MICROWAVE SPECTRA OF DEUTERIUM ISOTOPOLOGUES OF \textit{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 isotopologues of \textit{cis}-hexatriene have been synthesized in sub-millimole amounts. They include a mixture of the 1,1-d$_2$, \textit{cis}-1-d$_1$, and \textit{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. \textit{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 \textit{cis}-hexatriene were observed in natural abundance.\footnote{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).} Thus, we are close to having sufficient experimental information for determining a semiexperimental equilibrium structure for \textit{cis}-hexatriene. The principal goal is to assess the effect of pi-electron delocalization on the C$_6$ backbone in comparison with butadiene.