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$$CNC^+ + e^- \rightarrow CN + C \quad (1a)$$
$$\rightarrow C_2 + N \quad (1b)$$

Thermodynamic Data

$\Delta H^o_{298}(1a) \approx -469$ kJ mol^{-1}

$\Delta H^o_{298}(1b) \approx -317$ kJ mol^{-1}

All thermodynamical data were taken from Ref. [1]. Both reactions are enough exoergic to prevent small errors in the thermodynamic data to affect the viability of the processes.

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
None			
Rate Coefficient Reviews and Evaluations			
$3.0 \times 10^{-7}(T/300)^{-0.5}$	10 – 300	UMIST database	
$3.0 \times 10^{-7}(T/300)^{-0.5}$		OSU website	
Branching Fraction Measurements			
None			
Branching Fraction Reviews and Evaluations			
1(a) = 1	10 – 300	UMIST database and OSU website	
1(b) = 0			

Comments

Two isomers of these ions exist, CCN^+ and CNC^+. Both have comparatively high enthalpies of formation, CNC^+ being the mores stable one by 95 kJ/mol. We therefore limit our discussions to this species.

Albeit no experimental measurements exist for the title reaction, there are several measurements of other ions consisting of three heavier atoms (other than hydrogen). Such studies exist, amongst others for CO_2^+, N_2O^+, SO_2^+ and OCS^+ [2-6]. From the data available for these systems, some conclusions about the behaviour of NCN^+ upon dissociative recombination can be derived.

The dissociative recombination rates of ions containing three ions are often in the range of 3-5 × 10^{-7}cm^{3}s^{-1}. For CO_2 a recent storage ring experiment yielded 4.2 × $10^{-7}(T/300)^{-0.75}$ cm^{3}s^{-1}, which is in agreement with most previous afterglow studies [3,7,8]. Only a storage ring measurements at ASTRID yielded a somewhat higher value [2]. For

N_2O^+ a rate constant k = 3.34 × $10^{-7}(T/300)^{-0.57}$ cm^3s^{-1} was obtained in a CRYRING study, for SO_2^+ the respective figure was k = 4.6 × $10^{-7}(T/300)^{-0.52}$ cm^3 s^{-1}. In the case of OCS^+, the Stockholm team measured a rate constant of 3.5 × $10^{-7}(T/300)^{-0.62}$ cm^3s^{-1}. Only for the ozone cation a higher rate constant of 7.37 ×$10^{-7}(T/300)^{-0.55}$ cm^3s^{-1} was observed [9]. Therefore, we can with some confidence recommend a rate constant of 4 × $10^{-7}(T/300)^{-0.6}$ for the dissociative recombination of CNC^+, applying a somewhat median value for both the rate constant and the thermal coefficient among three-atomic ions.

Some of the ions show a three-body break-up, which is endothermic in the dissociative recombination of CNC^+. In neither the OCS^+ nor the CO_2^+ ion a considerable contribution of the channel leading to ejection of the central ion (producing C+O_2 or C+ SO, respectively) can be found (in OCS^+ the branching fraction of this channel is only 0.03). In the case of CO_2^+, the ring experiments somewhat disagree: in the ASTRID study the C+O_2 pathway shows a branching fraction of 0.09, whereas the CRYRING experiment yielded that this product channel is non-existing. We therefore assume that the branching fraction of the corresponding reaction pathway (N + C_2) in the title reaction does not exceed 0.05, which we recommend as a value.

Recommended rate constant:
k =4.0 × $10^{-7}(T/300)^{-0.6}$$cm^3$ $molecule^{-1}$ s^{-1}

Recommended branching fractions:
(1a) = 0.95
(1b) = 0.05

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