IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx16

This datasheet updated: 23th July 2003.

$Cl + NO_3 \rightarrow ClO + NO_2$

$\Delta H° = -60.2$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.6 \pm 0.5) \times 10^{-11}$	298	Mellouki, Le Bras, and Poulet, 1987[1]	DF-EPR/MS
$(2.26 \pm 0.17) \times 10^{-11}$	298	Becker *et al*., 1991[2]	DF-MS

Preferred Values

$k = 2.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 200 K to 300 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

$\Delta(E/R) = \pm 400$ K.

Comments on Preferred Values

The preferred value at room temperature is based on the studies of Mellouki *et al*.[1] and Becker *et al*.[2] The results of these direct absolute rate studies are preferred over those of earlier relative rate studies,[3-5] in which NO_3 was monitored in the photolysis of Cl_2-$ClONO_2$-N_2 mixtures. The agreement among these earlier studies[3-5] is not good and probably arises from complications in the chemistry of the systems used. This radical-radical reaction is expected to have a negligible temperature dependence, which is consistent with the results of Cox *et al*.[5] over the temperature range 278 K to 338 K.

References

1 A. Mellouki, G. Le Bras, and G. Poulet, J. Phys. Chem. **91**, 5760 (1987).

2 E. Becker, U. Wille, M. M. Rahman R. N. Schindler, Ber. Bunsenges. Phys. Chem. **95**, 1173 (1991).

3 R. A. Cox, R. A. Barton, E. Ljundstrom, and D. W. Stocker, Chem. Phys. Lett. **108**, 228 (1984).

4 J. P. Burrows, G. S. Tyndall, and G. K. Moortgat, J. Phys. Chem. **89**, 4848 (1985).

5 R. A. Cox, M. Fowles, D. Moulton, and R. P. Wayne, J. Phys. Chem. **91**, 3361 (1987).