Supplementary Material for the paper

The influence of natural and anthropogenic secondary sources on the glyoxal global distribution

Myriokefalitakis S.[1], Vrekoussis M.[2], Tsigaridis K.[3], Wittrock F.[2], Richter A.[2], Brühl, C.[4], Volkamer R.[5], Burrows J.P.[2], Kanakidou M.[1,*]

[1] Environmental Chemical Processes Laboratory, Department of Chemistry, University of Crete, Voutes Campus, P.O.Box 2208, 71003 Heraklion, Greece

[2] Institute of Environmental Physics and Remote Sensing, IUP, University of Bremen, Germany

[3] Laboratoire des Sciences du Climat et de l'Environnement (LSCE), CNRS-CEA, 91191 Gif-sur-Yvette, France

[4] Max Planck Institute, Atmospheric Chemistry Division, Mainz, Germany

[5] Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado, USA

*Corresponding author: mariak@chemistry.uoc.gr

Table 1. Photolysis reactions in TM4-ECPL and related references

#	reaction			refs.
j1	$O_3 + h\nu$	→	$O(^1D) + O_2$	1
j2	$H_2O_2 + h\nu$	→	$2OH$	1
j3	$NO_2 + h\nu$	→	$NO + O$	1
j4	$NO_3 + h\nu$	→	$NO_2 + O$	1
j5	$NO_3 + h\nu$	→	$NO + O_2$	1
j6	$HONO_2 + h\nu$	→	$NO_2 + OH$	1
j7	$HO_2NO_2 + h\nu$	→	$NO_2 + HO_2$	1
j8	$N_2O_5 + h\nu$	→	$NO_2 + NO_3$	1
j9	$CH_3OOH + h\nu + O_2$	→	$HCHO + HO_2 + OH$	1
j10	$CH_3ONO_2 + h\nu + O_2$	→	$HCHO + HO_2 + NO_2$	1
j11	$HCHO + h\nu$	→	$CO + H_2$	1
j12	$HCHO + h\nu + 2O_2$	→	$CO + 2HO_2$	1
j13	$C_2H_5OOH + h\nu + O_2$	→	$CH_3CHO + HO_2 + OH$	2
j14	$C_2H_5ONO_2 + h\nu + O_2$	→	$CH_3CHO + HO_2 + NO_2$	1
j15	$CH_3CHO + h\nu + 2O_2$	→	$CH_3O_2 + CO + HO_2$	1
j16	$CH_3C(O)O_2NO_2 + h\nu$	→	$CH_3COO_2 + NO_2$	1
j17	$CH_3COO_2H + h\nu + O_2$	→	$CH_3O_2 + CO_2 + OH$	2
j18	$C_3H_7O_2prim + h\nu + O_2$	→	$1\text{-}C_2H_5CHO + HO_2 + OH$	2
j19	$C_3H_7ONO_2prim + h\nu$	→	$1\text{-}C_2H_5CHO + HO_2 + NO_2$	4
j19	$C_2H_5CHOprim + h\nu + O_2$	→	$C_2H_5O_2 + CO + HO_2$	7
j20	$C_3H_7O_2sec + h\nu + O_2$	→	$CH_3COCH_3 + HO_2 + OH$	2
j21	$C_3H_7ONO_2sec + h\nu$	→	$CH_3COCH_3 + HO_2 + NO_2$	4
j22	$CH_3COCH_3 + h\nu + 2O_2$	→	$CH_3COO_2 + CH_3O_2$	5
j23	$CH_3COCHO + h\nu + 2O_2$	→	$0.3*(CH_3O_2 + 2CO + HO_2) + 0.7*(CH_3COO_2 + CO + HO_2)$	1
j24	$CH_3COCH_2OOH + h\nu + O_2$	→	$CH3COCHO + OH + HO_2$	2
j25	$HOCH_2CH_2OOH + h\nu + O_2$	→	$OH + e(2HCHO + HO_2) + f(CH_2OHCHO + HO_2)$	2, 8
j26	$HOCH_2CH_2ONO2 + h\nu + O_2$	→	$NO_2 + e(HCHO + HO2) + f(CH_2OHCHO + HO2)$	1, 8
j27	$HOCH_2CHO + h\nu + 2O_2$	→	$HCHO + CO + 2HO_2$	1
j28	$CHOCHO + h\nu$	→	$2CO + 2HO_2$	1
j29	$C_4H_9ONO_2 + h\nu + O_2$	→	$NO_2 + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO)$	4
j30	$C_4H_9OOH + h\nu + O_2$	→	$OH + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO)$	2
j31	$CH_3CH_2COCH_3 + h\nu + 2O_2$	→	$CH_3COO_2 + C_2H_5O_2$	5
j32	$CH_3CHONO_2COCH_3 + h\nu + O_2$	→	$CH_3CHO + CH_3COO_2 + NO_2$	4
j33	$CH_3CHOOHCOCH_3 + h\nu + O_2$	→	$CH_3CHO + CH_3COO_2 + OH$	2
j34	$CH_3COCOCH_3 + h\nu + 2O_2$	→	$2CH_3COO_2$	6
j35	$ISOOH + h\nu + O_2$	→	$HCHO + OH + HO_2 + 0.64MVK + 0.36MACR$	2
j36	$NITRATES + h\nu + O_2$	→	$HCHO + HO_2 + NO_2 + 0.64MVK + 0.36MACR$	4
j37	$MVKOOH + h\nu + O_2$	→	$CH_3COO_2 + CH_2OHCHO + OH$	2
j38	$MACROOH + h\nu + O_2$	→	$CH_3COCH_2OH + CO + OH + HO2$	2
j39	$CH_2ONO_2CH_2OOH + h\nu$	→	$OH + NO_2 + 2HCHO$	2
j40	$CH_2ONO_2CH_2OOH + h\nu$	→	$CH_3CHO + HCHO + NO_2 + OH$	2
j41	$CH_3COCOOH + h\nu$	→	$CH_3CHO + CO_2$	2
j43	$MACR + h\nu$	→	$0.67HO_2 + 0.33MACRO_2 + 0.67CH_2O + 0.67CH_3COO_2 + 0.33OH$	1
j44	$MVK + h\nu$	→	$0.3CH_3CO_3 + 0.7C_3H_6 + 0.7CO + 0.3CH_3O_2$	1

