

**Vibrational spectra and potential energy distributions for 3-cyclopropenecarboxaldehyde by density functional and normal coordinate calculations.** Badawi, H. M.; Forner, W

**Abstract**

The structural stability and internal rotation in 3-cyclopropenecarboxaldehyde were studied by ab initio calcns. with 6-311++G\*\* basis set. The calcns. were carried out at the RHF (HF) and the D. Functional B3LYP levels. The vibrational frequencies were computed at HF and DFT-B3LYP levels. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the cis and the trans conformers of the mol.