IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx3

This data sheet updated: 9th March 2002.

$O + HO \rightarrow O_2 + H$

$\Delta H^\circ = -68.4$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$3.35 \times 10^{-11} (T/300)^{-0.36}$	221-499	Lewis and Watson, 1980[1]	DF-RF (a)
$3.84 \times 10^{-11} (T/300)^{-0.5}$	250-500	Howard and Smith, 1981[2]	DF/FP-RF
3.52×10^{-11}	298	Temps, 1983[3]	DF-LMR
3.1×10^{-11}	298	Brune, Schwab and Anderson, 1983[4]	DF-LMR/RA/RF
$4.1 \times 10^{-11} (T/300)^{-0.6}$	158-294	Smith and Stewart, 1994[5]	DF/PLP-RF
Relative Rate Coefficients			
3.4×10^{-11}	298	Keyser,1983[6]	DF-RF (b)

Comments

(a) "Best-fit" values for 300 K from this work are preferred.

(b) Measurements relative to the reaction $O + HO_2 \rightarrow HO + O_2$ evaluated with $k(O+HO_2) = 5.8 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

$k = 3.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

$k = 2.4 \times 10^{-11} \exp(110/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 150-500 K.

Reliability

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

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

Comments on Preferred Values

The recommended temperature dependence is based on a least-squares fit of the data of Lewis and Watson[1] and Howard and Smith,[2] which are in close agreement. The preferred value for 300 K is the

average of data obtained near 300 K in refs. 1-5. The reaction has also been the subject of numerous theoretical studies, see Miller and Klippenstein[7] or Troe and Ushakov[8].

References

1 R. S. Lewis and R. T. Watson, J. Phys. Chem. **84**, 3495 (1980).
2 M. J. Howard and I. W. M. Smith, J. Chem. Soc. Faraday Trans. 2, **77**, 997 (1981).
3 F. Temps, Ph. D. Dissertation, Göttingen (1983).
4 W. H. Brune, J. J. Schwab, and J. G. Anderson, J. Phys. Chem. **87**, 4503 (1983).
5 I. W. M. Smith and D. W. A. Stewart, J. Chem. Soc. Faraday Trans. **90**, 3221 (1994).
6 L. F. Keyser, J. Phys. Chem. **87**, 837 (1983).
7 J. A. Miller and S. J. Klippenstein, Int. J. Chem. Kinet. **31**, 753 (1999).
8 J. Troe and V. G. Ushakov, J. Chem. Phys. **115**, 3621 (2001).