IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx4

This data sheet updated: 3rd July 2005.

$I + O_3 \rightarrow IO + O_2$

$\Delta H° = -134$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(9.6 \pm 3.0) \times 10^{-13}$	303	Jenkin and Cox, 1985	MM-AS (a)
$(9.5 \pm 1.5) \times 10^{-13}$	298	Sander, 1986	FP-AS (b)
$2.3 \times 10^{-11} \exp[-(886 \pm 15)/T]$	231-337	Buben et al., 1990	DF-RF (c)
$(1.2 \pm 0.1) \times 10^{-12}$	298		
$2.3 \times 10^{-11} \exp[-(860 \pm 100)/T]$	240-370	Turnipseed et al., 1995	PLP-LIF (d)
$(1.38 \pm 0.08) \times 10^{-12}$	298		
$1.6 \times 10^{-11} \exp[-(750 \pm 194)/T]$	243-295	Hölscher et al., 1998	PLP-LIF (d)
$(1.2 \pm 0.1) \times 10^{-12}$	295		
$(1.28 \pm 0.06) \times 10^{-12}$	298	Tucceri et al., 2005	PLP-RF (c)

Comments

(a) Modulated photolysis of I_2-O_3 mixtures at 570 nm and a total pressure of 34 mbar. IO radicals were monitored in absorption at 426.9 nm.
(b) Detection of IO in absorption at 427.2 nm. A non-linear dependence of the pseudo first-order decay constant on the O_3 concentration was observed.
(c) Direct detection of I atom reactant in excess O_3.
(d) Detection of IO product by LIF.

Preferred Values

$k = 1.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 2.1 \times 10^{-11} \exp(-830/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 230-370 K.

Reliability

$\Delta \log k = \pm 0.05$ at 298 K.
$\Delta(E/R) = \pm 150$ K.

Comments on Preferred Values

The most recent studies of this reaction (Buben et al., 1990; Turnipseed et al., 1995; Hölscher et al., 1998; Tucceri et al., 2005) are in excellent agreement and indicate somewhat higher rate coefficients than those obtained previously. A weighted, average value of $(1.28 \pm 0.08) \times 10^{-12}$

cm^3 $molecule^{-1}$ s^{-1} is derived from these four studies, and provides the basis of the recommendation.

The preferred Arrhenius expression for k is obtained by combining the mean of the values of E/R from the studies of Buben et al. (1990), Turnipseed et al. (1995) and Hölscher et al. (1998) with a pre-exponential factor adjusted to give the preferred value of k at 298 K.

References

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Hölscher, D., Fockenberg, Chr. and Zellner, R.: Ber. Bunsenges. Phys. Chem., 102, 716, 1998.

Jenkin, M. E. and Cox, R. A.: J. Phys. Chem., 89, 192, 1985.

Sander, S. P.: J. Phys. Chem., 90, 2194, 1986.

Tucceri, M. E., Dillon, T. J. and Crowley, J. N.: Phys. Chem. Chem. Phys. 7, 1657, 2005.

Turnipseed, A. A., Gilles, M. K., Burkholder, J. B. and Ravishankara, A. R.: Chem. Phys. Lett., 242, 427, 1995.