ANALYSIS OF ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF *cis*-1,3,5-HEXATRIENE

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The high-resolution infrared spectrum has been recorded for two C-type bands of *cis*-1,3,5-hexatriene. The resolution (0.0013 $cm^{-1}$) and the Doppler width (0.0012 $cm^{-1}$ at 900 $cm^{-1}$) are barely adequate for observing detailed rotational structure of this heavy molecule in a spectrum recorded at room temperature. An additional complication is the extensive hot band structure arising from excited states of the low frequency C-C torsional modes. A preliminary analysis of rotational structure yielded ${}^{R}R_{K}$ and ${}^{P}P_{K}$ series in each of the two bands, centered at 908 $cm^{-1}$ and 586 $cm^{-1}$. However, ground state combination differences (GSCDs) failed to fit a rotational Hamiltonian. Subsequent microwave spectroscopic measurements gave ground state rotational constants. Reliable GSCDs computed from the ground state rotational constants led to revisions in assignments of some of the sub-band series in the infrared spectrum and to a convincing assignment.