

Photophysical and Antimicrobial Studies of Ni (II) Salen Complex

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Abstract

In this study, a novel Ni(II)–salen complex (Ni–SBL1) was synthesized and comprehensively characterized to explore its structural, photophysical and antimicrobial properties. The crystalline nature of the complex was confirmed by X-ray diffraction (XRD), while surface morphology studies using FE-SEM revealed randomly shaped, petal-like structures with small sizes. UV–Vis analysis confirmed effective metal–ligand interactions through d– π^* transitions. Photoluminescence studies exhibited dual emission peaks at 544 nm and 601 nm upon excitation at 225 nm, highlighting the complex's notable luminescent behavior. Biological evaluation demonstrated moderate antibacterial activity against *Bacillus subtilis* and antifungal activity against *Aspergillus niger*, with inhibition zones of 7–8 mm over the tested concentrations. The combination of well-defined structural features, photophysical properties and antimicrobial activity indicates that Ni–SBL1 is a promising candidate for multifunctional applications in material science and biomedical fields.

Keywords: Photophysical Study; Antimicrobial Study; Schiff Base; Ni(II) Salen

1. Introduction

Transition metal complexes play a pivotal role in modern chemistry due to their diverse applications in catalysis, material science and medicine. Among these, Schiff base ligands and their metal complexes have attracted significant attention because of their structural versatility, ease of synthesis and tunable chemical and physical properties. Ni(II)–salen complexes, in particular, are of great interest owing to their unique coordination geometry, electronic features, and ability to interact with biomolecules. These complexes often exhibit intriguing photophysical properties such as strong absorption in the UV–Vis region and notable fluorescence, making them useful in sensing, imaging and photochemical applications. Additionally, the antimicrobial and antibiofilm potential of Ni(II)–salen complexes highlights their relevance in developing new therapeutic agents, especially against antibiotic-resistant bacterial strains.

Recent studies have highlighted the significance of Schiff base ligands and their metal complexes in medicinal and photophysical applications. Raj et al. synthesized five novel imine-linked ligands (H₂L₁, H₄L₂ and L₃–L₅) via two-step reactions and fully characterized them using spectroscopic techniques. The coordination of Ni²⁺ ions to these ligands induced substantial photophysical modulations, enabling tunable coordination geometries, variable stereochemistry, and electrostatic interactions crucial for biomolecular recognition. These Ni(II) complexes demonstrated notable antibacterial activity against *Staphylococcus aureus* and methicillin-resistant *S. aureus* (MRSA), with SEM studies indicating cell wall inhibition as the primary mechanism of bacterial cell death. Furthermore, cytotoxicity assays on HeLa cells confirmed high biocompatibility, showing 85–90% cell viability after 24 hours. This study illustrates the potential of Ni(II)-Schiff base complexes as sustainable antimicrobial agents with low cytotoxicity, combining photophysical properties with biomedical applications [1].

Salophen-based Ni(II) complexes have recently garnered attention for their multifaceted electrochemical, spectroscopic, and biological properties. Kamga et al. performed a comprehensive study on a Ni(II)-salophen complex and its tetradentate salophen ligand precursor using ¹H/¹³C NMR, FT-IR,

UV-Vis, ESI-MS, thermogravimetric analysis, and molar conductance measurements, confirming coordination through nitrogen and oxygen atoms. Electrochemical studies, including cyclic voltammetry (CV), differential pulse voltammetry (DPV), and rotating disk electrode (RDE) measurements, demonstrated reversible redox behavior and highlighted electropolymerization on electrode surfaces. Biological evaluations revealed that both the free ligand (H₂L) and Ni(II) complex exhibited notable antimicrobial, antifungal, and antioxidant activities, suggesting potential applications in pharmacology and biomedical research. The study underscores the relevance of Ni(II)-salophen complexes as multifunctional agents combining electrochemical tunability with bioactivity [2].

Schiff base metal complexes have been widely explored for their structural diversity and biological activity. Kargar et al. synthesized mononuclear Ni(II), Cu(II), and Zn(II) complexes using a tetradentate Schiff base ligand, N,N'-bis(3,5-dibromosalicylidene)-1,3-diaminopropane (H₂L). Characterization was performed via FT-IR, ¹H NMR, elemental (CHN) analysis, and single-crystal X-ray diffraction (SC-XRD). SC-XRD data revealed that Ni(II) and Cu(II) complexes adopt a monoclinic crystal system with square planar geometry, while Zn(II) forms an orthorhombic distorted octahedral geometry due to additional coordination by water molecules. The antimicrobial activity of both the ligand and complexes was evaluated against Gram-positive (*Staphylococcus aureus*, *Bacillus cereus*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria, showing significant inhibitory effects. This study underscores the importance of Schiff base coordination in modulating both the geometry and biological activity of metal complexes [3].

