MICROWAVE SPECTRA OF *cis*-1,3,5-HEXATRIENE AND ITS ^{13}C ISOTOPOMERS; AN r_s SUBSTITUTION STRUCTURE FOR THE CARBON BACKBONE

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Based on the presumed effects of π-electron delocalization, the adjustments in "C=C" and "C-C" bond lengths should increase with increasing length of polyene molecules. Thus, the adjustments in these bond lengths relative to localized bond lengths should increase from butadiene to hexatriene. Despite its weak dipole moment (0.05 D estimate from B3LYP/cc-pVTZ model), microwave spectra have been recorded for *cis*-1,3,5-hexatriene on the FT pulsed-jet broadband and cavity spectrometers at the University of Virginia. The small inertial defect (Δ = 0.16700 uÅ^2) shows that this molecule is planar. Spectra have also been recorded for the three ^{13}C isotopomers in natural abundance on the cavity instrument. An r_s substitution structure of the carbon backbone fitted to ground state rotational constants gives 1.343 Å for the C_1=C_2 bond, 1.457 Å for the C_2-C_3 bond, and 1.335 Å for the C_3=C_4 bond in partial agreement with expectations. After synthesis of deuterium isotopomers of hexatriene and investigation of their microwave spectra, we intend to obtain a semi-experimental equilibrium (r_e) structure for direct comparison with theoretical predictions and full assessment of the structural effects of π-electron delocalization.