FORMATION OF INTERSTELLAR HCCCCC VIA NEUTRAL-NEUTRAL REACTION OF GROUND STATE CARBON ATOM C(3P) WITH DIACETYLENE (HCCCCH)

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The interstellar reaction of ground-state carbon atom with the simplest polyyne, diacetylene (HCCCCH), is investigated theoretically to explore probable routes to form hydrogen-deficient carbon clusters at ultra-low temperature in cold molecular clouds. The isomerization and dissociation channels for each of the three collision complexes 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, are determined. Subsequently the corresponding rate equations are solved that the evolutions of concentrations of collision complexes, intermediates, and products versus time are obtained. As a result, the final products and yields are identified. This study predicts that three collision complexes, c1, c2, and c3, would produce a single final product, 2,4-pentadiynylidyne, HCCCCC, C5H (p1) + H, via the most stable intermediate, carbon chain HC5H (i4). Our investigation indicates the title reaction is efficient to form astronomically observed 2,4-pentadiynylidyne in cold molecular clouds, where a typical translational temperature is 10 K, via a single, bimolecular gas phase reaction.