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Synthesis, Spectroscopic, Computational and Biological Studies of Ni(II) Mixed-Ligand Complex Of (E)-1-((Phenylimino)Methyl)Naphthalen-2-Ol

Demehin, Abidemi Iyewumi [1,*], Oladipo, Mary Adelaide [2], Semire, Banjo [2]

[1],**Department of Chemistry, Adeyemi Federal University of Education, P.M.B. 520, Ondo, Ondo State, Nigeria.*

[2]*Department of Pure and Applied Chemistry, Faculty of Pure and Applied Chemistry, Ladoke Akintola University of Technology, P.M.B. 4000, Ogbomoso, Oyo State, Nigeria.*

[2]*Department of Pure and Applied Chemistry, Faculty of Pure and Applied Chemistry, Ladoke Akintola University of Technology, P.M.B. 4000, Ogbomoso, Oyo State, Nigeria.*

(*)Corresponding Author's: demehinai@gmail.com, +2348050415759

Abstract

The Schiff base compound (E)-1-((phenylimino)methyl)naphthalen-2-ol and the mixed Ni(II) complex were synthesized and characterized by elemental analysis, IR, UV-Vis, ^{1}H and ^{13}C NMR spectroscopies. Computational calculations were also performed on the modelled and optimized structure of the Ni(II) complex via Density functional theory (DFT) employing Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional (B3LYP) and the Empirical Density Functional 1 methods (EDF1) with 6-31G** basis set. The IR, UV-Vis, ^{1}H and ^{13}C NMR spectra of the Ni(II) complex were calculated and the results compared with the corresponding experimental spectra to improve the experimental structural elucidation. The ^{1}H NMR spectrum revealed that the Schiff base coordinated to the nickel(II) ion through the deprotonated phenolic oxygen and azomethine nitrogen atoms. The comparison between the calculated and experimental data provided a very good agreement which supported the proposed structure. The antibacterial studies showed that the Ni(II) complex exhibited better inhibitory activities than the Schiff base ligand.

Keywords: Antibacterial, antioxidant, computational, Nickel(II) ion, Schiff base.

Introduction

(E)-1-((phenylimino)methyl)naphthalen-2-ol is a Schiff base synthesized from the reaction of 2-hydroxyl-1-naphthaldehyde and aniline. Schiff bases are compounds like aldehyde or ketone except that the carbonyl group (C=O) in the compounds are being replaced by an imine or azomethine, (HC=N) group and have the general formula $RR_1C{=}N{-}R_2$ [1-3]. If R equals hydrogen, alkyl or aryl, R_1 hydrogen and R_2 alkyl or aryl; the compounds are referred to as aldimines ($R_1{-}CH{=}NR_2$) while compounds where both R and R_1 are alkyl or aryl groups are called ketimines. R_2 can either be an alkyl or aryl group [4-6].

Schiff bases can also be called azomethines or imines [7, 8]. They are significant chelating ligands in coordination chemistry and the chemical properties can be altered by varying the substituents on either the carbonyl or the amine ring. Intra- and intermolecular hydrogen bonds can be formed from Schiff bases obtained from salicylaldehyde and its different derivatives which usually determine their chemical and physicochemical properties [3, 9, 10]. They have vital donor atoms like nitrogen and oxygen which make them resemble living systems and display different biological properties. The ensuing imines in Schiff bases are involved in binding with metal ions via nitrogen lone pair of electrons, these can bind to the central metal ions as monodentates and polydentates [5, 8, 11]. The imine groups are important for the biological activities of Schiff bases and are very useful active centres of many biological systems [7, 12]. Schiff bases lead to the formation of many mononuclear and binuclear complexes with different coordination modes and stereochemistry [13, 14].

Schiff bases have played essential roles in understanding the coordination chemistry of transition metal ions. Studies showed that Schiff bases derived from 2-hydroxyl-1-naphthaldehyde and complexes with some transition metals displayed significant biological properties which make them gain attention. Some of the reported significant biological properties are antibacterial, antifungal, antimalarial, anthelmintic, anti-inflammatory, analgesic, anticonvulsant, antioxidants, anticancer, antiviral, antiparasitic and antitumor activities [1, 2, 5-8, 10, 12, 14-23]. Several Schiff base complexes have been synthesized due to the marked biological activities. Nevertheless, literatures search indicated that reports on complexes bearing ammonia are really limited. Therefore this study, which investigated the synthesis, spectroscopic, computational and biological studies of Ni(II) mixed-ligand complex of (E)-1-((phenylimino)methyl)naphthalen-2-ol with ammonia as co-ligand. Presently, with the development of computational methods, it is possible to reliably modelled and determine the molecular properties of different compounds to help augment experimental observations. Therefore, the molecular structure of the complex was modelled and DFT calculations were carried out on the optimized structure. A consideration of the resemblances between the theoretical and experimental spectra of the complex could further be used for the structural elucidation.

Materials and Methods

Reagents

Aniline, 2-hydroxy-1-naphthaldehyde, nickel(II) acetate tetrahydrate, methanoic acid and ammonium hydroxide were purchased from Merck (Germany) and used as supplied. The solvents were of analytical grade.

