

Synthesis, Characterization of Fe(III), Zr(OH)₂(IV), MoO₂(IV) and Cd(II) complexes, Biological Activity, DFT and Molecular Docking Studies

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Abstract:

A series of novel metal complexes of Fe(III), Zr(OH)₂(IV), MoO₂(IV) and Cd(II) were synthesized through the condensation reaction of a Schiff base, derived from thiosemicarbazide and p-chlorobenzaldehyde with their respective metal salts. The synthesized ligand and its metal complexes were characterized using FT-IR, UV-Vis, ¹H NMR and mass spectroscopy. Additionally, molar conductivity, magnetic moment measurements and elemental analyses were conducted to further confirm the structures. The molecular structures of the ligand and its complexes were optimized using Gaussian 09 and the resulting structural parameters were analyzed. Quantum chemical properties of these compounds were predicted and discussed in detail. Furthermore, the antimicrobial activity of the synthesized compounds was evaluated against fungal and bacterial strains. Molecular docking studies were performed with DNA and human serum albumin (HSA) using Autodock4 to investigate their potential biological interactions.

Keywords: Schiff base, thiosemicarbazone, metal complexes, antibacterial activity, antifungal activity, molecular docking.