

Potential function scans and potential energy distributions for 3-chloro and 3-fluoropropanals

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Abstract: The conformational behavior and structural stability of 3-chloropropanal and 3-fluoropropanal were investigated by ab initio calculations. The 6-311++G** basis set was employed to include polarization and diffuse functions in the calculations at B3LYP level. The compounds were predicted to exist as a complex mixture of stable conformers. The conformers with minimum interaction between the halogen atoms and the carbonyl oxygen were predicted to be the lower energy forms for the two molecules. The potential function scans were calculated from which the rotational barriers could be estimated.