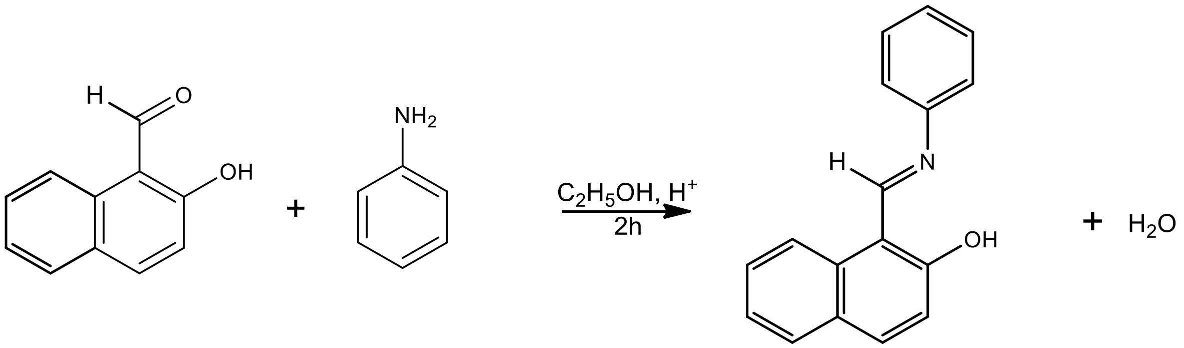
Instruments

The melting points of the synthesized compounds were recorded in open capillaries in Stuart Melting point, SMP10 apparatus. A Thermo Finnigan Flash EA 1112 Series was used for the elemental analyses (C, H, N). The Infrared spectroscopy analyses were carried out using the attenuated (ATR) technique with a Perkin-Elmer 400 FT-IR/FT-FIR spectrometer. A MPD Mitamura Riken Kogyo (Japan) electrothermal was used to determine the melting points. The nuclear magnetic resonance spectra were carried out on a Bruker Avance III 600 Spectrometer in solution with deuterated chloroform and DMSO using tetramethylsilane (TMS) as internal standard at 600 MHz. The UV-Visible spectra were recorded in 1.0 x 10^{-4} M DMSO solution using Shimadzu UV-2600 Spectrophotometer in the range 250-900 nm.

Syntheses

Synthesis of the Schiff base

5.0 mmol of the corresponding amine in 10 mL of ethanol was added in drops to 5.0 mmol of the 2-hydroxy-1-naphthaldehyde in 20 mL of the same solvent. The resulting solution was stirred for 2 hours on addition of three drops of methanoic acid. The coloured solids precipitated were separated by filtration and recrystallized from hot ethanol.



Scheme 1: Synthetic route of (E)-1-((phenylimino)methyl) naphthalen-2-ol

(E)-1-((phenylimino)methyl)naphthalen-2-ol ($C_{17}H_{13}NO$; L): Yield: 85%, colour: yellow solid, mol wt:: 247.29 g/mol. Elemental analysis, % (Found) C: 82.58, H: 5.30, N: 5.67. Calculated, C: 82.57, H: 5.30, N: 5.67. FT-IR (ATR, cm^{-1}): 3550, 3151, 2318, 2159, 2040, 1961, 1620, 1546, 1489, 1408, 1347, 1336, 1318, 1214, 1143, 1101, 1088, 1079, 1043, 1027, 982, 969, 907, 866, 839, 757, 688, 664, 648, 569, 544, 528, 519, 494, 479, 467. ^{1}H NMR (DMSO-d_6, δ, ppm): 13.05 (s, 1H, OH), 9.29 (s, 1H, −HC=N), 8.07-7.06 (m, 9H, aromatic). ^{13}C NMR (DMSO-d_6, ppm): 154.32, 144.94, 139.32, 137.04, 133.34, 129.72, 129.49, 128.26, 127.26, 126.69, 124.56, 123.53, 122.69, 120.26, 118.80. UV-Vis (DMSO, cm^{-1}): 31348 ($n-\pi^*$), 22676 ($\pi-\pi^*$).

Synthesis of the Ni(II) complex

A methanolic solution of $Ni(CH_3COO)_2.4H_2O$ (0.5 mmol) was added in drops to the corresponding Schiff base solution (1.0 mmol) while stirring in 10 mL of the same solvent. Some drops of aqueous ammonia were added to modify the pH of the resulting mixture to 7-7.5 and refluxed at 60°C for 4 hours. The brown solid precipitated was filtered by vacuum filtration, washed with distilled water, diethyl ether and methanol. This was dried over silica gel in a desiccator for two days and recrystallized from DMSO.

$$Ni(CH_3COO)_2.4H_2O \ + \ 2\,L \ \xrightarrow[p^H = 7\text{-}7.5]{NH_4OH} \ Ni(L)_2(NH_3)_2 \ + \ 2CH_3COOH \ + \ 5H_2O$$

Scheme 2: Synthetic route of the Ni(II) complex.

$Ni(L)_2(NH_3)_2$ ($NiC_{34}H_{30}N_4O_2$): Yield: 73%, brown solid, mol wt.: 585.32, m.pt: >260°C. Elemental analysis, % (Found) C: 68.96, H: 4.62, N: 9.39. Calculated, C: 69.77, H: 5.17, N: 9.57. FT-IR (ATR, cm^{-1}): 3339, 3281, 3238, 3162, 3016, 2925, 1904, 1820, 1613, 1600, 1578, 1532, 1510, 1475, 1456, 1428, 1409, 1397, 1361, 1344, 1312, 1292, 1280, 1261, 1251, 1205, 1170, 1111, 1097, 1041, 1029, 986, 964, 948, 912, 869, 855, 835, 826, 817, 775, 756, 690, 669, 652, 586, 562, 552, 507, 495, 471. ^1H NMR (DMSO-d_6, ppm): 9.25 (s, 1H, −HC=N), 8.50-6.44 (m, 9H, aromatic), 2.37 (s, 3H, $-NH_3$). ^{13}C NMR (DMSO-d_6, ppm): 166.88, 163.21, 142.02, 140.78, 134.03, 129.91, 128.46, 127.98, 127.73, 124.10, 122.89, 118.61, 115.99, 114.16. UV-Vis (DMSO, cm^{-1}): 30675, 22472, 21321.