Ni(II)-salen complexes have demonstrated significant catalytic potential in the synthesis of biologically active compounds. Patra et al. synthesized four unsymmetrical Ni(II)-salen complexes ([NiL1-4]) via reflux of Ni(Ac)₂·4H₂O with corresponding ligands (H₂L1-4), and characterized them through spectroscopic and physicochemical methods, including single-crystal X-ray diffraction for [NiL1], [NiL2] and [NiL4]. Optimization studies revealed excellent conversions with yields up to 98% within 1 h. The catalytic efficiency was influenced by the electronic nature of substituents on aromatic aldehydes, with electron-withdrawing groups enhancing conversion rates. The order of catalytic performance was found to be [NiL1] > [NiL3] > [NiL2] > [NiL4] [4].

Abdalla et al. synthesized a salen-based ligand, (2,2'-{1,2-ethanediylbis[nitrilo(E)methylidene]}diphenol, S), and its binary (MS) and ternary (MSI) complexes with Co(II), Ni(II), Cu(II), Cd(II), Al(III) and La(III). Antimicrobial screening indicated that CdS and CuSI exhibited the highest activity, outperforming standard antibiotics, with efficacy trends following CdS > gentamicin > CuS > NiS > CoS > LaS > AlS > S for MS complexes and CuSI > gentamicin > CdSI > NiSI > CoSI > LaSI > AlSI > S for MSI complexes. In vitro cytotoxicity assays showed that CuSI and CdSI demonstrated superior activity against Hep-G2 and MDA-MB231 cell lines compared to cisplatin. These findings highlight the potential of salen and salen/imidazole complexes as multifunctional agents for antimicrobial and anticancer applications [5].

Baydeniz et al. synthesized a series of azomethine ligands based on naphthalene or phenylmethane cores and their Co(II), Ni(II), Cu(II) and Zn(II) complexes. Biological evaluations demonstrated significant antibacterial and antibiofilm activities against clinically relevant strains. Notably, the Cu(II) complex of ligand-2 showed the highest inhibition of biofilm formation for MRSA and MSSA, while Co(II) complexes selectively inhibited *P. mirabilis* biofilms. These findings suggest that π -conjugated azomethine metal complexes combine favorable photophysical properties with potent antibacterial and antibiofilm activity, making them promising candidates for medical and healthcare applications [6].

Despite extensive studies on the synthesis, structural characterization and biological activities of Ni(II)–salen complexes, systematic investigations linking their photophysical properties to antimicrobial efficacy remain limited. Understanding how electronic and geometric features influence antibacterial and antibiofilm activities can provide crucial insights for the rational design of next-generation bioactive materials. In this context, the present study focuses on the synthesis of novel Ni(II)–salen complexes, comprehensive photophysical characterization and evaluation of their antimicrobial. The findings aim to bridge the knowledge gap between photophysical behavior and biological performance, offering a framework for designing Ni(II)–salen complexes with enhanced multifunctional properties.

2. Experimental Details

The Ni(II) complex of the Schiff base ligand SBL1 (Ni–SBL1) was synthesized by refluxing the preformed ligand with nickel(II) acetate tetrahydrate in ethanol. The dried ligand SBL1 (5.0 mmol) was dissolved in 20 mL of ethanol under constant stirring, followed by the dropwise addition of an ethanolic solution of nickel(II) acetate tetrahydrate $[\text{Ni}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}]$ (5.0 mmol, 1.245 g in 10 mL ethanol). The reaction mixture was refluxed for 1 hour, during which the color gradually changed to deep red–brown, indicating complex formation. After completion, the mixture was cooled to room temperature, and the precipitated complex was filtered, washed thoroughly with ethanol and distilled water to remove unreacted reagents, and dried at 60 °C for 4 hours. The final product was obtained as an air-stable, non-hygroscopic red–brown crystalline solid. Figure 1 illustrates the schematic synthesis of N,N'-ethylene-bis(salicylideneiminato) nickel(II) (Ni–SBL1).

