AB INITIO CALCULATION OF THE FIR TORSIONAL SPECTRUM CORRESPONDING TO THE METHYL AND ALDEHYDE TORSION IN STANDARD PROPANAL WITH THE ZPE CORRECTION

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The potential energy function for the simultaneous methyl and aldehyde torsion in propanal was determined with the 6-311(3df,p) basis set at the MP2/RHF level and corrected for the vibrational zero energy point (ZPE) with respect to the remaining vibration modes. With this potential, the kinetic parameters, and the dipole moment variations with the transition, the far infrared (FIR) frequencies and intensities for the methyl and aldehyde torsions were determined theoretically. It is found that the two-dimensional calculation yields not only methyl and aldehyde torsion bands for the cis-conformer, but also furnishes combination bands. Most of these transitions occur in the 220-100 cm^{-1} region and are responsible for the complexity of the spectrum. The results are compared with the previous ones obtained without the ZPE corrections, as well as with the experimental data. A much better agreement is observed.