## **IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet NOx7**

Website: <a href="http://www.iupac-kinetic.ch.cam.ac.uk/">http://www.iupac-kinetic.ch.cam.ac.uk/</a>. See website for latest evaluated data. Datasheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. This datasheet updated: 9<sup>th</sup> March 2002.

$$O(^{1}D) + N_{2}O \rightarrow N_{2} + O_{2}$$

$$\rightarrow 2NO$$
(1)
(2)

$$\Delta H^{\circ}(1) = -521.0 \text{ kJ} \cdot \text{mol}^{-1}$$
  
 $\Delta H^{\circ}(2) = -340.4 \text{ kJ} \cdot \text{mol}^{-1}$ 

# Rate coefficient data $(k = k_1 + k_2)$

k/cm³ molecule-1 s-1	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $(1.1 \pm 0.2) \times 10^{-10}$ $(1.20 \pm 0.1) \times 10^{-10}$ $(1.17 \pm 0.12) \times 10^{-10}$	204-359 295 298	Davidson <i>et al.</i> , 1977 <sup>1</sup> Amimoto <i>et al.</i> , 1979 <sup>2</sup> Wine and Ravishankara, 1981 <sup>3</sup>	PLP (a) PLP-RA (b) PLP-RF (b)
Branching Ratios $k_2/k = 0.62 \pm 0.02$ $k_2/k = 0.62 \pm 0.09$ $k_2/k = 0.61 \pm 0.08$	298 177-296 296	Marx, Bahe and Schurath, 1979 <sup>4</sup> Lam <i>et al.</i> , 1981 <sup>5</sup> Cantrell, Shetter and Calvert, 1994 <sup>6</sup>	P-GC/CL P-CL (c)

### **Comments**

- (a)  $O(^{1}D)$  atoms were monitored by time-resolved detection of  $O(^{1}D) \rightarrow O(^{3}P)$  emission.
- (b) O(<sup>3</sup>P) atom product monitored.
- (c) Static photolysis of  $N_2O$ - $O_3$  mixtures at  $\lambda$ >240 nm with product analysis by FTIR spectroscopy. The amount of NO formed in reaction (2) was determined from the yield of HNO<sub>3</sub> formed by total oxidation and hydration of  $NO_x$  products, corrected for losses to the wall. The value of  $k_2/k$  obtained from the experimental data was  $0.57 \pm 0.08$ ; the value given in the table was obtained by averaging the experimental value with selected literature data.

#### **Preferred Values**

 $k_1 = 4.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 200-350 K.  $k_2 = 7.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 200-350 K.

## Reliability

$$\Delta \log k_1 = \Delta \log k_2 = \pm 0.1$$
 at 298 K.  
  $\Delta (E_1/R) = (E_2/R) = \pm 100$  K.

### Comments on Preferred Values

The data and recommendation for the branching ratio at room temperature of  $k_2/k = 0.61 \pm 0.08$  given by Cantrell *et al.*<sup>6</sup> are in accord with the earlier results of Marx *et al.*<sup>4</sup> and Lam *et al.*<sup>5</sup> The overall rate coefficient values at room temperature are the average of the results of Davidson *et al.*, Amimoto *et al.*<sup>2</sup> and Wine and Ravishankara, all of which are in close agreement (see also data by Volltrauer *et al.*<sup>8</sup>). The temperature independence reported by Davidson *et al.*<sup>1,7</sup> is accepted.

#### References

- <sup>1</sup> J. A. Davidson, H. I. Schiff, G. E. Streit, J. R. McAfee, A. L. Schmeltekopf, and C. J. Howard, J. Chem. Phys. **67**, 5021 (1977).
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- W. Marx, F. Bahe, and U. Schurath, Ber. Bunsenges. Phys. Chem. 83, 225 (1979).
- <sup>5</sup> L. Lam, D. R. Hastie, B. A. Ridley, and H. I. Schiff, J. Photochem. **15**, 119 (1981).
- <sup>6</sup> C. A. Cantrell, R. E. Shetter, and J. G. Calvert, J. Geophys. Res. **99**, 3739 (1994).
- J. A. Davidson, C. J. Howard, H. I. Schiff and F. C. Fehsenfeld, J. Chem. Phys. 70, 1697 (1979).
- <sup>8</sup> H. N. Volltrauer, W. Felder, R. J. Pirkle, and A. Fontijn, J. Photochem. **11**, 173 (1979).