Formation of octatetrayne (HC_8H) from the reaction of butadiynyl (C_4H) with butadiyne (HC_4H)

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Abstract

We investigated the dynamics of reaction $C_4H + C_4H_2 \rightarrow C_8H_2 + H$ by interrogating the time-of-flight (TOF) spectra, the laboratory angular distribution, and the photoionization-efficiency (PIE) spectrum of product C_8H_2.

Reactants C_4H and HC_4H were synthesized from 1% C_2H_2/He in two crossed molecular beams by pulsed high-voltage discharge. We measured the angle-specific time-of-flight spectra and the photoionization-efficiency spectrum of product C_8H_2 using a crossed-molecular-beam quadrupole-mass apparatus and synchrotron vacuum-ultraviolet photoionization. The C_8H_2 product has translational energy stretching to the energetic limit of producing $HC_8H + H$ and has an ionization threshold 9.0 ± 0.1 eV in good agreement with that of HC_8H. The quantum-chemical calculations are in accord with the experimental results. This work demonstrates that octatetrayne can be synthesized from the reaction $C_4H + HC_4H \rightarrow HC_8H + H$.

HC_8H

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