References:

1. IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, Web Version February, http://www.iupac-kinetic.ch.cam.ac.uk/ summary/ IUPACsumm_web_Feb2006.pdf, 2006

2. $j = j13$

3. $j = 1.7 \times j22$

4. $j = j10$

5. $j = 3 \times 10^{-4} \times j3$

6. $j = 0.285 \times j3$

7. $j = (2.58 \times 10^{-4} + 1.2 \times 10^{-5}) \times j3$

8. $R1 = 2.7 \times 10^{14} \exp(-6350/T)$
   $R2 = 6.3 \times 10^{-14} \exp(-550/T)$
   $e = R1/(R1 + R2 \times [O_2])$, $f = 1 - e$
   T= temperature, lumping as in

   Poisson, N., Kanakidou, M., and Crutzen, P. J.: Impact of Non Methane Hydrocarbons on tropospheric chemistry and particular the oxidizing power of the global troposphere: 3-Dimensional Modelling results, J. Atmos. Chem., 36, 157-230, 2000.

Table 2. Thermal reactions in TM4-ECPL as related references.

#	reaction			rate coefficient	refs
k1	$O_3 + OH$	$\rightarrow$	$HO_2 + O_2$	$1.7 \times 10^{-12}\exp(-940/T)$	1
k2	$HO_2 + O_3$	$\rightarrow$	$OH + O_2$	$2.03 \times 10^{-16} (T/300)^{4.57} \exp(693/T)$	1
k3	$HO_2 + HO$	$\rightarrow$	$H_2O + O_2$	$4.8 \times 10^{-11}\exp(250/T)$	1
k4	$HO_2 + HO_2$	$\rightarrow$	$H_2O_2 + O_2$	$1.9 \times 10^{-33} [N2] \exp(980/T)$	1
k5	$H_2O_2 + OH$	$\rightarrow$	$H_2O + HO_2S$	$2.9 \times 10^{-12}\exp(-160/T)$	1
k6	$HO_2 + NO$	$\rightarrow$	$NO_2 + HO$	$3.6 \times 10^{-12}\exp(270/T)$	1
k7	$NO + O_3$	$\rightarrow$	$NO_2 + O_2$	$1.4 \times 10^{-12}\exp(-1310/T)$	1
k8	$NO + NO_3$	$\rightarrow$	$2NO_2$	$1.8 \times 10^{-11}\exp(110/T)$	1
k9	$NO_2 + O_3$	$\rightarrow$	$NO_3 + O2$	$1.4 \times 10^{-13}\exp(-2470/T)$	1
k10	$NO_2 + OH + M$	$\rightarrow$	$HONO_2 + M$	$3.3 \times 10^{-30}(T/300)^{-3.0}[N_2]$ 4.1×10^{-11} $Fc = 0.4$	1
k11	$NO_2 + NO_3 + M$	$\rightarrow$	$N_2O_5 + M$	$3.6 \times 10^{-30}(T/300)^{-4.1}[N_2]$ $1.9 \times 10^{-12}(T/300)^{0.2}$ $Fc = 0.35$	1
k12	$NO_2 + HO_2 + M$	$\rightarrow$	$HO_2NO_2 + M$	$1.8 \times 10^{-31}(T/300)^{-3.2}[N_2]$ 4.7×10^{-12} $Fc = 0.6$	1
k13	$HO_2 + NO_3$	$\rightarrow$	$OH + NO_2 + O_2$	4.0×10^{-12}	1
k14	$HONO_2 + OH$	$\rightarrow$	$H_2O + NO_3$	1.5×10^{-13}	1
k15	$HO_2NO_2 + HO$	$\rightarrow$	$H_2O + O_2 + NO_2$	$3.2 \times 10^{-13}\exp(690/T)$	1
k16	$HO_2NO_2 + M$	$\rightarrow$	$HO_2 + NO_2 + M$	$4.1 \times 10^{-5}\exp(-10650/T)[N2]$ $4.8 \times 10^{15}\exp(-11170/T)$ $Fc = 0.6$	1
k17	$N_2O_5 + M$	$\rightarrow$	$NO_2 + NO_3 + M$	$1.3 \times 10^{-3}(T/300)^{-3.5}\exp(-11000/T)[N2]$ $9.7 \times 10^{14}(T/300)^{0.1}\exp(-11080/T)$ $Fc = 0.35$	1
k18	$CH_4 + OH$	$\rightarrow$	$H_2O + CH_3O_2$	$1.85 \times 10^{-12} \exp(-1690/T)$	1
k19	$CH_3O_2 + NO$	$\rightarrow$	$HCHO + HO_2 + NO_2$	$2.3 \times 10^{-12}\exp(360/T)$	1
k10	$CH_3O_2 + NO_3$	$\rightarrow$	$HCHO + HO_2 + NO_2$	1.3×10^{-12}	1
k21	$CH_3O_2 + HO_2$	$\rightarrow$	$CH_3OOH + O_2$	$3.8 \times 10^{-13}\exp(780/T)$	1
k22	$CH_3O_2 + CH_3O_2$	$\rightarrow$	k22a($2HCHO + 2HO_2 + O_2$) $+(1-k22a)(CH_3OH + HCHO + O_2)$	$k22 = 7.4 \times 10^{-13}\exp(-520/T)$ $k22a = 5.4\exp(0.870/T)$	1
k23	$CH_3OOH + OH$	$\rightarrow$	$CH_3O_2 + H_2O$	1.9×10^{-12}	1
k24	$CH_3OOH + OH$	$\rightarrow$	$H_2O + HCHO + OH$	3.6×10^{-12}	1
k25	$CH_3ONO_2 + OH$	$\rightarrow$	$HCHO + NO_2 + H_2O$	$4.0 \times 10^{-13}\exp(-845/T)$	1
k26	$HCHO + OH$	$\rightarrow$	$H_2O + CO + HO_2$	$5.4 \times 10^{-12}\exp(135/T)$	1
k27	$CH_3OH + OH$	$\rightarrow$	$H_2O + HCHO + HO_2$	$2.85 \times 10^{-12}\exp(-345/T)$	1
k28	$CO + OH$	$\rightarrow$	$HO_2 + CO_2$	$1.44 \times 10^{-13}(1 +[N2] / 4 \times 10^{19})$	1
k29	$C_2H_6 + OH + O_2$	$\rightarrow$	$H_2O + C_2H_5O_2$	$6.9 \times 10^{-12}\exp(-1000/T)$	1
k30	$C_2H_5O_2 + NO + O_2$	$\rightarrow$	$(1 - RTC2) \times [CH_3CHO + HO_2 + NO_2]$ $+ RTC2 \times C_2H_5ONO_2$	$k30 = 2.6 \times 10^{-12} \exp(380/T)$ $R1= 1.94 \times 10^{-22} [AIR]\exp(0.972)$ $R2 = 0.826(T/300)^{-8.1}$ $A = 1/(1+\log(R1/R2)^2)$ $RTC2 = 0.4R1/(1+R1/R2)0.411^A$	2
k31	$C_2H_5O_2 + HO_2$	$\rightarrow$	$C_2H_5OOH + O_2$	$3.8 \times 10^{-13}\exp(900/T)$	1

