Author: Ian Smith (University of Cambridge, UK)

$$H_3^+ + N(^4S°) \rightarrow NH_2^+ + H \qquad (1)$$

$$H_3^+ + N(^4S°) \rightarrow NH^+ + H_2 \qquad (2)$$

Thermodynamic Data

$\Delta H^o_{298}(1) = -98$ kJ mol^{-1} $\Delta H^o_{298}(2) = +82$ kJ mol^{-1}

Sources of thermodynamic data: see ref. 1, 3

Rate Coefficient Data

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
$(4.5 \pm 1.8) \times 10^{-10}$	295 ± 5	Scott *et al.*, 1997[2]	(a)
$< 5 \times 10^{-11}$	295 ± 5	Milligan *et al.*, 2000	(b)
too small to estimate	all temperatures	Bettens and Collins	(c)
Reviews and Evaluations			
this reaction is not included		UMIST database	
1×10^{-17} (i.e., effectively zero)		OSU website	

Comments

(a) Experiments using a selected ion flow tube. Because N_2 reacts rapidly with H_3^+ and the fraction of N atoms produced from N_2 by microwave discharge is small, a relative rate measurement is adopted by measuring the yields of NH_4^+ and N_2H^+.

(b) Measurements made by the same group as in (a) with an improved flowing afterglow/selected ion flow tube apparatus. No evidence was found for the formation of NH_2^+ or NH_3^+ and the upper limit for the rate coefficient was derived. A probable source of error in the earlier experiments was given.

(c) A detailed theoretical study using an *ab initio* potential energy surface and quasiclassical trajectories. NO trajectories leading to $NH_2^+ + H$ were found. The possibility of a non-adiabatic mechanism was discussed and rejected.

Preferred Values

This reaction is too slow to influence chemistry in cold ISCs and can be omitted from models.

Reliability

Comments on Preferred Values

Channel (2) is strongly endothermic. Theory (both Bettens and Collins and earlier work by Herbst *et al.*[4]) were unable to find a low energy path for channel (1). It seems safe to assume that this reaction will not occur in interstellar clouds. Other routes for the formation of NH_3 must exist.

References

[1] G. B. I. Scott, D. A. Fairley, C. G. Freeman and M. J. McEwan, Chem. Phys. Lett. **269**, 88 (1997).
[2] D. B. Milligan, D. A. Fairley and M. J. McEwan, Int. J. Mass Spectrom., **202**, 351 (2000).
[3] R. P. A. Bettens and M. A. Collins, J. Chem. Phys., **109**, 9728 (1998).
[4] E. Herbst, D. J. DeFrees and A. D. Maclean, Astrophys. J. **321**, 898 (1987).

(29.03.11)