REACTION OF GROUND STATE CARBON ATOM C(3P) WITH DIACETYLENE (HCCCCH) AT ULTRA-LOW TEMPERATURE

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The barrierless reaction of ground-state carbon atom with the simplest polyyne, diacetylene (HCCCCH) are investigated theoretically to explore probable routes, particularly at ultra-low temperature. Three collision complexes are located. The isomerization and dissociation channels for each collision complex are characterized by utilizing the unrestricted B3LYP/6-311G(d,p) level of theory and the CCSD(T)/cc-pVTZ calculations. With facilitation of RRKM and variational RRKM rate constants at collision energies of 0-10 kcal/mol, the most probable paths, thus reaction mechanism, for the titled reactions are determined. Subsequently, the corresponding rate equations are solved numerically that the concentrations of collision complexes, intermediates, and products, v.s. time are obtained. The three reaction cross-sections for formation of the three collision complexes, respectively, are estimated. As a result, the final products and yields identified.