Ab initio calculations of vibrational frequencies, potential functions of internal rotations and vibrational infrared and Raman spectra for 3,3,3-trifluoropropanal. Forner, Wolfgang; Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Journal of Molecular Modeling (2000), 6(2), 99-111.

Abstract

The conformational behavior and structure of 3,3,3-trifluoropropanal were studied by using ab initio calcns. with the 6-31G** basis set (valence double zeta basis with polarization functions on all atoms) at the restricted Hartree Fock (RHF), 2nd-order Moller-Plesset perturbation (MP2), and D. Functional (B3LYP) levels. The mol. is predicted to have a cis .tautm. gauche conformational equil. Full optimization of the transition states was performed and the rotational barriers of both the CHO and CF3 rotors were calcd. Vibrational frequencies were computed at the 3 levels and the zero-point corrections were included into the calcd. asym. CHO rotational barrier. Complete vibrational assignments were made from normal coordinate calcns. for both stable conformers of the mol.