IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx105; VII.A5.27

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$HO + C_2F_5C(O)OH \rightarrow C_2F_5C(O)O + H_2O$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.54 \pm 0.17) \times 10^{-13}$	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 CH_3ONO in $C_2F_5C(O)OH/CH_3ONO/NO/$ (C_2H_2 or C_2H_4) mixtures in 700 Torr (933 mbar) of air. The loss of the reference compounds (C_2H_2 or C_2H_4) was monitored by FTIR spectroscopy. The loss of $C_2F_5C(O)OH$ was small and difficult to observe directly. The loss of $C_2F_5C(O)OH$ was calculated from the formation of COF_2 observed by FTIR spectroscopy (assumed quantitative). Experiments performed using $C_2F_5C(O)OH$, $C_3F_7C(O)OH$, and $C_4F_9C(O)OH$ gave indistinguishable values of the rate coefficient ratio $k(HO+C_xF_{2x+1}C(O)OH)/k(HO+reference)$. Analysis of the composite data set gave $k(HO+C_xF_{2x+1}C(O)OH)/k(HO+C_2H_2) = 0.197 \pm 0.022$ and $k(HO+C_xF_{2x+1}C(O)OH)/k(HO+C_2H_4) = 0.0198 \pm 0.0014$. Using $k(HO+C_2H_2) = 7.8 \times 10^{-13}$ and $k(HO+C_2H_4) = 7.9 \times 10^{-12}$ (Atkinson et al., 2006) gives the values of $k(HO+ C_xF_{2x+1}CHO)$ listed in the table above.

Preferred Values

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

Comments on Preferred Values

The recommendation is based on the study by Hurley et al. (2004). The $C_2F_5C(O)O$ radical decomposes rapidly to give CO_2 and a C_2F_5 radical. As discussed by Ellis et al. (2005), the C_2F_5 radical will be converted mainly into COF_2 with $CF_3C(O)OH$ formed as a minor product. As might be expected from their similar molecular structure, the reactivity of $C_2F_5C(O)OH$, $C_3F_7C(O)OH$, and $C_4F_9C(O)OH$ 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.