Potential function scans and potential energy distributions for 3-chloro and 3-fluoropropanals. Badawi, H. M.; Forner, W

Abstract

The conformational behavior and structural stability of 3-chloropropanal and 3-fluoropropanal were studied by ab initio calcns. The 6-311++G** basis set was employed to include polarization and diffuse functions in the calcns. at B3LYP level. The compds. were predicted to exist as a complex mixt. of stable conformers. The conformers with min. interaction between the halogen atoms and the carbonyl O were predicted to be the lower energy forms for the two mols. The potential function scans were calcd. from which the rotational barriers could be estd.