



Synthesis, Characterization and Theoretical Study of New Schiff Bases Derived from 1,8-Diaminonaphthalene and Their Ni(II) Complexes

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Authors' contributions

This work was carried out in collaboration between all authors. All authors read and approved the final manuscript.

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ABSTRACT

In this study, we report the synthesis and characterization of some new Schiff base compounds (L1H₂, L2H₂ and L3H₂) derived from the condensation reaction of 1,8-diaminonaphthalene with substituted benzaldehydes (3-NO₂, 3,4-OMe and 4-CN) and their nickel (II) complexes. The characterization and nature of bonding have been attained by a means of elemental analysis (C, H and N) and spectral analysis (FT-IR, ¹H-NMR and ¹³C-NMR). The analytical and spectral data are in good agreement with the suggested structures and show a 1:1 molar ratio of the ligand to metal and reveal that the Schiff base ligands are bidentate and coordinate with the Ni (II) ion via the two azomethine nitrogen atoms. Theoretical modeling of prepared Schiff base complexes have been conducted using DFT calculations and the obtained results are in good agreement with the experimental data. The computational structural features and relative energies for all the prepared complexes were performed at B3LYP/6-31G(d) and B3LYP/6-31+G(d,p) levels of theory.

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Keywords: Schiff base; metal complexes; DFT calculation; 1,8-diaminonaphthalene; benzaldehyde.

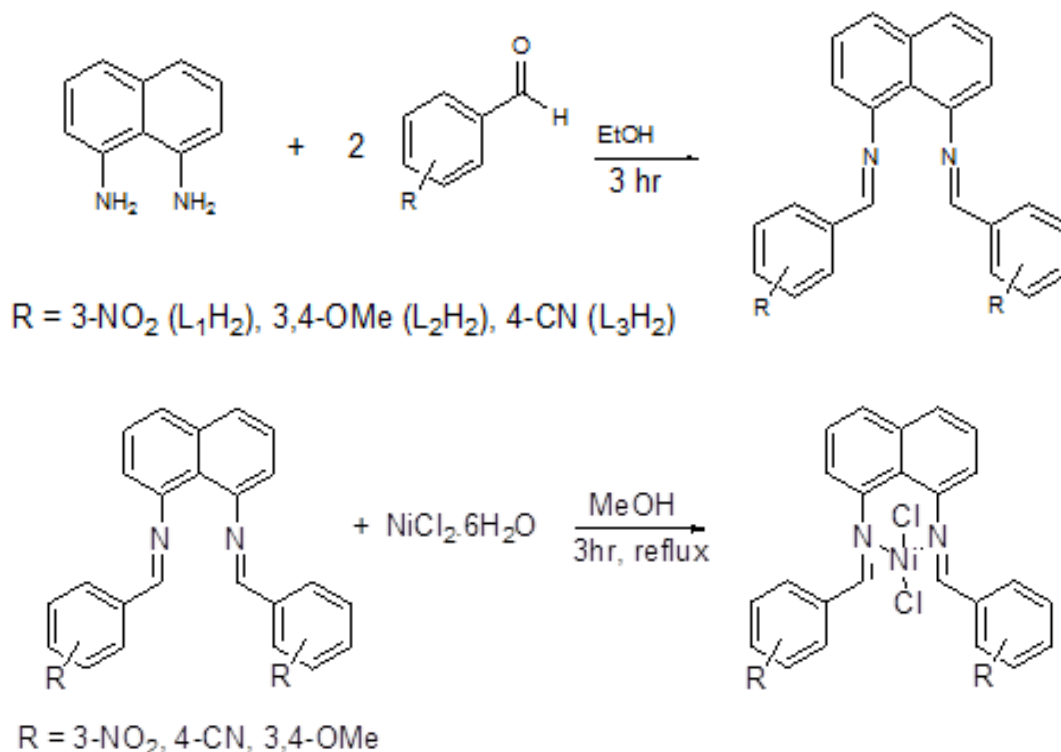
1. INTRODUCTION

Schiff's bases were first reported by Hugo Schiff in 1864 [1]. Schiff's bases are condensation of primary amines with carbonyl compounds such as aldehyde or ketone. Schiff's bases are important compounds owing to their wide range of industrial applications [2]. Furthermore, Schiff bases and their metal complexes have been extensively investigated and studied for many years to help the understanding of interactions between metal ions and proteins. This significant interest stems primarily from the unique chemical and biological properties exhibited by this class of compounds.

