Potential energy distributions and potential scans for the internal rotation of two rotors in 3,3-dichloro and 3,3,3-trichloropropanals. Badawi, H. M.; Forner, W

Abstract

The conformational behavior and structural stability of 3,3-dichloropropanal (I) and 3,3,3-trichloropropanal (II) were investigated by ab initio calcns. The 6-311++G** basis set was employed to include polarization and diffuse functions in the calcns. at B3LYP level. From the calcn., the trans conformer of II was predicted to be the predominant conformer with about 2 kcal mol-1 of energy lower than the cis form. Addnl., I was predicted to exist as a mixt. of three stable conformers. The potential function scans were calcd. for the two mols. from which the rotational barriers could be estd. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calcns. for the conformers of the two mols. Raman and IR spectra of the mixt. of the stable conformers were computed at 300 K.