$ $+7.51\text{E}-16*\text{EXP}(-1521./\text{temp}))$	Pöschl et al. (2000)
G4406	TrGC	$\text{MVK} + \text{OH} \rightarrow \text{MVKO}_2$	$.5*(4.1\text{E}-12*\text{EXP}(452./\text{temp})$ $+1.9\text{E}-11*\text{EXP}(175./\text{temp}))$	Pöschl et al. (2000)
G4407	TrGC	$\text{MVKO}_2 + \text{HO}_2 \rightarrow \text{MVKOOH}$	$1.82\text{E}-13*\text{EXP}(1300./\text{temp})$	Pöschl et al. (2000)
G4408	TrGNC	$\text{MVKO}_2 + \text{NO} \rightarrow \text{NO}_2 + .25 \text{CH}_3\text{C}(\text{O})\text{OO} + .25$ $\text{CH}_3\text{COCH}_2\text{OH} + .75 \text{HCHO} + .25 \text{CO} + .75 \text{HO}_2 + .5$ $\text{CH}_3\text{COCHO}$	$2.54\text{E}-12*\text{EXP}(360./\text{temp})$	Pöschl et al. (2000)
G4409	TrGNC	$\text{MVKO}_2 + \text{NO}_2 \rightarrow \text{MPAN}$	$.25*k\_3\text{rd}(\text{temp}, \text{cair}, 9.7\text{E}-29, 5.6,$ $9.3\text{E}-12, 1.5, 0.6)$	Pöschl et al. (2000)*
G4410	TrGC	$\text{MVKO}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{COCHO} + .375$ $\text{CH}_3\text{COCH}_2\text{OH} + .125 \text{CH}_3\text{C}(\text{O})\text{OO} + 1.125 \text{HCHO}$ + .875 $\text{HO}_2 + .125 \text{CO} + .25 \text{CH}_3\text{OH}$	2.E-12	von Kuhlmann (2001)
G4411	TrGC	$\text{MVKO}_2 + \text{MVKO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{CH}_3\text{COCHO} +$ .5 $\text{CO} + .5 \text{HCHO} + \text{HO}_2$	2.E-12	Pöschl et al. (2000)
G4412	TrGC	$\text{MVKOOH} + \text{OH} \rightarrow \text{MVKO}_2$	3.E-11	Pöschl et al. (2000)
G4413	TrGC	$\text{CH}_3\text{COC}_2\text{H}_5 + \text{OH} \rightarrow \text{MEKO}_2$	$1.3\text{E}-12*\text{EXP}(-25./\text{temp})$	Atkinson et al. (1999)

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

#	labels	reaction	rate constant	reference
G4414	TrGC	MEKO2 + HO <sub>2</sub> → MEKOOH	k_Pr02_H02	see note
G4415	TrGNC	MEKO2 + NO → .985 CH <sub>3</sub> CHO + .985 CH <sub>3</sub> C(O)OO + .985 NO <sub>2</sub> + .015 ONIT	k_Pr02_NO	see note
G4416	TrGC	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	k_CH300H_OH	see note
G4417	TrGNC	ONIT + OH → CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub> + NO <sub>2</sub> + H <sub>2</sub> O	1.7E-12	Atkinson et al. (1999)*
G4500	TrGC	ISOP + O <sub>3</sub> → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 CH <sub>3</sub> C(O)OO + .14 CO + .58 HCHO + .09 H <sub>2</sub> O <sub>2</sub> + .08 CH <sub>3</sub> O <sub>2</sub> + .25 OH + .25 HO <sub>2</sub>	7.86E-15*EXP(-1913./temp)	Pöschl et al. (2000)
G4501	TrGC	ISOP + OH → ISO2	2.54E-11*EXP(410./temp)	Pöschl et al. (2000)
G4502	TrGNC	ISOP + NO <sub>3</sub> → ISON	3.03E-12*EXP(-446./temp)	Pöschl et al. (2000)
G4503	TrGC	ISO2 + HO <sub>2</sub> → ISOOH	2.22E-13*EXP(1300./temp)	Boyd et al. (2003)*
G4504	TrGNC	ISO2 + NO → .88 NO <sub>2</sub> + .88 MVK + .88 HCHO + .88 HO <sub>2</sub> + .12 ISON	2.54E-12*EXP(360./temp)	Pöschl et al. (2000)*
G4505	TrGC	ISO2 + CH <sub>3</sub> O <sub>2</sub> → .5 MVK + 1.25 HCHO + HO <sub>2</sub> + .25 CH <sub>3</sub> COCHO + .25 CH <sub>3</sub> COCH <sub>2</sub> OH + .25 CH <sub>3</sub> OH	2.E-12	von Kuhlmann (2001)
G4506	TrGC	ISO2 + ISO2 → 2 MVK + HCHO + HO <sub>2</sub>	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 <sub>3</sub> COCH <sub>2</sub> OH + NACA	1.3E-11	Pöschl et al. (2000)
G0004	TrG	HO <sub>2</sub> → Dummy	Khet_H02*DUSTYESNO	see note
G0008	TrG	H <sub>2</sub> O <sub>2</sub> → Dummy	Khet_H202*DUSTYESNO	see note