Several reports have concluded the biological activities of Schiff bases [3,4]. In addition to being important in organic synthesis, Schiff base metal complexes have played a major role in the advancement of

coordination chemistry. Schiff base complexes with different metal ions such as nickel, cobalt and copper have been studied and reported in details for their several crystallographic features, structure-redox relationships, enzymatic reactions, mesogenic characteristics and catalytic properties [5-7]. Several studies have shown unique properties of Schiff bases and their complexes such as their ability to reversibly bind oxygen [8], as second-order nonlinear optical materials [9] and as ferromagnetic materials [10].

In the present study, we report the preparation and characterization of Ni(II) complexes of the Schiff bases derived from the condensation of 1,8-diaminonaphthalene with substituted benzaldehydes at different positions in the benzene ring (Scheme 1). Theoretical modeling of the prepared complexes has also been carried out using DFT calculations.



Scheme 1. Synthesis scheme for the preparation of the Schiff base ligands and Ni(II) complexes

2. EXPERIMENTAL

2.1 Materials and Physical Measurements

All solvents used were of analytical grade purchased from Sigma Aldrich Chemical Company and were used without further purification. Nickel (II) chloride hexahydrate $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ was purchased from Sigma Aldrich Chemical Company and used as received. 1,8-diaminonaphthalene, 3-nitrobenzaldehyde, 3,4-dimethoxybenzaldehyde and 4-cyanobenzaldehyde were purchased from Merck Schuchardt.

^1H NMR and ^{13}C NMR spectra of the ligands were recorded on a Bruker AVANCE-400 MHz NMR spectrometer. Spectra were taken in DMSO- d_6 using TMS as an internal reference. Carbon, nitrogen and hydrogen analyses were performed using a Vario EL elemental analyzer. IR spectra were recorded on a Shimadzu FT-IR-8300 on KBr pellets in the wavenumber range of 400-4000 cm^{-1} .

2.2 Synthesis of Ligands

L₁H₂: A solution of 1,8-diaminonaphthalene (0.5 g, 3.16 mmol) in absolute ethanol (25 ml) was added dropwise to a stirred solution of 3-nitrobenzaldehyde (0.96 g, 6.32 mmol) in absolute ethanol (25 ml). The mixture was stirred at room temperature for 4 h. A red brown precipitate was formed and collected by simple filtration, washed with cold ethanol, and air dried: (1.1 g, yield 82%). Anal. Calc. ($\text{C}_{24}\text{H}_{16}\text{N}_4\text{O}_4$): C: 67.92, H: 3.80, N: 13.20, Found: C: 67.62, H: 3.73, N: 13.07%, IR (KBr disk): 1628 cm^{-1} (C=N), ^1H -NMR (DMSO, 400MHz) chemical shift (σ ppm): 8.87 (s, 2H, CH=N), 6.16–8.27 (m, 14H, H-aromatic), ^{13}C -NMR (DMSO, 400MHz) chemical shift (σ ppm): 158.9 (-C=N), 155.3 (m-nitro), 117.1, 135.9, 134.7, 125.6, 121.2 (benzene), 150.8, 144.3, 142.4, 137.4, 115.6, 114.1 (naphthalene).

L₂H₂: (0.45 g, 2.84 mmol) of 1,8-diaminonaphthalene in absolute ethanol (20 ml) was added dropwise to a solution of 3,4-dimethoxybenzaldehyde (0.95 g, 5.68 mmol) in absolute ethanol (20 ml). The reaction mixture was stirred and refluxed for 6 h. After cooling, gray precipitate was formed and collected by filtration, washed with cold ethanol, and air dried: (0.98 g, yield 76%). Anal. Calc. ($\text{C}_{28}\text{H}_{26}\text{N}_2\text{O}_4$): C: 73.99, H: 5.77, N: 6.16, Found: C: 73.82, H: 5.72,