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k32	$C_2H_5O_2 + CH_3O_2$	→	$(1 - k32a)(CH_3CHO + HCHO + 2HO_2 - O2) +$ $k32a(CH_3CHO + CH_3OH + O_2)$	R1=0.45 $k32a = 0.5((1-k22a)+(1-R1))$	2
k33	$C_2H_5OOH + OH$	→	$C_2H_5O_2 + H_2O$	$k33 = 2.6 \times 10^{-12} \exp(190/T)$	2
k34	$C_2H_5OOH + OH$	→	$CH_3CHO + OH + H_2O$	$k34 = 4.5 \times 10^{-18} T^2 \exp(1069/T)$	2
k35	$C_2H_5ONO_2 + OH$	→	$CH_3CHO + NO_2 + H_2O$	$k35 = 6.7 \times 10^{-13} \exp(-395/T)$	1
k36	$CH_3CHO + HO + O_2$	→	$CH_3COO_2 + HO_2$	$4.4 \times 10^{-12} \exp(365/T)$	1
k37	$CH_3COO_2 + HO_2$	→	$CH_3COOOH + O_2$	$5.2 \times 10^{-13} \exp(980/T)$	1
k38	$CH3COO_2 + HO_2$	→	$CH_3COOH + O_3$	$1.04 \times 10^{-13} \exp(983/T)$	2
k39	$CH3COO_2 + NO + O_2$	→	$CH_3O_2 + CO_2 + NO_2$	$7.5 \times 10^{-12} \exp(290/T)$	1
k40	$CH_3COO_2 + NO_2 + M$	→	$CH_3CO_3NO_2 + M$	$2.7 \times 10^{-28}(T/300)^{-7.1}[N_2]$ $1.2 \times 10^{-11}(T/300)^{-0.9}$ $Fc = 0.3$	1
k41	$CH_3COO_2 + CH_3O_2$	→	$HCHO + HO_2 + CH_3O_2 + CO_2$	9.9×10^{-12}	1
k42	$CH_3COO_2 + CH_3O_2$	→	$CH_3COOH + HCHO + O_2$	1.1×10^{-12}	1
k43	$CH_3COO_2 + CH_3COO_2 + O_2$	→	$2(CH_3O_2 + CO_2)$	$2.9 \times 10^{-12} \exp(500/T)$	1
k44	$CH_3COO_2NO_2 + OH$	→	$HCHO + CO_2 + NO_2 + H_2O$	3×10^{-14}	1
k45	$CH_3COO_2NO_2$	→	$CH_3COO_2 + NO_2$	$4.9 \times 10^{-3} \exp(-12100/T)[N2]$ $5.4 \times 10^{16} \exp(-13830/T)$ $Fc = 0.3$	1
k46	$CH_3COO_2NO_2$	→	$CH_3ONO_2 + CO_2$	$2.1 \times 10^{12} \exp(-12525/T)$	2
k47	$CH_3COO_2H + OH$	→	$CH_3COO_2 + H_2O$	like k36	2
k48	$CH_3COOH + OH + O_2$	→	$CH_3O_2 + CO_2 + H_2O$	$4.2 \times 10^{-14} \exp(855/T)$	1
k49	$C_3H_8 + OH + O_2$	→	$(0.3)C_3H_7O_2prim + (0.7) C_3H_7O_2sec + H_2O$	$7.6 \times 10^{-12} \exp(-585/T)$	1
k50	$C_3H_7O_2prim + NO + O_2$	→	$(1 - RTC3P) \times [C_2H_5CHO + HO_2 + NO_2]$ $+ RTC3P \times C_3H_7ONO_2prim$	$2.9 \times 10^{-12} \exp(350/T)$	1
k51	$C_3H_7O_2sec + NO + O_2$	→	$(1 - RTC3S) \times [CH_3COCH_3 + HO_2 + NO_2]$ $+ RTC3S \times C_3H_7ONO_2sec$	$2.7 \times 10^{-12} \exp(360/T)$	1
k52	$C_3H_7O_2prim + HO_2$	→	$C_3H_7OOHprim + O_2$	$k52 = 3.4 \times 10^{-15} \cdot \exp(100/T)$	1
k53	$C_3H_7O_2prim + CH_3O_2$	→	$(1 - k32a)(C_2H_5CHO + HCHO + 2HO_2 + O_2)$ $+ k32a(C_2H_5CHOprim + CH_3OH + O_2)$	$R1 = 2.5 \times 10^{-13}$ $k56 = 2(R1 \cdot k25)^{0.5}$	2
k54	$C_3H_7OOHprim + OH$	→	$C_3H_7O_2prim + H_2O$	like k33	
k55	$C_3H_7OOHprim + OH$	→	$C_2H_5CHO prim + OH + H_2O$	like k34	
k56	$C_3H_7ONO_2prim + OH$	→	$C_2H_5CHO prim + NO_2 + H_2O$	5.8×10^{-13}	1
k57	$C_2H_5CHO + OH$	→	$1/2 (3CH_3COO_2 + H_2O + HO_2)$	$k57 = 5.1 \times 10^{-12} \exp(405/T)$	1
k58	$C_2H_5CHO + NO_3 + O_2$	→	$HNO_3 + CH_3CH_2O_2 + CO$	6.5×10^{-15}	1
k59	$C_3H_7O_2sec + HO_2$	→	$C_3H_7OOHsec + O_2$	$6.2 \times 10^{-13} \exp(-230/T)$	1
k60	$C_3H_7O_2sec + CH_3O_2$	→	$(1 - k60a)(CH_3COCH_3 + HCHO + 2HO_2$ $+ O_2) + k60a(CH_3COCH_3 + CH_3OH + O_2)$	$R1 = 5 \times 10^{-15}$ $k60a = 0.5((1-k22a) + (1-0.45))$ $k60 = 2((R1k_{25})^{0.5}$	2
k61	$C_3H_7OOHsec + OH$	→	$C_3H_7O_2sec + H_2O$	like k33	2
k62	$C_3H_7OOHsec + OH$	→	$CH_3COCH_3 + OH + H_2O$	$2.12 \times 10^{-18} \cdot T^2 \exp(688/T)$	2
k63	$C_3H_7ONO_2sec + OH$	→	$CH_3COCH_3 + NO_2 + H2O$	$6.2 \times 10^{-13} \exp(-230/T)$	1
k64	$CH_3COCH_3 + OH + O_2$	→	$CH_3COCH_2O_2 + H2O$	$\{8.8 \times 10^{-12} \exp(-1320/T)$ $+ 1.7 \times 10^{-14} \exp(420/T)\}$	1
k65	$CH_3COCH_2O_2 + NO + O_2$	→	$CH_3COCHO + NO_2 + HO_2$	like k50	2
k66	$CH_3COCH_2O_2 + HO_2$	→	$CH_3COCH_2OOH + O_2$	like k52	2
k67	$CH_3COCHO + OH + O_2$	→	$CH_3COO_2 + CO + H_2O$	1.5×10^{-11}	1
k68	$CH_3COCH_2OOH + OH$	→	$CH_3COCH_2O_2 + H_2O$	like k33	2

