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Synthesis, crystal structure, thermal stability and biological study of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel (II) complex

S. Sindhu^a, S. Arockiasamy^{b,*}

^a Physics Division, School of Advanced Sciences, Vellore Institute of Technology, Chennai, 127, India
 ^b Chemistry Division, School of Advanced Sciences, Vellore Institute of Technology, Chennai, 127, India

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ABSTRACT

A Schiff base complex of nickel, bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel (II) was synthesised by condensing bis(2-hydroxy-3-methoxybenzaldehyde) nickel (II) and n-propylamine in methanolic medium. Single crystal X-ray diffraction analysis of the complex revealed it to possess planar geometry with a monoclinic crystal system. The non-isothermal TG/ DTA runs on this complex in a high purity (99.99 %) nitrogen environment at atmospheric pressure confirmed the absence of any coordinated water. A sharp endotherm in its DTA shows a melting temperature range of 168–171 °C. It is thermally stable up to 243 °C and decomposes in two steps, yielding NiO and carbon as residue. In addition to the methoxy group (-OCH₃), infrared analysis (IR) confirmed the presence of the characteristic azomethine group (-CC=N-) which is also responsible for the biological action. It was further analysed by elemental analyser (C, H, N), ¹H and ¹³C NMR as well as mass spectrometry. It showed considerable antibacterial activity towards *Escherichia coli* and *Staphylococcus aureus* when the concentration exceeds 200 µg/ml. The antifungal study shows significant inhibition with the antifungal drug imidazole as a positive control (PC). Small values of MIC, MBC/MIC indicate a lesser quantity of complex is required to inhibit the growth of micro-organisms.

1. Introduction

Schiff base complexes of nickel with varying structural features exhibit variety of applications in various fields such as catalytic, biological and nanomaterials preparation. The modular synthesis of Schiff base complexes of various metals allows one to control the nature of donor atoms (N, O) [1] in the coordination sphere, denticity, chelating ability, steric and thermal properties [2]. Schiff bases complexes are among the most widely studied compounds for over several decades as they show a wide range of applications such as in food industry [3], as dye [4,5], polymer stabilizers [6,7], intermediates in organic synthesis [8,9], catalysis [10,11], chemo-sensors [12] and in pigments [10,13]. In addition, Schiff base complexes show excellent catalytic activities for organic transformations reactions [14,15], electroluminescent properties [16], biological activities such as antibacterial [17], antifungal [18,19], anti-inflammatory activities [20], as urease inhibitors [21], optical properties [22,23], chromotropic behaviour [24] and precursors for chemical vapour deposition (CVD) [25–27].

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^{*} Corresponding author. Vellore Institute of Technology-Chennai campus, Chennai-600127, India. *E-mail address:* arockiasamy.s@vit.ac.in (S. Arockiasamy).

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In the past decades, coordination chemistry has seen a huge growth in novel reactions and complexes and as a result of which chemists are now able to fine-tune the coordination sphere of a metal to prepare the desired complexes for various applications. The azomethine (-C==N-R) group present in the coordination sphere of the Schiff base complex instead of keto (-C==O) or aldehyde (-CHO) play a crucial role for them to exhibit a broad range of biological activities [28–30] and thermal stability [2].

Evaluation of thermal stability and physicochemical properties is essential for any compound to be used in biomedical applications [31]. Thermogravimetric analysis (TGA) is a powerful analytical tool to investigate and predict the thermal stability, and shelf-life of biologically active compounds in pharmaceutical, food, environmental field etc., under controlled conditions of temperature and atmosphere [32]. The importance of thermal analysis of newly developed biologically active compounds or drugs stems from the fact that they require appropriate storage conditions [33]. In addition, TGA is widely used in pharmaceutical field to assess the compatibility of active pharmaceutical ingredients (API) and excipient, moisture content [34] and sterilisations condition [35]. Thermal analysis can also provide theoretical support for the preparation and process optimisation of such compounds. Among the various nickel compounds studied for biological activity, the Schiff base complex of nickel containing the ligand, bis {(2-methoxy-6-[(E)-(propylimino)methyl]phenol have never been described.

As a result, we present here for the first time the single crystal X-ray diffraction, FTIR, NMR, C, H, N analysis, mass spectrometry, TG/DTA, biological, minimum inhibition concentration (MIC) and Minimum bactericidal concentration (MBC) studies on the mononuclear bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) complex.

