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$$N(^4S) + CH(^2\Pi) \rightarrow CN(X^2\Sigma^+) + H(^2S) \qquad (1a)$$

$$\rightarrow CN(A^2\Pi) + H(^2S) \qquad (1b)$$

Thermodynamic Data

$\Delta H^o_{298}(1a) = -414$ kJ mol^{-1} Thermochemical data are taken from ref. (*)

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	*T* / K	Reference	Comments
Rate Coefficient Measurements			
$(2.1 \pm 0.5) \times 10^{-11}$	298	Messing *et al*. 1981	(1)
$(1.66 \pm 0.12) \times 10^{-10}$ (T/298)$^{(-0.09\pm0.2)}$	216 - 584	Brownsword *et al*., 1996	(2)
$(1.4 \pm 0.4)\times 10^{-10}$ (T/298)$^{(0.41\pm0.05)}$	56-296	Daranlot et al, 2013	(3)
Reviews and Evaluations			
$(1.66 \pm 0.12) \times 10^{-10}$ (T/298)$^{(-0.09\pm0.2)}$	222 – 584	UMIST database	
$(1.66 \pm 0.12) \times 10^{-10}$ (T/298)$^{(-0.09\pm0.2)}$	all temperatures	OSU website	

Comments

The reactants correlate with triplet and quintet states, the products with only triplet states. The potential energy surfaces for this reaction are discussed in detail by Rayez et al. (4). A $^3A'$ PES connects the reactants with ground state products (reaction (1a)) and a $^3A''$ PES connects the reactants with CN(B$^2\Pi$) + H (reaction (1b)). Therefore, there is an electronic degeneracy factor of *ca*. 3/8. The reaction probably proceeds *via* energised intermediates (excited triplet states of HCN).

Calculations have been performed (5) using long-range transition state theory (6). The long-range interaction between reactants is assumed to arise from dispersion forces and dipole-induced dipole forces. Spin-orbit effects are ignored and the rotation of CH is treated quasi-classically. The calculated rate constants between 10 and 320 K fit: $k(T) = 1.87 \times 10^{-10}$ (T/298)$^{0.18}$ cm^3 molecule^{-1} s^{-1}. The results in the temperature range covered in the measurements in ref. (3) agree quite well with the experimental values.

The experiments of Brownsword et al. (2) should be reliable. The large values of the observed rate coefficients, and their agreement with the values calculated by long-range transitions state theory, suggest that the reaction rate is determined by capture under the influence of long-range forces. We recommend the calculated rate constant scaled to the experimental results at 298K.

Preferred Values

Between 56 and 300 K :
$k(T) = 1.4 \times 10^{-10} \times$ (T/298)$^{0.41}$ cm^3 molecule^{-1} s^{-1}

Reliability
F = 1.3, g = 4.0

Comments on Preferred Values

The UMIST and OSU data bases adopt the rate coefficients measured by Brownsword et al. (2) – and their *T*-dependence. The reason for the 'low' values reported by Messing et al. (1) is not clear. We recommend the new rate constant obtained in CRESU experiment. For temperatures below 56 K, the rate constant is more uncertain so we introduced a large “g”.

References

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