Theoretical calculation of potential energy distributions and potential functions for the two rotors internal rotation in 2,2,3,3,3-pentafluoropropanal

Author(s): Badawi HM, Forner W

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 545 **Pages:** 137-149

Abstract: The conformational behavior and structural stability of 2,2,3,3,3-pentafluoropropanal 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 and MP2 levels. From the calculation, the molecule was predicted to exist in gauche <----> cis conformational equilibrium. The potential function scans were calculated out at B3LYP/6-311 + +G** level for the molecule, from which the rotational barriers were estimated. The vibrational frequencies were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calculations for the two stable conformers of 2,2,3,3,3-pentafluoropropanal. Vibrational Raman and infrared spectra of the mixture of the gauche and cis conformers were computed at 300 K.