IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx6

This data sheet last updated: 2nd May 2008 (with revision of preferred values).

$$O(^1D) + H_2 \rightarrow HO + H \quad (1)$$
$$\rightarrow O(^3P) + H_2 \quad (2)$$

$\Delta H^\circ(1) = -182.7$ kJ·mol^{-1}
$\Delta H^\circ(2) = -189.7$ kJ·mol^{-1}

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(9.9 \pm 3) \times 10^{-11}$	204-352	Davidson et al., 1976, 1977	(a)
$(1.18 \pm 0.12) \times 10^{-10}$	297	Wine and Ravishankara, 1981	PLP-RF (b)
$(1.0 \pm 0.1) \times 10^{-10}$	298	Force and Wiesenfeld, 1981	(c)
$(1.2 \pm 0.1) \times 10^{-10}$	298	Talukdar and Ravishankara, 1996	PLP-RF (d)
$(1.49 \pm 0.1) \times 10^{-10}$	295	Blitz et al., 2004	PLP-VUV-LIF (e)
$(1.54 \pm 0.1) \times 10^{-10}$	195		

Comments

(a) Pulsed laser photolysis of O_3 at 266 nm, with $O(^1D)$ atoms being monitored by time-resolved emission at 630 nm.
(b) $O(^3P)$ atoms were monitored by time-resolved resonance fluorescence.
(c) Pulsed laser photolysis of O_3 at 248 nm. H and $O(^3P)$ atoms were monitored by time-resolved absorption spectroscopy.
(d) $O(^3P)$ and H atom products were monitored by resonance fluorescence.
(e) Pulsed laser photolysis of N_2O at 193 nm. $O(^1D)$ atoms were monitored directly by time-resolved resonance fluorescence at 115.2 nm.

Preferred Values

$k = 1.2 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 200-350 K.

Reliability

$\Delta \log k = \pm 0.1$ at 298 K.
$\Delta(E/R) = \pm 50$ K.

Comments on Preferred Values

The recent measurement of Blitz et al (2004) using direct monitoring of $O(^1D)$ is in good agreement with the earlier measurements of Davidson *et al*. (1976/1977)., Wine and Ravishankara (1981), Force and Wiesenfeld (1981), Talukdar and Ravishankara, (1996), and Blitz et al (2004), and confirms the absence

of significant temperature dependence. The recommended value is the mean of the values cited for room temperature and is independent of temperature. Channel (1) appears to be the dominant pathway (>95%) for the reaction.

Absolute rate constants and isotopic branching ratios have recently been reported by Wine and Ravishankara (1982) for the reaction of $O(^1D)$ with HD. The *k* values were insignificantly different from the recommendation for H_2, with a branching ratio OH/OD = 1.35 ± 0.20 (Laurent et al, 1995)

References

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