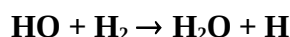


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx8

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: 2nd October 2001.



$$\Delta H^\circ = -62.0 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
7.0×10^{-15}	300	Greiner, 1969 ¹	FP-RA
$(7.1 \pm 1.1) \times 10^{-15}$	298	Stuhl and Niki, 1972 ²	FP-RF
7.6×10^{-15}	298	Westenberg and deHaas, 1973 ³	DF-EPR
$1.8 \times 10^{-11} \exp(-2330/T)$	210-460	Smith and Zellner, 1974 ⁴	FP-RA
7.1×10^{-15}			
$(5.79 \pm 0.26) \times 10^{-15}$	300	Overend, Paraskevopoulos and Cvetanovic, 1975 ⁵	FP-RA
$5.9 \times 10^{-12} \exp[-(2008 \pm 151)/T]$	298-425	Atkinson, Hansen and Pitts, 1975 ⁶	FP-RF
$(6.97 \pm 0.70) \times 10^{-15}$	298		
$4.12 \times 10^{-19} T^{2.44} \exp(-1281/T)$	298-992	Tully and Ravishankara, 1980 ⁷	FP-RF
$(6.08 \pm 0.37) \times 10^{-15}$	298		
6.1×10^{-15}	298	Zellner and Steinert, 1981 ⁸	DF-RF
$(4.9 \pm 0.5) \times 10^{-12}$	250-400	Ravishankara <i>et al.</i> , 1981 ⁹	FP-RF
$\exp[-(1990 \pm 340)/T]$			
$(5.64 \pm 0.60) \times 10^{-15}$	295		
$7.2 \times 10^{-20} T^{2.69} \exp(-1150/T)$	230-420	Talukdar <i>et al.</i> , 1996 ¹⁰	FP/PLP-LIF(a)
$(6.65 \pm 0.36) \times 10^{-15}$	298		

Comments

- (a) Both flash lamp and pulsed laser photolysis were used. The OH radical reactions with HD and D₂ were also studied.

Preferred Values

$k = 6.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k = 7.7 \times 10^{-12} \exp(-2100/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 200-450 K.

Reliability

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

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

There are several studies in good agreement concerning both the temperature dependence and absolute values of the rate coefficient. The preferred value of k at 298 K is the mean of the results of Greiner,¹ Stuhl and Niki,² Westenberg and deHaas,³ Smith and Zellner,⁴ Overend *et al.*,⁵ Atkinson *et al.*,⁶ Tully and Ravishankara,⁷ Zellner and Steinert⁸ and Ravishankara *et al.*⁹ The preferred value of E/R is the mean of the values of Smith and Zellner,⁴ Atkinson *et al.*⁶ and Ravishankara *et al.*⁹ The pre-exponential factor in the rate expression is calculated to fit the preferred value of k at 298 K and that of E/R . The results of Talukdar *et al.*¹⁰ are in excellent agreement with this recommendation. There have been many quantum mechanical calculations of the rate coefficient for this reaction, and these are in reasonable agreement with experiment.^{11,12} Brownsword *et al.*¹³ have recently measured the branching ratio for H₂O/HOD product formation of (1.2 ± 0.2) in the OH + HD reaction in a PLP/VUV-LIF study under single collision conditions.

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