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$N(^4S) + C_3(^1\Sigma_g^+) \rightarrow CN(^2\Sigma^+) + C_2(^1\Sigma_g^+); C_2(^3\Pi)$, (1)

Thermodynamic Data

$\Delta H^o_{298}(1) = -54.0$ kJ mol^{-1}; -45.4 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			
No records in the NIST data base			
Reviews and Evaluations			
No information	Baulch *et al.*, 2005	(*)	
1.0×10^{-13}	10 – 300	UMIST database	
1.0×10^{-13}	no *T*-dependence	OSU website	

Comments

This radical-radical reaction is exothermic. Reaction to the ground ($^1\Sigma_g^+$) state of C_2 is spin-forbidden. However, reaction to $C_2(^3\Pi)$ is exothermic and spin-allowed. On the other hand, $N(^4S)$ atoms are generally not reactive to other species in singlet states and C_3 is also not very reactive, even to other radicals such as NO and O_2 (Baulch et al. (*)).

If we consider C_3 to be an 'honorary' unsaturated hydrocarbon, then by the 'rules' proposed by Smith et al. (a), this reaction would be slow (N atoms have a negative electron affinity). In agreement with this conclusion, preliminary *ab initio* calculations (b) suggest that there is barrier of *ca*. 1 eV preventing the addition of $N(^4S)$ to $C_3(^1\Sigma_g^+)$.

It seems that this reaction is probably slow at 298 K and very slow indeed at 10 K. The origin of the values of *k*(*T*) in the UMIST and OSU data bases is unknown.

Preferred Values

$k(298\text{ K}) \leq 1 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}
$k(10\text{ K}) = 0$

Comments on Preferred Values

We adopt the rate coefficient at 298 K given in previous databases as an upper limit. At 10 K, it seems safe to assume that the reaction has a negligible rate.

References

(*) D. L. Baulch *et al.*, J. Phys. Chem. Ref. Data **34**, 575 (2005).
(a) I. W. M. Smith *et al.* Faraday Discuss., **133**, 137 (2006).
(b) J.-C. Loison, unpublished.

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