MICROWAVE SPECTRA OF DEUTERIUM ISOTOPOLOGUES OF *cis*-HEXATRIENE

NORMAN C. CRAIG, HANNAH A. FUSON, HENGFENG TIAN, and HERMAN VAN BESIEN, *Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074*; ANDREW A. CONRAD AND MICHAEL J. TUBERGEN, *Department of Chemistry, Kent State University, Kent, OH 44242*.

Several deuterium isototopologues of *cis*-hexatriene have been synthesized in sub-millimole amounts. They include a mixture of the 1,1-d_2, *cis*-1-d_1, and *trans*-1-d_1 species and a sample of the 2-d_1 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-d_2 species, 11 lines were found, and for each of the two 1-d_1 species, 9 lines were observed. For the 2-d_1 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 ^{13}C 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 C_6 backbone in comparison with butadiene.

[a] R. D. Suenram, B. H. Pate, A. Lesarri, J. L. Neill, S. Shipman, R. A. Holmes, M. C. Leyden, N. C. Craig J. Phys. Chem. A 113, 1864-1868 (2009).