Vibrational spectra and potential energy distributions for 3-cyclopropenecarboxaldehyde by density functional and normal coordinate calculations

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Abstract: The structural stability and internal rotation in 3-cylopropenecarboxaldehyde were: investigated by ab initio calculations with 6-311++G** basis set. The calculations were carried out at the restricted Hartree-Fock (HF) and the Density Functional B3LYP levels. The vibrational frequencies were computed at HF and DFT-B3LYP levels. Normal coordinate calculations were carried out and potential energy distributions were calculated for the cis and the trans conformers of the molecule.