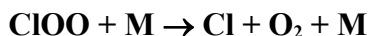


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx11

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: 9th March 2005.



$$\Delta H^\circ = 23.8 \text{ kJ}\cdot\text{mol}^{-1}$$

Low-pressure rate coefficients Rate coefficient data

| k_0/s^{-1} | Temp./K | Reference | Technique/ Comments |
|--|---------|-----------------------|---------------------|
| <i>Absolute Rate Coefficients</i> | | | |
| $1.9 \times 10^{-14} [\text{O}_2]$ | 185.4 | Nicovich et al., 1991 | PLP-RF (a) |
| $2.8 \times 10^{-10} \exp(-1820/T) [\text{N}_2]$ | 160-260 | Baer et al., 1991 | PLP-UVA |
| $6.2 \times 10^{-13} [\text{N}_2]$ | 298* | | (a) |
| $6.3 \times 10^{-10} \exp(-2030/T) [\text{O}_2]$ | 160-260 | Baer et al., 1991 | PLP-UVA |
| $1.1 \times 10^{-14} [\text{O}_2]$ | 185.4 | | (a) |

Comments

(a) From measurements of the reverse reaction and the equilibrium constant.

Preferred Values

$$k_0 = 6.2 \times 10^{-13} [\text{N}_2] \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_0 = 2.8 \times 10^{-10} \exp(-1820/T) [\text{N}_2] \text{ s}^{-1} \text{ over the temperature range } 160\text{-}300 \text{ K.}$$

Reliability

$$\Delta \log k_0 = \pm 0.3 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 200 \text{ K.}$$

Comments on Preferred Values

The preferred values are based on the extensive data of Baer et al. (1991). No deviations from third-order behavior were observed at pressures below 1 bar. The reaction probably does not proceed via an energy-transfer mechanism (see comments on the reverse reaction $\text{Cl} + \text{O}_2 + \text{M} \rightarrow \text{ClOO} + \text{M}$), but rather by a radical-complex mechanism.

References

- Baer, S., Hippler, H., Rahn, R., Siefke, M., Seitzinger, N. and Troe, J.: J. Chem. Phys., 95, 6463, 1991.
Nicovich, J. M., Kreutter, K. D., Shackelford, C. J. and Wine, P. H.: Chem. Phys. Lett., 179, 367, 1991.