

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx35

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Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i> $(1.2 \pm 0.6) \times 10^{-12}$	296	Hayman and Battin-Leclerc, 1995	LP-UVA (a)

Comments

- (a) Flash photolysis of H_2O_2 in the presence of $\text{CF}_3\text{CHF}_2\text{-O}_2\text{-N}_2$ mixtures at a total pressure of 1013 mbar. Decays in transient absorption signals (with contributions from $\text{CF}_3\text{CF}_2\text{O}_2$, HO_2 and CF_3O_2) were recorded in the wavelength range 220 nm and 230 nm. k derived from simulations of the decay traces using a 16 reaction mechanism.

Preferred Values

$$k = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.5 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

While the above value of the rate coefficient seems reasonable, it has been derived from the analysis of a complex chemical system and requires independent verification to reduce the recommended error limits. It is interesting to note that k is substantially smaller than that recommended for the reaction of HO_2 with $\text{C}_2\text{H}_5\text{O}_2$. This confirms a deactivating influence of $\alpha\text{-F}$ and $\alpha\text{-CF}_3$ groups, observed for the reactions of a number of halogenated peroxy radicals with HO_2 .

References

Hayman, G. and Battin-Leclerc, F.: J. Chem. Soc. Farad. Trans. 91, 1313, 1995.