Computational method

The structure of the Ni(II) complex was modelled and optimized using Gaussian 09 and Spartan '14 computational software packages. It was modelled based on the electronic spectrum and elemental analysis data. Density Functional Theory was employed for the geometry optimization, chemical shifts and electronic transitions calculations of the Ni(II) complex. The DFT calculations were performed on the optimized geometries in the ground states using Becke's three-parameter hybrid functional employing the Lee-Yang-Parr correlation functional (B3LYP) and the Empirical Density Functional 1 methods (EDF1) with 6-31G** basis set [9, 24, 25].

Antibacterial study

The antibacterial potentials of the Schiff base ligand and Ni(II) complex were measured against some Gram-positive and Gram-negative bacterial strains by agar-well diffusion method. The Gram-positive bacterial strains were *Streptococcus agalactiae and Staphylococcus aureus while Escherichia coli, Klebsiella pneumoniae, Proteus mirabilis, Pseudomonas aeruginosa and Salmonella typhimurium* were the Gram-negative bacterial strains used. The Nutrient agar medium was used to sub-culture the isolates of bacterial strains which were nurtured at 37°C for 24 hours. 20 mL of disinfected Nutrient agar medium was dispensed in each germfree Petri dish after modifying the bacterial strains cultures to 0.5 McFarland standards, these were allowed to gel. The dishes were swabbed with the inocula of the bacterial strains and left for 15 minutes to adsorb unto the gel. Varying concentrations of the samples (5 mg/mL, 10 mg/mL and 15 mg/mL) were filled into the wells that were drilled on the seeded agar dishes by a sterile cork borer of 6 mm diameter. These were kept for 1 hour in the refrigerator to allow for thorough circulation of the samples into the medium and then nurtured for 24 hours at 37ºC observing the inhibition zones. Antimicrobial activities were expressed as inhibition diameter zones in millimeter (mm). Standard Gentamycin (10 µg/ml) was employed as control [24, 26].

Phosphomolybdate Total Antioxidant Capacity (PTAC) Assay

The total antioxidant capacities (TAC) of the compounds were determined by phosphomolybdenum assay and ascorbic acid was used as the standard. 1.0 mL of reagent (0.6 M sulphuric acid, 28 µM sodium phosphate and 4 µM ammonium molybdate) was reacted with a fractional part of the extract solution (1.0 mL of 1000 µg). The covered tubes were incubated at 95ºC in a water bath for 90 minutes after which the samples were cooled to room temperature and a UV spectrophotometer was used to measure the absorbance of the aqueous solution of each at 695 nm. The procedure was repeated for an empty solution containing 1.0 mL of reagent solution. The TAC studies were performed three times and the mean was expressed as equivalents of ascorbic acid [27].

Results and discussion

The synthesized Schiff base and Ni(II) complex were stable and coloured solids. The Ni(II) complex was not soluble in water and almost all organic solvents except in DMSO and DMF. The melting point of the complex was greater than 260ºC. Elemental analyses data indicated the formation of 1:2:2 [metal: Schiff base: ammonia] molar ratio for the complex. The crystals obtained in DMSO were not suitable for X-ray crystallography study. No crystal was obtained in DMF. Attempts to isolate single crystal suitable for X-ray crystallography study were not successful.

Spectroscopic studies

Infrared spectra

The spectrum of the free Schiff base ligand presented in Fig. 1 displayed the azomethine ν(−HC=N) band at 1614 cm^{-1}, this band shifted to lower wavenumber 1600 cm^{-1} in the spectrum of the Ni(II) complex (Fig. 2). This revealed the involvement of the azomethine nitrogen atom in coordination with the Ni(II) ion and the formation of metal−ligand bond. The absorption band at 1143 cm^{-1} in the spectrum of the free Schiff base ligand was assigned to the phenolic (C−O) stretching vibration. This band shifted to higher wavenumber 1261 cm^{-1} in the Ni(II) complex which revealed the participation of the phenolic oxygen atom in coordination with the Ni(II) ion. The free Schiff base ligand displayed hydroxyl ν(O−H) absorption band around 3550–3151 cm^{-1}, this band was absent in the Ni(II) complex which further confirmed the deprotonation of the phenolic group and the coordination of phenolic oxygen atom to the Ni(II) ion [6, 18, 23, 24, 28]. The complex exhibited the ν(C−H) stretching vibration around 3281-2920 cm^{-1} and the aromatic ν(C=C) vibration in the range

1578-1409 cm^{-1}. The aromatic ν(C−H) bending vibrations appeared around 869-652 cm^{-1}. The new bands exhibited at 3339 cm^{-1} in the spectrum of the Ni(II) complex was assigned to ν(N−H) stretching vibration of –NH_3 groups, which revealed the presence of –NH_3 groups in the complex and the participation of nitrogen atom of –NH_3 groups in coordination with the Ni(II) ion [24, 29, 30]. The bands at 495-471cm^{-1} and 586-507 cm^{-1} in the complex were assigned to the stretching vibrations of the metal–oxygen, ν(M−O) and metal–nitrogen, ν(M−N) bands respectively. These confirmed the attachment of the Schiff base to the Ni(II) ion through the phenolic oxygen and the azomethine nitrogen atoms [11, 24, 31].

