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

This datasheet last evaluated: November 2017; last change in preferred values: June 2012

$O + NO + M \rightarrow NO_2 + M$

$\Delta H° = -306.2$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.55 \times 10^{-32} \exp[(584 \pm 35)/T]$ [N_2]	217-250	Whytock et al., 1976	FP-RF
$(1.18 \pm 0.15) \times 10^{-31} (T/300)^{-1.82}$ [N_2]			
$8.8 \times 10^{-32} (T/300)^{-1.44}$ [N_2]	200-370	Schieferstein et al., 1983	FP-CL

Preferred Values

$k = 1.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} in 1 bar of N_2 at 300 K.
$k_0 = 1.0 \times 10^{-31} (T/300)^{-1.6}$ [N_2] cm^3 molecule^{-1} 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_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$5 \times 10^{-11} (T/300)^{-0.3}$	200-400	Hippler et al., 1999	LP-A (a)
Relative Rate Coefficients			
$3 \times 10^{-11} (T/300)^{0.3}$	200-300	Hippler et al., 1975	P (b)

Comments

(a) Measurements between 2 and 200 bar of N_2. Oxygen atoms from laser flash photolysis of N_2O at 193 nm, NO_2 detected by light absorption at 405 nm. Falloff curves constructed with $F_c = 0.85$.
(b) Steady-state photolysis of NO_2-NO mixtures between 1 and 1000 bar of N_2 with analysis of NO_2 photolysis quantum yields. Falloff curve evaluated with $F_c = 0.85$.

Preferred Values

$k_\infty = 5 \times 10^{-11} (T/300)^{-0.3}$ cm^3 molecule^{-1} 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.

Preferred Values

Parameter	Value	T/K
k_0/cm^3 molecule^{-1} s^{-1}	$1.0 \times 10^{-31} (T/300)^{-1.6}$ [N_2]	200-300
k_∞/cm^3 molecule^{-1} s^{-1}	$5 \times 10^{-11} (T/300)^{-0.3}$	200-400
k(1 bar N_2)/cm^3 molecule^{-1} s^{-1}	1.5×10^{-12}	300
F_c	0.85	200-400
Reliability		
$\Delta \log k_0$	± 0.1	298
Δn_0	± 0.3	200-300
$\Delta \log k_\infty$	± 0.1	298
Δn_∞	± 0.2	200-400

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of k:

=((1.0e-31*(T/300)^-1.6)*M*(5e-11*(T/300)^-0.3))/((1.0e-31*(T/300)^-1.6)*M+(5e-11*(T/300)^-0.3))*10^(log10(0.85)/(1+(log10((1.0e-31*(T/300)^-1.6)*M/(5e-11*(T/300)^-0.3))/(0.75-1.27*log10(0.85)))^2))

The molecular density, M = 7.243×10^{21}P(bar)/T(K)

References

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