BIOMEMETIC MOLECULES AND INTERNAL ROTOR SPLITTINGS

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Recent improvements and modifications in the NIST Fourier Transform microwave spectrometers now allow us to obtain broad spectral survey scans of low vapor pressure molecules. Typically these surveys can be obtained in unattended overnight scans. We have applied these instruments to the study of a number of biologically relevant molecular systems which contain one or two peptide (HNCO) linkages. These systems serve as fundamental model systems for protein conformations that can be used to test the validity of various theoretical algorithms which are being applied to larger systems.

In addition to the interesting conformational possibilities that arise with these systems, most also exhibit reasonably large spectral splittings that are caused by the one or more methyl tops in the molecules. These methyl tops typically have low barriers ($100cm^{-1}$) to internal rotation if they are attached to the acetyl or N-methyl end of the molecules. We have been successful in using the spectral fitting program, jb95, to fit the AE-states of these molecules within the high-barrier approximation. The geometrical parameters are often obtained with sufficient accuracy to determine the V_3 barriers and rotor axis orientation angles in the principal axis frame. In some cases, this information leads to the assignment of conformational structure. In this talk, we will summarize some of the data obtained for these systems during the past year.