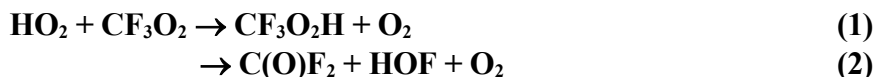


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet of FOx33

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This data sheet updated: 29th March 2005.



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>			
$\leq 2 \times 10^{-12}$	296	Hayman and Battin-Leclerc, 1995	FP-UVA (a)
$(4.0 \pm 2.0) \times 10^{-12}$	295	Sehested et al., 1997	PR-UVA (b)
$\leq 3 \times 10^{-12}$	296	Biggs et al., 1997	DF-LIF (c)

Comments

- (a) Flash photolysis of H_2O_2 in the presence of $\text{CF}_3\text{CH}_2\text{F-O}_2\text{-N}_2$ mixtures at a total pressure of 1013 mbar. Primary investigation of CF_3CHFO_2 radical kinetics, with CF_3O_2 radicals generated from the decomposition of product CF_3CHFO radicals. Decays in transient absorption signals (with contributions from CF_3CHFO_2 , HO_2 and CF_3O_2) were recorded in the wavelength range 220 nm to 240 nm. Upper limit k derived from simulations of the decay traces using a 15 reaction mechanism. Good fits could not be obtained if the $\text{CF}_3\text{O}_2 + \text{HO}_2$ was occurring appreciably under the experimental conditions.
- (b) Pulse radiolysis study of $\text{CHF}_3\text{-H}_2\text{-O}_2\text{-SF}_6$ mixtures at a total pressure of 1013 mbar. CF_3O_2 and HO_2 radicals were monitored by UV absorption spectroscopy at 230 nm. Decays in transient absorption signals (with contributions from HO_2 and CF_3O_2) were recorded at 230 nm. The cited value of k was derived from simulation of the decay in absorption, using a 13 reaction chemical mechanism.
- (c) Experiments performed at 2.7 mbar. CF_3O_2 and HO_2 radicals were produced by the $\text{F} + \text{CHF}_3$ and $\text{F} + \text{CH}_3\text{OH}$ reactions, with subsequent addition of O_2 . Both CF_3O_2 and HO_2 were monitored by titration to NO_2 following reaction with excess NO , with detection of NO_2 by LIF. Upper limit k derived from simulations of the decay in radical concentration, using an explicit reaction mechanism. Actual values obtained varied in the range $(< 1 \text{ to } 3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

No recommendation

Comments

Although the results of Sehested et al. (1997) and Biggs et al. (1997) provide evidence for the occurrence of the reaction of HO_2 with CF_3O_2 , the rate coefficient is not well-determined in any of the reported studies. No recommendation can be made until further kinetics and product studies of this reaction are available.

References

Biggs, P., Canosa-Mas, C.E., Shallcross, D.E., Vipond, A. and Wayne, R.P.: J. Chem. Soc.

Farad. Trans. 93, 2701, 1997.

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

Sehested, J., Mogelberg, T., Fagerstrom, K., Mahmoud, G. and Wallington, T. J.: Int. J. Chem. Kinet. 29, 673, 1997.