MICROWAVE SPECTRA, HEAVY ATOM STRUCTURE, AND AB INITIO CALCULATIONS ON CYCLOPROPYL CARBINOL

REBECCA A. PEEBLES, JOSH J. NEWBY and SEAN A. PEEBLES, *Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920 USA*.

The rotational spectra of the normal and deuterated isotopomers of cyclopropyl carbinol (cyclopropane methanol) have been remeasured with Fourier-transform microwave spectroscopy providing refined rotational and centrifugal distortion constants. The spectra of five additional isotopic species have also been measured, and the resulting inertial data has been used to derive a heavy atom structure in which the H-O-C-C and O-C-C-C dihedral angles both assume gauche conformations. The hydroxyl hydrogen atom interacts with one side of the cyclopropyl ring through an intramolecular hydrogen bond. *Ab initio* calculations at the MP2/6-311+G(d,p) level have given remarkable agreement with the experimental data. Our derived spectroscopic constants are in good agreement with a previous microwave study[a] except that our A rotational constant for the normal isotopic species is about 15 MHz lower than the value reported by Sastry, *et al*. For those transitions falling within the range of our spectrometer we were unable to observe $b-$ and $c-$type lines at the previously reported frequencies, but did locate the transitions between 5 and 16 MHz away. It is possible that the $b-$ and $c-$type assignments in the earlier work belong to an excited vibrational state. The heavy atom structure of this molecule will be presented and compared to *ab initio* results.

[a] A. Bhaumik, W. V. F. Brooks, S. C. Dass and K. V. L. N. Sastry *Can. J. Chem.* **48**, 2949 (1970)