IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet III.A2.53 iClOx38

This data sheet last evaluated: March 2005.

$Cl_2O_3 + M \rightarrow ClO + OClO + M$

$\Delta H° = 43.2$ kJ·mol^{-1}

Low-pressure rate coefficients

No direct measurements are available.

Preferred Values

$k_0 = 1.6 \times 10^{-19} \exp(-3810/T)$ [N_2] s^{-1} over the temperature range 200-300 K.

Reliability

$\Delta \log k_0 = \pm 0.5$ at 240 K.

$\Delta E/R = \pm 500$ K.

Comments on Preferred Values

The preferred values are from the preferred values for the reverse reaction $k_0 = 6.2 \times 10^{-32} (T/300)^{-4.7}$ [N_2] cm^3 molecule^{-1} s^{-1}, which were based on the measurements by Parr et al. (1990) and Burkholder et al. (1993), and the equilibrium constant $K_C = 9.7 \times 10^{-24} \exp(4940/T)$ cm^3 molecule^{-1} from Burkholder et al. (1993) and Hayman and Cox (1989).

High-pressure rate coefficients
Rate coefficient data

No direct measurements are available.

Preferred Values

$k_\infty = 2.5 \times 10^{12} \exp(-4940/T)$ [N_2] s^{-1} over the temperature range 200-300 K.

Reliability

$\Delta \log k_\infty = \pm 0.5$ at 240 K.

$\Delta E/R = \pm 500$ K.

Comments on Preferred Values

See comments on Preferred Values for k_0. Based on k_∞ for the reverse reaction of $k_\infty = 2.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}. Falloff curves constructed with $F_c = 0.6$.

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of k:

=((1.6e-19*exp(-3810/*T*))*M*(2.5e12*exp(-4940/*T*)))/((1.6e-19*exp(-3810/*T*))*M+(2.5e12*exp(-4940/*T*)))*10^(log10(0.6)/(1+(log10((1.6e-19*exp(-3810/*T*))*M/(2.5e12*exp(-4940/*T*)))/(0.75-1.27*log10(0.6)))^2))

The molecular density, $M = 7.243\times10^{21}$P(bar)/T(K)

References

Burkholder, J. B., Mauldin III, R. L., Yokelson, R. J., Solomon, S. and Ravishankara, A. R.: J. Phys. Chem., 97, 7597, 1993.

Hayman, G. D. and Cox, R.A.: Chem. Phys. Lett., 155, 1, 1989.

Parr, A. D., Wayne, R. P., Hayman, G. D., Jenkin, M. E. and Cox, R. A.: Geophys. Res. Lett., 17, 2357, 1990.