IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx10

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This datasheet last evaluated: 28th June 2007; no revision of preferred values.

$HO + I_2 \rightarrow HOI + I$

 $\Delta H^{\circ} = -62.5 \text{ kJ} \cdot \text{mol}^{-1}$

Rate coefficient data

k/cm³ molecule-1 s-1	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $(1.6^{+1.6}_{-0.8}) \times 10^{-10}$ $(2.10 \pm 0.60) \times 10^{-10}$	298 240-348	Loewenstein and Anderson, 1985 Gilles et al., 1999	DF-RF PLP-LIF (a)
Relative Rate Coefficients $(2.3 \pm 0.3) \times 10^{-10}$	294	Jenkin et al., 1984	RR (b)

Comments

- (a) From measurements of the rate coefficients at 240 K, 293-295 K and 348 K, a least-squares analysis led to $k = 1.97 \times 10^{-10} \exp[(21 \pm 318)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The temperature independent expression cited in the table was preferred by Gilles et al. (1999).
- (b) Steady-state photolysis of HONO-I₂-ethene-air (or N₂) mixtures at 1 bar total pressure. A rate coefficient ratio $k(\text{HO} + \text{I}_2)/k(\text{HO} + \text{ethene}) = 26.5 \pm 3.5$ was obtained from the rate of disappearance of ethene as a function of the I₂ concentration. This rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(\text{HO} + \text{ethene}) = 8.69 \times 10^{-12} \text{ cm}^3$ molecule⁻¹ s⁻¹ at 294 K and 1 bar of air (Atkinson, 1997).

Preferred Values

 $k = 2.1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 240-350 K.

Reliability

 $\Delta \log k = \pm 0.15 \text{ at } 298 \text{ K.}$ $\Delta (E/R) = \pm 300 \text{ K.}$

Comments on Preferred Values

The reported room temperature rate coefficients of Jenkin et al. (1984), Loewenstein and Anderson (1985) and Gilles et al. (1999) agree well, noting the large quoted error limits associated with the Loewenstein and Anderson (1985) data. The preferred values are based on the most recent and extensive study of Gilles et al. (1999). Loewenstein and Anderson (1985) determined that the exclusive products are HOI and I.

References

Atkinson, R.: J. Phys. Chem. Ref. Data 26, 215, 1997.

Gilles, M. K., Burkholder, J. B. and Ravishankara, A. R.: Int. J. Chem. Kinet. 31, 417, 1999. Jenkin, M. E., Clemitshaw, K. C. and Cox, R. A.: J. Chem. Soc. Faraday Trans. 2, 80, 1633, 1984.

Loewenstein, L. M. and Anderson, J. G.: J. Phys. Chem. 89, 5371, 1985.