MOLECULAR ORBITAL STUDY OF THE DISSOCIATIVE RECOMBINATION; $HC_3NH^+ + e^-$. IS IT POSSIBLE TO PRODUCE ALL OF ISOMERS OF CYANOACETYLENE?

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The dissociative recombination reaction between HC_3NH^+ and an electron is one of the major route to produce cyanoacetylene, HC_3N, in interstellar clouds. We have studied various pathways of this recombination reaction producing HC_3N and its isomers, HNC_3, HCCNC, and HCNCC, theoretically. Potential energy surfaces for the processes from neutralized HC_3NH are examined by using the *ab initio* molecular orbital method. The calculated result shows that HCCNC is also produced via the isomerization processes in addition to the products HC_3N and HNCCC from the direct hydrogen dissociation. Several product channels C_2H + HNC, C_2H + HCN, NH + C_3H, CN + C_2H_2, C_3 + NH_2 and C_3N + H_2 are shown to be energetically possible based on the thermochemical relationships.