2. Experimental

2.1. Materials and syntheses

The chemicals, 2-hydroxy-3-methoxybenzaldehyde (Merck), NiCl₂·6H₂O (Merck) and n-propylamine, methanol, ethanol, liqammonia (all from SD fine, India) were used as received without any further purification. The preparation of the title compound was carried out by slightly modifying the reported procedure [36,37]. First, a parent compound of bis (2-hydorxy-3-methoxybenzaldehyde) nickel (II) was prepared as prescribed here. NiCl₂.6H₂O (1.2 g) was dissolved in 10 cm³ of water, and 1.5 g of 2-hydroxy-3-methoxybenzaldehyde in 10 cm³ of absolute ethanol was added drop-wise under constant stirring in a 1 : 2 mol ratio. To this reaction mixture, liq. ammonia (1 cm³) was added drop-wise by continuously monitoring the formation of a greenish yellow precipitate. This precipitate (Scheme 1) was digested at 60 °C, over a water bath for 0.5 h. It was filtered, washed with ethanol several times and dried under vacuum overnight before being employed in the second stage. The yield was found to be 76 %. For the preparation of Schiff base complex, bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II), 1 mL of n-propylamine was added dropwise to a warm suspension of 0.3–0.5 g of bis(2-hydorxy-3-methoxybenzaldehyde)nickel(II) in aqueous methanol at 40 °C over a water bath until the solution turned olive green. The reaction mixture was then carefully transferred into an RB flask and refluxed for 0.5 h. The resulting olive-green crystals were filtered, washed with ethanol and vacuum dried overnight. These crystals were recrystallised several times from methanol and were used for single crystal analysis.

The Schiff base compound was characterised further and the spectral characterisation results are summarised below.



2-hydorxy-3-methoxybenzaldehyde

bis(2-hydorxy-3-methoxybenzaldehyde)nickel(II)



bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II)

Scheme 1. Synthesis of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II).

 $T_{\rm mp}$: 168–171 °C. Anal. calcd. for C₂₂H₂₈O₄N₂Ni (M = 443.2 g mol⁻¹, Ni: 13.2 %), (%): C, 59.56; H, 6.31; N, 6.31. Found (%): C, 60.01; H, 6.91; N, 6.80. $\delta_{\rm H}$, ¹H NMR (25 °C, 500 MHz, CDCl₃): 10.17 (s, 2H, N=HC-C₆H₅), 7.26–6.29 (m, 6H, 2C₆H₃), 4.26–4.29 (s, 4H, N-H₂C-C₂H₅), 3.72 (s, 6H, H₃C–O-C₆H₅), 1.88–1.95 (m, 4H, N–CH₂–H₂C–CH₃), 0.97–1.00 (s, 6H, N–C₂H₄–H₃C).

 $δ_{\rm C}$, ¹³C NMR (25 °C, 500 MHz, CDCl₃): 163.28 (s, -CH-C₆H₅), 149.62 (s, -C₆H₅), 122.65–111.84 (m, C₆H₅), 60.62–55.44 (s, -N-CH₂C₂H₅), 26.81 (s, N-CH₂-CH₂-CH₂), 11.36 (s, N-C₂H₄CH₃). CDCl₃ peaks at 76.82–77.33. FTIR (KBr pellet), cm⁻¹, 2830–3003 ($ν_{\rm C}$ -H), 1616 $ν_{\rm (C=N)}$, 1439, 1455,1552 $ν_{\rm (C=C)}$, 1354 $ν_{\rm (phenolic C=O)}$, 528 $ν_{\rm (Ni=N)}$, 458 $ν_{\rm (Ni=O)}$. Mass, (L: [CH₃O-C₆H₅(O)CHN(C₃H₇)]⁺, (Fragments, *m/z*), ([NiL₂]⁺, 443), ([L]⁺, 194), ([NiL₃]⁺, 636), ([NiL₄]⁺, 885). Crystallized in a monoclinic system, space group P 2₁/c, with a = 10.77647(7) Å, b = 7.3599(4) Å, c = 13.7225(7) Å, β = 91.009(2)°, α = γ = 90°, Z = 2, R1 = 0.0584, wR2 = 0.1006.

