

An investigation of internal rotations and analysis of vibrational spectra of dichloroacetyl isocyanate

Author(s): [Badawi HM](#), [Forner W](#), [Oloriegbe YS](#)

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 583 **Pages:** 153-162

Abstract: The conformational stability and vibrational infrared and Raman spectra of dichloroacetyl isocyanate ($\text{CHCl}_2\text{CONCO}$) 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 in both the halomethyl and the isocyanate rotors, the molecule was predicted to exist in the cis-cis double left right arrow cis-trans conformational equilibrium. The cis-cis (the hydrogen atom of the CHCl_2 group and the NCO group, both eclipse the carbonyl $\text{C}=\text{O}$ bond) form was predicted to be the predominant conformation at ambient temperature. Vibrational wavenumbers were computed for the molecule at DFT-B3LYP/6-311++G** level. Normal coordinate calculations were carried out to obtain the potential energy distributions among the symmetry coordinates of the normal modes for the molecule. The theoretical vibrational assignments were compared with experimental ones and the ratio of observed to calculated wavenumbers of about 0.97-1.04 was obtained.