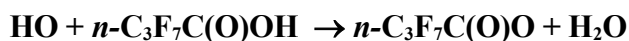


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of FOx106; VII.A5.28

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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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$T/\text{K}$	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  $\text{CH}_3\text{ONO}$  in  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{OH}/\text{CH}_3\text{ONO}/\text{NO}/(\text{C}_2\text{H}_2 \text{ or } \text{C}_2\text{H}_4)$  mixtures in 700 Torr (933 mbar) of air. The loss of the reference compounds  $\text{C}_2\text{H}_2$  or  $\text{C}_2\text{H}_4$  was monitored by FTIR spectroscopy. The loss of  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{OH}$  was small and difficult to observe directly. The loss of  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{OH}$  was calculated from the formation of  $\text{COF}_2$  observed by FTIR spectroscopy. Experiments performed using  $\text{C}_2\text{F}_5\text{C}(\text{O})\text{OH}$ ,  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{OH}$ , and  $\text{C}_4\text{F}_9\text{C}(\text{O})\text{OH}$  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	$T/\text{K}$
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.5 \times 10^{-13}$	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  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{O}$  radical decomposes rapidly to give  $\text{CO}_2$  and a  $\text{C}_3\text{F}_7$  radical. As discussed by Ellis et al. (2005), the  $\text{C}_3\text{F}_7$  radical will be converted mainly into  $\text{COF}_2$  with  $\text{CF}_3\text{C}(\text{O})\text{OH}$  and  $\text{C}_2\text{F}_5\text{C}(\text{O})\text{OH}$  formed as minor products. As might be expected from their similar molecular structure, the reactivity of  $\text{C}_2\text{F}_5\text{C}(\text{O})\text{OH}$ ,  $\text{C}_3\text{F}_7\text{C}(\text{O})\text{OH}$ , and  $\text{C}_4\text{F}_9\text{C}(\text{O})\text{OH}$  towards HO radicals are indistinguishable.

### References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M.

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.