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k69	$C_2H_4 + OH + O_2 + M$	$\rightarrow$	$CH_2OHCH_2O_2 + M$	$k_0 = 8.6 \times 10^{-29}(T/300)^{-3.1}[N_2]$ $k_\infty = 9 \times 10^{-12}(T/300)^{-0.85}$ $Fc = 0.48$	1
k70	$C_2H_4 + O_3 + 2O_2$	$\rightarrow$	$(0.0044)CHOCHO + (1.37)HCHO + (0.43)CO + (0.26)HO_2 + (0.12)OH + (0.002)H_2O_2 + (0.13)H_2 + (0.31)H_2O + (0.2)CO_2$	$9.1 \times 10^{-15}\exp(-2580/T)$	1
k71	$HOCH_2CH_2O_2 + NO + O_2$	$\rightarrow$	$(1-RTC2) \times [NO_2 + e(2HCHO + HO_2) + f(CH_2OHCHO + HO_2)] + RTC2 \times HOCH_2CH_2ONO_2$	$R1 = 2.7 \times 10^{14}\exp(-6350/T)$ $R2 = 6.3 \times 10^{-14}\exp(-550/T)$ $e = R1/(R1 + R2 [O_2])$, $f = 1 - e$ $k71 = 9 \times 10^{-12}$	1
k72	$HOCH_2CH_2O_2 + HO_2$	$\rightarrow$	$HOCH_2CH_2OOH + O_2$	1.2×10^{-11}	1
k73	$HOCH_2CH_2O_2 + CH_3O_2$	$\rightarrow$	$(1 - k32a)(HOCH_2CHO + HCHO + 2HO_2 + O_2) + k32a(HOCH_2CHO + CH_3OH + O_2)$	like k32	2
k74	$HOCH_2CH_2OOH + OH$	$\rightarrow$	$HOCH_2CH_2O_2 + H_2O$	like k33	2
k75	$HOCH_2CH_2OOH + OH$	$\rightarrow$	$HOCH_2CHO + OH + H_2O$	like k34	2
k76	$HOCH_2CH_2ONO_2 + OH$	$\rightarrow$	$HOCH_2CHO + NO_2 + H_2O$	like k35	2
k77	$HOCH_2CHO + OH$	$\rightarrow$	$CO_2 + HCHO$	8.8×10^{-12}	1
k79	$HOCH_2CHO + OH + O_2$	$\rightarrow$	$CHOCHO + HO_2 + H_2O$	2.2×10^{-12}	1
k80	$CHOCHO + OH + O_2$	$\rightarrow$	$2CO + HO_2 + H_2O$	$2.8 \times 10^{-12}\exp(340/T)$	3
k81	$CHOCHO + NO_3 + O_2$		$HNO_3 + HO_2 + 2CO$	$1. \times 10^{-15}$	4
k82	$C_3H_6 + OH + O_2$	$\rightarrow$	$HOC_3H_6O_2$	$8 \times 10^{-27}(T/300)^{-3.5}[N_2]$ $3.0 \times 10^{-11}(T/300)^{-1.0}$ $Fc = 0.5$	1
k83	$C_3H_6 + O_3 + 2O_2$	$\rightarrow$	$0.5(HCHO + 0.15CH_3COOH + 0.71CH_3O_2 + 0.68CO + 0.54OH + 0.17HO_2) +$	$5.5 \times 10^{-15}\exp(-1880/T)$	1
k84	$HOC_3H_6O_2 + NO$	$\rightarrow$	$(1 - 0.35RTC3P - 0.65RTC3S)$ $\times [CH_3CHO + HCHO + HO_2 + NO_2 + O_2] + 0.35RTC3P \times C_3H_7ONO_2prim + 0.65RTC3S \times C_3H_7ONO_2sec$	like k30	2
k85	$HOC_3H_6O_2 + HO_2$	$\rightarrow$	$HOC_3H_6OOH + O_2$	like k52	2
k86	$HOC_3H_6O_2 + CH_3O_2$	$\rightarrow$	$(1 - k60a)(CH_3CHO + 2HCHO + 2HO_2 + O_2) + k60a(CH_3COCH_2OH + CH_3OH + O_2)$	like k53	2
k87	$HOC_3H_6OOH + OH$	$\rightarrow$	$HOC_3H_6O_2 + H_2O$	2×10^{-11}	2
k88	$C_4H_{10} + OH + O_2$	$\rightarrow$	$C_4H_9O_2 + H_2O$	$9.1 \times 10^{-12}\exp(-405/T)$	
k89	$C_4H_9O_2 + NO$	$\rightarrow$	$(1 - RTC4S) \times [NO_2 + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO + O_2] + RTC4S \times C_4H_9ONO_2)$	like k30 $R1 = 1.94 \times 10^{-22} [AIR] \exp(0.9740$ $R2 = 0.826(T/300)^{-8.1}$ $A = 1/(1 + \log(R1/R2)^2)$ $RTC4P = 0.4R1/(1+R1/R2)0.411^A$ $RTC4S = 0.45*k33*R1/(1+R1/R2)0.411^A$	1
k90	$C_4H_9O_2 + HO_2$	$\rightarrow$	$C_4H_9OOH + O_2$	like k52	2
k91	$C_4H_9O_2 + CH_3O_2$	$\rightarrow$	$(1 - k60a)[HCHO + HO_2 + 0.67(CH_3CH_2C(O)CH_3 + HO_2 + O_2) + 0.33(CH_3CHO + CH_3CH_2O_2 + O2)] + k60a(CH_3CH_2COCH_3 + CH_3OH + O_2)$	like k60	2
k92	$C_4H_9ONO_2sec + OH$	$\rightarrow$	$CH_3CH_2COCH_3 + NO_2 + H_2O$	1.71×10^{-12}	2
k93	$C_4H_9OOH + OH$	$\rightarrow$	$C_4H_9O_2 + H_2O$	like k33	2
k94	$C_4H_9OOH + OH$	$\rightarrow$	$CH_3CH_2COCH_3 + OH + H_2O$	$2.12 \times 10^{-18}*T^2\exp(1131/T)$	2
k95	$CH_3CH_2COCH_3 + OH + 0.5O_2$	$\rightarrow$	$CH_3CHO_2COCH_3$	$1.3 \times 10^{-12}\exp(-25/T)$	1