N: 6.06%, IR (KBr disk): 1638 cm^{-1} (C=N), ^1H -NMR (DMSO, 400MHz) chemical shift (σ ppm): 8.45 (s, 2H, CH=N), 3.77 (s, 6H, m-OCH₃), 3.83 (s, 6H, p-OCH₃), 6.46-8.74 (m, 12H, H-aromatic), ^{13}C -NMR (DMSO, 400MHz) chemical shift (σ ppm): 160.5 (-C=N), 158.2, 144.3, 134.3.1, 126.7, 115.7, 121.5 (benzene), 157.8, 143.6, 128.8, 125.3, 112.2, 104.7 (naphthalene), 55.2, 55.6 (methoxy).

L₃H₂: To an ethanolic solution (20 ml) of 4-cyanobenzaldehyde (0.66 g, 5.03 mmol) a solution of 1,8-diaminonaphthalene (0.40 g, 2.52 mmol) in absolute ethanol (15 ml) was added dropwise. The reaction was stirred at room temperature for 4 h. A brown precipitate was formed and collected by simple filtration, then washed with cold ethanol and air dried: (0.88 g, yield 87%). Anal. Calc. ($\text{C}_{26}\text{H}_{16}\text{N}_4$): C: 81.23, H: 4.20, N: 14.57, Found: C: 81.18, H: 4.12, N: 14.42%, IR (KBr disk): 1635 cm^{-1} (C=N), ^1H -NMR (DMSO, 400MHz) chemical shift (σ ppm): 8.65 (s, 2H, CH=N), 5.84–8.77 (m, 14H, H-aromatic), ^{13}C -NMR (DMSO, 400MHz) chemical shift (σ ppm): 156.8 (-C=N), 142.2 (p-CN), 118.7, 134.3, 132.2, 126.9, 118.7 (benzene), 117.3 (CN), 153.8, 137.3, 127.4, 125.2, 112.3, 104.5 (naphthalene).

2.3 Synthesis of Complexes

L₁H₂-Ni: (0.5 g, 1.18 mmol) of the ligand (L₁H₂) was dissolved in 15 ml of absolute ethanol in a 50 ml round-bottom flask. A solution of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.28 g, 1.18 mmol) in 10 ml absolute ethanol was added dropwise using a dropping funnel, then the reaction mixture was refluxed for 6 hour at 80°C. After the reaction mixture was cooled, the red precipitate was filtrated, washed with ether and air dried. (0.54 g, yield 83%), Anal. Calc. ($\text{C}_{24}\text{H}_{16}\text{Cl}_2\text{N}_4\text{NiO}_4$): C: 52.03, H: 2.91, N: 10.11%, Found: C: 51.98, H: 2.86, N: 10.09%, IR (KBr disk): 1612 cm^{-1} (C=N).

L₂H₂-Ni: (0.5 g, 1.10 mmol) of the ligand (L₂H₂) was dissolved in 15 ml of absolute ethanol in a 50 ml round-bottom flask. A solution of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.26 g, 1.10 mmol) in 10 ml absolute ethanol was added dropwise using a dropping funnel, then the reaction mixture was refluxed for 6 hour at 80°C. After the reaction mixture was cooled, the brown precipitate was filtrated, washed with ether and air dried. (0.51 g, yield 80%), Anal. Calc. ($\text{C}_{28}\text{H}_{26}\text{Cl}_2\text{N}_2\text{NiO}_4$): C: 57.57, H: 4.49, N: 4.80%, Found: C: 57.55, H: 4.46, N: 4.78%, IR (KBr disk): 1619 cm^{-1} (C=N).

L₃H₂-Ni: (0.45 g, 1.17 mmol) of the ligand (L₃H₂) was dissolved in 15 ml of absolute ethanol in a 50 ml round-bottom flask. A solution of NiCl₂.6H₂O (0.28 g, 1.17 mmol) in 10 ml absolute ethanol was added dropwise using a dropping funnel, then the reaction mixture was refluxed for 6 hour at 80°C. After the reaction mixture was cooled, the red precipitate was filtrated, washed with ether and air dried. (0.46 g, yield 77%), Anal. Calc. (C₂₆H₁₆Cl₂N₄Ni): C: 60.75, H: 3.14, N: 10.90, Found: C: 60.71, H: 3.09, N: 10.81, IR (KBr disk): 1623 cm⁻¹ (C=N).

