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Investigation of reactions of CnH (n = 1 –6) radicals with propyne using synchrotron VUV ionization

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Carbon is the fourth most abundant element in our solar system and in the universe. Hydrocarbon chemistry plays an important role in planetary atmospheres, interstellar environments, and fuel combustions. Thus, the study of dynamics of hydrocarbon reactions can facilitate the understanding of stellar evolution, air pollution, etc. A crossed molecular-beam apparatus combined with synchrotron vacuum-ultraviolet ionization has been demonstrated to be a powerful tool in the investigation of dynamics of elementary chemical reactions. Recently, we have explored the dynamics of C/H and C/X exchanges in the reactions of 3P carbon atoms with ethene (C2H4), vinyl fluoride (C2H3F), vinyl chloride (C2H3Cl), and propene (C3H6) using the crossed molecular-beam apparatus established at NSRRC; X = F, Cl or CH3. The success encourages us to investigate the reactions of hydrocarbon radicals (e.g., CH, C2H, C3H, C4H, C5H, and C6H) with unsaturated hydrocarbons (e.g. C3H4). Those free radicals were produced from a mixture of 1% ethyne (C2H2) seeded in He by pulsed high-voltage discharge. We will present some of the experimental results of the reactions of CnH (n = 1 –6) radicals with propyne (C3H4) leading to product Cn+3H4 + H. The mechanisms of production of methylpolyynes were investigated by interrogating translational-energy distributions, angular distributions, and photoionization spectra of products Cn+3H4. Furthermore, the potential-energy surfaces of reactions CnH + C3H4 -> Cn+3H4 + H were established with ab-initio methods. The combination of crossed-beam experiments and quantum-chemical calculations gives an outline for the mechanisms of reactions of CnH radicals with propyne.

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