DFT INVESTIGATION ABOUT ELECTRONIC AND VIBRATIONAL PROPERTIES OF CHROMONE SCHIFF BASE LIGANDS WITH METAL COMPLEXES, SQM ANALYSIS

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This research attempts to electronic and vibrational properties of metal complexes of chromone Schiff base ligands were calculated using the gauge independent atomic orbital (GIAO) method. Using time-dependent density functional theory, the theoretical electronic absorption spectra were determined. To obtain information about the ability of the molecule to react with chemicals, Frontier Molecular Orbital properties, energies, descriptors, and total/partial state density diagram were obtained. The charge distribution and chemical reactivity sites were visualized monitored by mapping electron density isosurface with electrostatic potential surfaces (ESP). To learn nonlinear optical properties (NLO), the polarizability and hyper polarizability tensors of the complexes were computed using density functional (DFT) theory at mPW1PW91 6-311+G(d,p) and LanL2DZ level. The study's second section focused on vibrational spectroscopic analysis. To fit the calculated harmonic wavenumbers with the observed Fourier Transform Infrared (FT-IR) and Raman spectra in the solid phase of the complexes, the calculated harmonic force constants were refined using the Scaled Quantum Mechanical Force Field (SQM-FF) procedure. When combined with the results of the SQM approach, it is possible to create a comprehensive assignment of the observed spectra.