IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx79

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

$HO_2 + CF_3CCl_2O_2 \rightarrow O_2 + CF_3CCl_2O_2H$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.9 \pm 0.7) \times 10^{-12}$	298	Hayman et al., 1994	LP-UVA (a)

Comments

(a) Laser flash photolysis-UV absorption study of CF_3CCl_3-CH_3OH-O_2-N_2 mixtures. The kinetic data were obtained by analyzing two sets of transient decays for $CF_3CCl_2O_2$ and HO_2 radicals on the basis of a mechanism consisting of 10 reactions.

Preferred Values

$k = 1.9 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ 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. It is interesting to note, by comparison with data for analogous halogenated RO_2 radicals, that while the α-substitution of Cl appears to reduce the rate coefficient slightly, the presence of the CF_3 group causes a much larger reduction in the value of k.

References

Hayman, G. D., Jenkin, M. E., Murrells, T. P. and Johnson, C. E.: Atmos. Environ. 28A, 421, 1994.