FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF N-METHYLPROPIONAMIDE

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In order to clarify the dynamical behavior of the peptide bond, we have undertaken a systematic study of ′ peptide molecules ′, which consist of (a) peptide bond(s) with internal-rotation groups at the both ends of the bond(s). In the present investigation we focused attention to the molecule (NMPA) shown in the title, which has an ethyl group (CH_3 of which is referred to as C-CH_3) at the carbonyl side and a methyl group (called N-CH_3) at the amide side, and aimed at unveiling how the two CH_3 groups interact with each other through the peptide bond. We have derived a rotational Hamiltonian including the two CH_3 internal rotations, and have treated the C-CH_3 internal rotation by a conventional PAM, while applying a more sophisticated approach to the N-CH_3 internal rotation. NMPA may be regarded to belong to group G_{18}, even if its skeleton executes large-amplitude ′ out-of-plane ′ motions. The group consists of 6 species: A_1, A_2, E_1, E_2, E_3, and E_4. We have observed and analyzed A_1 (or A_2) and E_2 spectra, but have not detected any lines due to the first excited state of the CH_3CH_2-CO torsion of A_2 symmetry, indicating that the internal-rotation splitting is quite large. The potential barrier to the C-CH_3 internal rotation was determined to be 799 cm^{-1}, which may be compared with that of N-CH_3 of about 81 cm^{-1}. The coupling between the two CH_3's is being analyzed by observing E_1, E_3, and E_4 spectra.