2.4 Computational Method

All electronic structure calculations were performed using the Gaussian09 suite of programs [11]. Optimized geometries of all structures were fully optimized at using the hybrid DFT of B3LYP which employs the three parameter Becke exchange functional, B3 [12,13] with the Lee-Yang-Parr nonlocal correctional functional LYP [14] along with the polarized 6-31G(d) [15,16] basis set in gas phase. Analysis of the vibrational frequencies for all structures is used to ensure the absence of imaginary values in the vibrational mode calculations of the minima. The 6-31+G(d,p) [17] basis set at B3LYP level of theory has also been utilized to examine the effect of diffuse and polarization functions and to confirm the reliability of the 6-31G(d) basis set. The principal reason for employing different levels of theory is to assure that they give similar results for such systems and the relative stabilities remain independent of the used method. The GaussView5 program was used for preprocessing, structure modification, and post-processing analyses of structures, frequencies, and forces.

3. RESULTS AND DISCUSSION

The Schiff base ligands (L1H2, L2H2, and L3H2) were prepared by condensation of 1,8-

diaminonaphthalene with 3-nitrobenzaldehyde, 3,4-dimethoxybenzaldehyde, and 4-cyanobenzaldehyde in a 1:2 stoichiometric ratio in ethanol (Scheme 1). All of the isolated Schiff bases are stable at room temperature and soluble in most organic solvents. The elemental analysis and other properties of the ligands are listed in Table 1. The elemental compositions (C, H and N) of the L1H2, L2H2, and L3H2 ligands are in good agreement with the calculated values based on proposed molecular formulas. The reaction of the Schiff base ligands with Ni(II) yields complexes with the general formula LNiCl₂ where L is L1H2, L2H2 and L3H2 (Scheme 1). Analytical data show a 1:1 ratio of the ligand to metal. Additionally, the compositions of C, H and N are in good agreement with the suggested formulas. Their results along with some other physical properties of the complexes are listed in Table 2. The synthesized complexes are stable in the solid state and are generally soluble in DMSO and DMF.

The most characteristic infrared spectral band of Schiff bases belongs to the imine bond. The IR spectra of L1H2, L2H2 and L3H2 ligands reveal frequencies of 1628, 1638 and 1635 cm⁻¹, respectively, which are assigned to the (C=N) bond. The IR spectrum of 1,8-diaminonaphthalene shows characteristic peaks at 3370 cm⁻¹ and 3286 cm⁻¹ for ν (NH₂) and 1587 cm⁻¹ δ (NH) [18]. The absence of ν (NH₂) and benzaldehyde derivative ν (C=O) peaks in the spectra of the ligands indicates the complete formation of the imine product by the condensation from 1,8-diaminonaphthalene and the benzaldehyde derivative. Upon complexation with Ni(II), the C=N bands shift to 1612, 1619 and 1623 cm⁻¹, respectively, which indicates that the metal is coordinated to the Schiff base via the nitrogen atom of the azomethine group [19]. This was confirmed by the appearance of new bands at 520, 518 and 525 cm⁻¹, respectively, related to ν (Ni-N).

Table 1. Elemental analyses results and other physical properties of the prepared Schiff base ligands (L1H2, L2H2 and L3H2)

Ligand	Formula	FW (g/mol)	Color	Yield (%)	Elemental analyses calculated (Found) (%)		
					C	H	N
L1H2	C ₂₄ H ₁₆ N ₄ O ₄	424.41	Red-brown	82	67.92 (67.62)	3.80 (3.73)	13.20 (13.07)
L2H2	C ₂₈ H ₂₆ N ₂ O ₄	454.52	Gray	76	73.99 (73.82)	5.77 (5.72)	6.16 (6.06)
L3H2	C ₂₆ H ₁₆ N ₄	384.43	Brown	87	81.23 (81.18)	4.20 (4.12)	14.57 (14.42)

