IUPAC Task Group on Atmospheric Chemicl Kinetic Data Evaluation – Data Sheet NOx20

This data sheet updated: 16th July 2001.

$NH_2 + O_3 \rightarrow$ Products

Rate coefficient data

k / cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate coefficients			
$4.2 \times 10^{-12} \exp[-(1250 \pm 250)/T]$	298-380	Kurusawa and Lesclaux, 1980	FP/LIF
$(6.3 \pm 1.0) \times 10^{-14}$	298		
$(1.2 \pm 0.3) \times 10^{-13}$	298	Bulatov et al., 1980	FP (a,b)
$2.01 \times 10^{-12} \exp[-(710 \pm 50)/T]$	250-358	Hack, Horie, and Wagner, 1981	DF-LIF (b)
$(1.84 \pm 0.16) \times 10^{-13}$	295		
$1.57 \times 10^{-11} \exp[-(1151 \pm 123)/T]$	272-348	Patrick and Golden, 1984	PLP-RA
$(3.25 \pm 0.27) \times 10^{-13}$	298		
$(1.5 \pm 0.3) \times 10^{-13}$	298	Cheskis et al., 1985	PLP-LIF (c)

Comments

(a) [NH_2] monitored by intracavity laser spectroscopy.
(b) Deviation from first order kinetics observed at high O_3 pressures, and interpreted as due to formation of NH_2O, which regenerates NH_2 by reaction with O_3.
(c) The rate coefficients of reaction of vibrationally excited NH_2 with O_3 were also measured and found to be a factor of 10 greater than that of NH_2 in its ground vibrational state.

Preferred Values

$k = 1.7 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 4.9 \times 10^{-12} \exp(-1000/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 250-380 K.

Reliability

$\Delta \log k = \pm 0.5$ at 298 K.
$\Delta(E/R) = \pm 500$ K.

Comments on Preferred Values

The reported rate coefficients at 298K vary by a factor of 5. There is no convincing argument for rejecting any of the studies and, therefore, the preferred rate coefficient at 298 K is taken as the average of the results of Kurasawa and Lesclaux (1980), Bulatov et al. (1980), Hack et al. (1981), Patrick and Golden (1984) and Cheskis et al. (1985). The temperature dependence of k is obtained by averaging the values of Kurasawa and Lesclaux (1980), Hack et al. (1981) and Patrick and Golden (1984). Although the products of the reaction have not been characterized, the most likely process is transfer of an oxygen atom to form $NH_2O + O_2$. It has been suggested (Bulatov et al., 1980; Hack et al., 1981) that NH_2 may be regenerated by reaction with O_3, but the study of Patrick and Golden (1984) indicates that this reaction must be slow.

References

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Hack, W., Horie, O. and Wagner, H. Gg.: Ber. Bunsenges. Phys. Chem., 85, 72, 1981.

Kurasawa, H. and Lesclaux, R.: Chem. Phys. Lett., 72, 437, 1980.

Patrick, R. and Golden, D. M.: J. Phys. Chem., 88, 491, 1984.