INFLUENCE OF THE VIBRATIONAL ZERO POINT CORRECTION ON THE AMINE INVERSION BARRIER AND THE FIR SPECTRUM OF METHYLAMINE

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In the present communication the vibrational zero point corrections for the methyl torsion and amine hydrogen wagging potential energy function are determined, and the corresonding spectrum calculated. It is found that the amine inversion barrier increases from 1727 cm^{-1} up to 1850.65 cm^{-1} in better agreement with respect to the value of 1937 cm^{-1} deduced from experiment. In addition, the spitting values obtained for the fundamental band agree fairly well with the experimental data reported in the literature.