IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx3

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This data sheet updated: 6th June 2007.

$$I + HO_2 \rightarrow HI + O_2$$
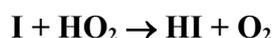
$\Delta H° = -94.9 \text{ kJ·mol}^{-1}$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.47 \times 10^{-11} \exp[-(1090 \pm 130)/T]$	283-353	Jenkin et al., 1990	PF-EPR
$(3.8 \pm 1.0) \times 10^{-13}$	298		MMS-UVA(a)

Comments

(a) Two experimental methods were used. The first technique involved a discharge flow system with EPR detection of I atoms (directly) and of HO$_2$ radicals after conversion to HO radicals (by reaction with NO). The first-order decays of HO$_2$ radicals in excess I atoms were measured, resulting in a rate coefficient of $k = (3.1 \pm 1.2) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K. The second technique, which provided the temperature dependence, employed the molecular modulation method with UV absorption detection of HO$_2$ radicals, and with the I atom concentration being determined from the observed modulation of the I$_2$ absorption at 500 nm. Excess I atoms were employed, and the HO$_2$ radical self-reaction competed with the I + HO$_2$ reaction. The best analysis gave $k = (4.17 \pm 0.4) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K. The Arrhenius expression was obtained from the mean of the discharge flow and molecular modulation determinations at 298 K and the E/R obtained from a least-squares fit to the temperature-dependent data.

Preferred Values

$k = 3.8 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.5 \times 10^{-11} \exp(-1090/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 280 K to 360 K.

Reliability
$\Delta \log k = \pm 0.3$ at 298 K.
$\Delta(E/R) = \pm 500$ K.

Comments on Preferred Values
The preferred values are based on the two experimental studies reported by Jenkin et al. (1990) which are the only reported measurements for this reaction. The values of the rate coefficient at 298K from the two studies agree quite well, although both studies exhibited

significant experimental error. The Arrhenius expression suggested by Jenkin et al. (1990) is accepted for the temperature dependence.

References

Jenkin, M. E., Cox, R. A., Mellouki, A., Le Bras, G., and Poulet, G.: J. Phys. Chem., 94, 2927, 1990.