

Conformational analysis and comparison between theoretical and experimental vibrational spectra for chloroacetyl isocyanate

Author(s): Badawi HM, Forner W

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 59 **Issue:** 2 **Pages:** 335-344

Abstract: The conformational stability and vibrational infrared and Raman spectra of chloroacetyl isocyanate (CH₂ClCONCO) were investigated by ab initio MP2 and density functional B3LYP calculations 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 mixture 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 molecule were computed at DFT-B3LYP/6-311++G** level. Normal coordinate calculations 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 theoretical vibrational assignments are compared with experimental ones and a ratio of observed/calculated wavenumbers of about 0.97-1.04 was obtained.