

Cr(II), Co(II) and Cu(II) complexes with 2-aminodiphenylamine derived Schiff base ligand: Synthesis, characterization, DFT and biological insights

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Two Schiff bases viz. 2-(((2-(phenylamino)phenyl)imino)methyl)phenol (L^1H) and 2-methoxy-6-(((2-(phenylamino)phenyl)imino)methyl)phenol (L^2H) have been synthesized by the reaction of 2-aminodiphenylamine with salicylaldehyde and *o*-vanillin in 1:1 molar ratio. A series of transition metal complexes of Cr(II), Co(II) and Cu(II) have been synthesized using Schiff bases (L^1H) and (L^2H) in a 1:2 molar ratios. The newly synthesized ligands and metal complexes have been characterized by elemental analysis and different spectroscopic techniques including FT-IR, UV-Vis, NMR and mass spectrometry. The DFT method has been incorporated to get the electronic properties of ligands and their transition metal complexes. The spectroscopic analysis and computational method indicate distorted octahedral geometry around metal centers. The *in vitro* antimicrobial activities of synthesized ligands and transition metal complexes have been evaluated against *Escherichia coli* and *Staphylococcus aureus*. The results indicate that metal complexes exhibit higher antibacterial activity as compared to free Schiff bases and lower antibacterial activity as compared to the standard drug Gentamycin.

Keywords: Transition metal complexes; Schiff base; 2-aminodiphenylamine; UV-Vis; DFT; Antibacterial studies