LABORATORY DETECTION OF THE RING-CHAIN MOLECULE C5H2

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The highly polar ring-chain ethynylcyclopropenylidene, C_5H_2 [i.e., c- $C_3H(CCH)$], a carbene with a singlet electronic ground state, has been detected with a Fourier transform molecular beam microwave spectrometer in the same diacetylene-neon discharge in which the linear cumulene carbene H_2C_5 was recently found. Thirteen a and b-type rotational transitions between 6 and 27 GHz were measured to 5 kHz, and precise values of the three rotational constants and two centrifugal distortion constants were determined. The identity of the new molecule as C_5H_2 , already fairly certain because of the close agreement between the measured rotational constants and those calculated ab initio, is conclusively confirmed by detection of the totally deuterated and two partially deuterated isotopic species at exactly the expected isotope shifts. Other isomers of the same elemental composition will also be discussed.