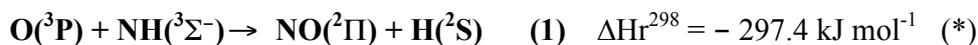


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Rate Coefficient Data $k = k_1 + k_2$

$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T / K	Reference	Comments
<i>Rate Coefficient Measurements</i>			
6.6×10^{-11}	295	Adamson <i>et al.</i> , 1994	(a)
$k_2 < 1.66 \times 10^{-13}$	298	Hack <i>et al.</i> , 1994	(b)
<i>Reviews and Evaluations</i>			
$1.8 \times 10^{-10} \exp(-300/T)$	295 – 3500	Baulch <i>et al.</i> , 2005	(*)
$k(298 \text{ K}) = 6.7 \times 10^{-11}$; $k_2(298 \text{ K}) < 1.7 \times 10^{-13}$			
$k_1 = k_2 = 1.16 \times 10^{-10}$	250 – 3000	UMIST database	
$k_1 = k_2 = 1.16 \times 10^{-10}$	all temperatures	OSU website	

Comments

Channel (1) is strongly exothermic and could occur via the ground (${}^1A'$) state of HNO (and possibly excited states). The reactants correlate with 27 states (${}^5A'$ + $2{}^5A''$, ${}^3A'$ + $2{}^3A''$, ${}^1A'$ + $2{}^1A''$), the products with 8 states (${}^3A'$ + ${}^3A''$, ${}^1A'$ + ${}^1A''$). Therefore, there is an electronic degeneracy factor of *ca.* 8/27.

There are scarcely any kinetic experiments on this reaction. The principal aim in the experiments described in (a) was to find the rate coefficient for O + NH₂. However, the interpretation of the observations to yield the rate coefficient for O + NH is quite direct and appears sound. Hidden in the text the authors propose a branching ratio into channel (2) of 7%. They also refer to an earlier measurement by Wagner's group in fair agreement with their value. Ref. (b) reports a very low branching ratio to channel (2) – in agreement with its lower exothermicity and the notion that reaction may occur *via* HNO.

Preferred Values

Rate coefficients (10 – 300 K)

$$k = k_1(298 \text{ K}) = 6.6 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k = k_1(10 \text{ K}) = 6.6 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_1(T) = 6.6 \cdot 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k_2(298 \text{ K}) = k_2(10 \text{ K}) = \text{zero}$$

Reliability

$$\Delta \log k(300 \text{ K}) = \pm 0.5$$

$$\Delta \log k(10 \text{ K}) = \pm 0.6$$

$$F_0 = 3 ; g = 2.97$$

Comments on Preferred Values

The value recommended for $k = k_1(298 \text{ K})$ is about what one would get by reducing a collisional rate coefficient by the factor of 8/27. I have assumed no temperature-dependence. I also believe that the branching ratio to channel (2) is likely to be small in agreement with the measurement in (b). I don't know where the values in the data bases come from. I recommend values that are lower by a factor of *ca.* 2.

References

- (*) D. L. Baulch *et al.*, J. Phys. Chem. Ref. Data **34**, 575 (2005).
(a) J. D. Adamson *et al.* J. Phys. Chem. **98**, 5665 (1994).
(b) W. Hack, H. Gg. Wagner and A. Zasytkin, Ber. Bunsch. Gesell. **98**, 156 (1994).