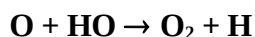


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx3

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: 9th March 2002.



$$\Delta H^\circ = -68.4 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$3.35 \times 10^{-11} (T/300)^{-0.36}$	221-499	Lewis and Watson, 1980 ¹	DF-RF (a)
$3.84 \times 10^{-11} (T/300)^{-0.5}$	250-500	Howard and Smith, 1981 ²	DF/FP-RF
3.52×10^{-11}	298	Temps, 1983 ³	DF-LMR
3.1×10^{-11}	298	Brune, Schwab and Anderson, 1983 ⁴	DF-LMR/RA/RF
$4.1 \times 10^{-11} (T/300)^{-0.6}$	158-294	Smith and Stewart, 1994 ⁵	DF/PLP-RF
<i>Relative Rate Coefficients</i>			
3.4×10^{-11}	298	Keyser, 1983 ⁶	DF-RF (b)

Comments

- (a) "Best-fit" values for 300 K from this work are preferred.
- (b) Measurements relative to the reaction $\text{O} + \text{HO}_2 \rightarrow \text{HO} + \text{O}_2$ evaluated with $k(\text{O} + \text{HO}_2) = 5.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

$$k = 3.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 2.4 \times 10^{-11} \exp(110/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 150\text{-}500 \text{ K.}$$

Reliability

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

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

Comments on Preferred Values

The recommended temperature dependence is based on a least-squares fit of the data of Lewis and Watson¹ and Howard and Smith,² which are in close agreement. The preferred value for 300 K is the

average of data obtained near 300 K in refs. 1-5. The reaction has also been the subject of numerous theoretical studies, see Miller and Klippenstein⁷ or Troe and Ushakov⁸.

References

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- ⁴ W. H. Brune, J. J. Schwab, and J. G. Anderson, *J. Phys. Chem.* **87**, 4503 (1983).
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- ⁶ L. F. Keyser, *J. Phys. Chem.* **87**, 837 (1983).
- ⁷ J. A. Miller and S. J. Klippenstein, *Int. J. Chem. Kinet.* **31**, 753 (1999).
- ⁸ J. Troe and V. G. Ushakov, *J. Chem. Phys.* **115**, 3621 (2001).