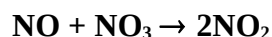


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO<sub>x</sub>27

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

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



$$\Delta H^\circ = -97.6 \text{ kJ mol}^{-1}$$

## Rate coefficient data

k / cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
1.55 x 10 <sup>-11</sup> exp[(195 ± 39)/T]	209-299	Hammer et al., 1986	DF-LIF (a)
(2.95 ± 0.16) x 10 <sup>-11</sup>	299-414		
1.59 x 10 <sup>-11</sup> exp(122/T)	224-328	Sander and Kircher, 1986	FP-A (b)
(2.41 ± 0.48) x 10 <sup>-11</sup>	298		
1.68 x 10 <sup>-11</sup> exp[(103 ± 50)/T]	223-400	Tyndall et al., 1991	DF-LIF (c)
(2.34 ± 0.24) x 10 <sup>-11</sup>	298		
(2.6 ± 0.2) x 10 <sup>-11</sup>	296	Brown et al., 2000	(d)

## Comments

- 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.
- [NO<sub>3</sub>] was monitored by optical absorption. Total pressure was varied over the range 67- 930 mbar (50-700 Torr) of He and N<sub>2</sub>.
- NO<sub>3</sub> was produced either by the F + HNO<sub>3</sub> reaction or the NO<sub>2</sub> + O<sub>3</sub> reaction. In these experiments [NO<sub>3</sub>] was monitored by LIF in an excess of NO. In other experiments the decay of [NO] in excess NO<sub>3</sub> was monitored by chemiluminescence. The value at 298 K is the mean of the values obtained in these different systems.
- NO<sub>3</sub> radicals were generated by pulsed laser photolysis of N<sub>2</sub>O<sub>5</sub> 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

$$k = 2.6 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

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

## Reliability

$$\Delta \log k = \pm 0.1 \text{ at } 298 \text{ K}$$

$$\Delta(E/R) = \pm 100 \text{ K.}$$

### *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.