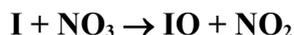


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet **iIOx7**

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This data sheet last evaluated: June 2008; last change in preferred values: June 2008.



$$\Delta H^\circ = -31.4 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(4.5 \pm 1.9) \times 10^{-10}$	298	Chambers et al., 1992	DF-RF (a)
$(1.0 \pm 0.3) \times 10^{-10}$	298	Dillon et al., 2008	PLP-LIF (b)

Comments

- (a) Discharge flow (2.7 mbar) with resonance fluorescence detection of I atoms in the presence of excess NO_3 radicals. NO_3 radicals and I atoms were produced by the $\text{F} + \text{HNO}_3$ and $\text{O} + \text{I}_2$ reactions, respectively. NO_3 radical concentrations were measured by visible absorption spectroscopy.
- (b) Experiments at 107- 120 mbar He. I atoms were generated in the 248 nm photolysis of CF_3I ; NO_3 was generated in the reaction of F atoms (248 nm photolysis of F_2) with HNO_3 . Kinetics of the title reaction were derived from IO-product profiles (with IO detected by LIF at 445 nm). The concentration of the excess reagent (NO_3) was calculated from measurements of laser fluence and $[\text{F}_2]$ and was associated with an uncertainty of 30 %. The yield of IO was determined relative to its yield in the reaction $\text{O}(^3\text{P}) + \text{CF}_3\text{I}$ and established as (1.0 ± 0.3) .

Preferred Values

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

Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

Both listed studies of this reaction agree that the rate coefficient is large, which contrasts the failure of Lancar et al. (1991) to observe a reaction (they report no upper limit to k). Whereas the experiment of Chambers et al. (1992) had the advantage of direct measurement of the NO_3 concentration, the I atom decays used to extract kinetic data were found to be non-exponential, which was attributed to establishment of a steady state concentration of I via an unknown process at long reactions times. In addition, wall losses of I were found to be fast and may have had some impact on the result obtained. For these reasons, we base our preferred value on the result of Dillon et al. (2008), which was obtained under true pseudo-

first order conditions and characterized by exponential kinetics. The uncertainty has been enhanced to partly reflect the significant divergence in the three reports of this reaction.

References

- Chambers, R. M., Heard, A. C., and Wayne, R. P.: *J. Phys. Chem.*, 96, 3321, 1992.
Dillon, T. J., Tucceri, M. E., Sander, R., and Crowley, J. N.: *Phys. Chem. Chem. Phys.*, 10, 1540, 2008.
Lancar, I. T., Mellouki, A., and Poulet, G.: *Chem. Phys. Lett.*, 177, 554, 1991.