k96	$CH_3CHO_2COCH_3 + NO + O_2$	$\rightarrow$	$(1 - RTC4S) \times [CH_3CHO + CH_3COO_2 + NO_2] + RTC4S \times CH_3CHONO_2COCH_3$	like k30	2
k97	$CH_3CHO_2COCH_3 + HO_2$	$\rightarrow$	$CH_3CHOOHCOCH_3 + O_2$	like k52	2
k98	$CH_3CHONO_2COCH_3 + OH$	$\rightarrow$	$CH_3COCOCH_3 + NO_2 + H_2O$	9.20×10^{-13}	2
k99	$CH_3CHOOHCOCH_3 + OH$	$\rightarrow$	$CH_3CHO_2COCH_3 + H_2O$	like k33	2
k100	$CH_3CHOOHCOCH_3 + OH$	$\rightarrow$	$CH_3COCOCH_3 + OH + H_2O$	$2.12 \times 10^{-18} *T^2 exp(983/T)$	2
k101	$ISOPRENE + OH \rightarrow$	$\rightarrow$	$0.99\ ISOPO_2 + 0.03\ CHOCHO$	$2.7 \times 10^{-11} exp(390/T)$	1
k102	$ISOPO_2 + NO + O_2$	$\rightarrow$	$(1 - RTC5S) \times [HCHO + HO_2 + NO_2 + 0.64\ MVK + 0.36\ MACR] + RTC5S \times NITRATES$	k102 = 0.45 * k30 R1=1.94×10^{-22} [AIR] exp(0.95*5) R2=$0.826(T/300)^{-8.1}$ A=$1/(1 + log(R1/R2)^2)$ RTC5P=$0.4R1/(1+R1/R2)0.411^A$ RTC5S=$0.45*k30*R1/(1+R1/R2)0.411^A$	2
k103	$ISOPO_2 + HO_2$	$\rightarrow$	$ISOOH + O_2$	like k52	2
k104	$ISOPO_2 + CH_3O_2 + O2$	$\rightarrow$	$(1 - k60a)(2(HCHO + HO_2) + 0.64\ MVK + 0.36\ MACR) + k60a(0.64\ MVK + 0.36\ MACR + 2O_2 + HCHO + CH_3OH)$	like k60	2
k105	$ISOOH + OH$	$\rightarrow$	$RO_2 + H_2O$	like k85	2
k106	$ISOOH + OH + 2O_2$	$\rightarrow$	$ISOPO_2 + H_2O$	2×10^{-11}	2
k107	$RO_2 + NO$	$\rightarrow$	$CH_2OHCHO + CH_3COCHO + HO_2 + NO_2$	like k30	2
k108	$RO_2 + HO_2$	$\rightarrow$	$CH_3COCHO + CH_2OHCHO + H_2O$	like k52	2
k109	$NITRATES + OH + O_2$	$\rightarrow$	$CH_3COCHO + CH_2OHCHO + H_2O + NO_2$	R1= $1.9 \times 10^{-11} exp(450/T)$ R2= $9.5 \times 10^{-12} exp(504/T)$ k=0.49k80+ 0.28R2 + 0.23R1	2
k110	$MVK + O_3$	$\rightarrow$	$0.38\ CH_3COCHO + 0.2088\ CH_3COO_2 + 0.26\ CH_3COCOOH + 0.26\ CO + 0.0432\ CH_3COOH + 0.108\ CH_3CHO + 0.62\ HCHO + 048\ CO_2 + 0.54\ HO_2 + 0.1008\ OH + 0.048\ H_2 + 0.116\ H_2O$	$8.5 \times 10^{-16} exp(-1520/T)$	2
k111	$MVK + OH$	$\rightarrow$	$MVKO_2$	$2.6 \times 10^{-12} exp(610/T)$	1
k112	$MVKO_2 + NO + O2$	$\rightarrow$	$CH_3COO2 + CH_2OHCHO + NO_2$	like k30	1
k113	$MVKO_2 + HO_2$	$\rightarrow$	$MVKOOH + O2$	like k52	2
k114	$MVKOOH + OH$	$\rightarrow$	$MVKO_2 + H_2O$	like k106	2
k115	$MVKOOH + OH + 3O2$	$\rightarrow$	$CH_3COO_2 + 2CO + OH + 2HO_2 + H_2O$	R1 = $2.12 \times 10^{-18} T^2 exp(1045/T)$ R2 = $4.5 \times 10^{-18} T^2 exp(1032/T)$ k115 = R1 + R2	2
k116	$MACR + O_3 + 1.476O_2$	$\rightarrow$	$0.2\ CH3COCHO + 1.6\ HCHO + 1.658\ CO + 0.142\ CO_2 + 1.116\ HO_2 + 0.72\ OH + 0.058\ H_2O + 0.024\ H_2$	$1.4 \times 10^{-15} exp(-2100/T)$	1
k117	$MACR + OH$	$\rightarrow$	$MACRO_2$	$8.0 \times 10^{-12} exp(380/T)$	1
k118	$MACRO_2 + NO + O_2$	$\rightarrow$	$CH_3COCH_2OH + CO + NO_2 + HO_2$	like k30	2
k119	$MACRO_2 + HO_2$	$\rightarrow$	$MACROOH + O_2$	like k52	2
k120	$MACROOH + OH$	$\rightarrow$	$MACRO_2$	like k33	2
k121	$MACROOH + OH + O_2$	$\rightarrow$	$CH_3COCHO + CO + 2\ HO_2 + OH + H_2O$	$4.5 \times 10^{-18} *T^2 exp(1032/T)$	2
k122	$MACROOH + OH$	$\rightarrow$	$CH_3COCH_2OH + CO + OH + H_2O$	like k57	2
k123	$CH_3COCH_2OH + OH$	$\rightarrow$	$CH_3COCHO + HO_2 + H_2O$	3.0×10^{-12}	1
k124	$ISOPRENE + O_3$	$\rightarrow$	$0.425\ MACR + 0.18\ MVK + 0.12\ CH_2CCH_3COOH + 0.12\ CH_3COCOOH + 0.84\ HCHO + 0.3\ CO + 0.24\ CO_2 + 0.24\ HCOOH +$	$1.03 \times 10^{-14} exp(-1995/T)$	1

