THE MICROWAVE SPECTRUM OF A PEPTIDE MIMETIC WITH THREE METHYL ROTORS: THE N-ACETYL ALANINE METHYL ESTER MOLECULE

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We report recent progress in measuring, assigning, and fitting the microwave spectrum of the ground torsional states of the methyl ester derivative of alanine dipeptide, $CH_3CONHCH(CH_3)C(O)OCH_3$. This study is part of a project undertaken to determine the conformational structures of various peptide mimetics from the fitted torsion-rotation parameters of the low-barrier methyl tops. Fourier-transform microwave data obtained at NIST between 9 GHz and 18 GHz are fit to an effective torsion-rotation Hamiltonian based on the PAM method and to a global RAM Hamiltonian for one methyl group in a non-planar frame. Torsional rotation splittings from two of the three methyl tops account for most of the observed lines. In addition to the AA-state, two E-states have been assigned and include an AE-state having a V_3 barrier of 400 cm^{-1} and an EA-state having a lower torsional barrier of 68 cm^{-1}. (The two letters indicate the symmetry species of the wave function with respect to the nuclear-permutation-inversion group for each of the two tops). A third set of splittings built off of the EA-state is likely associated with the two remaining EE-states. For each state, the observed-minus-calculated standard deviation for $>$100 assigned lines is $<$4 kHz. These results are derived from fits of individual symmetry species to effective Hamiltonians containing even and odd powers of the rotational angular momentum operators. Rotational transitions within the AA torsional state are thus fit separately from transitions within the AE and EA torsional states. The resulting constants are then compared in pairs, i.e., the (AA,AE) and the (AA,EA) sets, using perturbation theory applied to a one-top rotation-torsion Hamiltonian to determine the barriers and the directions of the methyl rotor axes in the principal axis system. We are presently undertaking fits using the RAM one-top global-fit method and attempting to identify the conformational structure of the molecule through comparisons with ab initio theory.