\*Notes:

G2110: The rate constant is:  $k_{H02\_H02} = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*zcon)*(1.0\_dp+1.4E-21*EXP(2200./temp)*C(KPP\_H20))$ . 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 constant is:  $k_{N03\_N02} = k_{3rd}(temp, zcon, 2.0E-30, 4.4, 1.4E-12, 0.7, 0.6)$ .

G3110: The rate constant is defined as backward reaction divided by equilibrium constant.

G3206: The rate constant is:  $k_{$

HN03\_OH =  $2.4E-14*EXP(460./temp)+1./((1./6.5E-34*EXP(1335./temp)*zcon)+(1./2.7E-17*EXP(2199./temp)))$

G3207: The rate constant is defined as backward reaction divided by equilibrium constant.

G4103: product distribution is from Elrod et al. (2001)

G4107: The rate constant is:  $k_{CH300H\_OH} = 3.8E-12*EXP(200./temp)$

G4109: same temperature dependence assumed as for CH<sub>3</sub>CHO+NO<sub>3</sub>

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

G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH<sub>3</sub>OO and C<sub>2</sub>H<sub>5</sub>OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

G4207: same value as for G4107: CH<sub>3</sub>OOH+OH assumed

G4213: The rate constant is:  $k_{PA\_N02} = k_{3rd}(temp, zcon, 8.5E-29, 6.5, 1.1E-11, 1.0, 0.6)$ .

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

G4218: same value as for G4107:  $\text{CH}_3\text{OOH}+\text{OH}$  assumed

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

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

G4221: The rate constant is:  $k_{\text{PAN}_M} = k_{\text{PA}_N\text{O}_2} / 9.\text{E-}29 * \text{EXP}(-14000./\text{temp})$ , i.e. the rate constant is defined as backward reaction divided by equilibrium constant.

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

G4304: The rate constant is:  $k_{\text{PrO}_2\text{H}_2\text{O}_2} = 1.9\text{E-}13 * \text{EXP}(1300./\text{temp})$ . Value for generic  $\text{RO}_2 + \text{HO}_2$  reaction from Atkinson (1997) is used.

G4305: The rate constant is:  $k_{\text{PrO}_2\text{NO}} = 2.7\text{E-}12 * \text{EXP}(360./\text{temp})$

G4306: The rate constant is:  $k_{\text{PrO}_2\text{CH}_3\text{O}_2} = 9.46\text{E-}14 * \text{EXP}(431./\text{temp})$ . The product distribution is from von Kuhlmann (2001).