2.2. Physical characterization

The crystal structure analysis of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) was done by using Bruker APEX 2 CCD diffractometer equipped with ω and φ scan mode with Mo K α ($\lambda = 0.71073$ Å) at T = 298(2) K. The Crystal structure was solved by SHELXL 2014/7 using the direct method and the refinement was performed by full matrix least squares of F² [38]. SAINT and SADABS programs were used to correct the data for Lorentzian, polarisation and absorption effects. EURO VECTOR EA 3000 was used for elemental analysis. Nicolet iS10-FTIR spectrometer was used for IR analysis in the range of 4000 - 450 cm⁻¹. NMR and mass spectral data were acquired by using Bruker Avance III 500 spectrometer and JMS-T100LC Accu ToF respectively. Thermal analysis was carried out using a Hitachi (model 7200) TG/DTA by passing a purge gas of high pure inert N₂ of 200 ml/min at a heating rate of 10 °C/min.

2.3. Anti-bacterial and anti-fungal study

Agar well diffusion method was used for testing the antimicrobial activity. Three different concentrations of $100 \mu g/ml$, $200 \mu g/ml$ and $300 \mu g/ml$ prepared using DMSO were used for evaluating the effect on test organisms such as *Escherichia coli* and *Staphylococcus aureus* by well diffusion method. The test cultures were inoculated in a sterile Nutrient broth and allowed to attain the growth for 24–48 h. Sterile Mueller-Hinton Agar plates were prepared and allowed to solidify. Swabs were used to evenly spread 0.1 % inoculum suspensions of the test organism over the agar surface in each case. On the agar surface of each NA plate, 6 mm wells were cut while maintaining sterility. The wells were filled with about 20 µl of each concentration, and the plates were then incubated for 24 h at 37 °C. In all of the inoculated NA plates, the antimicrobial activity was measured in terms of the zone of inhibition surrounding the wells. The millimetre measurements and records of the inhibition clear zones were made. The resultant zones were contrasted with the streptomycin positive and DMSO negative controls.

To study antifungal activity, imidazole was selected as positive antifungal agent (PC) and DMSO was used as negative control (NC). Each sample was evaluated against the test organisms by well diffusion method. All the test cultures (*Aspergillus niger* and *Candida albicans*) were inoculated in a sterile nutrient broth (Annexure 1) and allowed to attain the growth for 24–48 h. Sterile Mueller-Hinton agar (Annexure 1) plates were prepared and allowed to solidify. About 0.1 % inoculum suspensions of the test organism (*Aspergillus niger* and *Candida albicans*) were swabbed uniformly over the agar surface separately. Under sterile conditions, 6 mm wells were cut on the agar surface of each NA plates. About 20 μ l of each sample was loaded into the well and the plates were incubated at 37 °C for 24 h. The antifungal activity was evaluated in terms of zone of inhibition around the wells in all the inoculated NA plates. The inhibition clear zones were measured and recorded in millimetre. All the values were compared with positive control and negative control.



Fig. 1. ORTEP diagram drawn with 30 % probability of ellipsoid for bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II).

3. Results and discussion

3.1. Synthesis and crystal structure of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II)

Bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) was prepared by treating n-propylamine with bis(2-hydroxy-3methoxybenzaldehyde)nickel (II) as shown in Scheme 1, resulting in the coordination of azomethine group (-C=N-R) with the nickel centre. The olive-green needle type crystals of this complex were analysed by single crystal-X-ray diffraction. The ORTEP diagram is shown in Fig. 1 and the crystal data summary is given in Table 1. Table 2 shows the specified bond lengths (Å) and angles (°). The bidentate ligand is linked to nickel through one phenolato-O and one imine-N donor sites in trans-positions to each other in the coordination sphere of nickel and the nickel is situated on inversion centres (NiN_2O_2) to form a distorted square plane [39]. The sp² hybridization and centre of symmetry (i) of the two nitrogen atoms around nickel has led to the planar geometry of the coordination sphere with the sum of bond angles of (O(1)-Ni(1) - O#(1) and N(1)-Ni(1) - N#(1)) to 360° (Table 2) which is same as few other complexes of nickel reported earlier [40]. When compared to its parent compound without nitrogen coordination, the increase in covalent nature could be attributed to a decrease in bond length of Ni(1)-O(2) from 2.03 to 1.915(2) Å (Ni(1)-N(1)) as a result of nitrogen coordination [41]. The bond angle of Ni(1)–N(1)–C(8) is $120.84 (20)^{\circ}$ and the rotational motion [42] of n-propyl group block the water molecules (c.f. Scheme 1) from coordinating to nickel which resulted in a coordinatively saturated bis {(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II). The packing patterns are given in Fig. 2a and b showing no interactions between molecules. The absence of intermolecular hydrogen bonds and intermolecular $\pi \dots \pi$ interactions within in the wan der walls radii, indicates that the crystal packing (Fig. 2a and b) was essentially formed by weak van der waals forces and non-covalent interactions. The ligand-molecular arrangement and anti-parallel arrangement of the molecular planes show a one-dimensional chain along the crystallographic a-axis (Fig. 2a). The basal plane of the square plane is bound by two N atoms from (-C=N) and two O atoms from the phenolic group forming a tetradentate N2O2-donor, bis-Schiff base complex, thus forming two six membered chelate rings [Ni (1)-N(1)-C(7)-C(5)-C(6)-O(1)] and [Ni(1)-N(1)' - C(7)' - C(5)' - C(6)' - O(1)'] as shown in Fig. 3.

