

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NOx5

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



$$\Delta H^\circ = -356.9 \text{ kJ}\cdot\text{mol}^{-1}$$

Low-pressure rate coefficients Rate coefficient data

$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.8 \pm 0.8) \times 10^{-36} (T/300)^{-0.88}$	220-300	Estupiñán et al., 2002	(a)
<i>Relative Rate Coefficients</i>			
$2.8 \times 10^{-36} [\text{N}_2]$	300	Gaedtke et al., 1973	(b)
$6.5 \times 10^{-37} [\text{N}_2]$	296	Kajimoto and Cvetanovic, 1976	(c)
$(8.8 \pm 3.3) \times 10^{-37} [\text{N}_2]$	298	Maric and Burrows, 1992	(d)

Comments

- Laser flash photolysis of O_3 generating $\text{O}({}^1\text{D})$ and diode laser absorption spectroscopy in a multipass cell detecting N_2O .
- Steady-state photolysis of $\text{O}_3\text{-O}_2$ mixtures at 260 nm in the presence of 1-200 bar of N_2 . The rate of N_2O formation was measured relative to O_3 consumption and analyzed in terms of the ratio $k/k[\text{O}({}^1\text{D}) + \text{O}_3 \rightarrow 2 \text{O}_2]$.
- See comment (b), measurements between 25 and 115 bar.
- Steady-state photolysis of synthetic air at 185 and 254 nm.

Preferred Values

Parameter	Value	T/K
$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.8 \times 10^{-36} [\text{N}_2]$	298
<i>Reliability</i>		
$\Delta \log k_0$	± 0.5	298

Comments on Preferred Values

The slow rate of the reaction, in competition with the fast electronic quenching reaction $O(^1D) + N_2 \rightarrow O(^3P) + N_2$, makes the measurement of the N_2O yield a difficult task. The differences between the various studies reflect this experimental problem. Because of the agreement of the results from Estupiñán et al. (2002) and Gaedtke et al. (1973), these are preferred, however, allowing for a large uncertainty. A theoretical analysis should be made in relation to the thermal decomposition of $N_2O \rightarrow N_2 + O(^3P)$ in the low- and high-pressure ranges.

References

- Estupiñán, E. G., Nicovich, J. M., Li, J., Cunnold, D.M., and Wine, P. H.: *J. Phys. Chem. A* 106, 5880, 2002.
- Gaedtke, H., Glänzer, K., Hippler, H., Luther, K., and Troe, J.: *Proc. Combust. Inst.* 14, 295, 1973.
- Kajimoto, O., and Cvetanovic, R. J.: *J. Chem. Phys.* 64, 1005, 1976.
- Maric, D., and Burrows, J. P.: *J. Photochem. Photobiol. A* 66, 291, 1992.