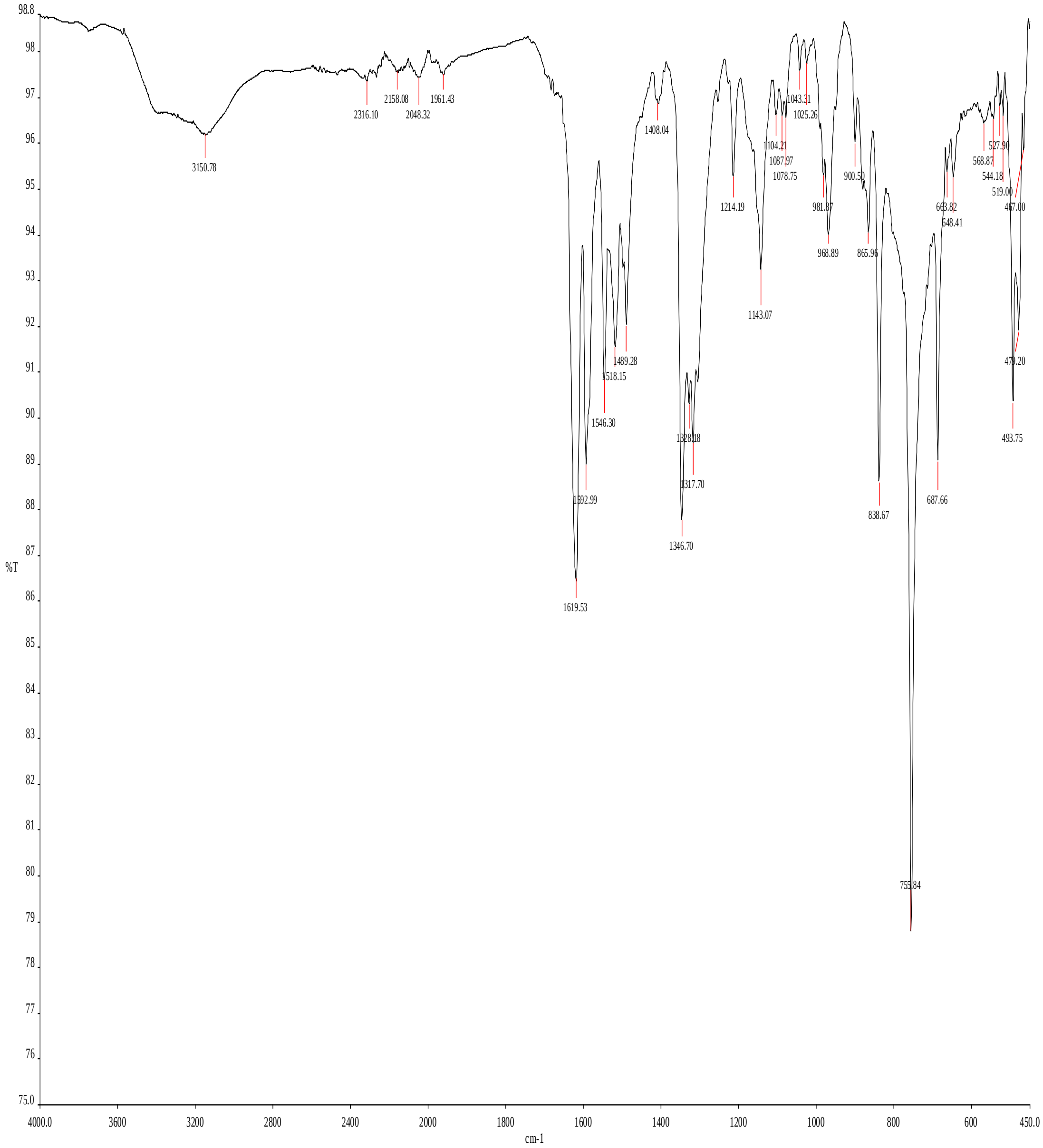


Fig 1: FT-IR spectrum of Schiff base ligand

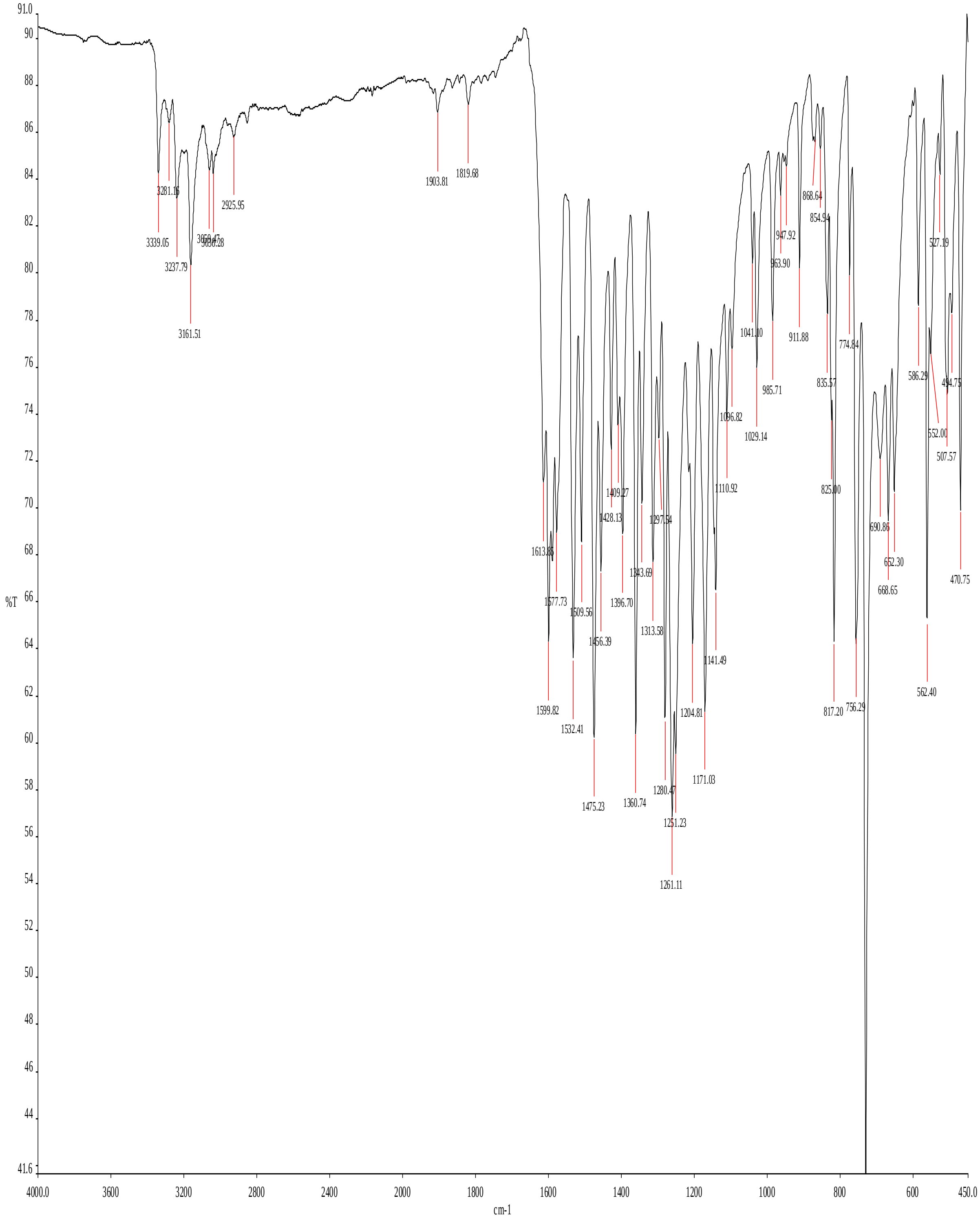
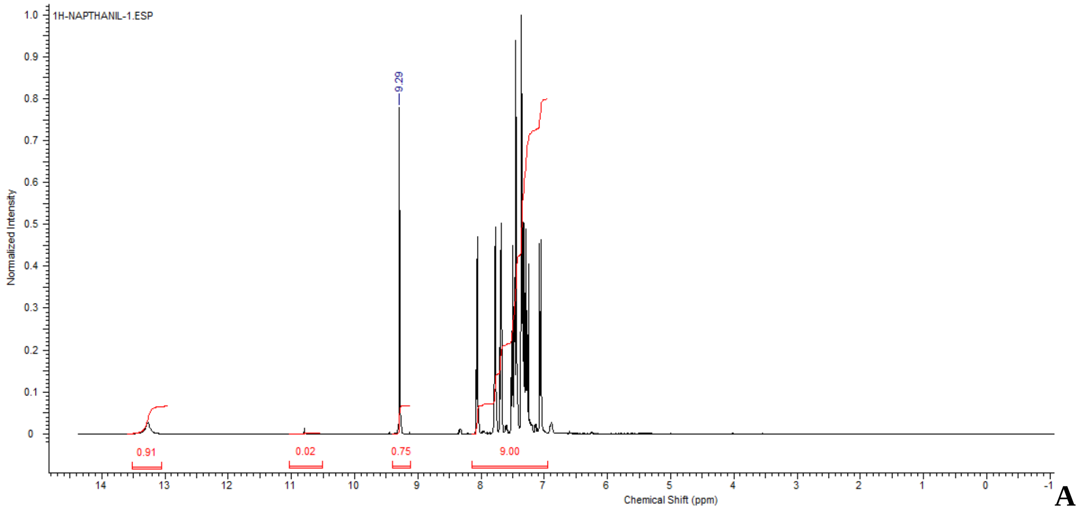


Fig 2: FT-IR spectrum of Ni(II) complex

NMR spectra

The ^{1}H NMR spectrum of the free Schiff base ligand displayed a singlet signal at δ 13.30 ppm and δ 9.29 ppm assigned to the phenolic (–OH) and azomethine (−HC=N) protons respectively. The signals for aromatic protons appeared as multiplets at δ 8.07-7.06 ppm [1, 20, 24]. A comparison of the ^{1}H NMR spectra of the free Schiff base ligand and the Ni(II) complex in Fig. 3 showed that the phenolic –OH proton in the parent Schiff base was absent in the complex. This indicated the detachment of the Schiff base –OH proton before coordinating to the Ni(II). It also corroborated the coordination of oxygen atoms to the metal ions. Additionally, the coordination of the azomethine nitrogen atoms of the parent Schiff base to the Ni(II) were indicated by the displacements of the chemical shift of the azomethine proton to 9.25 ppm. The aromatic protons in the complex appeared as multiplets at δ 8.50-6.44 ppm [18, 22, 29]. The new singlet signals at δ 2.37 ppm in the Ni(II) complex were assigned to the three hydrogen atoms of $–NH_3$ groups [24, 32]. Signals at 3.33 ppm and 2.46 ppm in the spectrum of the complex were for H_2O/DMSO and DMSO respectively. The ^{1}H NMR revealed the coordination of the Schiff base ligand to the central Ni(II) ion.

The ^{13}C NMR spectrum of the Ni(II) complex was in accord with the ^{1}H NMR. The ^{13}C NMR spectrum of Ni(II) complex (Fig. 4) exhibited a peak at δ 166.88 ppm which confirmed the presence of azomethine carbon in the complex. The peaks for the aromatic carbons were displayed around 163.21-114.16 ppm [24, 29].