3.2. TG/DTA study

The TG/DTA study reveals the physico-chemical properties such as thermal stability/resistivity, decomposition temperature,

IIICKEI(II).	
Crystal data	
Identification code	Ni(3meO-salPrN) ₂
Empirical formula	C22 H28 N2 NiO4
Formula weight	443.17
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_{1}/c$
Unit cell dimensions	
	a = 10.7647(7) Å
	b = 7.3599(4) Å
	c = 13.7225(7) Å
	$lpha=90^{\circ}.$
	$\beta = 91.009(2)^{\circ}.$
	$\gamma = 90^{\circ}$.
Volume	1087.03(11) Å3
Z	2
Density (calculated)	1.354 Mg/m3
Absorption coefficient	0.922 mm-1
F(000)	468
Crystal size	$0.350\times0.300\times0.250~\text{mm}^3$
Theta range for data collection	2.969–25.998°.
Index ranges	$-11 \le h <= 13, -9 \le k <= 9, -16 \le l <= 16$
Reflections collected	11080
Independent reflections	2130 [R(int) = 0.0373]
Completeness to theta =	25.242° 99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.796 and 0.720
Refinement method	Full-matrix least-squares on F2
Data/restraints/parameters	2130/0/133
Goodness-of-fit on F2	1.110
Final R indices [I > 2sigma(I)]	R1 = 0.0392, $wR2 = 0.0864$
R indices (all data)	R1 = 0.0584, wR2 = 0.1006
Largest diff. peak and hole	0.529 and -0.276 e.Å-3

 Table 1

 Crystal data and structure refinement for bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato} nickel(II).

Table 2

Selected Bond lengths	A] and angles	[°] for bis{(2-methoxy	-6-[(E)-(propylimind	o)methyl]phenolato}nickel(II)
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Bond	[Å]	Bond	[°]
N(1)–Ni(1)	1.915(2)	C(7)-N(1)-Ni(1)	123.0(2)
O(1)–Ni(1)	1.830(2)	C(8)-N(1)-Ni(1)	120.84(18)
(C6)–O(1)	1.304(3)	O(1)-Ni(1)-O(1)#	180.00(13)
C(7)–N(1)	1.286(3)	N(1)#-Ni(1)-N(1)	180.00(11)
(C5)–C(6)	1.403(4)	C(2)-C(1)-O(2)	124.9(3)
C(5)–C(7)	1.432(4)	C(2)-C(1)-C(6)	120.7(3)
C(8)–N(1)	1.477(3)	O(2)-C(1)-C(6)	114.4(3)
C(1)–C(2)	1.371(4)	C(1)-C(2)-C(3)	121.0(3)
C(1)–O(2)	1.371(4)	C(4)-C(5)-C(6)	120.4(3)
C(1)–C(6)	1.418(4)	C(4)-C(5)-C(7)	119.8(3)
C(2)–C(3)	1.397(5)	C(6)-O(1)-Ni(1)	126.08(18)
C(3)–C(4)	1.365(4)	C(1)-O(2)-C(11)	118.0(3)
C(4)–C(5)	1.399(4)	O(1)-C(6)-C(5)	123.9(3)
C(8)–C(9)	1.505(5)	C(5)-C(6)-C(1)	117.6(3)
C(9)–C(10)	1.518(5)	N(1)-C(7)-C(5)	126.7(3)
C(11)–O(2)	1.390(4)	C(7)-N(1)-C(8)	116.1(2)



