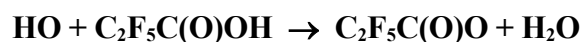


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of FOx105; VII.A5.27

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The citation for the preferred values in this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.

This datasheet last evaluated: June 2014; last change in preferred values: June 2009.



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(1.54 \pm 0.17) \times 10^{-13}$	296	Hurley et al. (2004)	RR (a)
$(1.56 \pm 0.11) \times 10^{-13}$			

Comments

- (a) HO radicals were generated by the photolysis of CH₃ONO in C₂F₅C(O)OH/CH₃ONO/NO/(C₂H₂ or C₂H₄) mixtures in 700 Torr (933 mbar) of air. The loss of the reference compounds (C₂H₂ or C₂H₄) was monitored by FTIR spectroscopy. The loss of C₂F₅C(O)OH was small and difficult to observe directly. The loss of C₂F₅C(O)OH was calculated from the formation of COF₂ observed by FTIR spectroscopy (assumed quantitative). Experiments performed using C₂F₅C(O)OH, C₃F₇C(O)OH, and C₄F₉C(O)OH gave indistinguishable values of the rate coefficient ratio $k(\text{HO} + \text{C}_x\text{F}_{2x+1}\text{C}(\text{O})\text{OH})/k(\text{HO} + \text{reference})$. Analysis of the composite data set gave $k(\text{HO} + \text{C}_x\text{F}_{2x+1}\text{C}(\text{O})\text{OH})/k(\text{HO} + \text{C}_2\text{H}_2) = 0.197 \pm 0.022$ and $k(\text{HO} + \text{C}_x\text{F}_{2x+1}\text{C}(\text{O})\text{OH})/k(\text{HO} + \text{C}_2\text{H}_4) = 0.0198 \pm 0.0014$. Using $k(\text{HO} + \text{C}_2\text{H}_2) = 7.8 \times 10^{-13}$ and $k(\text{HO} + \text{C}_2\text{H}_4) = 7.9 \times 10^{-12}$ (Atkinson et al., 2006) gives the values of $k(\text{HO} + \text{C}_x\text{F}_{2x+1}\text{CHO})$ listed in the table above.

Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.5×10^{-13}	298
<i>Reliability</i>		
$\Delta \log k$	0.12	298

Comments on Preferred Values

The recommendation is based on the study by Hurley et al. (2004). The C₂F₅C(O)O radical decomposes rapidly to give CO₂ and a C₂F₅ radical. As discussed by Ellis et al. (2005), the C₂F₅ radical will be converted mainly into COF₂ with CF₃C(O)OH formed as a minor product. As might be expected from their similar molecular structure, the reactivity of C₂F₅C(O)OH, C₃F₇C(O)OH, and C₄F₉C(O)OH towards HO radicals are indistinguishable.

References

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E., Rossi, M. J., and Troe, J.: *Atmos. Chem. Phys.*, 6, 3625, 2006; IUPAC Subcommittee for Gas Kinetic Data Evaluation, <http://iupac.pole-ether.fr>.
Ellis, D. A., Martin, J. W., De Silva, A. O., Mabury, S. A., Hurley, M. D., Sulbaek Andersen, M. P., and Wallington, T. J.: *Environ. Sci. Tech.*, 38, 3316, 2004.
Hurley, M. D., Wallington, T. J., Ellis, D. A., Martin, J. W., and Mabury, S. A.: *J. Phys. Chem. A*, 108, 615, 2004.