IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx12 I.A3.42

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

$HO + NO + M \rightarrow HONO + M$

$\Delta H° = -207.0\ kJ \cdot mol^{-1}$

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.1 \pm 0.1) \times 10^{-30}$ [N_2]	293	Burrows et al., 1983	DF-RF
$(7.0 \pm 2.0) \times 10^{-31}(T/300)^{-(2.6 \pm 0.3)}$ [N_2]	90-220	Atkinson and Smith, 1994	DF-LIF (a)
$8.9 \times 10^{-31} (T/298)^{-2.1}$ [N_2]	23-301	Sharkey et al., 1994	PLP-LIF (b)
$(0.93 \pm 0.02) \times 10^{-30}$ [N_2]	298	Liessmann et al., 2011	FP-LIF (c)
$(5.4 \pm 0.78) \times 10^{-30}$ [N_2]	135		
$(6.44 \pm 0.78) \times 10^{-30}$ [N_2]	116		

Comments

(a) HO radicals were generated by a cold cathode discharge and detected by LIF. The experiments were carried out in a supersonic expansion at total pressures corresponding to 10^{16} to 10^{18} molecule cm^{-3}.
(b) Experiments were carried out in a cryogenically cooled cell and in a supersonic expansion. At 52 K, rate coefficients have been determined at total gas densities from 5.1×10^{16} to 8.2×10^{17} molecule cm^{-3}.
(c) Flow tube (298 K) and Laval nozzle (61 – 135 K) experiments. Enhancement of the reaction by added water.

Preferred Values

$k = 9.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} in 1 bar of N_2 at 300 K.
$k_0 = 7.4 \times 10^{-31} (T/300)^{-2.4}$ [N_2] cm^3 molecule^{-1} s^{-1} over the temperature range 200-400 K.

Reliability

$\Delta \log k_0 = \pm 0.10$ at 298 K.
$\Delta n = \pm 0.5$.

Comments on Preferred Values

The preferred values are derived following the analysis given in Forster et al. (1995) of data Burrows et al. (1983), Atkinson and Smith (1994), Sharkey et al. (1994), Anderson and Kaufman (1972), Stuhl and Niki (1972), Morley and Smith (1972), Westenberg and deHaas (1972), Anderson et al. (1974), Howard and Evenson (1974), Harris and Wayne (1975), Atkinson et al (1975), Overend et al. (1976), Anastasi and Smith (1978), and Liessmann et al. (2011) and from measurements of the falloff curve with M=He from Forster et al. (1995), using a theoretical value of F_c = 0.81, and other bath gases from Zabarnick (1993). For measurements of k_0 in the bath gas SF_6, see Pagsberg et al. (1997). Experiments between 60 and 300 K from Liessmann et al. (2011) illustrate a marked influence of M = H_2O on the rate at low temperatures.

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
3.0×10^{-11}	298	Zabarnick, 1993	PLP-LIF (a)
3.3×10^{-11}	298	Forster et al., 1995	PLP-LIF (b)
$3.3 \times 10^{-11}(T/300)^{-0.3}$	250-400	Fulle et al., 1998	PLP-LIF (c)

Comments

(a) Falloff extrapolations with M=Ar and SF_6 at pressures below 1 bar.
(b) Measurements in He up to 200 bar using saturated LIF for detection.
(c) see (b); measurements in the bath gas He over the range 5-150 bar.

Preferred Values

$k_\infty = 3.3 \times 10^{-11} (T/300)^{-0.3}$ cm^3 molecule^{-1} s^{-1}, over the temperature range 200-400 K.

Reliability

$\Delta \log k_\infty = \pm 0.2$ over the temperature range 200-400 K.

Comments on Preferred Values

The preferred values are taken from the determination and analysis of the complete falloff curve from Forster et al. (1995) and Fulle et al. (1998). The falloff curve is represented with calculated F_c (300 K) = 0.81. Measurements at pressures below 1 bar in the low pressure part of the falloff curves from Zabarnick (1993) and Donahue et al. (1997) are consistent with the given representation of the falloff curve.

Preferred Values

Parameter	Value	T/K
k_0/cm^3 molecule^{-1} s^{-1}	7.4 x 10^{-31} (T/300)$^{-2.4}$ [N_2]	200-400
k_∞/cm^3 molecule^{-1} s^{-1}	3.3 x 10^{-11} (T/300)$^{-0.3}$	200-400
k(1 bar N_2)/cm^3 molecule^{-1} s^{-1}	9.7 x 10^{-12}	298
F_c	0.81	200-400
Reliability		
$\Delta\log k_0$	± 0.1	298
Δn_0	± 0.5	200-400
$\Delta\log k_\infty$	± 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*:

=((7.4e-31*(*T*/300)^-2.4)*M*(3.3e-11*(*T*/300)^-0.3))/((7.4e-31*(*T*/300)^-2.4)*M+(3.3e-11*(*T*/300)^-0.3))*10^(log10(0.81)/(1+(log10((7.4e-31*(*T*/300)^-2.4)*M/(3.3e-11*(*T*/300)^-0.3))/(0.75-1.27*log10(0.81)))^2))

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

References

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