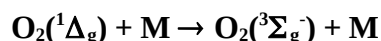


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox7

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.



$$\Delta H^\circ = -94.3 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	M		Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>				
$(1.51 \pm 0.05) \times 10^{-18}$	O ₂	298	Borrell, Borrell and Pedley, 1977 ¹	DF-CL (a)
$(1.47 \pm 0.05) \times 10^{-18}$	O ₂	298	Leiss <i>et al.</i> , 1978 ²	(b)
$(1.65 \pm 0.07) \times 10^{-18}$	O ₂	298	Raja, Arora and Chatha, 1986 ³	DF-CL (a)
$3.15 \times 10^{-18} \exp(-205/T)$	O ₂	100-450	Billington and Borrell, 1986 ⁴	DF-CL (a)
1.57×10^{-18}		298		
1.4×10^{-19}	N ₂	300	Collins, Husain and Donovan, 1973 ⁵	FP-VUVA (c)
5.6×10^{-18}	H ₂ O	298	Findlay and Snelling, 1971 ⁶	(d)
$<1.5 \times 10^{-20}$	CO ₂	298		
$(4 \pm 1) \times 10^{-18}$	H ₂ O	298	Becker, Groth and Schurath, 1971 ⁷	(e)

Comments

- Discharge flow system. O₂(¹Δ) was monitored by dimol emission at 634 nm or from O₂(¹Σ) emission at 762 nm.
- Large static reactor. O₂(¹Δ) was monitored by emission at 1.27 μm.
- O₂(¹Δ) was detected by time-resolved absorption at 144 nm.
- Flow system, with photolysis of C₆H₆-O₂ mixtures at 253.7 nm to produce O₂(¹Δ). O₂(¹Δ) was measured by 1.27 μm emission.
- As (b) but using dimol emission at 634 nm.

Preferred Values

$k = 1.6 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for M = O₂ at 298 K.

$k = 3.0 \times 10^{-18} \exp(-200/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for M = O₂ over the temperature range 100-450 K.

$k \leq 1.4 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for M = N₂ at 298 K.

$k = 5 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for M = H₂O at 298 K.

$k \leq 2 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for $M = \text{CO}_2$ at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ for $M = \text{O}_2$ at 298 K.

$\Delta(E/R) = \pm 200 \text{ K}$ for $M = \text{O}_2$.

$\Delta \log k = \pm 0.3$ for $M = \text{H}_2\text{O}$ at 298 K.

Comments on Preferred Values

The preferred value for $k(M = \text{O}_2)$ is based on the data of Borrell *et al.*,¹ Leiss *et al.*,² Raja *et al.*³ and Billington and Borrell,⁴ which also gives the temperature dependence adopted. For other quenching gases the recommendation for $k(M = \text{N}_2)$ is based on the data of Collins *et al.*,⁵ for $k(M = \text{H}_2\text{O})$ on the data of Findlay and Snelling⁶ and Becker *et al.*,⁷ and for $k(M = \text{CO}_2)$ on the data of Leiss *et al.*² and Findlay and Snelling.⁶

References

- ¹ P. Borrell, P. M. Borrell, and M. B. Pedley, *Chem. Phys. Lett.* **51**, 300 (1977).
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- ⁶ F. D. Findlay and D. R. Snelling, *J. Chem. Phys.* **55**, 545 (1971).
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