IUPAC Task Group on Atmospheric Chemical kinetic Data Evaluation – Data Sheet III.A4.85 iIOx6

This data sheet last evaluated: March 2005.

$$\mathbf{I + NO_2 + M \rightarrow INO_2 + M}$$

$\Delta H° = -79.8$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
1.5×10^{-31} $(T/300)^{-1}$ [He]	320-450	van den Bergh and Troe, 1976	PLP-UVA (a)
1.62×10^{-31} [He]	330	van den Bergh, Benoit-Guyot and Troe, 1977	PLP-UVA (b)
2.6×10^{-31} [N_2]	330		
$(9.5 \pm 3.5) \times 10^{-32}$ [He]	298	Mellouki et al., 1989	DF-EPR (c)
3.1×10^{-31} [N_2]	298	Buben et al., 1990	FP-RF (d)

Comments

(a) Derived from the NO_2 catalyzed recombination of I atoms, with I atoms being produced by photolysis of I_2 at 694 nm. The falloff curve was measured from 1 200 bar of He, and only a short extrapolation to k_0 was required.
(b) As in comment (a). The efficiencies of 26 bath gases were studied.
(c) Measurements performed over the pressure range 0.8 to 2.9 mbar.
(d) I atoms generated by photolysis of CH_3I in a flow system with NO_2-N_2 mixtures. The bath gases N_2, O_2, Ar and He were studied at total pressures between 0.7 and 13 mbar.

Preferred Values

$k_0 = 3.0 \times 10^{-31}$ $(T/300)^{-1}$ [N_2] cm^3 molecule^{-1} s^{-1} over the temperature range 290-450 K.

Reliability

$\Delta \log k_0 = \pm 0.2$ at 298 K.
$\Delta n = \pm 1$.

Comments on Preferred Values

The preferred values are based on the results of the studies of van den Bergh and Troe (1976), van den Bergh et al. (1977) and Buben et al. (1990). The data of Mellouki et al. (1989) for M

= He are also consistent with these data Falloff extrapolations are made with a fitted value of $F_c = 0.63$ from van den Bergh and Troe (1976).

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
6.6 x 10^{-11}	320-350	van den Bergh and Troe, 1976	PLP-UVA (a)

Comments

(a) See comment (a) for k_0. Extrapolation of the falloff curve towards the high pressure limit uses a fitted value of $F_c = 0.63$.

Preferred Values

k_∞ = 6.6 x 10^{-11} cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 290-450 K.

Reliability

$\Delta \log k_\infty = \pm 0.3$ over the temperature range 300-400 K.

Comments on Preferred Values

The preferred values are based on the results of the study of van den Bergh and Troe (1976). Falloff curves are represented with $F_c = 0.63$.

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:

=((3.0e-31*(*T*/300)^-1)*M*(6.6e-11))/((3.0e-31*(*T*/300)^-1)*M+(6.6e-11))*10^(log10(0.63)/(1+(log10((3.0e-31*(*T*/300)^-1)*M/(6.6e-11))/(0.75-1.27*log10(0.63)))^2))

The molecular density, M = 7.243×10^{21}P(bar)/T(K)

References

Buben, S. N., Larin, I. K., Messineva, N. A. and Trofimova, E. M.: Kinet. Catal., 31, 854, 1990; original pages 973-977, 1990.

Mellouki, A., Laverdet, G., Jourdain, J. L. and Poulet, G.: Int. J. Chem. Kinet., 21, 1161, 1989.

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