Fig. 2a. Packing pattern along a-axis does not show any intermolecular interactions.

melting point, presence/absence of water of hydration in the coordination sphere etc., of the biologically active metal chelates [43]. The non - isothermal TG/DTA pattern of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) is reproduced in Fig. 4. No detectable endothermic peak was obtained from DTA (Fig. 4) till 100 °C indicating the absence of water molecules. Thus, the coordination sphere formed by the azomethine (-C=N–R) group coordinating to nickel atom had not only improved the thermal stability but the rotational motion of n-propyl group also prevented water molecules from approaching the nickel centre [44]. It melts at temperatures ranging from 168 to 171 °C, as evidenced by a sharp endo in the DTA curve (Fig. 4) and no corresponding weight loss in the TG curve. The solid phase is stable from 40 to 168 °C and the liquid phase is stable from 171 to 443 °C before decomposing. As seen from its TG curve, it loses only 2 % of its weight between 40 and 243 °C demonstrating its thermal stability even after melting and



Fig. 2b. Packing pattern along b-axis.



Fig. 3. Six membered chelate ring formed by the Schiff base ligands in bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II).

subsequently decomposes in two steps. The loss of two fragmented ligand moieties $[C_6H_4(OCH_3)CH=N(CH_2-)]$ could be attributed to the experimental weight loss of 68 % (calc.: 67.2 %) in the temperature range of 243–373 °C [45,46]. This was followed by a gradual trailing step caused by the removal of residual organic moieties, resulting in a greenish black end residue of NiO/C at 519 °C (exp.:17 %, calcd.: 16.86 %), as reported earlier for a similar type of complexes [46–49] under inert N₂ environment.

3.3. Anti-bacterial and anti-fungal study

The results on antibacterial performance are presented in Table 3. Among three concentrations taken for the study, $100 \mu g/ml$ did not show any activity against two test bacteria (*Escherichia coli* and *Staphylococcus aureus*). The 200 µg/ml concentration showed inhibition zones 19 mm and 20 mm against both test bacteria. The 300 µg/ml concentration showed more antibacterial activity in terms of inhibition zones of about 21 mm and 22 mm against *Escherichia coli* and *Staphylococcus aureus* respectively. The zones are almost similar to standard antibiotics which were about 22 mm and 23 mm for the respective organisms. These results obtained are comparable with the reported results of a similar complex of 2 – hydroxy – 3 – methoxy-benzaldehyde [50].

The complex was screened for its anti-fungal activity against *Aspergillus niger* and *Candida albicans*. Imidazole was selected as the positive antifungal agent (PC) and DMSO was used as negative control (NC). The disc diffusion assay data and the minimum inhibition

Table 3



Fig. 4. TG/DTA pattern of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) recorded at a linear heating rate of 10 °C/min in N₂ environment.

Antibacterial activity of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) using agar well diffusion method.

S. No.	Samples	Zone of Inhibition (i	in mm)
centerSamples		E. coli	S. aureus
1	1 (100 μg/ml)	0	0
2	2 (200 μg/ml)	19	20
3	3 (300 μg/ml)	21	22
4	PC (Streptomycin, 4 µg/ml)	22	23
5	NC (DMSO)	0	0

PC- Positive control, NC-Negative control.

concentration (MIC) and minimum bactericidal concentration (MBC) results were recorded and are given in Table 4. Among the three samples, the zone of inhibition was measured almost similarly ranging from 19 mm to 22 mm. The obtained results were found significant as the inhibitory zones were comparatively good with a positive control antifungal agent (Imidazole). It is found to be more bactericidal towards gram-positive that are tested. Such a selective activity was observed by Ishak et al. [51] for mixed ligand type Schiff base complex of nickel.

