Vibrational infrared and Raman spectra and density functional calculation of C-S rotational barrier in vinylsulfonyl chloride and fluoride. Badawi, H. M.; Forner, W

Abstract

The structure and conformational stability of vinylsulfonyl chloride and fluoride were investigated using ab initio calcns. at DFT-B3LYP/6-311++G** level. From the calcns. the mols. were predicted to exist predominantly in the non-planar gauche conformations with the vinyl C:C group being nearly eclipsing one of the sulfonyl S:O groups as a result of significant conjugation between the two moieties. The asym. potential function for the internal rotation was detd. for the mol. The vibrational frequencies were calcd. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the two mols. in the gauche conformation.