IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx98; VII.A5.17

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$HO + C_2F_5CHO \rightarrow C_2F_5CO + H_2O$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
$2.56 \times 10^{-12} \exp[-(458\pm36)/T]$	263-358	Antinolo et al. (2014)	PLP-LIF (a)
$(5.57 \pm 0.14) \times 10^{-13}$	298		
Relative Rate Coefficients			
$(4.63 \pm 0.51) \times 10^{-13}$	296	Sulbaek Andersen et al. (2003)	RR (b)
$(5.10 \pm 0.29) \times 10^{-13}$			

Comments

(a) HO radicals were produced by 248 nm (KrF eximer laser) photolysis of HNO_3 in 50-205 Torr (67-273 mbar) of helium diluent at 263-358 K. HO radicals were monitored by LIF. No effect of total pressure was reported over the range studied

(b) HO radicals were generated by the photolysis of CH_3ONO in 700 Torr (933 mbar) of air in the presence of NO. In separate experiments C_2H_2 and C_2H_4 were used as reference compounds. The loss of C_2F_5CHO and the reference compounds were monitored using FTIR spectroscopy. Rate coefficient ratios of $k(HO+C_2F_5CHO)/k(HO+C_2H_2) = 0.593 \pm 0.065$ and $k(HO+C_2F_5CHO)/k(HO+C_2H_4) = 0.0646 \pm 0.0037$ were reported. Scaling these ratios 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 $k(HO+C_2F_5CHO) = (4.63 \pm 0.51) \times 10^{-13}$ and $(5.10 \pm 0.29) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	5.2×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$2.52 \times 10^{-12} \exp(-470/T)$	250-360
Reliability		
$\Delta \log k$	0.10	298
$\Delta E/R$	± 200	298

Comments on Preferred Values

The results reported by Sulbaek Andersen et al. (2003) and Antinolo et al. (2014) near room temperature are in agreement within the likely experimental uncertainties. Taking an average of the results from the two studies gives the recommended value of $k(OH+C_2F_5CHO) = 5.2 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K. Fitting the Arrhenius expression to the data from Antinolo et al. (2014) and

adjusting the A-factor to reproduce the recommended value at 298 K gives $k(OH+C_2F_5CHO) = 2.52 \times 10^{-12} \exp(-470/T)$ cm^3 molecule^{-1} s^{-1}. The reaction proceeds via abstraction of the aldehydic hydrogen to give $C_2F_5C(O)$ radicals.

References

Antinolo, M., Jiménez, E., Gonzalez, S., and Albaladejo, J.: J. Phys. Chem. A, 118, 178, 2014.

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.

Sulbaek Andersen, M. P., Hurley, M. D., Wallington, T.J., Ball, J. C., Martin, J. W., Ellis, D.A., Mabury, S. A., and Nielsen, O. J.: Chem. Phys. Lett., 379, 28, 2003.