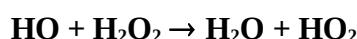


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx12

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

This data sheet updated: 2<sup>nd</sup> October 2001.



$$\Delta H^\circ = -129.1 \text{ kJ}\cdot\text{mol}^{-1}$$

## Rate coefficient data

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

## Preferred Values

$$k = 1.7 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

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

### Reliability

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

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

### Comments on Preferred Values

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

## References

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