Two-dimensional surface scan and analysis of vibrational spectra of 3,3-difluoropropanal based on ab initio and normal coordinate calculations. Forner, W.; Badawi, H. M

Abstract

The conformational behavior and structure of 3,3-difluoropropanal were investigated by utilizing ab initio calcns. with 6-31G** basis set at RHF, MP2, and B3LYP levels. The mol. was predicted to exist in a complex mixt. of conformers at ambient temps. Two-dimensional single point surface scan for the rotations of both the CHO and CHF2 rotors was calcd. at RHF and MP2 levels. Full optimization was then performed at the possible min. and at the transition states. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calcns. for the three most stable cis-gauche, gauche-cis and gauche-gauche conformers of the mol. Vibrational Raman and IR spectra of the mixt. of the stable conformers were computed at 300 K.