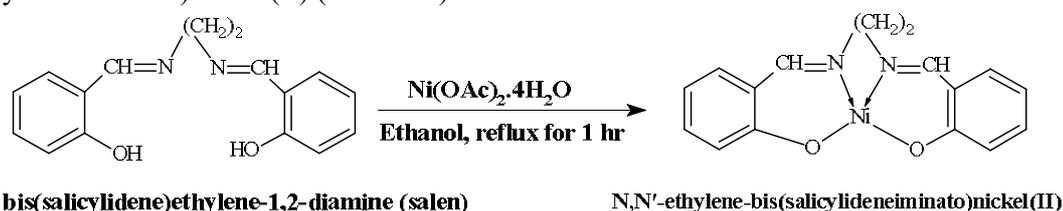


Figure 1: Schematic pathway showing the preparation of the N,N'-ethylene-bis(salicylideneiminato) nickel(II) (Ni–SBL1) complex.

The Ni–SBL1 complex was comprehensively characterized using various spectroscopic and analytical methods to confirm its structural, morphological, and optical properties. Its crystalline nature was examined via XRD using a Rigaku MiniFlex 600 diffractometer with Cu-K α radiation ($\lambda = 1.5406$ Å). Surface features were analyzed through FE-SEM on a JEOL JSM-7600F instrument. Vibrational modes and bonding characteristics were investigated using Raman spectroscopy with a Bruker MultiRAM FT-Raman spectrometer. The optical behavior, including UV–Vis absorption, was recorded on a Shimadzu UV-1800 spectrophotometer, while PL properties were studied using a HITACHI F-7000 Fluorescence Spectrophotometer. The biological activity of Ni–SBL1 was assessed by evaluating its antibacterial effect against *Bacillus subtilis* and antifungal activity against *Aspergillus niger*, measured through the zone of inhibition. Table 1 summarizes the characterization techniques and key findings for Ni–SBL1 complex.

Table 1: Summary of characterization techniques and key findings for Ni–SBL1 complex.

Technique	Property Studied	Outcome
XRD	Crystalline nature	Confirmed crystalline nature of Ni–SBL1

FE-SEM	Surface morphology	Revealed particle shape and surface features
Raman Spectroscopy	Vibrational modes / bonding	Verified functional groups and metal-ligand coordination
UV-Vis Spectroscopy	Optical absorption / electronic transitions	Identified characteristic absorption peaks of ligand and complex
PL Spectroscopy	Fluorescence behavior / photophysical property	Demonstrated emission properties
Antimicrobial Testing	Biological activity (antibacterial & antifungal)	Inhibition zones observed against <i>Bacillus subtilis</i> and <i>Aspergillus niger</i>

3. Results and Discussion

Figure 2 illustrates the structural characterization of the Ni-SBL1 complex. The XRD pattern (Figure 2a) confirms the crystalline nature of the complex, showing distinct reflections at 17.7° , 20.3° , 23.1° , 26.3° and 29.8° , indicative of a well-defined crystalline phase [7]. The FE-SEM image (Figure 2b) reveals the surface morphology of the complex, exhibiting randomly shaped, petal-like structures with relatively small particle sizes. These morphological features suggest that the complex forms aggregated nanostructures, which may influence its surface area and interaction with other molecules, potentially impacting its photophysical and antimicrobial properties [8].

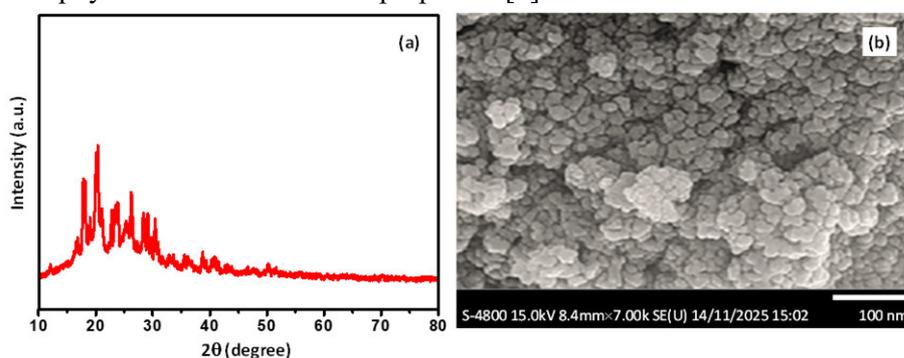


Figure 2: Structural characterization of Ni-SBL1: (a) XRD pattern showing crystallinity and (b) SEM image depicting surface morphology.

