

Three rotor potential energy scans, conformational equilibrium constants and vibrational analysis of 3-fluoro-1-propanol CH₂FCH₂CH₂OH. Badawi, Hassan M.; Foerner, Wolfgang; Ali, Shaikh A. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. *Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy* (2008), 69A(1), 263-271.

Abstract

The conformational stability and the three rotor internal rotations in 3-fluoro-1-propanol were investigated by the DFT-B3LYP/6-311 + G** and the ab initio MP2/6-311 + G** levels of theory. The calcd. potential energy curves of the mol. at both levels of theory were consistent with complex conformational equil. of about 12 min., all of which were predicted to have real frequencies at both the B3LYP and the MP2 levels. The lowest energy min. in the potential curves of 3-fluoro-1-propanol was predicted to correspond to the Gauche-gauche-trans (Ggt) conformer in excellent agreement with microwave and electron diffraction results. The equil. consts. for the conformational interconversion of the mol. were calcd. and found to correspond to an equil. mixt. of about 33% Ggt, 14% Ggg1 and 13% Gg1g and about 43% Ggt, 12% Ggg1 and 10% Gg1g distribution by the B3LYP/6-311 + G** and the MP2/6-311 + G** calcns., resp., at 298.15 K. The vibrational frequencies of each mol. in its three stable forms were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calcns. and comparison with exptl. data of the mol.