IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx12

This data sheet updated: 3rd February 2004.

$$\mathbf{FO + FO \rightarrow 2F + O_2} \quad \mathbf{(1)}$$
$$\mathbf{\rightarrow FO_2 + F} \quad \mathbf{(2)}$$
$$\mathbf{\rightarrow F_2 + O_2} \quad \mathbf{(3)}$$

$\Delta H°(1) = -59$ kJ·mol^{-1}
$\Delta H°(2) = -113$ kJ·mol^{-1}
$\Delta H°(3) = -218$ kJ·mol^{-1}

Rate coefficient data ($k = k_1 + k_2 + k_3$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(8.5 \pm 2.8) \times 10^{-12}$	298	Clyne and Watson, 1974[1]	DF-MS
$1.0 \times 10^{-11} (T/300)^{0.85\pm0.5}$	300-435	Bedzhanyan, Markin, and Gershenzon, 1993[2]	DF-LMR

Preferred Values

$k = 1.0 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 290 K to 440 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.
$\Delta(E/R) = \pm 250$ K.

Comments on Preferred Values

The recommended value is based on the results of Clyne and Watson[1] and Bedzhanyan *et al.*[2] In a less direct study, Wagner *et al.*[3] reported a factor of 3 higher value. Although Bedzhanyan *et al.*[2] reported a weak temperature dependence, a temperature-independent rate coefficient fits their data equally well and is recommended in this evaluation. The study of Bedzhanyan *et al.*[2] showed that the predominant reaction channel is that to produce $2F + O_2$.

References

[1] M. A. A. Clyne and R. T. Watson, J. Chem. Soc. Faraday Trans. 1, **70**, 1109 (1974).

[2] Yu. R. Bedzhanyan, E. M. Markin, and Yu. M. Gershenzon, Kinet. Catal. **33**, 601 (1993); original pages 753-759 (1992).

[3] H. Gg. Wagner, C. Zetzsch, and J. Warnatz, Ber. Bunsenges. Phys. Chem. **76**, 526 (1972).