Figure 3 presents the spectroscopic characterization of the Ni-SBL1 complex. The Raman spectrum (Figure 3a) exhibits characteristic vibrational bands at 1167 , 1235 and 1341 cm^{-1} , with the most intense peak observed at 1576 cm^{-1} . These features are indicative of the coordination environment around the Ni^{2+} center, suggesting a square-planar or octahedral geometry typical of Ni(II)-Schiff base complexes. The vibrational modes confirm the involvement of the azomethine (C=N) and phenolic (C-O) groups in metal binding [9].

The UV-Vis spectrum (Figure 3b) of Ni-SBL1 shows a minor dip at 235 nm, corresponding to π - π^* transitions of the ligand framework, and a broad absorption in the 240 - 600 nm range, which can be attributed to metal-to-ligand (d - π^*) charge transfer transitions. The observed spectral behavior supports effective coordination between the Ni^{2+} ion and the ligand, consistent with the expected electronic interactions in square-planar or octahedral Ni(II) complexes. These findings collectively confirm the successful formation of the Ni-SBL1 complex with well-defined structural and electronic characteristics [10].

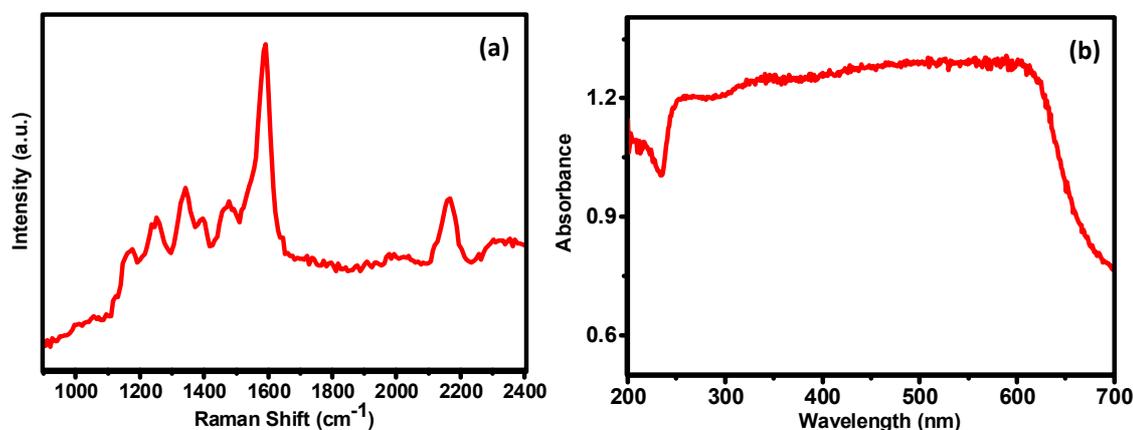


Figure 3: Spectroscopic characterization of Ni-SBL1: (a) Raman spectrum and (b) UV-Vis spectrum.

Figure 4 depicts the PL spectrum of the Ni-SBL1 complex, highlighting its luminescent properties. The complex exhibits two prominent emission peaks at 544 nm and 601 nm upon excitation at 225 nm. These emission bands can be attributed to ligand-centered $\pi-\pi^*$ and metal-to-ligand charge transfer (MLCT) transitions, indicating efficient electronic communication between the Ni^{2+} center and the Schiff base ligand [11]. The dual emission peaks suggest the presence of multiple emissive states, which may arise from different coordination environments or vibrational relaxation pathways within the complex. The observed luminescence confirms that Ni-SBL1 possesses notable photophysical activity, which could be exploited for applications in sensing, imaging, or as a functional bioactive material.

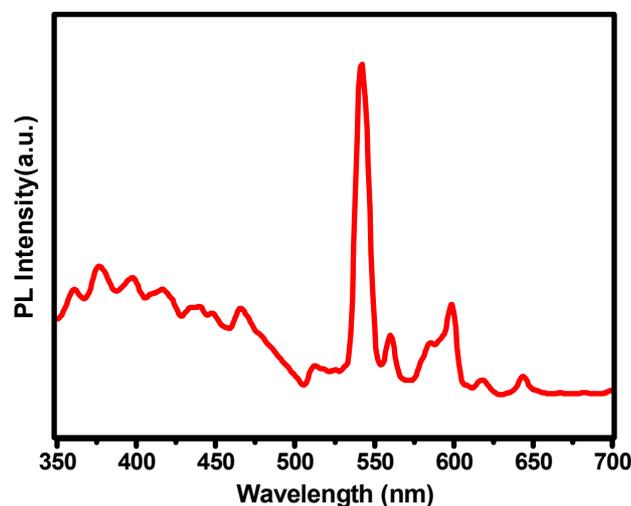


Figure 4: PL spectrum showing the luminescent properties of Ni-SBL1.

