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Synthesis, spectral characterization, DFT, and molecular docking studies of metal(II) complexes derived from thiophene-2-carboxaldehyde and 2-amino-6-picoline

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ABSTRACT

A novel series of metal complexes ML_2Cl_2 [M = Co(II), Ni(II), Cu(II), and Zn(II), L = Schiff base] have been synthesized by the interaction of the ligand derived from the condensation of thiophene-2-carboxaldehyde with 2-amino-6-picoline. Molar conductance measurements indicate that the complexes are non-electrolytes. Infrared data indicate that the ligand is monodentate and binds to the metal ion via azomethine nitrogen atom. Electronic spectral data and magnetic measurements reveal tetrahedral and square planar geometries for the metal complexes. The redox behavior of complex $[CuL_2Cl_2]$ has been investigated using cyclic voltammetry. Thermal decomposition profiles are consistent with the proposed formulation of the complexes. The XRD and SEM results indicate that ligand and complexes $[CuL_2Cl_2]$ and $[ZnL_2Cl_2]$ are nanocrystalline. The metal complexes showed higher photocatalytic efficiency under sunlight as evidenced by photocatalytic studies using methylene blue dye. Molecular structures of the ligand and its complexes have been optimized by DFT computations. Binding affinity of ligand and its complexes with target protein have been examined by molecular docking study. The in vitro antimicrobial activity of the synthesized compounds has been tested against certain bacterial and fungal species. Furthermore, in vitro cytotoxicity of complexes $[CoL_2Cl_2]$ and $[CuL_2Cl_2]$ have been tested against L929 fibroblast.

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