Table 2. Elemental analyses results and other physical properties of the prepared Schiff base complexes (L1H2-Ni, L2H2-Ni and L3H2-Ni)

Complex	Formula	FW (g/mol)	Color	Yield (%)	Elemental analyses calculated (Found) (%)		
					C	H	N
L1H2-Ni	C ₂₄ H ₁₆ Cl ₂ N ₄ NiO ₄	554.01	Red	83	52.03 (51.98)	2.91 (2.86)	10.11 (10.09)
L2H2-Ni	C ₂₈ H ₂₆ Cl ₂ N ₂ NiO ₄	584.12	Brown	80	57.57 (57.55)	4.49 (4.46)	4.80 (4.78)
L3H2-Ni	C ₂₆ H ₁₆ Cl ₂ N ₄ Ni	514.03	Red	77	60.75 (60.71)	3.14 (3.09)	10.90 (10.81)

From the IR results, it may be concluded that the Schiff base ligands are bidentate and coordinate with the Ni (II) ion via the two azomethine nitrogen atoms [20].

The ¹H-NMR spectrum of Schiff bases were recorded in DMSO-d₆ solution. The ¹H-NMR spectrum of Ni(II) complexes (L1H2-Ni, L2H2-Ni and L3H2-Ni) showed approximately the same peaks as to those in the free ligands. The ¹H-NMR spectra of L1H2, L2H2, and L3H2 ligands showed a singlet at 8.87, 8.45, 8.65 ppm, attributed to CH=N protons; while multiplet were in the range of 6.16–8.27, 6.46–8.74, and 5.84–8.77 ppm due to the aromatic hydrogens, respectively. The L2H2 ligand additionally shows two singlets at 3.77 and 3.83 ppm corresponding to the protons of the two methoxy groups. The

absence of any signals related to 1,8-diaminonaphthalene and benzaldehyde derivatives in ¹H-NMR spectra of prepared Schiff base ligands (L1H2, L2H2 and L3H2) indicates that the condensation reaction is complete with no remaining starting materials.

The ¹³C-NMR spectrum of Schiff bases were recorded in DMSO-d₆ solution. The ¹³C-NMR spectra of L1H2, L2H2 and L3H2 ligands showed peaks at 158.9, 158.9 and 156.8 ppm, respectively, due to -C=N carbons. The ¹³C-NMR spectra of the ligands reveal peaks assigned to carbon atoms of the benzene ring such that: *L1H2*: 155.3 (m-nitro), 117.1, 135.9, 134.7, 125.6, 121.2, *L2H2*: 158.2, 144.3, 134.3.1, 126.7, 115.7, 121.5 and *L3H2*: 142.2 (p-CN), 118.7, 134.3, 132.2, 126.9, 118.7 ppm.

Table 3. Selected bond lengths (Å), Angles (°), and Dihedral Angles (Torsions) (°) of L1H1-Ni

Bonds	B3LYP/ 6-31G(d)	B3LYP/ 6-31+G(d,p)
Ni49–N18	1.8746	1.9265
Ni49–Cl50	2.1923	2.1896
N18–C21	1.2937	1.2927
N18–C5	1.4300	1.4268
C21–C33	1.4581	1.4614
N45–O47	1.2303	1.2318
N45–C36	1.4734	1.4751
Angles		
C5–C4–C11	130.2457	130.0735
C5–N18–Ni49	106.2916	109.0781
Cl50–Ni49–Cl51	157.0067	160.3484
Cl50–Ni49–C18	95.7121	95.4539
Ni49–N17–C19	132.6695	130.0762
C36–N45–O46	117.5566	117.6611
O46–N45–O47	124.8669	124.6544
Torsions		
C11–C4–C5–N18	-19.3526	-19.1356
N18–Ni49–N17–C19	149.3621	149.9015
Ni49–N17–C19–C23	27.2369	25.9870
N17–C19–C23–C24	15.2667	18.4835
Cl50–Ni49–Cl51–N17	120.0656	122.9218
C34–C36–N45–O46	179.3181	179.2283
N18–Ni49–N17–C19	149.3621	149.9015

Additionally the ^{13}C -NMR spectra of the ligands show peaks attributed to carbon atoms of the naphthalene ring such that: L1H2: 150.8, 144.3, 142.4, 137.4, 115.6, 114.1, L2H2: 157.8, 143.6, 128.8, 125.3, 112.2, 104.7 and 153.8, 137.3, 127.4, 125.2, 112.3, 104.5 ppm. Furthermore, the methoxy groups in L2H2 ligand show two peaks at 55.2, 55.6 ppm whereas the L3H2 ligand is distinguished by the peak appearance at 117.3 ppm due to the carbon of the cyano group (-CN).

