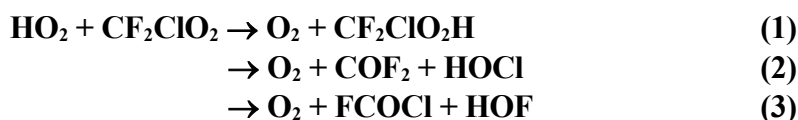


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx75

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

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



Rate coefficient data ($k = k_1 + k_2 + k_3$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(3.4 \pm 1.7) \times 10^{-12}$	296	Hayman and Battin-Leclerc, 1995	LP-UVA (a)

Comments

- (a) Flash photolysis of H_2O_2 in the presence of $\text{CHF}_2\text{Cl-O}_2\text{-N}_2$ mixtures at a total pressure of 1013 mbar. Decays in transient absorption signals (with contributions from CF_2ClO_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

$$k = 3.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

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.

The rate coefficients for the reactions of HO_2 with a number of halogenated peroxy radicals suggest that the presence of an $\alpha\text{-F}$ atom has a deactivating influence. Consistent with this, k is apparently somewhat lower than those for the corresponding reactions of CH_3O_2 , CH_2ClO_2 , CHCl_2O_2 and CCl_3O_2 , which all lie in the range $5\text{-}6 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

References

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