

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx1 I.A3.31

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$$\Delta H^\circ = -306.2 \text{ kJ}\cdot\text{mol}^{-1}$$

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>			
$1.55 \times 10^{-32} \exp[(584 \pm 35)/T] [\text{N}_2]$	217-250	Whytock et al., 1976	FP-RF
$(1.18 \pm 0.15) \times 10^{-31} (T/300)^{-1.82} [\text{N}_2]$			
$8.8 \times 10^{-32} (T/300)^{-1.44} [\text{N}_2]$	200-370	Schieferstein et al., 1983	FP-CL

Preferred Values

$k = 2.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ in 1 bar of N_2 at 300 K.

$k_0 = 1.0 \times 10^{-31} (T/300)^{-1.6} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 200-300 K.

Reliability

$\Delta \log k_0 = \pm 0.1$ at 298 K.

$\Delta n = \pm 0.3$.

Comments on Preferred Values

The preferred values are based on the data from Whytock et al. (1976) and Schieferstein et al. (1983), combined with measurements from Yarwood et al. (1991), Michael et al. (1976), Atkinson et al. (1977), Anderson and Stephens (1979), and Umemoto et al., (2001), and the relative efficiencies determined in Schieferstein et al. (1983).

High-pressure rate coefficients Rate coefficient data

$k_\infty/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$5 \times 10^{-11} (T/300)^{-0.3}$	200-400	Hippler et al., 1999	LP-A (a)
<i>Relative Rate Coefficients</i>			
$3 \times 10^{-11} (T/300)^{0.3}$	200-300	Hippler et al., 1975	P (b)

Comments

- (a) Measurements between 2 and 200 bar of N₂. Oxygen atoms from laser flash photolysis of N₂O at 193 nm, NO₂ detected by light absorption at 405 nm. Falloff curves constructed with $F_c = 0.85$.
- (b) Steady-state photolysis of NO₂-NO mixtures between 1 and 1000 bar of N₂ with analysis of NO₂ photolysis quantum yields. Falloff curve evaluated with $F_c = 0.85$.

Preferred Values

$k_\infty = 5 \times 10^{-11} (T/300)^{-0.3} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 200-400 K.

Reliability

$\Delta \log k_\infty = \pm 0.1$ over the temperature range 200-400 K.

$\Delta n = \pm 0.2$.

Comments on Preferred Values

The results from Hippler et al., (1999) are in good agreement with theoretical data from Harding et al. (1999) and measurements of vibrational relaxation rates for NO($v=1$) + O \rightarrow NO($v=0$) + O from Fernando and Smith (1979). Falloff curves are represented with $F_c = 0.85$ independent of the temperature.

References

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