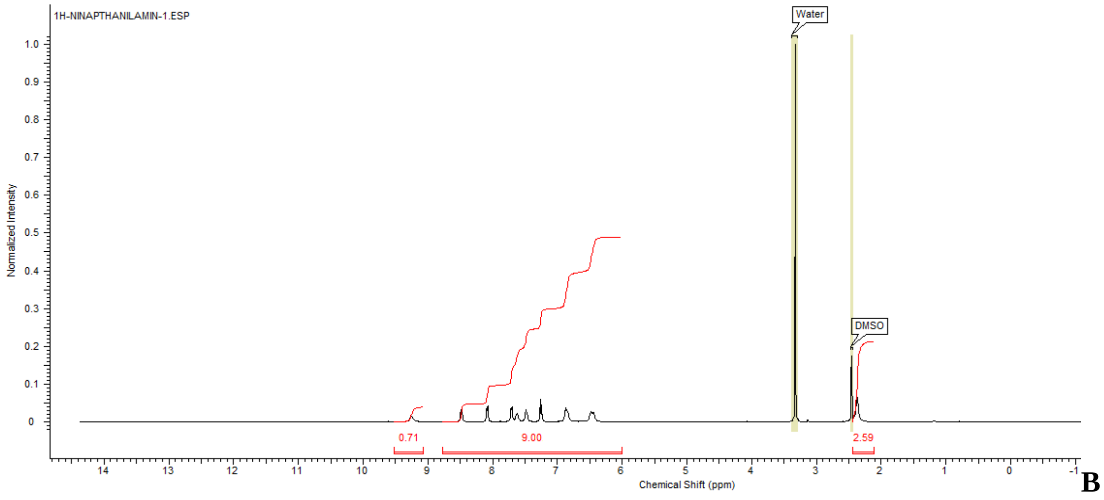


Fig. 3: ^{1}H NMR spectra of Schiff base ligand (A) and Ni(II) complex (B).

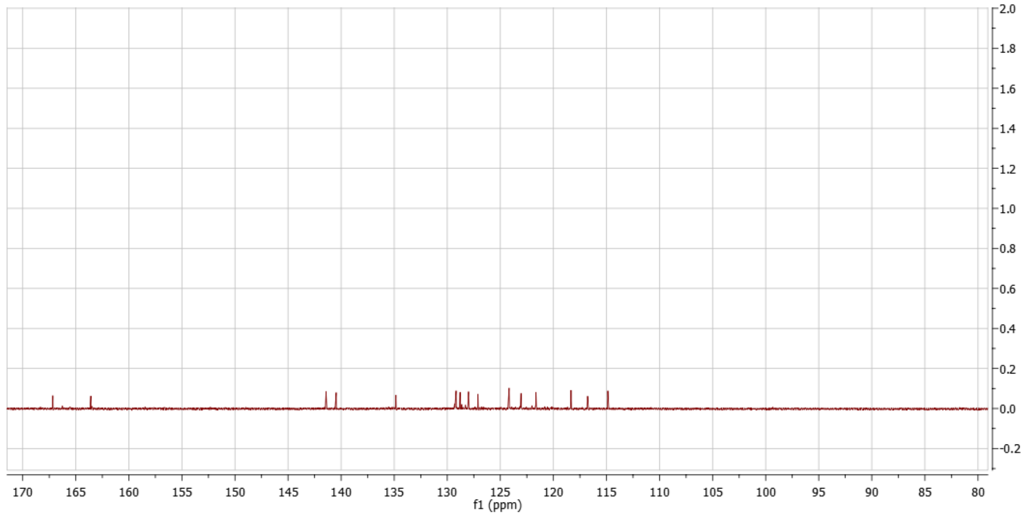


Fig. 4: ^{13}C NMR spectrum of Ni(II) complex.

Electronic spectrum

The electronic spectra were recorded in 1.0 x 10^{-4} M DMSO solution in the range 250-900 nm. The spectrum of the Ni(II) complex exhibited three bands at 30675 cm^{-1}, 22472 cm^{-1} and 21321 cm^{-1} attributed to LMCT, $^{3}A_{2(g)}(F)\rightarrow{}^{3}T_{1(g)}(P)$, $^{3}A_{2(g)}(F)\rightarrow{}^{3}T_{1(g)}(F)$ transitions respectively [3, 33-35]. Owing to these, an octahedral geometry was proposed for the complex the complex.

Theoretical IR spectra

The theoretical IR vibrational frequency values of the Ni(II) complex (Table 1) were in good agreement with the experimental values. The azomethine ν(−HC=N) absorption band of the complex was observed around 1624 cm^{-1} and 1619 cm^{-1} at B3LYP/6-31G** level while it appeared at 1600 cm^{-1} experimentally. The phenolic C−O stretching vibrations in the theoretical data were shown in the range 1345-1112 cm^{-1}; however, the stretching vibration was observed around 1261 cm^{-1} experimentally.

Table 1: Some selected theoretical IR data of the Ni(II) complex.

