IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iClOx28

This data sheet updated: 3rd February 2004.

$NO_3 + HCl \rightarrow HNO_3 + Cl$

$\Delta H° = 4.8$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$<7 \times 10^{-18}$	298	Cantrell *et al*., 1987[1]	(a)
$\leq 5 \times 10^{-17}$	298	Mellouki *et al*., 1989[2]	DF-EPR (b)
$<2.4 \times 10^{-17}$	298	Canosa-Mas *et al*., 1989[3]	DF-A (c)

Comments

(a) NO_3 radical concentrations were derived from the measured NO_2 and N_2O_5 concentrations in N_2O_5-NO_2-NO_3-HCl-air mixtures, using the equilibrium constant of Graham and Johnston.[4] The upper limit to the rate coefficient cited above was derived from computer fits of the time-concentration data for reactants and products monitored by FTIR absorption spectrometry.

(b) The upper limit to the rate coefficient cited above was derived from fitting the measured upper limit to the ClO radical concentration (determined by EPR after conversion to Cl atoms) to a complex mechanism.

(c) No reaction was observed at room temperature, leading to the upper limit to the rate coefficient cited above. At higher temperatures (333 K to 473 K), rate coefficients derived from fitting to a complex mechanism yielded the Arrhenius expression of $k = 4 \times 10^{-12} \exp(-3330/T)$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

$k < 5 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The preferred value is the upper limit to the rate coefficient reported by Mellouki *et al*.[2] in a study using the discharge flow-EPR technique. Somewhat lower upper limits have been reported by Cantrell *et al*.[1] and by Canosa-Mas *et al*.[3] Canosa-Mas *et al*.[3] also reported Arrhenius parameters at higher temperatures (over the range 333 K to 473 K). The preferred value indicates that this reaction is not important in the chemistry of the atmosphere.

References

[1] C. A. Cantrell, J. A. Davidson, R. E. Shetter, B. A. Anderson, and J. G. Calvert, J. Phys. Chem. **91**, 6017 (1987).
[2] A. Mellouki, G. Poulet, G. Le Bras, R. Singer, J. P. Burrows, and G. K. Moortgat, J. Phys. Chem. **93**, 8017 (1989).
[3] C. E. Canosa-Mas, S. J. Smith, S. Toby, and R. P. Wayne, J. Chem. Soc. Faraday Trans. 2, **85**, 709 (1989).
[4] R. A. Graham and H. S. Johnston, J. Phys. Chem. **82**, 254 (1978).