

MICROWAVE SPECTRA OF DEUTERIUM ISOTOPOLOGUES OF *cis*-HEXATRIENE

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Several deuterium isotopologues of *cis*-hexatriene have been synthesized in sub-millimole amounts. They include a mixture of the 1,1-d₂, *cis*-1-d₁, and *trans*-1-d₁ species and a sample of the 2-d₁ species. Microwave spectra for *b*-type transitions were observed in the 12-21 GHz range on the jet-beam, mini-cavity FT instrument at Kent State University. *cis*-Hexatriene has a small dipole moment of approximately 0.05 D. For the 1,1-d₂ species, 11 lines were found, and for each of the two 1-d₁ species, 9 lines were observed. For the 2-d₁ species, 10 lines were measured. Ground state rotational constants were fitted to the transitions using quartic centrifugal distortion constants computed with the B3LYP/cc-pVTZ model for each isotopologue. In prior work, rotational constants for the ¹³C species of *cis*-hexatriene were observed in natural abundance.^a Thus, we are close to having sufficient experimental information for determining a semiexperimental equilibrium structure for *cis*-hexatriene. The principal goal is to assess the effect of pi-electron delocalization on the C₆ backbone in comparison with butadiene.

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