IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx77

This data sheet last evaluated: June 2015; last change in preferred values: December 2004.

$$HO_2 + CF_2ClCH_2O_2 \rightarrow O_2 + CF_2ClCH_2O_2H \quad (1)$$
$$\rightarrow O_2 + CF_2ClCHO + H_2O \quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(6.8 \pm 3.4) \times 10^{-12}$	296	Hayman and Battin-Leclerc, 1995	LP-UVA (a)

Comments

(a) Flash photolysis of H_2O_2 in the presence of CF_2ClCH_3-O_2-N_2 mixtures at a total pressure of 1013 mbar. Decays in transient absorption signals (with contributions from $CF_2ClCH_2O_2$ and HO_2) were recorded in the wavelength range 220 nm to 240 nm. k derived from simulations of the decay traces using a 10 reaction mechanism.

Preferred Values

$k = 6.8 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.5$ at 298 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. Within the uncertainty of the determination, k is indistinguishable from that recommended for the reaction of HO_2 with $C_2H_5O_2$, suggesting that the presence of the CF_2Cl group has only a minor influence on the reaction.

References

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