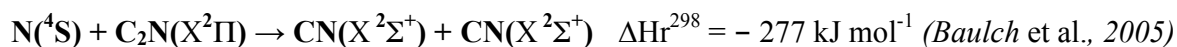


Author:

Ian Smith (University of Cambridge, UK)



Rate Coefficient Data k

$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T / K	Reference	Comments
<i>Rate Coefficient Measurements</i>			
1.0×10^{-10}	300 K	(a)	use the value given to model the time-dependence of CN in their experiments to find k for N + CN. It seems a reasonable value but is not a <i>measurement</i> . I doubt that their fitting is sensitive to the value assumed.
<i>Reviews and Evaluations</i>			
1.0×10^{-10}	10 - 300	UMIST database	
1.0×10^{-10}	no T -dependence	OSU website	

Comments

This radical-radical reaction is strongly exothermic. Reaction is spin-allowed (over triplet PESs). However, the reactants also correlate with quintet PESs.

Comments on Preferred Values

The UMIST and Ohio databases adopt the value given in (a). Despite my reservations about this experiment, I believe that the value they give is a reasonable estimate.

Preferred Values

Rate coefficient (10 – 300 K)

$$k(300 \text{ K}) = 1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k(10 \text{ K}) = 1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

$$k(T) = 1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

Reliability

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

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

$$F_0 = 3 ; g = 2.97$$

References

DL Baulch, CT Bowman, CJ Cobos, RA Cox, T Just, JA Kerr, MJ Pilling, D Stocker, J Troe, W Tsang, RW Walker, J Warnatz: *J. Phys. Chem. Ref. Data* 34 (2005) 757-1397. Thermochemical data for C₂N is evaluated from the paper by Mebel and Kaiser (b).

(a) A. R. Whyte and L. F. Phillips, *Bull. Chem. Soc. Belg.* **92**, 635 (1983); *Chem. Phys. Lett.* **98**, 590 (1983).

(b) A. M. Mebel and R. I. Kaiser, *Ap. J.* **564**, 787 (2002)