THEORETICAL STUDY OF DEUTERATED PROPANAL FIR SPECTRUM APPLYING THE ZERO POINT ENERGY CORRECTION

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In a previous work it has been shown that the Zero Point Energy (ZPE) correction is quite convenient to reproduce more precisely the FIR spectrum of methylamine and propanal. In this work the same procedure has been modified to be applied to the deuterated propanal where de ZPE correction is more imporant to reproduce the experimental spectrum reported. It has to be notice that the CH3 internal rotation motion is the most difficult to reproduce.