IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox4

This data sheet updated: 2nd October 2001.

$$O(^1D) + O_3 \rightarrow O_2 + 2O(^3P) \quad (1)$$
$$\rightarrow O(^3P) + O_3 \quad (2)$$
$$\rightarrow 2O_2(^1\Delta_g) \quad (3)$$
$$\rightarrow O_2(^1\Sigma_g^+) + O_2(^3\Sigma_g^-) \quad (4)$$
$$\rightarrow 2O_2(^3\Sigma_g^-) \quad (5)$$

ΔH° = -83.2 kJ·mol^{-1}
ΔH° = -189.7 kJ·mol^{-1}
ΔH° = -393.0 kJ·mol^{-1}
ΔH° = -424.7 kJ·mol^{-1}
ΔH° = -581.6 kJ·mol^{-1}

Rate coefficient data ($k = k_1 + k_2 + k_3 + k_4 + k_5$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
(2.4 ± 0.5) x 10^{-10}	103-393	Streit *et al*., 1976[1]	(a)
(2.5 ± 0.5) x 10^{-10}	300	Amimoto *et al*., 1978[2]; 1980[3]	PLP-RA (b)
(2.28 ± 0.23) x 10^{-10}	298	Wine and Ravishankara, 1981[4]	PLP-RF (b)
(2.5 ± 0.2) x 10^{-10}	298	Greenblatt and Wiesenfeld, 1983[5]	PLP-RF (b)
Branching Ratios			
$k_1/(k_3 + k_4 + k_5) = 1$	~298	Davenport *et al*., 1972[6]	FP-RF (b)
$k_1/k = 0.53$ $k_5/k = 0.47$	298	Cobos, Castellano, and Schumacher, 1983[7]	(c)

Comments

(a) $O(^1D)$ atoms produced by flash photolysis of O_3 in a flow system and detected by emission at 630 nm.

(b) The product $O(^3P)$ atoms were detected by resonance absorption[2,3] or resonance fluorescence.[4,5]

(c) Steady-state photolysis of pure O_3 and O_3-inert gas mixtures. Ozone removal was monitored manometrically at high pressures and spectrophotometrically at lower pressures. The quantum yield of O_3 removal was interpreted in terms of a complex reaction scheme.

Preferred Values

$k = 2.4 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 100-400 K.
$k_1/k = k_5/k = 0.5$ at 298 K.

Reliability

$\Delta \log k = \pm 0.05$ over the temperature range 100-400 K.
$\Delta k_1/k = \Delta k_5/k = \pm 0.1$ at 298 K.

Comments on Preferred Values

The recommendation for the rate coefficient is based on the data of Streit *et al*.,[1] Amimoto *et al*.,[2,3] Wine and Ravishankara[4] and Greenblatt and Wiesenfeld.[5] The branching ratios are based on these studies plus the work of Davenport *et al*.[6] and Cobos *et al*.[7]

References

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