

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

NORMAN C. CRAIG, and MATTHEW C. LEYDEN, *Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074*; TONY MASIELLO, *Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352*.

The high-resolution infrared spectrum has been recorded for two C-type bands of *cis*-1,3,5-hexatriene. The resolution ( $0.0013\text{ cm}^{-1}$ ) and the Doppler width ( $0.0012\text{ cm}^{-1}$  at  $900\text{ cm}^{-1}$ ) 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  $908\text{ cm}^{-1}$  and  $586\text{ cm}^{-1}$ . 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.