IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx12

This data sheet updated: 2nd October 2001.

$HO + H_2O_2 \rightarrow H_2O + HO_2$

$\Delta H^\circ = -129.1$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
2.96×10^{-12} exp[-(164 ± 52)/T]	250-459	Sridharan, Reimann and Kaufman, 1980[1]	DF-LIF
(1.69 ± 0.26) x 10^{-12}	298		
2.51×10^{-12} exp[-(126 ± 76)/T]	245-423	Keyser, 1980[2]	DF-RF
(1.64 ± 0.32) x 10^{-12}	298		
3.7×10^{-12} exp[-(260 ± 50)/T]	273-410	Wine, Semmes and Ravishankara, 1981[3]	PLP-RF
(1.59 ± 0.08) x 10^{-12}	297		
(1.67 ± 0.33) x 10^{-12}	296	Temps and Wagner, 1982[4]	DF-LMR
(1.81 ± 0.24) x 10^{-12}	298	Marinelli and Johnston, 1982[5]	PLP-RF
2.93×10^{-12} exp[-(158 ± 52)/T]	250-370	Kurylo *et al.*, 1982[6]	FP-RF
(1.79 ± 0.14) x 10^{-12}	296		
2.76×10^{-12} exp[-(110 ± 60)/T]	273-410	Vaghjiani, Ravishankara and Cohen, 1989[7]	PLP-LIF
(1.86 ± 0.18) x 10^{-12}	298		

Preferred Values

$k = 1.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 2.9 \times 10^{-12}$ exp(-160/T) cm^3 molecule^{-1} s^{-1} over the temperature range 240-460 K.

Reliability

$\Delta \log k = \pm 0.1$ at 298 K.
$\Delta(E/R) = \pm 100$ K.

Comments on Preferred Values

There are a number of studies in excellent agreement on the value of the rate coefficient k.[1-7] The recommended expression is a fit to the data in refs. 1-7. The high temperature study of Hippler *et al.*[8] shows that above 800 K there is a strong increase in k with temperature, the data being best represented by the biexponential expression $k = \{3.3 \times 10^{-12} \exp(-215/T) + 2.8 \times 10^{-6} \exp(-14800/T)\}$ cm^3 molecule^{-1} s^{-1} over the temperature range $240 \leq T \leq 1700$ K.

References

[1] U. C. Sridharan, B. Reimann, and F. Kaufman, J. Chem. Phys. **73**, 1286 (1980).
[2] L. F. Keyser, J. Phys. Chem. **84**, 1659 (1980).
[3] P. H. Wine, D. H. Semmes, and A. R. Ravishankara, J. Phys. Chem. **75**, 4390 (1981).
[4] F. Temps and H. Gg. Wagner, Ber. Bunsenges. Phys. Chem. **86**, 119 (1982).
[5] W. J. Marinelli and H. S. Johnston, J. Chem. Phys. **77**, 1225 (1982).
[6] M. J. Kurylo, J. L. Murphy, G. S. Haller, and K. D. Cornett, Int. J. Chem. Kinet. **14**, 1149 (1982).
[7] G. L. Vaghjiani, A. R. Ravishankara, and N. Cohen, J. Phys. Chem. **93**, 7833 (1989).
[8] H. Hippler, N. Neunaber, and J. Troe, J. Chem. Phys. **103**, 3510 (1995).