IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox10

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$$O_2(^1\Sigma_g^+) + O_3 \rightarrow 2O_2 + O \quad (1)$$
$$\rightarrow O_2(^1\Delta_g) + O_3 \quad (2)$$
$$\rightarrow O_2(^3\Sigma_g^-) + O_3 \quad (3)$$

$\Delta H^\circ(1) = -50.4$ kJ·mol^{-1}
$\Delta H^\circ(2) = -62.6$ kJ·mol^{-1}
$\Delta H^\circ(3) = -156.9$ kJ·mol^{-1}

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

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
(2.5 ± 0.5) x 10^{-11}	295	Gilpin, Schiff and Welge, 1971[1]	FP-CL (a)
(2.3 ± 0.5) x 10^{-11}	295	Snelling, 1974[2]	FP (a)
(2.2 ± 0.2) x 10^{-11}	300	Slanger and Black, 1979[3]	(a) (b)
(1.8 ± 0.2) x 10^{-11}	295	Amimoto and Wiesenfeld, 1980[4]	FP-RA
(2.2 ± 0.3) x 10^{-11}	295-361	Choo and Leu, 1985[5]	DF-CL (c)
(1.96 ± 0.09) x 10^{-11}	300	Shi and Barker, 1990[6]	PLP-CL (d)
(2.06 ± 0.22) x 10^{-11}	300	Turnipseed *et al*., 1991[7]	PLP-RF (e)

Comments

(a) $O_2(^1\Sigma_g^+)$ detected in emission.
(b) Flow system with $O_2(^1\Sigma_g^+)$ being produced by the modulated photolysis of O_2 at 147.0 nm to produce $O(^1D)$ atoms, followed by $O(^1D) + O_2 \rightarrow O(^3P) + O_2(^1\Sigma_g^+)$.
(c) Negligible temperature dependence was observed, with $E/R < \pm 300$ K.
(d) $O_2(^1\Sigma_g^+)$ generated by the reaction $O(^1D) + O_2 \rightarrow O + O_2\ (^1\Sigma_g^+)$, with $O(^1D)$ atoms being produced from 308 nm pulsed laser photolysis of O_3.
(e) Rate coefficient for global reaction of $O_2(^1\Sigma_g^+)$ with O_3 was derived by modeling the temporal behavior of $O(^3P)$ and $O(^1D)$ atoms.

Preferred Values

$k = 2.2 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 295-360 K.
$k_1 = 1.5 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.06$ at 298 K.
$\Delta \log k_1 = \pm 0.10$ at 298 K.
$\Delta(E/R) = \pm 300$ K.

Comments on Preferred Values

The preferred value at 298 K is based on all of the studies cited in the table,[1-7] which show very good agreement at room temperature. The temperature independence reported in the study of Choo and Leu[5] is adopted in the evaluation. Channel (1) accounts for 70 ± 20% of the total reaction.[3,4]

References

1 R. Gilpin, H. I. Schiff, and K. H. Welge, J. Chem. Phys. **55**, 1087 (1971).
2 D. R. Snelling, Can. J. Chem. **52**, 257 (1974).
3 T. G. Slanger and G. Black, J. Chem. Phys. **70**, 3434 (1979).
4 S. T. Amimoto and J. R. Wiesenfeld, J. Chem. Phys. **72**, 3899 (1980).
5 K. Y. Choo and M.-T. Leu, Int. J. Chem. Kinet. **17**, 1155 (1985).
6 J. Shi and J. R. Barker, Int. J. Chem. Kinet. **22**, 1283 (1990).
7 A. A. Turnipseed, G. L. Vaghjiani, T. Gierczak, J. E. Thompson, and A. R. Ravishankara, J. Chem. Phys. **95**, 3244 (1991).