IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx40

This data sheet updated: 23th July 2003.

$OClO + NO \rightarrow ClO + NO_2$

$\Delta H° = -50.0$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(3.4 \pm 0.5) \times 10^{-13}$	298	Bemand, Clyne, and Watson, 1973[1]	DF-MS
$1.04 \times 10^{-13}\exp[(347\pm58)/T]$	220-367	Li, Wuebbles, and Pylawka, 2002	DF-MS
$(3.55 \pm 0.3) \times 10^{-13}$	298		

Preferred Values

$k = 3.6 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.1 \times 10^{-13} \exp(350/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 220 – 370 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 K.
$\Delta(E/R) = \pm 200$.

Comments on Preferred Values

The two available studies of this reaction,[1,2] both using the same method, show good agreement at the common temperature, 298 K, and the recommendation at this temperature is the average result. The recommended temperature dependence is provided by the study of Li *et al*.[2] with a slight correction to the preexponential factor to match the preferred value at 298 K.

References

[1] P. P. Bemand, M. A. A. Clyne, and R. T. Watson, J. Chem. Soc. Faraday Trans. 1, **69**, 1356 (1973).
[2] Z. Li, R. D. Wuebbles, and N.J. Pylawka, Chem. Phys. Lett. **354**, 491 (2002).