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

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

$O(^1D) + N_2 + M \rightarrow N_2O + M$

$\Delta H° = -356.9$ kJ·mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.8 \pm 0.8) \times 10^{-36} (T/300)^{-0.88}$	220-300	Estupiñán et al., 2002	(a)
Relative Rate Coefficients			
2.8×10^{-36} [N_2]	300	Gaedtke et al., 1973	(b)
6.5×10^{-37} [N_2]	296	Kajimoto and Cvetanovic, 1976	(c)
$(8.8 \pm 3.3) \times 10^{-37}$ [N_2]	298	Maric and Burrows, 1992	(d)

Comments

(a) Laser flash photolysis of O_3 generating $O(^1D)$ and diode laser absorption spectroscopy in a multipass cell detecting N_2O.
(b) Steady-state photolysis of O_3-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 $k/k[O(^1D) + O_3 \rightarrow 2\ O_2]$.
(c) See comment (b), measurements between 25 and 115 bar.
(d) Steady-state photolysis of synthetic air at 185 and 254 nm.

Preferred Values

$k_0 = 2.8 \times 10^{-36}$ [N_2] cm^3 molecule^{-1} s^{-1} at 298 K.
$\Delta \log k_0 = \pm 0.5$ at 298 K.

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 four studies[1-4] 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.