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

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

$$HO_2 + CF_2ClO_2 \rightarrow O_2 + CF_2ClO_2H \quad (1)$$
$$\rightarrow O_2 + COF_2 + HOCl \quad (2)$$
$$\rightarrow O_2 + FCOCl + HOF \quad (3)$$

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

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

Comments

(a) Flash photolysis of H_2O_2 in the presence of CHF_2Cl-O_2-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

$k = 3.4 \times 10^{-12}$ 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.

The rate coefficients for the reactions of HO_2 with a number of halogenated peroxy radicals suggest that the presence of an α–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 5-6 x 10^{-12} cm^3 molecule^{-1} s^{-1}.

References

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