THEORETICAL AND EXPERIMENTAL VIBRATIONAL MODE ASSIGNMENTS ON FT-RAMAN, FT-IR OF A 1, 3-BIS (2-BENZIMIDAZYL) 2-THIAPROPANE AND ITS Zn(II) CHLORIDE COMPLEX

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The optimized geometries and vibrational wavenumbers of both ligand and complex were calculated using the DFT/RB3LYP method with a 3-21G basis set on the Gaussian 03 package program. The geometry optimization of the \([\text{Zn}(L)\text{Cl}_2]\) complex yields a distorted tetrahedral environment around Zn while the molecule clearly reveals the Cs symmetry. The assignment of the Raman and IR active vibrational modes of the title compounds is supported by total energy distribution (TED) calculations performed with the SCALE2 program \cite{1}. The non-redundant set of 108 internal coordinates has been defined as recommended by Pulay et al.\cite{2}. Each of the vibrational modes was assigned to one of the nine types of motion predicted by the point group analysis (stretching, in-plane bending, out-of-plane bending, torsion, rocking, twisting, wagging, scissoring, butterfly). In order to decrease overestimation of the calculated vibrational frequencies, vibrational wavenumbers were scaled with 0.9620. The simulated IR and Raman spectra of both ligand and Zn complex were plotted by using the Lorentz profile with band half-width (FWHH) of 7 cm\(^{-1}\).

![Optimized structure of the complex](image)

References