The potential function for the internal rotation and the derived potential energy distribution of the normal modes for 3-chloropropionyl chloride based on ab initio calculations. Badawi, Hassan M.; Forner, Wolfgang

Abstract

The conformational behavior and structure of ClCH2CH2COCl (I) were studied by ab initio calcns. The 6-311++G** basis set was used to include polarization and diffuse functions in the calcns. at RHF and MP2 levels. I was predicted to exist as a complex mixt. of stable conformers. The trans-cis conformation with min. Cl-Cl interaction was the lowest-energy form for the mol. From the potential scan, the barrier for internal rotation between the trans-cis and trans-gauche conformers was calcd. The vibrational frequencies were computed at the HF level. Normal coordinate calcns. were carried out, and potential-energy distributions among symmetry coordinates were calcd. for the stable conformers. Raman and IR spectra of both the individual conformers and their mixt. were computed at 300 K.