$0.04C_3H_6 + 0.34OH + 0.025H_2 + 0.19H_2O$

k125	$HCOOH + OH + O_2$	$\rightarrow$	$CO_2 + HO_2 + H_2O$	4.5×10^{-13}	2
k126	$C_4H_{10} + NO_3 + O_2$	$\rightarrow$	$C_4H_9O_2 + HNO_3$	$2.8 \times 10^{-12} \exp(-3280/T)$	1
k127	$HCHO + NO_3 + O_2$	$\rightarrow$	$HNO_3 + HO_2 + CO$	5.6×10^{-16}	1
k128	$CH_3CHO + NO_3 + O_2$	$\rightarrow$	$HNO_3 + CH_3O_2 + CO$	$1.4 \times 10^{-12} \exp(-1860/T)$	1
k129	$CH_3OH + NO_3 + O_2$	$\rightarrow$	$HNO_3 + HCHO + HO_2$	$9.4 \times 10^{-13} \exp(-2650/T)$	1
k130	$C_2H_4 + NO_3$	$\rightarrow$	CH_2ONOCH_2OO	$3.3 \times 10^{-12} \exp(-2880/T)$	1
k131	$CH_2ONO_2CH_2OO + NO$	$\rightarrow$	$2NO_2 + 2HCHO$	like k30	1
k132	$CH_2ONO_2CH_2OO + NO$	$\rightarrow$	$2NO_2 + CH_3CHO + HCHO$	like k30	
k133	$CH_2ONO_2CH_2OO + HO_2$	$\rightarrow$	$CH_2ONO_2CH_2O_2H + O_2$	$0.4 \times 3.5 \times 10^{-15} \exp(1000/T)$	
k134	$CH_2ONO_2CH_2OO + HO_2$	$\rightarrow$	$CH_2ONO_2CH_2O_2H + O_2$	$0.6 \times 3.5 \times 10^{-15} \exp(1000/T)$	
k135	$CH_2ONO_2CH_2O_2H + OH$	$\rightarrow$	$NO_2 + HCHO + CO + 2HO_2 + OH$	like k34	
k136	$CH_2ONO_2CH_2O_2H + OH$	$\rightarrow$	$CH_2ONO_2CH_2OO + H_2O$	like k33	
K137	$C_3H_6 + NO_3$	$\rightarrow$	$CH_3CHONO_2CH_2OO$	$4.6 \times 10^{-13} \exp(-1155/T)$	1
k138	$ISOPRENE + NO_3$	$\rightarrow$	$NITRATES$	$3.15 \times 10^{-12} \exp(-450/T)$	1
k139	$MACR + NO_3$	$\rightarrow$	$HNO_3 + MACRO_2$	3.4×10^{-15}	1
k140	$CH_3O_2 + HO_2$	$\rightarrow$	$0.5CH_2O + 0.5CH_3O_2H$	$3.8 \times 10^{-13} \exp(780/T)$	1
k141	$CH_3COCOOH + OH$	$\rightarrow$	$CH_3C(O)OO + CO_2 + H_2O$	$4.9 \times 10^{-14} \exp(276/T)$	7
k142	$DMS + OH$	$\rightarrow$	$0.995CH_3O_2 + HCHO + 0.995SO_2 + 0.005MSAg$	$1.13 \times 10^{-11} \exp(-253/T)$	1
k144	$DMS + OH$	$\rightarrow$	$DMSO$	$1.0 \times 10^{-39}[O_2] \exp(5820/T) / \{1 + 5.0 \times 10^{-30}[O_2] \exp(6280/T)\}$	1
k144	$DMS + NO_3$	$\rightarrow$	$CH_3O_2 + HNO_3 + HCHO + SO_2$	$1.9 \times 10^{-13} \exp(520/T)$	1
k145	$DMSO + OH$	$\rightarrow$	$MSIA$	8.7×10^{-11}	11
