DEUTERATED PROPANAL FIR SPECTRUM

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In previous work, the zero point energy correction has been aplied to methylamine and propanal in order to reproduce more properly their FIR spectrum. In this work it will be shown the zero point energy correction applied to diffent deuterated species of propanal, and the FIR spectrum obtained experimentaly is going to be compared with experimental data reported in the literature. It is important to emphazise that the zero point energy correction method that has been used is a parametrized one, in order to improve the HF/(gaussian 98) energy and frequency calculations that have been obtained.