Theoretical analysis of two rotors internal rotation and vibrational spectra for 2,2,3,3,3-pentafluoropropionyl fluoride. Badawi, Hassan M.; Forner, Wolfgang. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Asian Journal of Spectroscopy (2000), 4(4), 159-171.

Abstract

The conformational behavior and structural stability of 2,2,3,3,3-pentafluoropropionyl fluoride 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 and MP2 levels. From the calcns., the mol. was predicted to exist in Gauche 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 of conformers of 2,2,3,3,3-pentafluoropropionyl fluoride. Vibrational Raman and IR spectra of the mixt. of the gauche and cis conformers were computed at 300 K.