IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx9

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

$F + HONO_2 \rightarrow HF + NO_3$

 $\Delta H^{\circ} = -143.9 \text{ kJ} \cdot \text{mol}^{-1}$

Rate coefficient data

k/cm³ molecule-1 s-1	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.7 \pm 0.5) \times 10^{-11}$	298	Mellouki et al., 1987	DF-EPR
$(2.1 \pm 1) \times 10^{-11}$	298	Rahman et al., 1988	DF-MS
$6.0 \times 10^{-12} \exp[(400 \pm 120)/T]$	260-320	Wine et al., 1988	PLP-A (a)
$(2.3 \pm 0.3) \times 10^{-11}$	298		
$(2.2 \pm 0.2) \times 10^{-11}$	298	Becker et al., 1991	DF-MS
$(2.3 \pm 0.2) \times 10^{-11}$	298	Becker et al., 1991	DF-EPR

Comments

(a) Pulsed laser photolysis of F_2 -HONO₂-He mixtures at 351 nm, with detection of NO₃ radicals by long-path laser absorption at 662 nm. At higher temperatures (335-373 K) the rate coefficient was observed to be independent of temperature with a value of $(2.0 \pm 0.3) \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹.

Preferred Values

 $k = 2.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}.$ $k = 6.0 \times 10^{-12} \exp(400/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 260-320 \text{ K}.$

Reliability

 $\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$ $\Delta (E/R) = \pm 200 \text{ K.}$

Comments on Preferred Values

The recommendation is based on the results of the temperature-dependent study of Wine et al. (1988) and the room temperature results of Mellouki et al. (1987), Rahman et al. (1988) and Becker et al. (1991). The values at room temperature are in good agreement. The study of Wine et al. (1988) was carried out over the temperature range 260-373 K; below 320 K the authors fitted their data with the Arrhenius expression recommended here, whereas at higher temperatures a temperature-independent value was found suggesting the occurrence of different mechanisms in the two temperature regimes.

References

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Mellouki, A., Le Bras, G. and Poulet, G.: J. Phys. Chem. 91, 5760, 1987.

Rahman, M. M., Becker, E., Benter, Th. and Schindler, R. N.: Ber. Bunsenges. Phys. Chem. 92, 91, 1988.

Wine, P. H., Wells, J. R. and Nicovich, J. M.: J. Phys. Chem. 92, 2223, 1988.