

Conformational analysis and comparison between theoretical and experimental vibrational spectra for chloroacetyl isocyanate. Badawi, H. M.; Forner, W

Abstract

The conformational stability and vibrational IR and Raman spectra of chloroacetyl isocyanate (CH₂ClCONCO) 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 of both the halomethyl and the isocyanate rotors, chloroacetyl isocyanate was predicted to exist predominantly in a mixt. of the cis-cis (chlorine atom and NCO group eclipse C:O bond) and the gauche-cis (one hydrogen atom and NCO group eclipse C:O bond) conformations with a comparable relative stability. The vibrational wavenumbers of each of the two conformers of the mol. were computed at 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 each of the stable conformers of chloroacetyl isocyanate. The theor. vibrational assignments are compared with exptl. ones and a ratio of obsd./calcd. wavenumbers of about 0.97-1.04 was obtained.