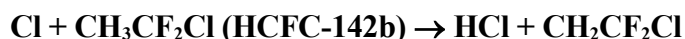


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx29

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. 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 Kinetic Data Evaluation, <http://iupac.pole-ether.fr>. This data sheet last evaluated: June 2015; last change in preferred values: November 2003.



Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference | Technique/ Comments |
|--|---------|-------------------------------|---------------------|
| <i>Absolute Rate Coefficients</i> | | | |
| $(5.3 \pm 1.1) \times 10^{-16}$ | 297 | Jourdain et al., 1977 | DF-MS |
| $(5.6 \pm 2.0) \times 10^{-16}$ | 297 | Sawerysyn et al., 1992 | DF-MS |
| $< 4.4 \times 10^{-15}$ | 298 | Warren and Ravishankara, 1993 | PLP-RF |
| $1.5 \times 10^{-12} \exp[-(2420 \pm 400)/T]$ | 296-438 | Talhaoui et al., 1996 | DF-MS |
| $(4.7 \pm 1.3) \times 10^{-16}$ | 296 | | |
| <i>Relative Rate Coefficients</i> | | | |
| $(3.90 \pm 0.52) \times 10^{-16}$ | 295 | Wallington and Hurley, 1992 | RR (a) |
| $(3.7 \pm 0.8) \times 10^{-16}$ | 298 | Tuazon et al., 1992 | RR (b) |

Comments

- (a) Cl atoms were generated by the photolysis of Cl_2 . The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).
- (b) Cl atoms were generated by the photolysis of Cl_2 . The decays of the reactant and reference organic were measured by FTIR spectroscopy. The measured rate coefficient is placed on an absolute basis by use of a rate coefficient of $k(\text{Cl} + \text{CH}_4) = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).

Preferred Values

| Parameter | Value | T/K |
|--|-------------------------------------|---------|
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | 4.1×10^{-16} | 298 |
| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $1.4 \times 10^{-12} \exp(-2420/T)$ | 296-440 |
| <i>Reliability</i> | | |
| $\Delta \log k$ | ± 0.15 | 298 |
| $\Delta(E/R)$ | ± 500 | |

Comments on Preferred Values

The preferred value of the rate constant at 298 K is based on the results reported by Wallington and Hurley (1992), Tuazon et al. (1992) and Talhaoui et al. (1996). The latter study supersedes

the work of Sawerysyn et al. (1992). The single temperature dependent study of Talhaoui et al. (1996) forms the basis for the recommendation of $k(T)$, with the A-factor adjusted to reproduce the recommended value of k at 298 K.

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