A DFT STUDY: SPECTROSCOPIC ANALYSIS OF SCHIFF BASE LIGAND WITH FE(II) COMPLEX

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In this study, the molecular geometry, electronic, magnetic, and vibrational spectra of Schiff base ligand with Fe(II) Complexes were simulated by using density functional theory hybrid methods. NMR, UV-Vis, Raman, Infrared Spectroscopic investigations were carried out. The calculated values have been compared with the corresponding experimental results. Molecular orbital properties, descriptors, the mapping molecular electrostatic potential surface (MEP), and nonlinear optical (NLO) properties have been reported for better understanding at the molecular level. Normal modes analysis and their vibrational assignments were searched by using the Scaled Quantum Mechanical Force Field (SQM-FF) method based on total energy distribution (TED).