

VIBRATIONAL SPECTROSCOPY INVESTIGATION AND HYBRID COMPUTATIONAL (HF &DFT) ANALYSIS ON THE STRUCTURE OF CHLORZOAZONE

S. HARIKRISHNAN & T. J. BHOOPATHY

PG and Research Department of Physics, Pachaiyappa's College, Chennai, Tamil Nadu, India

ABSTRACT

In this work, the spectral properties of 5-chloro-3H-benzoxazol-2-one (Chlorzoxazone) are studied using density functional theory (DFT) employing B3LYP/6-311++G (d,p) and ab initio HF/6-311++G(d,p) levels of theory. The optimized geometrical parameters obtained by B3LYP/6-311++G (d, p) method show good agreement with experimental X-ray data. Satisfactory vibrational assignments were made for the stable conformer of the molecule using Hartree–Fock (HF) and density functional theory DFT-B3LYP methods with the 6-311++G(d,p) basis set. Comparison of the observed fundamental vibrational wave numbers of the molecule and calculated results by RHF and DFT methods indicates that B3LYP is superior for molecular vibrational problems. A study on the electronic properties, such as HOMO and LUMO energies, is performed. The isotropic chemical shift computed by ¹H and ¹³C nuclear magnetic resonance (NMR) chemical shifts of the Chlorzoxazone calculated using the gauge invariant atomic orbital (GIAO) method also shows good agreement with ChemDraw Ultra. The natural bond order analysis and thermodynamic functions of the title molecule were also performed using the RHF and DFT methods.

KEYWORDS: FTIR, FT-Raman and UV Spectra, ab Initio and DFT, Chlorzoxazone, Chemical Shift