Supplement of Atmos. Chem. Phys. Discuss., 15, 2055–2084, 2015
http://www.atmos-chem-phys-discuss.net/15/2055/2015/
doi:10.5194/acpd-15-2055-2015-supplement

Atmospheric Chemistry and Physics Discussions

Supplement of

Understanding atmospheric peroxyformic acid chemistry: observation, modeling and implication

H. Liang et al.

Correspondence to: Z. M. Chen (zmchen@pku.edu.cn)

Table S1. $HC(O)O_2$ radical and PFA related chemistry in the form of CB6 mechanism.

Reactions	k_{298}	E/R
$HC(O)O_2$-chemistry		
HC(O)OO+HO2→0.4HC(O)OOH+0.2HC(O)OH+ 0.2O3 +0.4OH+0.4HO2+0.4CO2	1.40E–11	–980
HC(O)OO+HCHO→HC(O)OOH+HC(O)	5.00E–14	0
HC(O)OO+RO2→HC(O)OO	1.30E–11	–800
HC(O)OO+HC(O)OO→2HO2	1.60E–11	–500
HC(O)OO+CH3C(O)OO→HO2+HCHO+XO2H+RO2	1.60E–11	–500
HC(O)OO+CXO3→HO2+ALD2+XO2H+RO2	1.60E–11	–500
HC(O)OO+CH3O2→HCHO+1.8HO2+0.1HC(O)OH	1.10E–11	–500
HC(O)OO+XO2H→1.6HO2+0.2HC(O)OH	1.30E–11	–800
HC(O)OO+XO2→0.8HO2+0.2HC(O)OH	1.30E–11	–800
HC(O)OO+XO2N→1.6HO2+0.2HC(O)OH	1.30E–11	–800
HC(O)OO+ISO2→1.51HO2+0.2HC(O)OH	1.30E–11	–800
HC(O)OO+EPX2→1.48HO2+0.2HC(O)OH	1.30E–11	–800
HC(O)OO+BZO2→2HO2	1.30E–11	–800
HC(O)OO+TO2→2HO2	1.30E–11	–800
HC(O)OO+XLO2→2HO2	1.30E–11	–800
HC(O)OO+CAO2→2HO2	1.30E–11	–800
HC(O)OO+OPO3→HO2+XO2	1.60E–11	–500
HC(O)OO+NO→HO2+CO2+NO2	2.00E–11	–290
PFA-chemistry		
HC(O)OOH+OH→HC(O)OO+H2O	6.90E–13	–850
HC(O)OOH+hν→OH+HO2+CO2	0.28× $j(H_2O_2)$	
HC(O)OOH→HC(O)OH+0.5O2	3.70E–04	0

In Table S1, RO_2 is an operator to estimate the total organic peroxy radical; XO2 refers to the alkylperoxy radical which converts NO to NO_2; XO2H refers to the alkylperoxy radical which converts NO to NO_2 accompanied by HO_2 production; CXO3 refers to the acylperoxy radical with C≥3; XO2N refers to alkylperoxy radical which converts NO to organic nitrate; ISO2 refers to the peroxy radical from OH addition to isoprene; ALD2 refers to the aldehyde with C≥2; EPX2 refers to the peroxy radical from EPOX reaction with OH; BZO2, TO2 and XLO2 refer to the

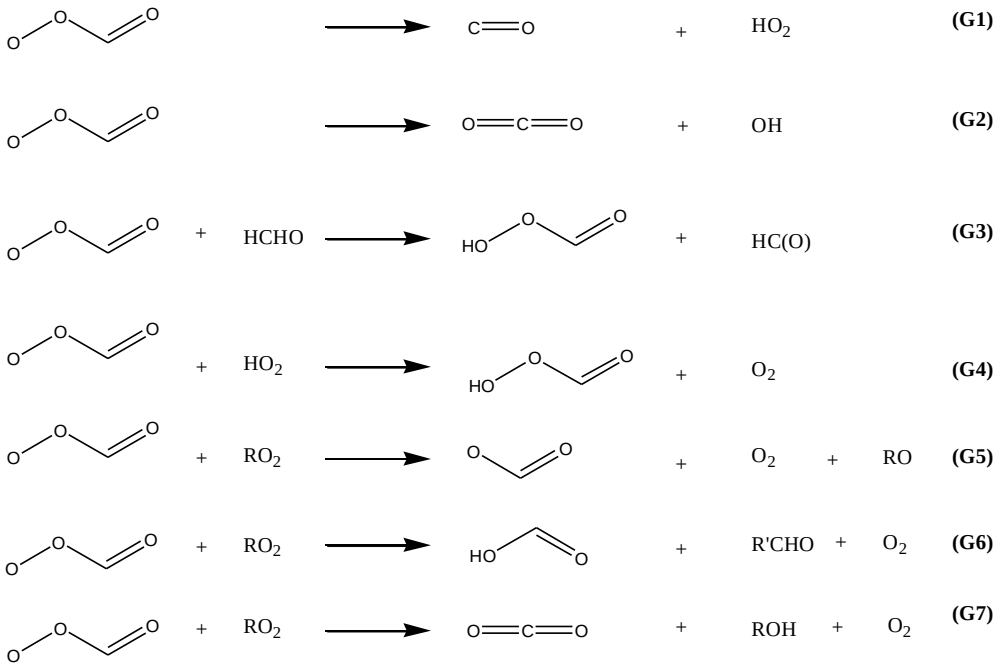
peroxy radical from OH addition to benzene, monoalkyl aromatics and polyalkyl aromatics, respectively; CAO2 refers to the peroxy radical from aromatic degradation products; OPO3 refers to the acylperoxy radical from aromatic ring opening product.

