IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox9

This data sheet updated: 2nd October 2001.

$$\mathbf{O_2(^1\Sigma_g^+) + M \rightarrow O_2(^3\Sigma_g^-) + M} \quad (1)$$
$$\mathbf{\rightarrow O_2(^1\Delta_g) + M} \quad (2)$$

$\Delta H^\circ(1) = -156.9$ kJ·mol^{-1}
$\Delta H^\circ(2) = -62.6$ kJ·mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	M	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients				
$(4.6 \pm 1) \times 10^{-17}$	O_2	294	Thomas and Thrush, 1975[1]	DF-CL
4.6×10^{-12}	H_2O	294		
$(4.0 \pm 0.4) \times 10^{-17}$	O_2	298	Martin, Cohen and Schatz, 1976[2]	FP-CL
$(2.2 \pm 0.1) \times 10^{-15}$	N_2	298		
$(3.8 \pm 0.3) \times 10^{-17}$	O_2	300	Lawton *et al*., 1977[3]	FP-CL
$(2.5 \pm 0.2) \times 10^{-17}$	O_2	298	Chatha *et al*., 1979[4]	DF-CL
$(1.7 \pm 0.1) \times 10^{-15}$	N_2	298		
$1.7 \times 10^{-15} \exp(48/T)$	N_2	203-349	Kohse-Höinghaus and Stuhl, 1980[5]	PLP (a)
$(8.0 \pm 2.0) \times 10^{-14}$	O	300	Slanger and Black, 1979[6]	FP (a)
4.4×10^{-13}	CO_2	298	Filseth, Zia and Welge, 1970[7]	FP (a)
$(3.0 \pm 0.5) \times 10^{-13}$	CO_2	298	Noxon, 1970[8]	FP (a)
$(4.1 \pm 0.3) \times 10^{-13}$	CO_2	298	Davidson, Kear and Abrahamson, 1972[9]	FP (a)
$(4.53 \pm 0.29) \times 10^{-13}$	CO_2	298	Avilés, Muller and Houston, 1980[10]	PLP (a)
$(5.0 \pm 0.3) \times 10^{-13}$	CO_2	298	Muller and Houston, 1981[11]	PLP (a)
$(3.4 \pm 0.4) \times 10^{-13}$	CO_2	293	Borrell, Borrell and Grant, 1983[12]	DF-CL
$(1.7 \pm 0.1) \times 10^{-15}$	N_2	298	Choo and Leu, 1985[13]	DF (a)(b)
$(4.6 \pm 0.5) \times 10^{-13}$	CO_2	245-262		
5.6×10^{-17}	O_2	302	Knickelbein *et al*., 1987[14]	PLP (a)
$(2.2 \pm 0.2) \times 10^{-15}$	N_2	298	Wildt *et al*., 1988[15]	PLP-CL (c)
$(2.4 \pm 0.4) \times 10^{-13}$	CO_2	298		
$<1.0 \times 10^{-16}$	O_2	298	Shi and Barker, 1990[16]	PLP-CL (d)
$(2.32 \pm 0.14) \times 10^{-15}$	N_2	298		
$(4.0 \pm 0.1) \times 10^{-13}$	CO_2	298		
$(4.25 \pm 0.52) \times 10^{-17}$	O_2	295	Kebabian and Freeman, 1997[17]	(e)

Comments

(a) Time-resolved emission from $O_2(^1\Sigma)$ measured near 762 nm.
(b) Negligible temperature dependence observed for quenching by CO_2 over the range 245-362 K, with $E/R < \pm 200$ K.

(c) Direct laser excitation of $O_2(^1\Sigma)$ from O_2 by photolysis at 600-800 nm.
(d) $O_2(^1\Sigma)$ formed by the reaction $O(^1D) + O_2 \rightarrow O(^3P) + O_2(^1\Sigma)$.
(e) Fluorescence following broadband excitation in an integrating sphere.

Preferred Values

$k = 4.1 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} for M = O_2 at 298 K.
$k = 2.1 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} for M = N_2 over the temperature range 200-350 K.
$k = 8.0 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} for M = $O(^3P)$ at 298 K.
$k = 4.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} for M = H_2O at 298 K.
$k = 4.1 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} for M = CO_2 over the temperature range 245-360 K.

Reliability

$\Delta\log k = \pm0.3$ for M = O_2, $O(^3P)$ and H_2O at 298 K.
$\Delta\log k = \pm0.10$ for M = N_2, CO_2 at 298 K.
$\Delta(E/R) = \pm200$ K for M = N_2, CO_2.

Comments on Preferred Values

The preferred value for $k(M=O_2)$ is based on the data of Thomas and Thrush,[1] Martin *et al*.,[2] Lawton *et al*.,[3] Chatha *et al*.[4], Knickelbein *et al*.[14] and Kebabian and Freeman.[17] For M = N_2 the value is based on the data of Kohse-Höinghaus and Stuhl,[5] Martin *et al*.,[2] Chatha *et al*.,[4] Choo and Leu,[13] Wildt *et al*.[15] and Shi and Barker.[16] The value of Slanger and Black[6] is adopted for M = $O(^3P)$ and the value of Thomas and Thrush[1] for M = H_2O. For $k(M = CO_2)$ the results of Choo and Leu,[13] Filseth *et al*.,[7] Noxon,[8] Davidson *et al*.,[9] Avilés *et al*.,[10] Muller and Houston,[11] Borrell *et al*.,[12] Wildt *et al*.[15] and Shi and Barker[16] are used.

References

1. R. G. O. Thomas and B. A. Thrush, J. Chem. Soc. Faraday Trans. 2, **71**, 664 (1975).
2. L. R. Martin, R. B. Cohen, and J. F. Schatz, Chem. Phys. Lett. **41**, 394 (1976).
3. S. A. Lawton, S. E. Novick, H. P. Broida, and A. V. Phelps, J. Chem. Phys. **66**, 1381 (1977).
4. J. P. S. Chatha, P. K. Arora, S. M. T. Nalini Raja, P. B. Kulkarni, and K. G. Vohra, Int. J. Chem. Kinet. **11**, 175 (1979).
5. K. Kohse-Höinghaus and F. Stuhl, J. Chem. Phys. **72**, 3720 (1980).
6. T. G. Slanger and G. Black, J. Chem. Phys. **70**, 3434 (1979).
7. S. V. Filseth, A. Zia, and K. H. Welge, J. Chem. Phys. **52**, 5502 (1970).
8. J. F. Noxon, J. Chem. Phys. **52**, 1852 (1970).
9. J. A. Davidson, K. E. Kear, and E. W. Abrahamson, J. Photochem. **1**, 307 (1972/73).
10. R. G. Avilés, D. F. Muller, and P. L. Houston, Appl. Phys. Lett. **37**, 358 (1980).
11. D. F. Muller and P. L. Houston, J. Phys. Chem. **85**, 3563 (1981).
12. P. M. Borrell, P. Borrell, and K. R. Grant, J. Chem. Phys. **78**, 748 (1983).
13. K. Y. Choo and M.-T. Leu, Int. J. Chem. Kinet. **17**, 1155 (1985).
14. M. B. Knickelbein, K. L. Marsh, O. E. Ulrich, and G. E. Busch, J. Chem. Phys. **87**, 2392 (1987).
15. J. Wildt, G. Bednarek, E. H. Fink, and R. P. Wayne, Chem. Phys. **122**, 463 (1988).
16. J. Shi and J. R. Barker, Int. J. Chem. Kinet. **22**, 1283 (1990).
17. P. L. Kebabian and A. Freeman, J. Phys. Chem. A **101**, 7765 (1997).