IR bands (cm^{-1})	$NiLNH_3$	
	B3LYP	EDF1
ν(N−H)	3590-3416	3539-3475
ν(C−H)	3209-3094	3292-3057
ν(C=N)	1624,1619	1624, 1622
ν(N−H) bending	1676-1631	1652-1630
ν(C=C)	1588-1403	1616-1405
ν(C−O)	1345-1112	1318-1147
ν(C−H) bending	991-762	989-719
ν(Ni−O)	549-510	545-503
ν(Ni−N)	667-559	650-545

Furthermore, the ν(N−H) stretching vibration of the $-NH_3$ groups were displayed at 3590-3416cm^{-1} theoretically while it was observed at 3339 cm^{-1} in the experimental spectrum. The characteristic ν(C=C) bands of the aromatic ring were observed at 1588-1403 cm^{-1} in the theoretical data while the bands were exhibited at 1578-1409 cm^{-1} experimentally. The ν(Ni−O) and ν(Ni−N) absorption bands were revealed in the range 549-510 cm^{-1} and 667-559 cm^{-1} in the theoretical spectrum, however, they appeared at 495-471 cm^{-1} and 586-507 cm^{-1} respectively in the experimental data. The observed theoretical IR data were within the expected range for the functional groups.

Theoretical NMR spectra

The theoretical values for the chemical shifts of the Ni(II) complex (Table 2) were in good agreement with the experimental results. The data obtained at B3LYP/6-31G** level revealed the aromatic protons in the Ni(II) complex as: H2, H7, H3, H10, H9, H8, H4, H6, H11, H12, H20, H22, H23, H24, H25, H26, H19, H28, H29, H30, H13, H21 which were displayed at 8.39, 8.42, 8.65, 8.14, 8.22, 8.10, 9.38, 9.38, 8.48, 8.48, 8.39, 8.42, 8.65, 8.14, 8.22, 8.10, 9.38, 9.38, 8.48, 8.48, 8.26, 8.26 ppm respectively in the theoretical spectrum, these aromatic protons appeared in the range 8.50-6.44 ppm in the experimental data. However, the azomethine (−HC=N) protons were shown at 10.00 ppm in the theoretical calculations while they appeared in the experimental spectrum at 9.25 ppm. The chemical shift of the three protons in the $-NH_3$ groups appeared at 1.70 ppm in the theoretical data and 2.37 ppm in the experimentally.

However, the aromatic carbons in the Ni(II) complex appeared in the range 159.45-113.80 ppm in the theoretical spectrum, these were observed experimentally in the range 163.21 -114.16 ppm. The azomethine carbon appeared at 169.69 ppm in the theoretical calculations and was observed experimentally at 166.88 ppm.

A comparison of the theoretical and experimental data of the complex revealed that the theoretical spectrum values were in good agreement with the experimental data. The agreement of the experimental and theoretical data supported the proposed structure for the complex

Table 2: Theoretical NMR spectra data of the Ni(II) complex

Positions of H & C	Ni(II) complex δ (ppm)			
	^{1}H NMR		^{13}CNMR	
	B3LYP	EDF1	B3LYP	EDF1
1	1.70	3.24	159.45	152.13
2	8.39	8.21	124.96	123.15
3	8.65	8.65	133.04	129.59
4	9.38	9.31	121.52	119.99
5	10.00	9.67	133.15	129.96
6	9.38	9.31	113.86	115.75
7	8.42	8.46	124.16	122.16
8	8.10	8.20	116.22	115.28
9	8.22	8.27	122.50	119.85
10	8.14	8.18	113.80	113.08
11	8.48	8.50	169.69	163.98
12	8.48	8.50	150.11	147.21
13	8.26	8.32	120.27	118.70
14	1.70	3.24	121.06	119.27
15	1.70	3.24	121.06	119.27
16	1.70	3.24	123.86	121.77
17	1.70	3.24	123.86	121.77
18	1.70	3.24	159.45	152.13
19	9.38	9.31	113.86	115.75
20	8.39	8.21	133.04	129.59
21	8.26	8.32	133.15	129.96
22	8.42	8.46	124.96	123.15
23	8.65	8.65	121.52	119.99
24	8.14	8.18	113.80	113.08
25	8.22	8.27	122.50	119.85
26	8.10	8.20	116.22	115.28
27	10.00	9.67	124.66	122.16
28	9.38	9.31	169.69	163.98

29	8.48	8.50	150.11	147.21
30	8.48	8.50	120.27	118.70
31	-	-	121.06	119.27
32	-	-	121.06	119.27
33	-	-	123.86	121.77
34	-	-	124.86	121.77

Geometry of the Ni(II) complex

In the absence available X-ray crystallographic data, the use of quantum chemical methods in determining the equilibrium geometry of the Ni(II) complex becomes an important tool. Table 3 showed the data from B3LYP/6-31G** and EDF1/6-31G** methods used to predict the geometry of the complex. The experimental and theoretical results earlier discussed have confirmed the formation of the complex. The two methods used for the calculations suggested a distorted octahedral geometry for the Ni(II) complex. The bond angles N2−Ni1−N3, N1−Ni1−N4, O1−Ni1−O2, N2−Ni1−N4, N4−Ni1−N3, N2−Ni1−O1, N2−Ni1−N1 at B3LYP/6-31G** are 179.87°, 179.79°, 179.80, 91.02°, 88.96°, 71.66°, 88.98° respectively. These values revealed that the coordination geometry of the nickel atom is distorted from a regular octahedral and are in the range of observed values for reported distorted octahedral geometry of Ni(II) complex [36-38]. Similarly, the bond distances Ni1−N1, Ni1−N2, Ni1−N3, Ni1−N4, Ni1−O1, Ni1−O2 are 1.937 Ȧ, 1.930 Ȧ, 1.931 Ȧ, 1.934 Ȧ, 2.653 Ȧ, 2.652 Ȧ respectively. Thus, the proposed and optimized structures of the Ni(II) complex were shown in Fig. 5.

