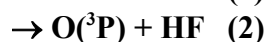


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx3

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

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This datasheet last evaluated: June 2014; last change in preferred values: July 2003.



$$\Delta H^\circ(1) = -49.0 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -189.7 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data ($k = k_1 + k_2$)

| $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | Temp./K | Reference | Technique/ Comments |
|--|---------|----------------------------|------------------------|
| <i>Relative Rate Coefficients</i> | | | |
| $(5.1 \pm 1.0) \times 10^{-11}$ | 298 | Sorokin et al., 1998; 1999 | PLP-LMR (a) |
| <i>Branching Ratios</i> | | | |
| $k_1/k = 0.30 \pm 0.02$ | 298 | Sorokin et al., 1998; 1999 | PLP-LMR (a) |
| $k_2/k = 0.70 \pm 0.02$ | 298 | | |

Comments

(a) Measured rate coefficient ratio of $k(\text{O}(^1\text{D}) + \text{HF})/k(\text{O}(^1\text{D}) + \text{NF}_3)$ was placed on an absolute basis by use of the rate coefficient for the reference reaction $k(\text{O}(^1\text{D}) + \text{NF}_3) = 1.15 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Sorokin et al., 1998; 1999). Pressure in the reactor was ~ 13 mbar.

Preferred Values

| Parameter | Value | T/K |
|--|-----------------------|-----|
| $k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | 5.1×10^{-11} | 298 |
| k_1/k | 0.30 | 298 |
| k_2/k | 0.70 | 298 |
| <i>Reliability</i> | | |
| $\Delta \log k$ | ± 0.2 | 298 |
| $\Delta(k_1/k) = \Delta(k_2/k)$ | ± 0.1 | 298 |

Comments on Preferred Values

The preferred values of k , k_1/k , and k_2/k are based on the results reported by Sorokin et al. (1998; 1999). These results are given in the only published journal articles presenting a systematic study of this system. In a published paper on the reactions of O(¹D) with HCl and HBr, Wine et al. (1986), because of uncertainties in the HF concentration, report for the reaction O(¹D) + HF only a highly uncertain rate constant in the range (6 to 24) x 10⁻¹¹ cm³ molecule⁻¹ s⁻¹ at room temperature. Chichinin (2000) has measured the deuterium isotope effect for the reaction of O(¹D) with DF. The effect on the rate of physical quenching was negligible.

References

- Chichinin, A. I.: Chem. Phys. Lett. 316, 425, 2000.
Sorokin, V. I., Gritsan, N. P. and Chichinin, A. I.: J. Chem. Phys. 108, 8995, 1998.
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Wine, P. H., Wells, J. R. and Ravishankara, A. R.: J. Chem. Phys. 84, 1349. 1986.