ANALYSIS OF ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF THE *TRANS*-HEXATRIENE-1,1-D_2 AND -*CIS*-1-D_1 SPECIES

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Hexatriene-1,1-d_2 with some admixture of the *cis*-1-d_1 and *trans*-1-d_1 species was synthesized by reaction of 2,4-pentadienal and (methyl-d_3)-triphenylphosphonium iodide (Wittig reagent). The *trans* isomer was isolated by preparative gas chromatography, and the high-resolution (0.0015 cm^{-1}) infrared spectrum was recorded on a Bruker IFS 125HR instrument. The rotational structure in two C-type bands for the 1,1-d_2 species was analyzed. For this species the bands at 902.043 and 721.864 cm^{-1} yielded composite ground state rotational constants of A_0 = 0.801882(1), B_0 = 0.041850(2), and C_0 = 0.039804(1) cm^{-1}. For the *cis*-1-d_1 species the C-type band at 803.018 cm^{-1} gave A_0 = 0.809384(2), B_0 = 0.043530(3), and C_0 = 0.041321(2) cm^{-1}. By iodine-catalyzed isomerization, we have obtained some of the much less favored *cis* isomer and hope to obtain microwave spectra for its three deuterium-substituted species. The rotational constants reported here contribute to data needed for determining a semi-experimental structure for *trans*-hexatriene, which should show that the structural consequences of *pi*-electron delocalization increase with the chain length of polyenes.