G4307: same value as for G4107:  $\text{CH}_3\text{OOH}+\text{OH}$  assumed

G4309: products are from von Kuhlmann (2001)

G4315: same value as for G4107:  $\text{CH}_3\text{OOH}+\text{OH}$  assumed

G4319: same value as for PAN assumed

G4401: same value as for propyl group assumed ( $k_{\text{PrO}_2\text{CH}_3\text{O}_2}$ )

G4402: same value as for propyl group assumed ( $k_{\text{PrO}_2\text{H}_2\text{O}_2}$ )

G4403: same value as for propyl group assumed ( $k_{\text{PrO}_2\text{NO}}$ )

G4404: same value as for G4107:  $\text{CH}_3\text{OOH}+\text{OH}$  assumed

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

G4414: same value as for propyl group assumed ( $k_{\text{PrO}_2\text{H}_2\text{O}_2}$ )

G4415: same value as for propyl group assumed ( $k_{\text{PrO}_2\text{NO}}$ )

G4416: same value as for G4107:  $\text{CH}_3\text{OOH}+\text{OH}$  assumed

G4417: value for  $\text{C}_4\text{H}_9\text{ONO}_2$  used here

G4503: same temperature dependence assumed as for other  $\text{RO}_2+\text{HO}_2$  reactions

G4504: Yield of 12 %  $\text{RONO}_2$  assumed as suggested in Table 2 of Sprengnether et al. (2002).

G0004: Heterogeneous removal reaction of  $\text{HO}_2$  on mineral dust aerosol. The calculation of the removal rate is described in the accompanying paper.

G0008: Heterogeneous removal reaction of  $\text{H}_2\text{O}_2$  on mineral dust aerosol. The calculation of the removal rate is described in the accompanying paper.

Table 2: Photolysis reactions

#	labels	reaction	rate constant	reference
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	J_01D	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	J_03P	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2 OH$	J_H2O2	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	J_NO2	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	J_NO20	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	J_NO02	see note
J3104	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	J_N205	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	J_HONO	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	J_HNO3	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	J_HNO4	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	J_CH300H	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	J_COH2	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	J_CHOH	see note
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	J_CH300H	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	J_CH3CHO	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	J_PAH	see note
J4203	TrGNCJ	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*J_CHOH	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	J_PAN	see note
J4300	TrGCJ	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	J_CH300H	see note
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	J_CH3COCH3	see note
J4302	TrGCJ	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*J_CHOH	see note
J4303	TrGCJ	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	J_CH3COCHO	see note
J4304	TrGCJ	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	J_CH300H	see note
J4305	TrGNCJ	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	J_PAN	see note
J4306	TrGNCJ	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*J_PAN	see note
J4400	TrGCJ	$C_4H_9OOH + h\nu \rightarrow OH + .67 CH_3COC_2H_5 + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	J_CH300H	see note
J4401	TrGCJ	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	0.019*J_COH2+.015*J_CH3COCHO	see note
J4402	TrGCJ	$MVKOOH + h\nu \rightarrow OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 CH_3C(O)OO + .25 CO$	J_CH300H	see note
J4403	TrGCJ	$CH_3COC_2H_5 + h\nu \rightarrow CH_3C(O)OO + C_2H_5O_2$	0.42*J_CHOH	see note
J4404	TrGCJ	$MEKOOH + h\nu \rightarrow CH_3C(O)OO + CH_3CHO + OH$	J_CH300H	see note
J4405	TrGCJ	$MeCOCO + h\nu \rightarrow 2 CH_3C(O)OO$	2.15*J_CH3COCHO	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate constant	reference
J4406	TrGNCJ	ONIT + $h\nu$ → NO <sub>2</sub> + .67 CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub> + .67 HO <sub>2</sub> + .33 C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> + .33 CH <sub>3</sub> CHO	3.7*J_PAN	see note
J4500	TrGCJ	ISOOH + $h\nu$ → MVK + HCHO + HO <sub>2</sub> + OH	J_CH300H	see note
J4501	TrGNCJ	ISON + $h\nu$ → MVK + HCHO + NO <sub>2</sub> + HO <sub>2</sub>	3.7*J_PAN	see note

\*Notes: J-values are calculated with an external module and then supplied to the MECCA chemistry



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