IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iIOx11

This data sheet updated: 3rd February 2004.

$NO_3 + HI \rightarrow HNO_3 + I$

$\Delta H° = -128.5$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.3 \times 10^{-12} \exp[-(1830 \pm 300)/T]$	298-373	Lancar, Mellouki and Poulet, 1991[1]	DF-EPR/MS (a)
$(2.5 \pm 0.8) \times 10^{-15}$	298		

Comments

(a) NO_3 radicals were generated by the reaction of F atoms with HNO_3. The rate coefficient was determined by measuring the decay rate of NO_3 radicals (by MS, correcting for the contribution of HNO_3 to the m/z = 62 ion signal) or by measuring the formation rate of I atoms (by EPR).

Preferred Values

No recommendation.

Comments on Preferred Values

Although the rate coefficients measured in the only study[1] of this reaction from the decay of NO_3 using MS and I atom production using EPR spectrometry were in agreement,[1] there is a serious potential for secondary chemistry occurring in the system leading to an overestimation of the rate coefficient for the elementary process. Lancar *et al.*[1] reported that the reaction of I + $NO_3 \rightarrow$ IO + NO_2 does not occur, while Chambers *et al.*[2] observed that the I + NO_3 reaction is rapid, with a measured rate coefficient of $k(I + NO_3) = 4.5 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K, and that I atoms are regenerated from subsequent reactions of IO radicals. Until this uncertainty is resolved, no recommendation can be made.

References

[1] I. T. Lancar, A. Mellouki, and G. Poulet, Chem. Phys. Lett. **177**, 554 (1991).

[2] R. M. Chambers, A. C. Heard, and R. P. Wayne, J. Phys. Chem. **96**, 3321 (1992).