

Potential energy distribution and vibrational spectra for cyclohexanecarboxaldehyde from ab initio and normal coordinate calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The vibrational frequencies were computed for the title mol. (I) at the Hartree-Fock level of calcns. using 6-311G* basis set. Normal coordinate calcns. were carried out and potential energy distributions among symmetry coordinates were calcd. for the stable gauche and trans conformers of I. Raman and IR spectra of both the individual conformers and the mixt. were computed at 300 K.