

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx35

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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>			
$1.16 \times 10^{-12} \exp[-(1800 \pm 150/T)]$ $(2.62 \pm 0.50) \times 10^{-15}$	276-376 298	Warren and Ravishankara, 1993	PLP-RF
<i>Relative Rate Coefficients</i>			
$(2.7 \pm 0.6) \times 10^{-15}$	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 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
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	2.7×10^{-15}	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.1 \times 10^{-12} \exp(-1800/T)$	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) 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 carried out over a range of temperatures.

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.
- Warren, R. F. and Ravishankara, A. R.: Int. J. Chem. Kinet., 25, 833, 1993.

