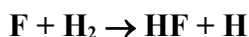


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx4

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be re-transmitted or disseminated either electronically or in hard copy without explicit written permission.

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



$$\Delta H^\circ = -134.7 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.0 \times 10^{-10} \exp[-(433 \pm 51)/T]$	190-359	Wurzberg and Houston, 1980	PLP-CL
$(2.27 \pm 0.18) \times 10^{-11}$	297		
$(2.55 \pm 0.11) \times 10^{-11}$	298	Clyne and Hodgson, 1985	DF-LIF (a)
$1.2 \times 10^{-10} \exp[-(470 \pm 30)/T]$	221-376	Stevens et al., 1989	DF-RF (b)
$(2.48 \pm 0.09) \times 10^{-11}$	298		

Comments

- (a) F atoms were reacted with Br₂ to form BrF, which was detected by LIF.
- (b) Discharge flow system. F atoms were converted to D atoms by reaction with D₂ downstream of the reaction zone, and the D atoms monitored by resonance fluorescence.

Preferred Values

$$k = 2.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 1.1 \times 10^{-10} \exp(-450/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 190\text{--}380 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 100 \text{ K.}$$

Comments on Preferred Values

This evaluation accepts the recommended values given in the critical review of Persky and Kornweitz (1997) of the literature data for this reaction. The preferred values are based on the results of Wurzberg and Houston (1980), Clyne and Hodgson (1985) and Stevens et al. (1989).

References

- Clyne, M. A. A. and Hodgson, A.: J. Chem. Soc. Faraday Trans. 2, 81, 443, 1985.
- Persky, A. and Kornweitz, H.: Int. J. Chem. Kinet. 29, 67, 1997.
- Stevens, P. S., Brune, W. H. and Anderson, J. G.: J. Phys. Chem. 93, 4068, 1989.
- Wurzberg, E. and Houston, P. L.: J. Chem. Phys. 72, 4811, 1980.