THE STRUCTURE OF CIS-HEX-3-ENE-1,5-DIYNE

ROBB J. WILSON, ROBERT L. KUCZKOWSKI, SEAN A. PEEBLES, Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109-1055, U.S.A.; ROBERT J. HALTER, RYAN L. FIMMEN, ROBERT J. McMAHON, Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706-1396, U.S.A.

The microwave spectrum of seven isotopes of cis-hex-3-ene-1,5-diyne has been observed using a pulsed-nozzle Fourier transform spectrometer. The inertial defect of 0.43 (amu- 3) indicates planarity, as expected for this π -conjugated system. The r_o and r_s structures will be discussed and compared to results from *ab initio* calculations. The evidence for non-linearity in the alkyne arms (CCCH) will be discussed, given that this highly unsaturated molecule is the prototype hydrocarbon which undergoes the Bergman cyclization to benzenoid diradicals.