

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx36

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Rate coefficient data

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference | Technique/ Comments |
|--|---------|-------------------------------|---------------------|
| <i>Absolute Rate Coefficients</i> | | | |
| $3.94 \times 10^{-12} \exp[-(1740 \pm 100)/T]$ | 276-382 | Warren and Ravishankara, 1993 | PLP-RF |
| $(1.15 \pm 0.30) \times 10^{-14}$ | 298 | | |
| <i>Relative Rate Coefficients</i> | | | |
| $(1.22 \pm 0.18) \times 10^{-14}$ | 295 | Wallington and Hurley, 1992 | RR (a) |
| $(1.4 \pm 0.3) \times 10^{-14}$ | 298 | Tuazon et al., 1992 | RR (a) |

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 was 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 |
|--|-------------------------------------|---------|
| $k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | 1.2×10^{-14} | 298 |
| $k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | $4.4 \times 10^{-12} \exp(-1740/T)$ | 270-380 |
| <i>Reliability</i> | | |
| $\Delta \log k$ | ± 0.1 | 298 |
| $\Delta(E/R)$ | ± 500 | 270-380 |

Comments on Preferred Values

The preferred value at 298 K is based on the results reported by Warren and Ravishankara (1993), Wallington and Hurley (1992), and Tuazon et al. (1992), which are in good agreement. The recommended temperature dependence is that reported by Warren and Ravishankara (1993), the only study of the temperature dependence.

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>
- Tuazon, E. C., Atkinson, R. and Corchnoy, S. B.: Int. J. Chem. Kinet., 24, 639, 1992.
- Wallington, T. J. and Hurley, M. D.: Chem. Phys. Lett., 189, 437, 1992.
- Warren, R. F. and Ravishankara, A. R.: Int. J. Chem. Kinet., 25, 833, 1993.

