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

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$HO + HO \rightarrow H_2O + O$

ΔH° = -71.2 kJ·mol^{-1}

Rate coefficient data

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

Preferred Values

k = 1.48 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K.
k = 6.2 x 10^{-14} (T/298)$^{2.6}$ exp(945/T) cm^3 molecule^{-1} s^{-1} over the temperature range 200-350 K.

Reliability

$\Delta \log k$ = ±0.15 at 298 K.
$\Delta(E/R)$ = ±250 K.

Comments on Preferred Values

There are a number of measurements of k at temperatures close to 298 K,[1-6,9-12] falling in the range (1.4-2.3) x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}. The more recent studies[3,5-7] support the lower values for k(298) near 1.4 x 10. The negative temperature dependence reported by Bedjanian *et al*.[7] in the low temperature region, which is in conflict with the earlier works of Wagner and Zellner[6] supports the theoretically derived temperature dependence recommended by IUPAC.[8] The current recommendation was the IUPAC 1998 expression with the temperature independent term adjusted to give a k298 value of 1.5 x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}.

References

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