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$O(^3P) + HNO(^1A') \rightarrow NO_2(^2A_1) + H(^2S)$ (1) $\Delta Hr^{298} = -\ 105.3$ kJ mol^{-1} *(Baulch* et al.*, 2005)*

$\rightarrow NO(^2\Pi) + OH(^2\Pi)$ (2) $\Delta Hr^{298} = -\ 227.2$ kJ mol^{-1} *(Baulch* et al.*, 2005)*

$\rightarrow O_2(^3\Sigma_g^-) + NH(^3\Sigma^-)$ (3) $\Delta Hr^{298} = +\ 0.54$ kJ mol^{-1} *(Baulch* et al.*, 2005)*

Rate Coefficient Data $k = k_1 + k_2 + k_3$

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
$k = 3.8 \times 10^{-11}$	242-473	(a) Inomata and Washida.	O-atoms produced in flow-discharge, NH_2 from laser photolysis of NH_3. NH_2 and HNO concentrations followed by photoionisation mass spec.
Reviews and Evaluations			
$k_1 = 1 \times 10^{-12}$	10 – 300	UMIST database	
$k_2 = 6 \times 10^{-11}$	10 – 2500	UMIST database	
k_3 negligible	116 – 300	UMIST database	
$k_1 = 1 \times 10^{-12}$	no T-dependence	OSU website	
$k_2 = 3.8 \times 10^{-11}$	no T-dependence	OSU website	

Comments

The reactions via channels (1) and (2) are strongly exothermic and spin-allowed. It should be noted that HNO is a singlet in its electronic ground state, so the main reaction, (2), is an H-atom abstraction (rather than one proceeding through an adduct). The experimental measurement in (a) seems reliable and provides an overall rate coefficient. There is some theoretical evidence (b) to support the idea that (2) is the dominant channel. Inomata and Washida (a) find no T-dependence over the range studied. The UMIST and OSU data bases assume a very small contribution from channel (1) but the grounds for this are unclear.

Preferred Values

Rate coefficient (10 – 300 K)

k(300 K) = 3.8x10^{-11} cm^3 molecule^{-1} s^{-1}

k(10 K) = 5x10^{-11} cm^3 molecule^{-1} s^{-1}

$k(T) = 3.8\text{x}10^{-11}\ (T/300)^{-0.08}$ cm^3 molecule^{-1} s^{-1}

Branching Ratios

$k_2 / (k_1 + k_2 + k_3) = 1.0$

$k_1 / (k_1 + k_2 + k_3) = k_3 / (k_1 + k_2 + k_3) = 0.0$

Reliability

$\Delta \log k$ (300 K) = ± 0.3

$\Delta \log k$ (10 K) = ± 0.6

$F_0 = 2$; $g = 7$

Comments on Preferred Values

For k(300 K), the value of k measured in (a) is recommended. The T-dependence is hard to predict. I have assumed no barrier and allowed for a small negative T-dependence at lower temperatures.

References

D. L. Baulch *et al.*, J. Phys. Chem. Ref. Data **34**, 575 (2005).

(a) S. Inomata and N. Washida, J. Phys. Chem. *A* **103**, 5023 (1999).

(b) B. Du, W. Zhang, C. Feng and Z. Zhou, J. Mol. Struct., **712**, 101 (2004).