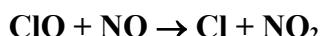


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx31

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 re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet updated: 23th July 2003.



$$\Delta H^\circ = -37.4 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.7 \pm 0.2) \times 10^{-11}$	298	Clyne and Watson, 1974	DF-MS
$5.72 \times 10^{-12} \exp[(296 \pm 20)/T]$	227-415	Leu and DeMore, 1978	DF-MS
$(1.53 \pm 0.11) \times 10^{-11}$	299		
$(1.61 \pm 0.16) \times 10^{-11}$	295	Clyne and MacRobert, 1980	DF-MS
$(1.72 \pm 0.2) \times 10^{-11}$	298	Ray and Watson, 1981	DF-MS
$7.1 \times 10^{-12} \exp[(270 \pm 50)/T]$	202-393	Lee et al., 1982	DF-LMR
$(1.84 \pm 0.03) \times 10^{-11}$	297		

Preferred Values

$$k = 1.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 6.2 \times 10^{-12} \exp(295/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 200 \text{ K to } 420 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 100 \text{ K.}$$

Comments on Preferred Values

The room temperature rate coefficients reported by Clyne and Watson (1974), Leu and DeMore (1978), Clyne and MacRobert (1980), Ray and Watson (1981) and Lee et al. (1982) are in good agreement and are ~30% lower than the value reported by Zahniser and Kaufman (1977) from a competitive study. The preferred values are derived from a least-squares fit to the data reported by Clyne and Watson (1974), Leu and DeMore (1978), Clyne and MacRobert (1980), Ray and Watson (1981) and Lee et al. (1982).

References

- Clyne, M. A. A. and Watson, R. T.: J. Chem. Soc. Faraday Trans. 1, 70, 2250, 1974.
Clyne, M. A. A. and MacRobert, A. J.: Int. J. Chem. Kinet. 12, 79, 1980.
Lee, Y. P., Stimpfle, R. M., Perry, R. A., Mucha, J. A., Evenson, K. M., Jennings, D. A. and Howard, C. J.: Int. J. Chem. Kinet. 14, 711, 1982.
Leu, M. T. and DeMore, W. B. : J. Phys. Chem. 82, 2049, 1978.

Ray, G. W. and Watson, R. T.: J. Phys. Chem. 85, 2955, 1981.
Zahniser, M. S. and Kaufman, F.: J. Chem. Phys. 66, 3673, 1977.