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$C(^3P) + NH_2(^2B_1)$ → $HCN(X\ ^1\Sigma^+) + H(^2S)$ (1) ΔHr_{298} = − 554 kJ/mol refs (2) and (3)

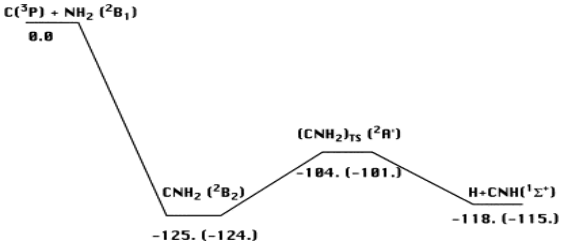
→ $HNC(X\ ^1\Sigma^+) + H(^2S)$ (2) ΔHr_{298} = - 499 kJ/mol refs (2) and (3)

Rate Coefficient Data ($k = k_1 + k_2$)

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
No data was found			
Calculations			
$k = 2.3\ 10^{-10}$	10	Herbst et al. (2000)	
$k = 1.6\ 10^{-10}$	20	Herbst et al. (2000)	
$k = 6.8\ 10^{-11}$	300	Herbst et al. (2000)	
Reviews and Evaluations			
k_1 (T) = 3.26 x 10^{-11} (T/300)$^{-0.36}$	10-300	UMIST database	
k_2 (T) = 3.26 x 10^{-11} (T/300)$^{-0.36}$	10-300	UMIST database	
k_1 (T) = 3.26 x 10^{-11} (T/300)$^{-0.36}$		OSU database	
k_2 (T) = 3.26 x 10^{-11} (T/300)$^{-0.36}$		OSU database	

Comments

To our knowledge no experimental studies have been undertaken to determine rate coefficients for these reactions. The only known reaction rates are from the dynamical calculations of Herbst et al (1). Using the potential energy surface calculated by D. Talbi & Y Ellinger (2) by means of accurate ab initio methods, Herbst et al. (1) have determined the rate coefficients given above. The dynamical study has also revealed that the products (HCN and HNC) are formed with so much excess of energy that efficient isomerization occurs leading to an equal production rate for HNC and HCN from both reactions.



The Energy profiles are for surfaces of doublet multiplicity. Relative energies, given in kcal/mol, have been calculated at the PMP4SDTQ/6-311++G(3df,3pd)//MP2/6-31G(d,p) and CCSD(T)/6-311++G(3df,3pd)//MP2/6-31G(d,p) (numbers in brackets) levels. In all cases, relative energies are corrected for the ZPE and for spin contamination from higher spin state

Preferred Values

Rate coefficient (10 – 300 K)

k_1 (T) = $3\times10^{-11}(T/300)^{-0.2}e^{-6/T}$ cm^3s^{-1}

k_2 (T) = $3\times10^{-11}(T/300)^{-0.2}e^{-6/T}$ cm^3s^{-1}

Reliability

F_0 = 1.5 ; g = 0

Comments on Preferred Values

References

(1) E. Herbst, R. Terzieva and D. Talbi, *MNRAS,* **311**, 869 (2000)

(2) D. Talbi *Chem. Phys. Letters*, **313**, 626 (1999)

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