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

This data sheet updated: 2nd October 2001.

$$O_2(^1\Delta_g) + M \rightarrow O_2(^3\Sigma_g^-) + M$$

ΔH° = -94.3 kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	M		Reference	Technique/ Comments
Absolute Rate Coefficients				
(1.51 ± 0.05) x 10^{-18}	O_2	298	Borrell, Borrell and Pedley, 1977[1]	DF-CL (a)
(1.47 ± 0.05) x 10^{-18}	O_2	298	Leiss *et al*., 1978[2]	(b)
(1.65 ± 0.07) x 10^{-18}	O_2	298	Raja, Arora and Chatha, 1986[3]	DF-CL (a)
3.15 x 10^{-18} exp(-205/T)	O_2	100-450	Billington and Borrell, 1986[4]	DF-CL (a)
1.57 x 10^{-18}		298		
1.4 x 10^{-19}	N_2	300	Collins, Husain and Donovan, 1973[5]	FP-VUVA (c)
5.6 x 10^{-18}	H_2O	298	Findlay and Snelling, 1971[6]	(d)
<1.5 x 10^{-20}	CO_2	298		
(4 ± 1) x 10^{-18}	H_2O	298	Becker, Groth and Schurath, 1971[7]	(e)

Comments

(a) Discharge flow system. $O_2(^1\Delta)$ was monitored by dimol emission at 634 nm or from $O_2(^1\Sigma)$ emission at 762 nm.
(b) Large static reactor. $O_2(^1\Delta)$ was monitored by emission at 1.27 μm.
(c) O_2 ($^1\Delta$) was detected by time-resolved absorption at 144 nm.
(d) Flow system, with photolysis of C_6H_6-O_2 mixtures at 253.7 nm to produce $O_2(^1\Delta)$. $O_2(^1\Delta)$ was measured by 1.27 μm emission.
(e) As (b) but using dimol emission at 634 nm.

Preferred Values

k = 1.6 x 10^{-18} cm^3 molecule^{-1} s^{-1} for M = O_2 at 298 K.
k = 3.0 x 10^{-18} exp(-200/T) cm^3 molecule^{-1} s^{-1} for M = O_2 over the temperature range 100-450 K.
$k \leq$1.4 x 10^{-19} cm^3 molecule^{-1} s^{-1} for M = N_2 at 298 K.
k = 5 x 10^{-18} cm^3 molecule^{-1} s^{-1} for M = H_2O at 298 K.

$k \leq 2 \times 10^{-20}$ cm^3 molecule^{-1} s^{-1} for M = CO_2 at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ for M = O_2 at 298 K.

$\Delta(E/R) = \pm 200$ K for M = O_2.

$\Delta \log k = \pm 0.3$ for M = H_2O at 298 K.

Comments on Preferred Values

The preferred value for k(M = 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=N_2) is based on the data of Collins *et al*.,[5] for k(M = H_2O) on the data of Findlay and Snelling[6] and Becker *et al*.,[7] and for k(M = CO_2) on the data of Leiss *et al*.[2] and Findlay and Snelling.[6]

References

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3 N. Raja, P. K. Arora, and J. P. S. Chatha, Int. J. Chem. Kinet. **18**, 505 (1986).

4 A. P. Billington and P. Borrell, J. Chem. Soc. Faraday Trans. 2, **82**, 963 (1986).

5 R. J. Collins, D. Husain, and R. J. Donovan, J. Chem. Soc. Faraday Trans. 2, **69**, 145 (1973).

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