

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox1 I.A1.1

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$$\Delta H^\circ = -106.5 \text{ kJ}\cdot\text{mol}^{-1}$$

Low-pressure rate coefficients Rate coefficient data

$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$6.75 \times 10^{-35} \exp[(635 \pm 18)/T]$	262-319	Arnold and Comes, 1979	FP-RA
[O ₂]			
$(5.69 \pm 0.40) \times 10^{-34}$	298		
$1.82 \times 10^{-35} \exp[(995 \pm 37)/T]$	262-309		
[N ₂]			
$(5.13 \pm 0.60) \times 10^{-34}$	298		
$(6.9 \pm 1.0) \times 10^{-34}$	219-368	Klais et al., 1980	FP-RF
$(T/300)^{-(1.25 \pm 0.2)}$ [O ₂]			
$(6.2 \pm 0.9) \times 10^{-34}$	219-368		
$(T/300)^{-(2.0 \pm 0.5)}$ [N ₂]			
$(5.69 \pm 0.34) \times 10^{-34}$	227-353	Lin and Leu, 1982	FP-RF
$(T/300)^{-(2.37 \pm 0.37)}$ [O ₂]			
$(5.70 \pm 0.19) \times 10^{-34}$	218-366		
$(T/300)^{-(2.62 \pm 0.18)}$ [N ₂]			
$5.5 \times 10^{-34} (T/300)^{-2.6}$ [N ₂]	100-400	Hippler et al., 1990	PLP-UVA (a)
$5.2 \times 10^{-35} (T/1000)^{-1.3}$ [N ₂]	700-900		
$(6.5 \pm 1.1) \times 10^{-34}$ [N ₂]	296	Anderson et al., 1997	(b)

Comments

- (a) The O₃ product was monitored by UV absorption at 265 nm. Data for $T > 400$ K are based on dissociation experiments. The reaction is suggested to follow the energy transfer mechanism at high temperatures. The strong temperature dependence observed for low temperatures suggests that here a radical-complex mechanism dominates. Anomalous pressure dependences of the reaction are observed at pressures above 1 bar.

- (b) Steady-state photolysis of O₂ near 200 Torr monitoring O₃ absorption at 254 nm and following isotopic compositions by molecular beam mass spectrometric sampling. Isotope effects with ¹⁶O and ¹⁸O resolved.

Preferred Values

$k = 1.4 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in 1 bar of N₂ at 300 K.

$k_0 = 6.0 \times 10^{-34} (T/300)^{-2.6} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 200-300 K.

Reliability

$\Delta \log k_0 = \pm 0.05$ at 298 K.

$\Delta n = \pm 0.5$.

Comments on Preferred Values

The preferred values at 300 K are taken from Arnold et al. (1979), Klais et al. (1980), Lin and Leu (1982), Hippler et al., (1990) and from the detailed analysis of earlier results given by Luther et al. (2005). The temperature coefficients are from Hippler et al. (1990). The analysis of ozone recombination and dissociation data as well as theoretical treatments given by Luther et al. (2005) and Ivanov and Schinke (2006) confirm the presence of a radical-complex mechanism in addition to the energy-transfer mechanism such as suggested by Hippler et al. (1990). Luther et al. (2005) specify the respective contributions over the temperature range 80-1600 K. The preferred temperature dependences are only valid over the indicated temperature range.

References

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