

Theoretical calculation of potential energy distributions and potential functions for the two rotors internal rotation in 2,2,3,3,3-pentafluoropropanal. Badawi, H. M.; Forner, W

Abstract

The conformational behavior and structural stability of 2,2,3,3,3-pentafluoropropanal 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 and MP2 levels. From the calcn., the mol. was predicted to exist in gauche .tautm. cis conformational equil. The potential function scans were calcd. out at B3LYP/6-311++G** level for the mol., from which the rotational barriers were estd. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calcns. for the two stable conformers of 2,2,3,3,3-pentafluoropropanal. Vibrational Raman and IR spectra of the mixt. of the gauche and cis conformers were computed at 300 K.