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Synthesis, Characterization, and Theoretical Studies of Thiourea Ligands and its Cu(II) & Ni(II) Complexes as Antibacterial Agents

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Structured Abstract

Background: Antibiotics have revolutionized modern medicine in contributing to the saving of countless lives since the 1940s. However, thiourea compounds which are known for their wide applications in organic synthesis and pharmaceuticals has garnered significant interest in coordination chemistry due to their versatile bonding capabilities and potential biological activities. The formation of metal complexes with transition metals like Cu(II) and Ni(II) often enhances the properties of thiourea ligands, including their antibacterial efficacy.

Methods: Cu(II) and Ni(II) complexes derived from benzoyl thiourea ligands, 2-chlorobenzoyl chloride (**L1**), 4-chlorobenzoyl chloride (**L2**), and 4-methylbenzoyl chloride (**L3**) were synthesized under reflux conventional method for 3 hours with 1:1 ratio for ligands and 2:1 ratio for metal complexes. The structure of the synthesized compounds were confirmed by elemental analysis CHNS, FT-IR, UV-Visible, and ^{1}H NMR spectroscopic techniques. Their antibacterial properties were screened against both Gram-positive (MRSA 43300 and *Streptococcus mutans* ATCC 7006) and Gram-negative bacteria (*Acinetobacter nosocomialis* TDB35) by disk diffusion method. Lastly, Density Functional Theory (DFT) was employed to analyze their biological properties theoretically.

Results: Important peak corresponding to C=S and N-H of **L2** were observed at 1274 cm^{-1} and 3150 cm^{-1}, respectively for FTIR, ν(C=S) at 283 nm of **L3** for UV-Vis, and around 8.48–10.83 ppm attributed to N-H in ^{1}H NMR. The DFT studies revealed that even **L3** would have the highest inhibition due to its small band gap at 0.01169 eV yet, **L1** and **L2** exhibited better inhibition in the antibacterial results. It also showed that the copper complexes (**L1Cu** and **L2Cu**) were more active against the selected bacterial strains than its ligands and nickel complexes, highlighting their potential as potent antibacterial agents.

Conclusion: In conclusion, this research presents a detailed synthesis and characterization of thiourea ligands and their Cu(II) and Ni(II) complexes, highlighting their potential as potent antibacterial agents The successful development of such agents could lead to innovative antibacterial drugs, thereby benefiting public health in combating infectious diseases.

Keywords: Thiourea ligands, Copper(II) complexes, Nickel(II) complexes, DFT studies, Antibacterial agents

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