IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx67

 The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr
This datasheet last evaluated: June 2015; last change in preferred values: November 2003.

$HO + CF_2ClCHO \rightarrow H_2O + CF_2ClCO$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(9.5 \pm 0.5) \times 10^{-13}$	298 ± 2	Scollard et al., 1993	PLP-RF
Relative Rate Coefficients			
$(6.9 \pm 0.5) \times 10^{-13}$	298 ± 2	Scollard et al., 1993	RR (a)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO or C_2H_5ONO in CH_3ONO (or C_2H_5ONO)-CF_2ClCHO-ethanol-air mixtures at 987 ± 13 mbar pressure. The concentrations of CF_2ClCHO and ethanol were measured by GC and/or FTIR spectroscopy. Scollard et al. (1993) did not report a value for the rate coefficient ratio k(HO + CF_2ClCHO)/k(HO + ethanol). Dividing the reported value of k(HO + CF_2ClCHO) by the value of k(HO + ethanol) used by Scollard et al. (1993) gives k(HO + CF_2ClCHO)/k(HO + ethanol) = 0.214 ± 0.015 which is placed on an absolute basis in the table above using a rate coefficient of k(HO + ethanol) = 3.2×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	8.2×10^{-13}	298
Reliability		
$\Delta \log k$	± 0.25	298

Comments on Preferred Values

The preferred value is an average of the absolute and relative rate coefficients of Scollard et al. (1993).

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr

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