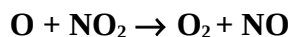


**IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet
NO_x2 I.A3.32**

Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this datasheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr/>.

This datasheet last evaluated: 1st June 2012; last change in preferred values: 1st June 2012.



$$\Delta H^\circ = -192.1 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments/
<i>Absolute Rate Coefficients</i>			
9.3×10^{-12}	296	Slanger et al., 1973	DF-CL (a)
1.05×10^{-11}	240		
$(1.0 \pm 0.1) \times 10^{-11}$	298	Ongstad and Birks, 1984	DF-CL (a)
$6.58 \times 10^{-12} \exp[(142 \pm 23)/T]$	224-354	Ongstad and Birks, 1986	DF-CL (a)
$(1.03 \pm 0.09) \times 10^{-11}$	298		
$5.21 \times 10^{-12} \exp[(202 \pm 27)/T]$	233-357	Geers-Müller and Stuhl, 1987	PLP-CL (b)
$(1.02 \pm 0.02) \times 10^{-11}$	301		
$(9.3 \pm 1.0) \times 10^{-12}$	298	Paulson et al., 1995	PLP-RF (c)
$5.26 \times 10^{-12} \exp[(209 \pm 35)/T]$	220-412	Gierczak et al., 1999	PLP-RF (d)
$(1.06 \pm 0.08) \times 10^{-11}$	298		
$4.21 \times 10^{-12} \exp[(273 \pm 18)/T]$	221-425	Estupiñán et al., 2001	PLP-RF (e)
$1.05 (\pm 0.06) \times 10^{-11}$	298		
$5.64 \times 10^{-12} \exp[(165 \pm 10)/T]$	216-413	Avallone, 2003	DF-RF (f)
$(9.93 \pm 0.19) \times 10^{-12}$	298		
$(9.3 \pm 0.9) \times 10^{-12}$	294	Dillon et al., 2006	PLP-LIF (g)

Comments

- (a) O(³P) atoms were monitored by O + NO chemiluminescence.
- (b) O(³P) atoms were generated by photolysis of NO. O(³P) were monitored by O + NO chemiluminescence. Values for $k(\text{O} + \text{N}_2\text{O}_4)$ and $k(\text{O} + \text{N}_2\text{O}_5)$ were also estimated from the results.
- (c) O(³P) atoms were generated by pulsed laser photolysis of NO₂ at 308 nm. NO₂ concentrations were determined by comparison of the UV absorption in pure NO₂ with that in the He/NO₂ mixtures which were flowed through the photolysis cell.
- (d) O(³P) atoms were generated by pulsed laser photolysis of NO₂ at 308 nm. Three methods were used to determine the NO₂ concentration: (i) UV absorption, (ii) flow measurements based on the drop in pressure from a calibrated volume, (iii) chemical titration using an excess of O₃ to convert a measured flow of NO to NO₂. The UV cross sections used were measured at 413 nm as a function of temperature and combined with those of Harder et al. (1997) with which they are in close agreement.
- (e) Oxygen atoms generated by laser photolysis of NO₂ at 355 nm.

- (f) Oxygen atoms generated by microwave discharge of O₂ and detected by resonance fluorescence.
- (g) LIF spectroscopy of IO in the presence of NO₂, O₃, and CF₃I. Oxygen atoms generated by excimer laser photolysis of O₃ at 248 nm.

Preferred Values

$k = 9.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k = 5.1 \times 10^{-12} \exp(198/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 220-420 K.

Reliability

$\Delta \log k = \pm 0.03$ at 298 K.

$\Delta(E/R) = \pm 80$ K.

Comments on Preferred Values

The preferred value of k at 298 K is the average of the values obtained by Slanger et al. (1973), Ongstad and Birks (1984, 1986), Geers-Müller and Stuhl (1987), Paulson et al. (1995), Gierczak et al. (1999), Estupiñán et al. (2001), Avallone (2003), and Dillon et al. (2006), and the temperature dependence is from an unweighted least squares fit to the data from the same studies (Slanger et al., 1973; Ongstad and Birks, 1984, 1986; Geers-Müller and Stuhl, 1987; Paulson et al., 1995; and Gierczak et al., 1999).

The earlier studies of Davis et al. (1973), and Bemand et al. (1974), are in satisfactory agreement with the other studies but show greater scatter than the more recent studies, and are not used in arriving at our preferred values.

References

- Avallone, L. M.: J. Photochem. Photobiol. A 157, 231, 2003.
- Bemand, P. P., Clyne, M. A. A. and Watson, R. T.: J. Chem. Soc. Faraday Trans. 2 70, 564, 1974.
- Davis, D. D., Herron, J. T. and Huie, R. E.: J. Chem. Phys. 58, 530, 1973.
- Dillon, T. J., Blitz, M. A. and Heard, D. E.: J. Phys. Chem. A 110, 6995, 2006.
- Estupiñán, E. G., Nicovich, J. M. and Wine, P. H.: J. Phys. Chem. A 105, 9697, 2001.
- Geers-Müller R. and Stuhl, F.: Chem. Phys. Lett. 135, 263, 1987.
- Gierczak, T., Burkholder, J. B. and Ravishankara, A. R.: J. Phys. Chem. A 103, 877, 1999.
- Harder, J. W., Brault, J. W., Johnston, P. V. and Mount, G. H.: J. Geophys. Res. 102, 3861, 1997.
- Ongstad, A. P. and Birks, J. W.: J. Chem. Phys. 81, 3922, 1984.
- Ongstad, A. P. and Birks, J. W.: J. Chem. Phys. 85, 3359, 1986.
- Paulson, S. E., Orlando, J. J., Tyndall, G. S. and Calvert, J. G.: Int. J. Chem. Kinet. 27, 997, 1995.
- Slanger, T. G., Wood, B. J. and Black, G.: Int. J. Chem. Kinet. 5, 615, 1973.