IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet III.A4.84 iIOx5

This data sheet last evaluated: June 2007.

I + NO + M → INO + M

$\Delta H° = -75.7$ 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			
(6.0 ± 2.5) x 10^{-33} (T/300)$^{-1.0}$ [He]	320-450	van den Bergh and Troe, 1976	PLP-UVA (a)
(1.6 ± 0.5) x 10^{-32} [N_2]	330	van den Bergh, Benoit-Guyot and Troe, 1977	PLP-UVA (b)
(9.5 ± 3) x 10^{-33} [Ar]	330		
(1.05 ± 0.3) x 10^{-32} [Ar]	298		
(1.03 ± 0.06) x 10^{-32} (T/300)$^{-1.1}$ [Ar]	298-328	Basco and Hunt, 1978	FP (c)

Comments

(a) Photolysis of I_2 at 694 nm in the presence of NO and He. The pressure of He was varied between 1 and 200 bar. I_2 and INO spectra were observed.

(b) As in comment (a). The rate coefficient for M = Ar at 298 K was calculated from the measured rate coefficient at 330 K and the temperature dependence reported by van den Bergh and Troe (1976).

(c) Photolysis of I_2 in the presence of NO and Ar.

Preferred Values

$k_0 = 1.8 \times 10^{-32} (T/300)^{-1.0}$ [N_2] cm^3 molecule^{-1} s^{-1} over the temperature range 290-450 K.

Reliability

$\Delta \log k_0 = \pm 0.1$ at 298 K.

$\Delta n = \pm 0.5$.

Comments on Preferred Values

The preferred values are based on the rate coefficients for M = Ar determined by van den Bergh et al. (1976) and Basco and Hunt (1978) which agree remarkably well.

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
≥1.7 x 10^{-11}	330	van den Bergh and Troe, 1976	PLP-UVA (a)

Comments

(a) As for comment (a) for k_0. Based on a falloff extrapolation with $F_c = 0.6$.

Preferred Values

$k_\infty = 1.7 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} over the temperature range 300 K to 400 K.

Reliability

$\Delta \log k_\infty = \pm 0.5$ over the temperature range 300 K to 400 K.
$\Delta n = \pm 1$.

Comments on Preferred Values

The preferred values are based on the only measurement by van den Bergh and Troe (1976), extrapolated by using a value of $F_c = 0.6$.

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:

=((1.8e-32*(*T*/300)^-1.0)*M*(1.7e-11))/((1.8e-32*(*T*/300)^-1.0)*M+(1.7e-11))*10^(log10(0.6)/(1+(log10((1.8e-32*(*T*/300)^-1.0)*M/(1.7e-11))/(0.75-1.27*log10(0.6)))^2))

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

References

Basco, N. and Hunt, J. E.: Int. J. Chem. Kinet., 10, 733, 1978.
van den Bergh, H. and Troe, J.: J. Chem. Phys., 64, 736, 1976.
van den Bergh, H., Benoit-Guyot, N. and Troe, J.: Int. J. Chem. Kinet., 9, 223, 1977.