IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx9

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

$HO + HI \rightarrow H_2O + I$

$\Delta H° = -198.8$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$(1.3 \pm 0.5) \times 10^{-11}$	295	Takacs and Glass, 1973	DF-EPR
$(2.7 \pm 0.2) \times 10^{-11}$	298	Mac Leod et al., 1990	PLP-RF
$(3.3 \pm 0.2) \times 10^{-11}$	298	Lancar et al., 1991	DF-EPR
$(7.0\ ^{+1.9}_{-0.4}) \times 10^{-11}(T/298)^{-(1.5 \pm 0.5)}$	246-353	Campuzano-Jost and Crowley, 1999	PLP-RF
$(6.5\ ^{+2}_{-0.4}) \times 10^{-11}$	294		

Preferred Values

$k = 1.6 \times 10^{-11} \exp(440/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 240-360 K.

$k = 7.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

$\Delta(E/R) = \pm 400$ K.

Comments on Preferred Values

The preferred values are based on the most recent and extensive study of Campuzano-Jost and Crowley (1999), in which, although the HI concentrations in the reaction cell were not monitored directly during the experiments, care was taken to remove potential impurities in the HI and a number of HO radical precursors were investigated before choosing H_2O_2 photolysis at 248 nm as the optimum. Additionally, two analyses using ion chromatography showed that the HI concentrations in the reaction cell were within ~20% to 25% of those expected (Campuzano-Jost and Crowley, 1999). The lower room temperature rate coefficients obtained in the studies of Mac Leod et al. (1990) and Lancar et al. (1991), which are more than a factor of two higher than the earlier results of Takacs and Glass (1973), may have suffered from unrecognized losses of HI due to reactions with the HO radical precursors used and/or (in the study of Lancar et al., 1991) from generation of vibrationally-excited HO radicals (Campuzano-Jost and Crowley, 1999).

References

Campuzano-Jost, P. and Crowley, J. N.: J. Phys. Chem. A 103, 2712, 1999.
Lancar, I. T., Mellouki, A. and Poulet, G.: Chem. Phys. Lett. 177, 554, 1991.
Mac Leod, H., Balestra, C., Jourdain, J. L., Laverdet, G. and Le Bras, G.: Int. J. Chem. Kinet. 22, 1167, 1990.
Takacs, G. A. and Glass, G. P.: J. Phys. Chem. 77, 1948, 1973.