k146	$MSIA + OH$	$\rightarrow$	$CH_3O_2 + SO_2$	$1. \times 10^{-10}$	11
k147	$DMSO$	$\rightarrow$	$MSAp$	$1. \times 10^{-10}$	11
k148	$MSIA$	$\rightarrow$	$MSAp$	$1. \times 10^{-10}$	11
k149	$MSAg$	$\rightarrow$	$MSAp$	4.5×10^{-5}	11
k150	$SO_2 + OH$	$\rightarrow$	$HO_2 + SO_4 + 2ACID$	$4.5 \times 10^{-31}(T/300)^{-3.9}[N_2]$ $1.3 \times 10^{-12} (T/300)^{-0.7}$ $Fc = 0.525$	1
k151	$ACID + NH_3$	$\rightarrow$	NH_4		9
k152	$NH_3 + OH$	$\rightarrow$	NH_2	$3.5 \times 10^{-12} \exp(-925/T)$	1
k153	$NH_2 + NO$	$\rightarrow$	$Products$	$1.6 \times 10^{-11}(T/298)^{-1.4}$	1
k154	$NH_2 + NO_2$	$\rightarrow$	$Products$	$2.0 \times 10^{-11}(T/298)^{-1.3}$	1
k155	$NH_2 + HO_2$	$\rightarrow$	$Products$	3.4×10^{-11}	10
k156	$NH_2 + O_2$	$\rightarrow$	$Products$	6×10^{-21}	1
k157	$NH_2 + O_3$	$\rightarrow$	$Products$	$4.3 \times 10^{-12} \exp(-930/T)$	10
k158	$a\text{-}PINENE + O_3$	$\rightarrow$	$TERO_2$	$6.3 \times 10^{-16} \exp(-580/T)$	1
k159	$a\text{-}PINENE + OH$	$\rightarrow$	$TERO_2$	$1.2 \times 10^{-11} \exp(440/T)$	1
k160	$a\text{-}PINENE + NO_3$	$\rightarrow$	$TERO_2 + HNO_3$	$1.2 \times 10^{-12} \exp(490/T)$	1
k161	$b\text{-}PINENE + O_3$	$\rightarrow$	$TERO2 + b1*HCHO + b2*HCHO$	1.5×10^{-17}	5
k162	$b\text{-}PINENE + OH$	$\rightarrow$	$TERO_2$	$2.38 \times 10^{-11} \exp(357/T)$	5
k163	$b\text{-}PINENE + NO_3$	$\rightarrow$	$TERO_2 + HNO_3$	$1.6 \times 10^{-10} \exp(-1248/T)$	5
k164	$BENZENE + OH$	$\rightarrow$	$0.64*(6/8)AROO_2 + 0.36CHOCHO$	$2.47 \times 10^{-12} \exp(-207/T)$	6
k165	$TOLUENE + O_3$	$\rightarrow$	$(7/8)*AROO_2 + c2*MGLY$	$2.34 \times 10^{-12} \exp(-6694/T)$	5
k166	$TOLUENE + OH$	$\rightarrow$	$0.65*(7/8)AROO_2 + 0.36CHOCHO + c2*MGLY$	5.69×10^{-12}	5
k167	$TOLUENE + NO_3$	$\rightarrow$	$(7/8)*AROO_2 + HNO_3$	6.8×10^{-17}	5
k168	$XYLENE + O_3$	$\rightarrow$	$AROO2 + d2 (MGLY + 1/4C_4H_9O_2)$	$(2.4 \times 10^{-13} \exp(-5586/T) + 5.37 \times 10^{-13} \exp(-6039/T) + 1.91 \times 10^{-13}$	5

