

Conformational stability and vibrational analyses of 1,1,3-trichloroacetone CHCl₂-CO-CH₂Cl. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Asian Journal of Spectroscopy (2007), 11(1), 23-34.

Abstract

The conformational stability of 1,1,3-trichloroacetone was investigated by DFT-B3LYP/6-311+G** and ab initio MP2/6-311+G** calcns. The calcd. potential energy curves of the mol. at DFT-B3LYP level were consistent with two distinct min. that correspond to cis-cis and gauche-gauche (G-g) conformers in the order of decreasing relative stability. The cis-cis conformation with C_s symmetry was calcd. to have an imaginary frequency and a near cis-cis with C₁ symmetry form was predicted to be the true lower energy min. for 1,1,3-trichloroacetone. A decrease of about 0.3 Debye in the total dipole moment was calcd. as going from the low energy Ncc conformer to the high energy Gg1 form. This small change in the dipole moment that supported by noticeable change in several of the skeletal bond and dihedral angles with changing conformation indicated that steric forces play more important role than dipolar interactions in controlling conformational stability of the mol. The vibrational frequencies of 1,1,3-trichloroacetone in its stable forms were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calcns. and comparison with exptl. IR and Raman spectra of the mol.