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


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·Å²) indicates planarity, as expected for this π-conjugated system. The \( r_N \) and \( r_g \) 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.