				exp(−5586/T))/3	
k169	XYLENE + OH	→	$0.68AROO2 + 0.32CHOCHO + d2$ (MGLY + $1/4C_4H_9O_2$)	1.72×10^{-11}	5
k170	XYLENE + NO$_3$	→	$AROO2 + HNO_3$	3.54×10^{-16}	5
k171	TERO$_2$ + NO +O$_2$	→	$[(X-a1-a2) +(X-b1-b2)]*[(1 - RTC5S) *(HCHO + HO_2+ NO_2 + 0.64\ MVK + 0.36MACR] + RTC5S * NITRATES]$	like k30	
k172	TERO$_2$ + HO$_2$	→	$[(X-a1-a2) +(X-b1-b2)]*[ISOOH + O_2]$	like k31	
k173	TERO$_2$ + CH$_3$O$_2$ + O$_2$	→	$[(X-a1-a2) +(X-b1-b2)]*[(1 − k60a)$ $(2(HCHO + HO_2) +$	like k60	
k174	TERO$_2$ +TERO$_2$	→	Products	like k53	
k175	AROO$_2$ + NO	→	$[(X-c1-c2) +(X-d1-d2)]*[(1-RTC4S) *[NO_2 + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO + O_2] + RTC4S *C_4H_9ONO_2)$	like 30	
k176	AROO$_2$ + HO$_2$	→	$[(X-c1-c2) +(X-d1-d2)]*[C_4H_9OOH+O2]$	like 52	
k177	AROO$_2$ + CH$_3$O$_2$	→	$[(X-c1-c2) +(X-d1-d2)]*[(1 - k60a)$ $[HCHO+HO_2+0.67(CH_3CH_2C(O)CH_3+HO_2 +O_2)$	like 60	
k178	AROO$_2$ + AROO$_2$	→	Products	like 53	
k179	C$_2$H$_2$ + OH	→	$0.635(CHOCHO + OH) + 0.365(HCOOH + CO + HO_2)$	$5 \times 10^{-30}(T/300)^{-1.5}[N_2]$	1
k180	CH$_3$COO$_2$ + CH$_3$COCH$_2$O$_2$	→	$CH_3COOH + CH_3COCHO + O_2$	2.5×10^{-12}	1
k181	CH$_3$COO$_2$ + CH$_3$COCH$_2$O$_2$	→	$CH_3O_2 + CH_3COCH_2OH + CO_2$	2.5×10^{-12}	1
k182	C$_2$H$_5$O$_2$ + CH$_3$COO$_2$	→	$C_2H_5O(CH_3CHO+HO_2) + CH_3O_2 + CO_2$	$0.5 * 4.4 \times 10^{-13}\exp(1070/T)$	1
k183	C$_2$H$_5$O$_2$ + CH$_3$COO$_2$	→	$CH_3CHO + CH_3COOH + O_2$	$0.5 * 4.4 \times 10^{-13}\exp(1070/T)$	1
k184	ISOPO$_2$ + NO$_3$	→	$HO_2 + NO_2 + HCHO + 0.36MACR + 0.64MVK$	$2.3\ 10^{-12}$	7
k185	RO$_2$ + NO$_3$	→	$HO_2 + HOCH_2CHO + CH_3COCHO + NO_2$	$2.3\ 10^{-12}$	7
k186	TERO$_2$ + NO$_3$	→	$HO_2 + NO_2 + 2(HCHO +0.36MACR + 0.64MVK)$	$2.3\ 10^{-12}$	7

For three bodies reactions:
$$k = \frac{ko}{1+\dfrac{ko}{k\infty}} xFc^{\dfrac{1}{1+\log(\frac{ko}{k\infty})^2}}$$

References:

1 Atkinson, R., Baulch, D., L., Cox, R., A., Crowley, J., N., Hampson, R., F., Hynes, R., G., Jenkin, M., E., Rossi, M., J., Troe, J., and IUPAC Subcommittee: Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II – gas phase reactions of organic species Atmos. Chem. Phys., 6, 3625-4055, 2006.

IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, Web Version February, http://www.iupac-kinetic.ch.cam.ac.uk/ summary/IUPACsumm_web_Feb2006.pdf, 2006.

2 Poisson, N., Kanakidou, M., and Crutzen, P. J.: Impact of Non Methane Hydrocarbons on tropospheric chemistry and particular the oxidizing power of the global troposphere: 3-Dimensional Modelling results, J. Atmos. Chem., 36, 157-230, 2000.

3 Feierabend, K., Zhu, L., Talukdar, R. K., and Burkholder, J. B.: Rate coefficients for the OH + HC(O)C(O)H (Glyoxal) reaction between 210 and 390 K, J. Phys. Chem. A, accepted, 2007.

4 upper limit, I. Barnes personal communication, September 2007

5 see references in Tsigaridis, K. and Kanakidou, M.: Global modeling of secondary organic aerosol in the troposphere: a sensitivity analysis, Atmos. Chem. Phys. 3, 1849-1869, 2003.

6 Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J., and Yarwood, G.: The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons, Oxford University Press, Oxford, 2002.

7 IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, Web Version 2001 http://www.iupac-kinetic.ch.cam.ac.uk/

8 Mellouki, W., and Mu, Y.: On the atmospheric degradation of pyruvic acid in the gas phase, J. of Photochemistry and Photobiology A: Chemistry ,157, 295-300, 2003.

9 Metzger, S., Dentener, F., Pandis, S., and Lelieveld, J.: Gas/aerosol partitioning: 1. A computationally efficient model, J. Geophysical Research, 107, D16, 10.1029/2001JD001102, 2002.

10 Sander, S.P., Ravishankara, A. R., Golden, D. M., Kolb, C. E, Kurylo, M. J., Molina, M. J., Moortgat, G. K., Finlayson-Pitts, B. J., Wine, P. H., Huie, R. E.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies Evaluation Number 15, JPL Publication 06-2 (2006). available on the web at http://jpldataeval.jpl.nasa.gov/

11 based on Barnes, I., Hjorth, J., and Mihalopoulos N.: Dimethyl Sulfide and Dimethyl Sulfoxide and Their Oxidation in the Atmosphere, Chem. Rev., 106, 940-975, 2006.