

Density functional calculations of vibrational wavenumbers, ring puckering, and asymmetric CHO potential functions for cyclobutanecarboxaldehyde: comparative study between theoretical and experimental spectra. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The structural parameters and energies of the trans-equatorial and gauche-equatorial conformers of cyclobutanecarboxaldehyde c-C₄H₇-CHO were investigated by quantum mech. DFT-B3LYP (D. Functional Theory-Becke 3 exchange and Lee-Yang-Parr correlation functional) calcns. using 6-311G** basis set. The potential functions for the CHO asym. torsion in the equatorial mol. and for the ring puckering inversion were derived. The vibrational wavenumbers were calcd. and the potential energy distributions PED among the symmetry coordinates of the normal modes were computed for the two stable conformers of the mol. The vibrational assignments on the basis of the calcd. PED values were compared to the reported ones from exptl. data. The vibrational IR and Raman spectra of the mixt. of the trans-equatorial and gauche-equatorial were plotted and the line intensities were compared to the corresponding exptl. ones.