Raman and infrared wavenumbers, normal coordinate analyses, barrier to internal rotation and ring inversion in 4-cyclopentenecarboxaldehyde based on ab initio calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The conformational stability of 4-cyclopentenecarboxaldehyde was studied by ab initio calcns. with the 6-311G* basis set. The calcns. were carried out at RHF and 2nd-order Moller-Plesset (MP2) levels. From the calcn., the mol. was predicted to exist as a complex mixt. of both axial and equatorial conformations at ambient temp. The potential function in the equatorial mols. was detd. for the CHO asym. torsion. The vibrational wavenos. were computed at the HF level and the zero-energy corrections were included in the calcd. barrier. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the trans-equatorial and gauche-equatorial conformers of the mol. The calcd. vibrational wavenos. for the 2 conformers were scaled and compared with those obsd. exptl. for similar mols.