Table S2. The emission rates of lumped volatile organic compounds.

VOC	Emission rate (molecules cm^{-2} s^{-1})
PAR	1.64E+12
OLE	5.32E+10
TOL	1.40E+11
XYL	1.64E+11
FORM	5.93E+10
ALD2	1.44E+10
ETH	1.02E+11
ISOP	6.99E+10
MEOH	7.92E+09
ETHA	8.44E+10
IOLE	6.30E+09
ALDX	1.63E+08
PRPA	7.43E+10
BENZ	3.78E+10
ETHY	8.23E+10
ACET	1.77E+10
KET	7.16E+08

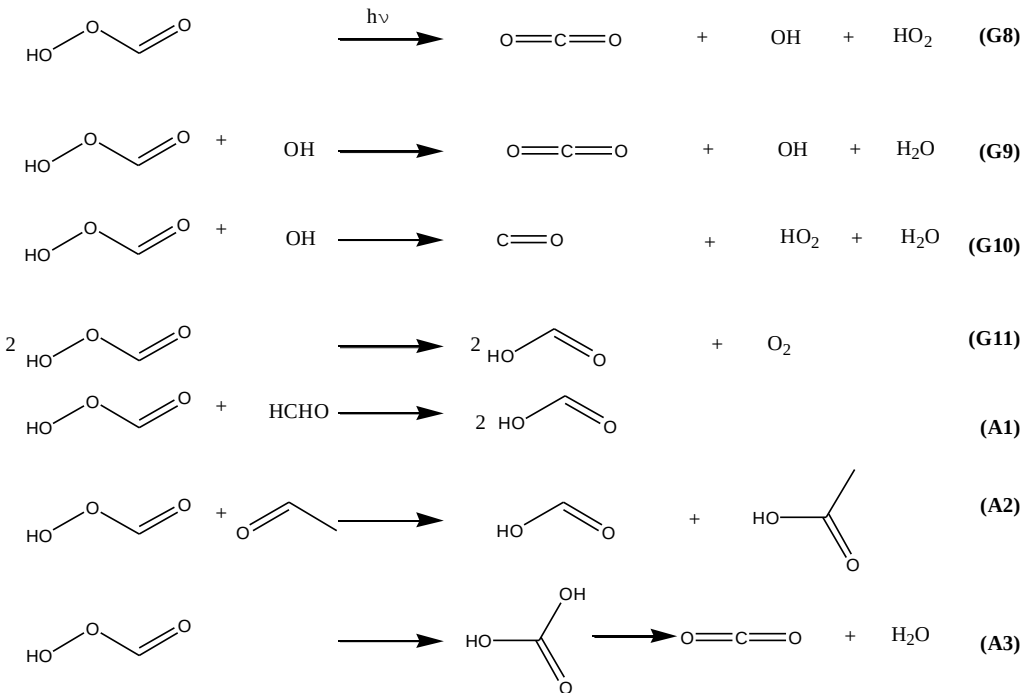
The exact meanings of the CB6 lumped VOC species in Column 1 in Table S2 can be found in Yarwood et al. (2010).

(a)



(G1) (G2) (G3) (G4) (G5) (G6) (G7)

(b)



(G8) (G9) (G10) (G11) (A1) (A2) (A3)

Scheme S1. Possible reaction of (a) $HC(O)O_2$ radical and (b) PFA. G and A in the parenthesis refer to gas and aqueous phase reactions, respectively.

References

Yarwood, G., Jung, J., Whitten, G. Z., Heo, G., Mellberg, J., and Estes, M.: Updates to the Carbon Bond mechanism for version 6 (CB6). In 2010 CMAS Conference, Chapel Hill, NC. October. (Download at http://www.cmascenter.org/conference/2010/abstracts/emery_updates_carbon_2010.pdf, last access: October 22, 2013).