Reactions of C_mH (m = 1 – 8) Radicals with Ethyne and Some Related Reactions

Shih-Huang Lee, Yi-Lun Sun, and Wen-Jian Huang

National Synchrotron Radiation Research Center (NSRRC), Hsinch, Taiwan

The dynamics of reactions of C + C_2H_4 [1], C_2 + C_2H_4 [2], C_2 + C_6H_2 [3], and C_3 + C_2H_2 [4] have been investigated in our laboratory. Recently, we are interested in the reactions of hydrocarbon radicals with unsaturated hydrocarbons such as ethyne (C_2H_2) and propyne (C_3H_4). The reactions of C_mH (m = 1 – 8) radicals with C_2H_2 were investigated in crossed-molecular beams by interrogating products $C_{m+2}H_2$. The C_mH radicals were synthesized from 1% C_2H_2/He by pulsed high-voltage discharge. Time-of-flight (TOF) spectra and photoionization-efficiency spectra of $C_{m+2}H_2$ were measured using tunable synchrotron vacuum-ultraviolet (VUV) ionization. Product's translational-energy and angular distributions of the hydrogen-loss channels were derived from the global fitting to product TOF spectra recorded at various laboratory angles. The C_mH (m = 1 – 8) + C_2H_2 reactions can be classified into two types of reactions $C_{2n-1}H$ + C_2H_2 and $C_{2n}H$ + C_2H_2; n = 1 – 4. In the $C_{2n-1}H + C_2H_2 \rightarrow C_{2n+1}H_2 + H$ reaction, singlet *c*-HC_{2n-1}(C)CH and triplet $HC_{2n+1}H$ are the most-possible product isomers justified by the maximal translational-energy release and the photoionization threshold. This work implies the formation of $C_{2n+1}H_2$ from the $C_{2n-1}H$ + C_2H_2 reaction though $C_{2n+1}H_2$ ($n \geq 2$) has yet been discovered in interstellar space and in combustion processes. In the $C_{2n}H + C_2H_2 \rightarrow C_{2n+2}H_2 + H$ reaction, the product $C_{2n+2}H_2$ has an ionization threshold in good agreement with the ionization energy of polyyne ($HC_{2n+2}H$, sometimes called polyacetylene). This work verifies that the $C_{2n}H$ + C_2H_2 reaction is a major source for the formation of various polyacetylenes, e.g., di-, tri-, tetra-, and penta-acetylene, observed in the interstellar medium and in combustion processes. Furthermore, the complementary quantum-chemical calculations indicate that the reactions $C_mH + C_2H_2 \rightarrow C_{m+2}H_2 + H$ have small or negligible entrance barriers in accord with the experimental observations. The reactions of $C_4H + C_4H_2 \rightarrow C_8H_2 + H$, $C_3H + C_6H_2 \rightarrow C_9H_2 + H$, and $C_4H + C_6H_2 \rightarrow C_{10}H_2 + H$ will also be stated in the talk.

References

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