IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx1

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$O + I_2 \rightarrow IO + I$

$\Delta H° = -89$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.38 \pm 0.44) \times 10^{-10}$	298	Ray and Watson, 1981	DF-MS (a)
$(1.4 \pm 0.4) \times 10^{-10}$	298	Laszlo et al., 1995	PLP-AS (b)
$(1.3 \pm 0.15) \times 10^{-10}$	295	Hölscher et al., 1998	PLP-LIF (c)
$(1.2 \pm 0.1) \times 10^{-10}$	298	Tucceri et al., 2005	PLP-RF (d)

Comments

(a) MS detection of I_2 in a large excess of O(^{3}P) atoms. The O(^{3}P) atom concentrations were determined by titration with NO_2. The total pressure was ~2.6 mbar.

(b) O(^{3}P) atoms were produced by pulsed laser photolysis of N_2O at 193 nm in the presence of I_2, at total pressures of ~260 mbar of N_2. The I_2 concentrations used were comparable to those of O(^{3}P) atoms. The I_2 and IO radical concentrations were monitored simultaneously by absorption spectroscopy at 530 nm and at 340 nm to 435 nm, respectively, and values of k were derived by modeling the I_2 and IO radical time-concentration profiles.

(c) O(^{3}P) atoms were produced by pulsed laser photolysis of N_2O at 193 nm in the presence of an excess of I_2, at total pressures of 40 mbar of N_2. IO radical concentrations were monitored by LIF at 445.05 nm.

(d) O(^{3}P) atoms were produced by pulsed laser photolysis of NO_2 at 351 nm in the presence of an excess of I_2, which was monitored in situ at 500 nm. Total pressures of 80 or 266 mbar of He or 80 mbar N_2 were used. The I atom product was monitored by RF.

Preferred Values

$k = 1.25 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The recommended rate coefficient is based on the data of Hölscher et al. (1998) and Tucceri et al. (2005), both of whom employed sufficiently sensitive detection schemes that the IO self reaction was unimportant, and a simple exponential behaviour of IO and I was therefore observed. Note that the recommended value is within the large errors limits presented by Ray

and Watson (1981) and Laszlo et al. (1995). The rate coefficient is large, approaching the gas kinetic collisional value and suggesting a near zero temperature dependence for *k*. This is in accord with the molecular beam study of the reaction by Parrish and Herschbach (1973).

References

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