IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx27

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This data sheet last evaluated: May 2008 (with no changes to the preferred values).

$NO + NO_3 \rightarrow 2NO_2$

ΔH° = -97.6 kJ mol^{-1}

Rate coefficient data

k / cm3 molecule-1 s-1	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.55 \times 10^{-11} \exp[(195 \pm 39)/T]$	209-299	Hammer et al., 1986	DF-LIF (a)
$(2.95 \pm 0.16) \times 10^{-11}$	299-414		
$1.59 \times 10^{-11} \exp(122/T)$	224-328	Sander and Kircher, 1986	FP-A (b)
$(2.41 \pm 0.48) \times 10^{-11}$	298		
$1.68 \times 10^{-11} \exp[(103 \pm 50)/T]$	223-400	Tyndall et al., 1991	DF-LIF (c)
$(2.34 \pm 0.24) \times 10^{-11}$	298		
$(2.6 \pm 0.2) \times 10^{-11}$	296	Brown et al., 2000	(d)

Comments

(a) Arrhenius behaviour was observed for k over the temperature range 209-299 K, but k was independent of temperature over the range 299-414 K.

(b) [NO_3] was monitored by optical absorption. Total pressure was varied over the range 67- 930 mbar (50-700 Torr) of He and N_2.

(c) NO_3 was produced either by the F + HNO_3 reaction or the NO_2 + O_3 reaction. In these experiments [NO_3] was monitored by LIF in an excess of NO. In other experiments the decay of [NO] in excess NO_3 was monitored by chemiluminescence. The value at 298 K is the mean of the values obtained in these different systems.

(d) NO_3 radicals were generated by pulsed laser photolysis of N_2O_5 at 248 nm in the presence of an excess of NO. and detected by cavity ring-down spectroscopy at wavelengths of 622 nm or 623 nm.

Preferred Values

$k = 2.6 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 1.8 \times 10^{-11} \exp(110/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 220-420 K.

Reliability

$\Delta \log k = \pm 0.1$ at 298 K
$\Delta(E/R) = \pm 100$ K.

Comments on Preferred Values

The preferred value of k at 298 K is the mean of the values reported by Hammer et al. (1986), Sander and Kircher (1986), Tyndall et al. (1991), and Brown et al. (2000), which are in excellent agreement. The preferred value of E/R is the average of the values obtained by Sander and Kircher (1986) and Tyndall et al. (1991). The pre-exponential factor in the Arrhenius expression is adjusted to fit the values of k at 298 K.

References

Brown, S. S., Ravishankara, A. R., and Stark, H.: J. Phys. Chem. A 104, 7044, 2000.

Hammer, P. D., Dlugokencky, E. J., and Howard, C. J.: J. Phys. Chem. 90, 2491, 1986.

Sander, S. P. and Kircher, C. C.: Chem. Phys. Lett. 126, 149, 1986.

Tyndall, G. S., Orlando, J. J., Cantrell, C. A., Shetter, R. E. and Calvert, J. G.: J. Phys. Chem. 95, 4381, 1991.