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Synthesis and Antimicrobial Studies of Metal Complexes Derived from Schiff Base 1-Phenyl-2,4-Dithiobiurets and AI Applications

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ABSTRACT

Artificial Intelligence (AI) has significantly advanced the field of chemistry, providing powerful tools for research, discovery, and optimization. Key applications include drug discovery and development, predicting molecular properties, virtual screening, and material science. AI also enhances spectroscopic data analysis, facilitating molecular structure and functional group identification.

This study focuses on the synthesis and spectroscopic characterization of metal complexes derived from Schiff bases. The Schiff bases were synthesized by condensing isonitroso acetophenone (HINAP) with dithiobiurets. The characterization of these complexes was performed using elemental analysis, molar conductivity, IR, electronic thermal analysis, and UV-visible spectroscopy. Antimicrobial activity was tested against Escherichia coli, Staphylococcus, Bacillus cereus, and Bacillus subtilis. Conductivity measurements indicated the non-electrolytic nature of the complexes. Thermal studies showed that they are thermally stable, insoluble in water, and soluble in organic solvents. Spectral analysis suggested an octahedral geometry for the metal complexes, further confirmed by electronic absorption and diffuse reflectance spectra.

Keywords: *Zn(II); Hg complexes; Schiff bases; Structural analysis; Spectral analysis; Antibacterial studies*

INTRODUCTION

Schiff base complexes play a crucial role in artificial intelligence applications, particularly in molecular modeling, machine learning, and materials science. Schiff bases, formed through the condensation of primary amines and carbonyl compounds, exhibit unique properties when coordinated with metal ions. Literature survey reveals their extensive use in catalysis, pattern recognition, data analysis, and environmental monitoring.

AI-driven chemical research has enabled the extraction of patterns from large datasets generated through experiments involving Schiff base complexes. The present study introduces novel ligands synthesized from phenyl/tolyl 2,4-dithiobiuret and HINAP, designated as HPEPDTB and HPETDTB, respectively.

EXPERIMENTAL SECTION

Synthesis of Metal Complexes

The metal complexes were synthesized by reacting equimolar amounts of ligands and metal halides. The resulting fine powdered solids were obtained through reactions of phenyl/tolyl 2,4-dithiobiuret with HINAP. These ligands exhibit variable solubility in organic solvents like chloroform, methanol, and carbon tetrachloride.

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Characterization

Elemental Analysis

The elemental analysis confirmed the empirical formulas of the synthesized compounds. HPETDTB exhibited a higher melting point than HPEPDTB, indicating greater thermal stability.

Infrared Spectroscopy (FTIR)

The FTIR spectra revealed complex bands due to multiple functional groups. Notably, the absence of a free or hydrogen-bonded carbonyl group was observed. The spectra suggested metal-ligand interactions via sulfur donors.

Electronic Absorption Spectra

The UV-visible spectra of the ligands exhibited high-intensity bands due to intra-ligand transitions. Minor shifts upon complexation confirmed coordination.

Proton Magnetic Resonance (PMR) Spectroscopy

PMR spectra provided insights into bonding. The Zn(II) complex showed a singlet for oximino proton at ~12.2 δ, indicating retention of the =NOH group. The aromatic protons appeared between 6.4-7.2 δ. Methyl protons in HPETDTB were observed at 2.4 δ.

Thermal Stability and Conductivity Measurements

Thermal analysis demonstrated stability up to 120°C. Molar conductance values (<1.0 ohm^{-1} cm^2 mol^{-1}) indicated non-electrolytic nature.

Antimicrobial Studies

The antibacterial activity of the Zn(II) and Hg(II) complexes was evaluated against E. coli, Staphylococcus aureus, B. cereus, and B. subtilis using the agar cup method. The inhibitory effects varied among complexes, with Zn(II) complexes displaying superior antibacterial activity.

Compound	B. subtilis (mm)	B. cereus (mm)	S. aureus (mm)	E. coli (mm)
$Zn_2(L_1)_2Cl_2$	14	11	20	20
$Zn_2(L_2)_2Cl_2$	13	11	13	12
$Hg(L_2)_2Cl_2$	13	12	13	17
$Hg(L_2)_2Cl_2$	14	12	13	17

CONCLUSION

The synthesized metal complexes exhibit octahedral coordination, as confirmed by spectral and thermal analysis. These Schiff base complexes are being further investigated using AI models to predict and design complexes with enhanced anticancer properties and improved therapeutic efficacy.

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