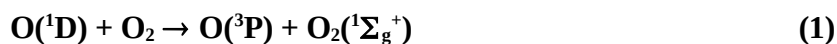


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox3

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.



$$\Delta H^\circ(1) = -32.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -95.4 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(3) = -189.7 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data ($k = k_1 + k_2 + k_3$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$2.9 \times 10^{-11} \exp[(67 \pm 11)/T]$	104-354	Streit <i>et al.</i> , 1976 ¹	(a)
3.6×10^{-11}	298		
$(4.2 \pm 0.2) \times 10^{-11}$	295	Amimoto <i>et al.</i> , 1979 ²	PLP-RA (b)
$(4.0 \pm 0.6) \times 10^{-11}$	298	Brock and Watson, 1979 ³	PLP-RF (b)
<i>Branching Ratios</i>			
$k_1/k = 0.77 \pm 0.2$	300	Lee and Slanger, 1978 ⁴	(c)
$k_2/k \leq 0.05$	300	Gauthier and Snelling, 1971 ⁵	(d)

Comments

- (a) O(¹D) atoms were produced by flash photolysis of O₃ and detected by O(¹D) → O(³P) emission at 630 nm.
- (b) O(³P) atom product detected by resonance absorption² or resonance fluorescence.³
- (c) O(¹D) atoms detected by O(¹D) → O(³P) emission at 630 nm. O₂(¹Σ_g⁺) was monitored from the O₂(¹Σ_g⁺) → O₂(³Σ_g⁻) (1-1) and (0-0) band emission. O₂(¹Σ_g⁺) is only formed in the v = 0 and 1 levels, with k(1)/k(0) = 0.7.
- (d) O(¹D) atom production by the photolysis of O₃.

Preferred Values

$$k = 4.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 3.2 \times 10^{-11} \exp(67/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 200\text{-}350 \text{ K.}$$

$k_1/k = 0.8$ at 298 K.

$k_2/k \leq 0.05$ at 298 K.

Reliability

$\Delta \log k = \pm 0.05$ at 298 K.

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

$\Delta(k_1/k) = \pm 0.1$ at 298 K.

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of the results from Streit *et al.*,¹ Amimoto *et al.*² and Brock and Watson.³ The temperature dependence is that measured by Streit *et al.*¹ The branching ratios of Lee and Slanger³ and Gauthier and Snelling⁴ are recommended.

References

- ¹ G. E. Streit, C. J. Howard, A. L. Schmeltekopf, J. A. Davidson, and H. I. Schiff, *J. Chem. Phys.* **65**, 4761 (1976).
- ² S. T. Amimoto, A. P. Force, R. G. Gulotty, Jr., and J. R. Wiesenfeld, *J. Chem. Phys.* **71**, 3640 (1979).
- ³ J. C. Brock and R. T. Watson, Reported at the NATO Advanced Study Institute on Atmospheric Ozone, Portugal (1979). See also G. K. Moortgat, in Report. No. FAA-EE.80-20 (1980).
- ⁴ L. C. Lee and T. Slanger, *J. Chem. Phys.* **69**, 4053 (1978).
- ⁵ M. Gauthier and D. R. Snelling, *J. Chem. Phys.* **54**, 4317 (1971).