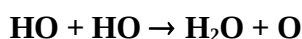


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx9

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.



$$\Delta H^\circ = -71.2 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.3 \pm 0.3) \times 10^{-12}$	350	Westenberg and deHaas, 1973 <sup>1</sup>	DF-EPR
$(2.1 \pm 0.5) \times 10^{-12}$	298	McKenzie, Mulcahy and Steven, 1973 <sup>2</sup>	DF-EPR
$(1.4 \pm 0.2) \times 10^{-12}$	300	Clyne and Down, 1974 <sup>3</sup>	DF-RF/RA
$(2.1 \pm 0.1) \times 10^{-12}$	300	Trainor and von Rosenberg, 1974 <sup>4</sup>	FP-RA
$(1.7 \pm 0.2) \times 10^{-12}$	298	Farquharson and Smith, 1980 <sup>5</sup>	DF-RF
$3.2 \times 10^{-12} \exp(-242/T)$	250-580	Wagner and Zellner, 1981 <sup>6</sup>	FP-RA
$(1.43 \pm 0.3) \times 10^{-12}$	298		
$(7.1 \pm 1.0) \times 10^{-13} \exp[(210 \pm 40)/T]$	233-360	Bedjanian, Le Bras and Poulet, 1999 <sup>7</sup>	DF-MS
$1.4 \times 10^{-12}$	298		
$1.9 \times 10^{-12}$	298	IUPAC, 1997 <sup>8</sup>	(a)
$7.9 \times 10^{-14} (T/298)^{2.6} \exp(945/T)$	200-500		

### Comments

- (a) Based on on 298 K values from refs. 1-6 and a temperature dependence from an ab-initio modelling study of Harding *et al.*<sup>13</sup>

### Preferred Values

$$k = 1.48 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 6.2 \times 10^{-14} (T/298)^{2.6} \exp(945/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 200\text{-}350 \text{ K.}$$

### Reliability

$$\Delta \log k = \pm 0.15 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 250 \text{ K.}$$

### Comments on Preferred Values

There are a number of measurements of  $k$  at temperatures close to 298 K,<sup>1-6,9-12</sup> falling in the range  $(1.4-2.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The more recent studies<sup>3,5-7</sup> support the lower values for  $k(298)$  near  $1.4 \times 10^{-12}$ . The negative temperature dependence reported by Bedjanian *et al.*<sup>7</sup> in the low temperature region, which is in conflict with the earlier works of Wagner and Zellner<sup>6</sup> supports the theoretically derived temperature dependence recommended by IUPAC.<sup>8</sup> The current recommendation was the IUPAC 1998 expression with the temperature independent term adjusted to give a  $k_{298}$  value of  $1.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .

### References

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- <sup>13</sup> L. B. Harding and A. F. Wagner, 22nd Symp. (Int.) on Combustion (Combustion Institute, Pittsburgh, 1988), p. 983.