PRELIMINARY RESULTS IN THE MICROWAVE SPECTRUM OF A PEPTIDE MIMETIC: THE ETHYL ACETAMIDOACETATE MOLECULE

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Last year, we presented some theoretical aspects and a newly written program aimed at analyzing the Fourier-transform microwave (FTMW) data taken at NIST for peptide mimetics containing one methyl internal rotor and belonging to the C_1 symmetry group. The first molecule chosen to test the quality of the theoretical method is ethyl acetamidoacetate, CH_3-CH_2-O-C(=O)-CH_2-NH-C(=O)-CH_3. The microwave spectrum between 10 GHz and 20 GHz has been measured and assigned to two different conformers, both exhibiting A and E symmetry states due to the facile internal rotation of the methyl top attached to the carbonyl carbon. The lowest energy conformer (I) for this molecule has a plane of symmetry in its equilibrium C_s configuration, and using the internal rotation RAM program which has now been applied to a number of internal rotors with a plane of symmetry, we have obtained an excellent fit for this conformer. This year, we dedicated our effort to increasing and fitting the data for the higher energy conformer (II), which does not possess a plane of symmetry, and thus requires use of the new program for molecules with C_1 point-group symmetry. Preliminary results for conformer II will be discussed. These results demonstrate that a number of new Hamiltonian terms are required due to the non-planarity of the molecule. The quality of the final fit is limited by the absence of b-type transitions within the E symmetry species.