

Vibrational frequencies, normal coordinate analyses and potential functions for internal rotations in 3,3,3-trifluoropropionyl fluoride and 3,3,3-trichloropropionyl chloride based on ab initio calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The conformational behavior and structure of 3,3,3-trifluoropropionyl fluoride and 3,3,3-trichloropropionyl chloride were investigated by utilizing ab initio calcns. with 6-31G* basis set at RHF and MP2 levels. The chloride was predicted to exist only in the cis conformation with min. chlorine-chlorine interaction. For the fluoride, the cis conformer was predicted by the two levels to be slightly the lower energy form than the gauche and trans conformations. Full optimization was performed at the transition state of the fluoride and the barrier to internal rotation between the cis and gauche conformers was calcd. The vibrational frequencies were computed at HF level and the zero energy corrections were included into the calcd. barrier. The sym. rotational barrier of each of the CCl₃ and the CF₃ rotors was calcd. Normal coordinate calcns. were carried out and potential energy distributions were calcd. for the stable conformers of the mols.