IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx14

This data sheet updated: 22th July 2003.

$FO_2 + NO \rightarrow FNO + O_2$

$\Delta H° = -182$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.5 \pm 0.1) \times 10^{-12}$	298	Sehested *et al*., 1994[1]	PR-UVA (a)
$7.5 \times 10^{-12} \exp[-(688 \pm 377)/T]$	190-298	Li, Friedl, and Sander, 1995[2]	DF-MS (b)
$(8.5 \pm 1.3) \times 10^{-13}$	298		

Comments

(a) Pulse radiolysis of NO-O_2-SF_6 mixtures at 1 bar SF_6. The formation of FNO was monitored in absorption at 310.5 nm. The yield of FNO was determined to be (100 ± 14)%.

(b) First-order decay rates of FO_2 in the presence of excess NO were monitored by mass spectrometry at a total pressure of 1.3 mbar He. The yield of FNO was found to be nearly 100%.

Preferred Values

$k = 7.5 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k = 7.5 \times 10^{-12} \exp(-690/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 190 K to 300 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.

$\Delta(E/R) = \pm 400$ K.

Comments on Preferred Values

The preferred values are based on results of the temperature-dependent study of Li *et al*.[2] The higher room temperature rate coefficient of Sehested *et al*.[1] is encompassed within the assigned uncertainty limits. The low barrier to form FNO may indicate that the reaction proceeds via formation of a short lived FOONO complex.[3]

References

[1] J. Sehested, K. Sehested, O. J. Nielsen, and T. J. Wallington, J. Phys. Chem. **98**, 6731 (1994).
[2] Z. Li, R. R. Friedl, and S. P. Sander, J. Phys. Chem. **99**, 13445 (1995).
[3] T. S. Dibble and J. S. Francisco, J. Am Chem. Soc. **119**, 2894 (1997).