The antibacterial and antifungal activities of Ni-SBL1 were evaluated against *Bacillus subtilis* and *Aspergillus niger* at different concentrations, as illustrated in Figure 5 and summarized in Table 2. The complex exhibited moderate antibacterial activity against *B. subtilis*, with zones of inhibition ranging from 7 to 8 mm across doses of 20–100 μg . Similarly, antifungal activity against *A. niger* was consistent, showing inhibition zones of 7 to 8 mm over the tested concentrations up to 120 μg . The results indicate that Ni-SBL1 is effective in restricting the growth of both bacterial and fungal strains, although the

activity does not increase proportionally with concentration, suggesting that the complex exerts a baseline inhibitory effect at relatively low doses. The observed antimicrobial behavior can be attributed to the coordination of Ni²⁺ with the Schiff base ligand, which may facilitate interactions with microbial cell walls, leading to disruption of cellular functions. These findings highlight the potential of Ni-SBL1 as a multifunctional agent with both antibacterial and antifungal properties [12].

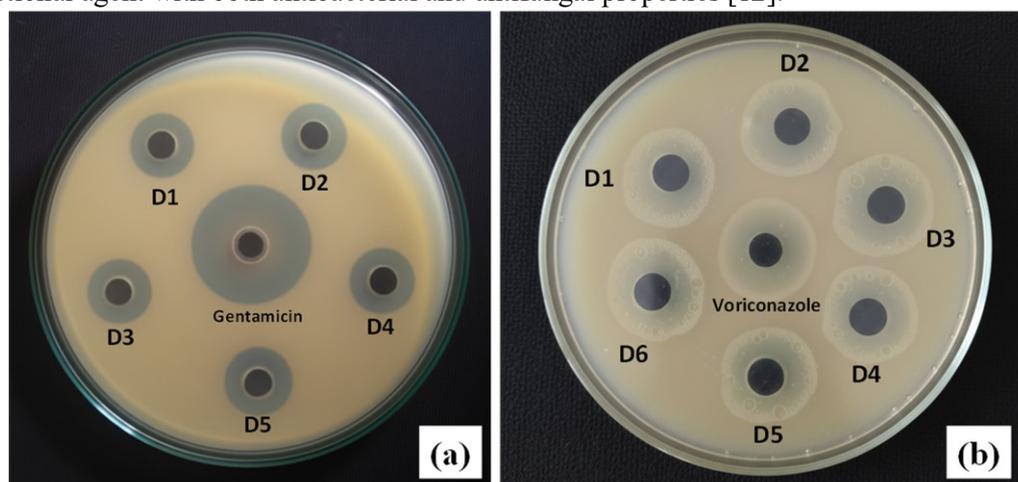


Figure 5: (a) Antibacterial activity of Ni-SBL1 towards the *Bacillus subtilis* for different doses (D1: 20 µg, D2: 40 µg, D3: 60 µg, D4: 80 µg, D5: 100 µg), (b) Antifungal activity of Ni-SBL1 towards the *Aspergillus niger* for different doses (D1: 20 µg, D2: 40 µg, D3: 60 µg, D4: 80 µg, D5: 100 µg, D6: 120 µg).

Table 2: Antibacterial activity of Ni-SBL1.

Sample	Zone of inhibition (mm)				
	20 µg	40 µg	60 µg	80 µg	100 µg
	D1	D2	D3	D4	D5
<i>Bacillus subtilis</i>					
Ni-SBL1	7	7	8	7	8
<i>Aspergillus niger</i>					
Ni-SBL1	7	7	7	7	8

4. Conclusions

The Ni(II)-salen complex Ni-SBL1 was successfully synthesized and thoroughly characterized, confirming its crystalline nature, defined surface morphology, and characteristic metal-ligand coordination. Spectroscopic studies revealed strong vibrational, UV-Vis, and photoluminescent properties, demonstrating the complex's robust photophysical behavior. Antimicrobial testing indicated moderate inhibitory effects against *Bacillus subtilis* and *Aspergillus niger*, establishing its potential as a bioactive material. Overall, the study highlights Ni-SBL1 as a multifunctional complex combining structural stability, luminescence, and antimicrobial efficacy, providing a foundation for future exploration in biomedical and photophysical applications.

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