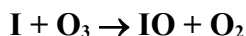


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IO_x4

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

This data sheet updated: 3rd July 2005.



$$\Delta H^\circ = -134 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(9.6 \pm 3.0) \times 10^{-13}$	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

- Modulated photolysis of $\text{I}_2\text{-O}_3$ mixtures at 570 nm and a total pressure of 34 mbar. IO radicals were monitored in absorption at 426.9 nm.
- 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.
- Direct detection of I atom reactant in excess O_3 .
- Detection of IO product by LIF.

Preferred Values

$$k = 1.3 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

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

Reliability

$$\Delta \log k = \pm 0.05 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 150 \text{ K.}$$

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 $(1.28 \pm 0.08) \times 10^{-12}$

$\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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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