

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.

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.