Potential scans and potential energy distributions of normal vibrational modes of trichloroacetyl isocyanate. Badawi, Hassan M.; Forner, Wolfgang; Abu-Sharkh, Basel F.; Oloriegbe, Yahya S. Dep. Chem., King Fahd Univ. Petroleum Minerals, Dhahran, Saudi Arabia. Journal of Molecular Modeling [online computer file] (2002), 8(2), 44-49.

Abstract

The conformational stability and IR and Raman spectra of trichloroacetyl isocyanate (CCl_3CONCO) were investigated by ab initio MP2 and d. functional B3LYP calcns. using the 6-311++G** basis set. From the potential energy scans of the internal rotations in both the halomethyl and the isocyanate rotors, the mol. was predicted to exist predominantly in the cis-cis conformation. The steric hindrance between the halomethyl group and the nitrogen lone-pair was found to favor the staggered configuration for the chlorine atom, while conjugation effects favor the planar configuration for the C=O and the NCO groups. Vibrational wavenumbers were computed for the mol. at the DFT-B3LYP/6-311++G** level. Normal coordinate calcns. were carried out to obtain the potential energy distributions (PED) among the symmetry coordinates of the normal modes for the mol. The theor. vibrational assignments were compared with exptl. ones and ratios of obsd. to calcd. wave nos. of about 0.97.-1.04 were obtained.