EXPERIMENTAL FT-IR, DISPERSIVE RAMAN AND THEORETICAL DFT CALCULATIONS ON CU(II) CHLORIDE COMPLEX OF P-TOLUIDINE

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In this study Cu(p-tol)2Cl2 (p-tol: p-toluidine) is prepared and characterized by elemental analysis, FT-IR, FT-FIR, and dispersive Raman spectral analysis. The molecular geometry and vibrational modes of p-tol and Cu(p-tol)2Cl2 are calculated using DFT- BVP86 and DFT-B3LYP methods with 6-311G+(d,p) basis set. The optimized geometries and calculated vibrational frequencies have been evaluated via comparison with experimental values, and the normal modes were assigned on the basis of the percent potential energy distribution (PED). The coordination effects on vibrational frequencies of p-tol are discussed by comparing the spectra of free p-tol and its Cu (II) chloride complex. A good agreement between calculated and experimental data is observed.
Keywords: IR and Raman spectra; DFT; p-toluidine; Copper (II) chloride complex