ANALYSIS OF ROTATIONAL STRUCTURE IN THREE C-TYPE BANDS IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF *TRANS*-1,3,5-HEXATRIENE

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We seek a semi-experimental equilibrium structure for *trans*-1,3,5-hextatriene, which should show structural evidence for increased pi-electron delocalization in comparison with butadiene. Despite the marginal resolution in the spectrum of *trans*-hexatriene, rotational structure of three C-type bands of trans-hexatriene in the high-resolution infrared spectrum (0.0015 cm^{-1}) has been analyzed as a first step. Strong bands are at 1010.95 and 901.910 cm^{-1}; a weaker band is at 683.45 cm^{-1}. The most extensive analysis was for the band at 901.910 cm^{-1}. The composite fit of 1628 ground state combination differences from the three bands gave the ground state rotational constants of A = 0.8742480(7), B = 0.0446600(10), and C = 0.0425099(8) cm^{-1}. For this near-symmetric top, κ = -0.99483. Procedures for synthesizing needed isotopomers are being explored.