MOLECULAR ORBITAL STUDY OF THE DISSOCIATIVE RECOMBINATION; \( \text{HC}_3\text{NH}^+ + e^- \). IS IT POSSIBLE TO PRODUCE ALL OF ISOMERS OF CYANOACETYLENE?

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The dissociative recombination reaction between \( \text{HC}_3\text{NH}^+ \) and an electron is one of the major route to produce cyanoacetylene, \( \text{HC}_3\text{N} \), in interstellar clouds. We have studied various pathways of this recombination reaction producing \( \text{HC}_3\text{N} \) and its isomers, \( \text{HNC}_3 \), \( \text{HCCNC} \), and \( \text{HCNCC} \), theoretically. Potential energy surfaces for the processes from neutralized \( \text{HC}_3\text{NH} \) are examined by using the \textit{ab initio} molecular orbital method. The calculated result shows that \( \text{HCCNC} \) is also produced via the isomerization processes in addition to the products \( \text{HC}_3\text{N} \) and \( \text{HNCCC} \) from the direct hydrogen dissociation. Several product channels \( \text{C}_2\text{H} + \text{HNC} \), \( \text{C}_2\text{H} + \text{HCN} \), \( \text{NH} + \text{C}_3\text{H} \), \( \text{CN} + \text{C}_2\text{H}_2 \), \( \text{C}_3 + \text{NH}_2 \) and \( \text{C}_3\text{N} + \text{H}_2 \) are shown to be energetically possible based on the thermochemical relationships.