The nickel complex was observed to exhibit better antibacterial activity than the un - chelated Schiff base compounds (ligands) suggesting that the metal ions reduce the polarity of the compounds through the partial sharing of positive charge with the donor atoms such as N and O of Schiff bases [52]. Hence, p - electron delocalisation upon chelation increases the lipophilic character of the central metal atom which allows nickel complexes to permeate strongly to enter the permeable membrane of the bacterial strains [53]. Thus, imine-based (-C=N–R) (R = alkyl, aryl groups) nickel complexes show better antibacterial activity than the complexes containing only aldehyde - based ligands [54]. The complex studied here seemed to be more bactericidal towards the gram-positive bacteria tested. The complex has small MIC and MBC values against a *Staphylococcus aureus* positive bacterium, suggesting that only small amounts of the metal complex were required to inhibit/kill the growth of the micro - organism as observed earlier for a similar type of complexes [55]. Similarly, it has a small MIC and MFC against Candida albicans fungi (Table 5) suggesting that a small quantity was sufficient to inhibit the growth of fungi micro-organism as well. The biological activity results obtained for this compound were compared with the literature data (Table 6 and references therein Refs. [56–61]), demonstrating its potential as a therapeutic agent. According to previous and current findings, cell growth suppression may be caused by azomethine linkage, atoms present in Schiff base ligands and metal centre. Thus, the azomethine linkage of Schiff base ligands plays crucial roles in several pharmacological

Table 4

Antifungal activity of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) using agar well diffusion method.

S. No.	Samples	Zone of Inhibition (in mm)	
Sample		A. niger	C. albicans
1	NC (DMSO)	0	0
2	PC (Imidazole)	23	22
3	S (Sample)	20	21

PC- Positive control, NC-Negative control.

Table 5

Results for minimum inhibitory concentration (MIC) and minimum bactericidal/fungicidal concentration (MBC, MFC). Results are in (µg/ml).

Sample	Escherichia coli		Staphylococcus aureus		Aspergillus niger		Candida albicans	
	MIC	MBC	MIC	MBC	MIC	MFC	MIC	MFC
Complex	400	400	300	300	400	400	300	300

Table 6

Comparison of biological activity of bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II).

Ref.	Complexes	Antibacterial (Zone of inhibition in mm)		Antifungal	Antifungal (Zone of inhibition in mm)	
		E. coli	S.aureus	A.niger	C.albicans	
[56]	[Ni ₂ (L ¹)Cl ₂ (H ₂ O) ₆].2H ₂ O	2	10	NA	NA	
[57]	C ₂₀ H ₁₂ BrN ₂ O ₂ Ni	15	10	16	3	
[58]	C24H24N6O3Ni	23	19	16	16	
[59]	[NiL(OAc) ₂]	20	NA	11	21	
[60]	$[Ni(C_{14}H_8N_2OClF)_2(H_2O)_2]Cl_2 \cdot 2H_2O$	15	24	22	28	
[61]	C ₃₆ H ₃₂ N ₆ O ₄ Ni	18.6	18.6	9.3	4.6	
This Work	C ₂₄ H ₂₈ N ₂ O ₄ Ni	21	22	20	21	

properties of complexes in the medical field [62].

4. Conclusion

A distorted square planar Schiff base complex, bis{(2-methoxy-6-[(E)-(propylimino)methyl]phenolato}nickel(II) was prepared and screened for its thermal stability and biological activity. The spectral analysis confirmed the coordination of phenolic oxygen and azomethine nitrogen to nickel atoms. The X - ray crystal structure determination revealed the complex to crystallise in a monoclinic crystal system with a square planar geometry. The n-propyl and methoxy groups have arranged in transposition to each other and show out of plane arrangement. The presence of the azomethine group (-C=N–R) which is bonded to nickel contributes in the redistribution of charge on the complex which enhances the biological activity and thermal stability. The complex shows good thermal stability till 243 °C which is a desirable property for any biologically active ingredients. The nickel complex showed better antibacterial activity when the concentration was increased from 100 μ g/ml to 300 μ g/ml for *Escherichia coli* and *Staphylococcus aureus*. It was found to show a selective bactericidal activity towards gram-positive. The small MIC and MFC indicate only a little amount of this complex is required to kill the bacteria.

Compliance with ethical standards

The authors confirm that the submitted manuscript is an outcome of a research work carried out in our laboratories on the title compound. The results were not published anywhere in part or in full. Further we, confirm that the manuscript is not under consideration for publication anywhere.

Research data policy and data availability

The datasets generated during and/or analysed during the current study are available from the corresponding author on reasonable request.

CRediT authorship contribution statement

S. Sindhu: Project administration, Formal analysis. **S. Arockiasamy:** Writing – review & editing, Writing – original draft, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.heliyon.2024.e24108.

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