

**Analysis of vibrational infrared and Raman spectra of 3-cyclopropenecarboxylic acid fluoride by density functional and normal coordinate calculations.** Badawi, Hassan M.; Forner, Wolfgang

### **Abstract**

The structural stability and internal rotation in 3-cyclopropenecarboxylic acid fluoride were investigated by ab initio density functional theory (DFT) calculations with the 6-311++G\*\* basis set. The vibrational frequencies were computed at Hartree-Fock (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. Using the calculated frequencies at the DFT-B3LYP level we plotted vibrational IR and Raman spectra of the molecules.