Table 3: Selected bond distances and bond angles of the Ni(II) complex

Bond Angles (°)	Ni(II) complex	
	B3LYP	EDF1
N2−Ni1−N3	179. 87	177.72
N1−Ni1−N4	179. 79	178.93
O1−Ni1−O2	179.80	177.61
N2−Ni1−N4	91.02	91.01
N4−Ni1−N3	88.96	88.54
N2−Ni1−O1	71.66	68.58
N1−Ni1−O1	75.47	74.64
N2−Ni1−N1	88.98	89.37
N1−Ni1−O2	104.60	106.54
N2−Ni1−O2	108. 14	113.26
N3−Ni1−O1	108.47	113.59
N3−Ni1−O2	71.72	64.47
N4−Ni1−O2	75.60	72.39
Bond Distance (Ȧ)		
Ni1−N1	1.937	1.907

Ni1−N2	1.930	1.917
Ni1−N3	1.931	1.911
Ni1−N4	1.934	1.906
Ni1−O1	2.653	2.937
Ni1−O2	2.652	2.764

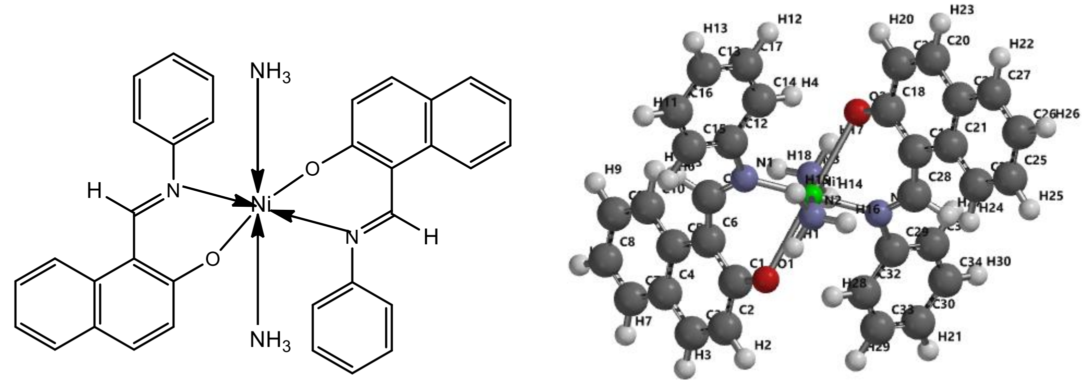


Fig. 5: **Proposed and Optimized structures of the Ni(II) complex at B3LYP/6-31G** level**

Antibacterial activity

The results of the antibacterial activities of the free Schiff base ligand and Ni(II) complex are summarized in Table 4. The antibacterial results revealed that the synthesized Schiff base ligand and Ni(II) complex exhibited antibacterial activities. The Ni(II) complex displayed better inhibitory effects compared to the free Schiff base ligand. The enhancement in the antibacterial activities of the complex can be explained on the basis of chelation theory and probably the presence of ammonia molecules in the Ni(II) complex. Chelation makes the Ni(II) complex more powerful and potent bactericidal agents; consequently, killing more bacteria than the free Schiff base ligand [2, 6, 10, 14, 15, 23]. In comparison with standard Gentamycin, the Ni(II) complex showed more potent activities against *S. agalactiae* than standard Gentamycin which was inactive against it.

Total antioxidant capacity

The results of the total antioxidant capacities of the Schiff base and Ni(II) complex are shown in Table 5. The free Schiff base ligand displayed higher total antioxidant capacities than the complex, though this was not expected. As literatures have reported that complexation of the system increases its capacity to stabilize unpaired electrons and consequently, to scavenge free radicals [39].

Table 4: Antibacterial activities of the Schiff base and Ni(II) complex

Bacterial strains	Concentration	Schiff base ligand	Ni(II) complex	Gentamycin standard
E. coli	5 mg/mL	-	16	20
	10 mg/mL	10	18	
	15 mg/mL	13	20	
K. pneumoniae	5 mg/mL	9	14	18
	10 mg/mL	12	15	
	15 mg/mL	12	18	
P. aeruginosa	5 mg/mL	10	19	20
	10 mg/mL	14	20	
	15 mg/mL	14	20	
S. agalactiae	5 mg/mL	6	14	-
	10 mg/mL	12	14	
	15 mg/mL	14	16	
S. aureus	5 mg/mL	7	16	20
	10 mg/mL	14	19	
	15 mg/mL	14	21	
S. typhimurium	5 mg/mL	7	14	17
	10 mg/mL	11	16	
	15 mg/mL	11	20	
P. mirabilis	5 mg/mL	7	13	20
	10 mg/mL	11	13	
	15 mg/mL	12	13	
DMSO	5 mg/mL	-	-	-
	10 mg/mL	-	-	
	15 mg/mL	-	-	

− = Resistant, not sensitive (< 8 mm), sensitive (9−14 mm), very sensitive (15−19 mm) and ultrasensitive (> 20 mm) [15].

Table 5: Total antioxidant capacity

Schiff bases/Complexes	TAC µg per mg AA
Schiff base ligand	0.87
Ni(II) complex	0.82

Conclusion

(E)-1-((phenylimino)methyl)naphthalen-2-ol and Ni(II) mixed-ligand complex were synthesized and characterized by different spectroscopic techniques. The elemental analyses, IR, ^{1}H NMR, ^{13}C NMR and UV-Visible confirmed the formation of the complex. Density functional theory calculations were performed on the optimized structure of the complex to obtain the IR and NMR spectra which were used to augment the experimental results. Based on the spectroscopic and DFT studies, a distorted octahedral geometry was proposed for the complex.

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