We have performed thorough calculations to find the most plausible and stable minimum for each prepared complexes. Figs. 1→3 depict the optimized ground state geometries for all

the prepared complexes at B3LYP/6-31G(d) level of theory. The selective structural parameters for L1H2-Ni optimized complex at B3LYP/6-31G(d) and B3LYP/6-31G(d,p) levels of theory are listed in Table 3, where the bond lengths are in Å and bond angles are in degrees. As you can see from Table 3, the structural parameters for both B3LYP/6-31G(d) and B3LYP/6-31G(d,p) levels of theory are very close differing by no more than 0.1Å for bond lengths and 3° for angels. The optimized Cartesian structures for all prepared complexes are available in the Supporting Information where the bonds and angles along with their relative energies can be seen in any visualization software.

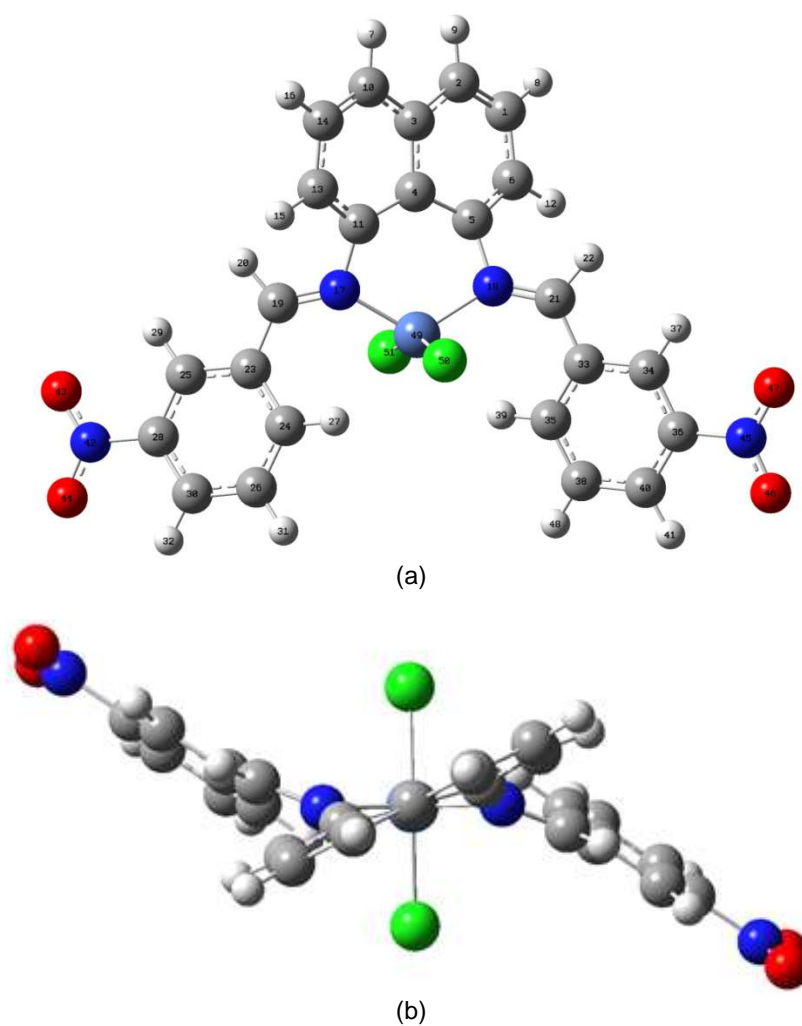


Fig. 1. The optimized ground state geometry for the L1H2-Ni complex at B3LYP/631G(d) level of theory. (a) and (b) correspond to the side- and top-view for the same structure

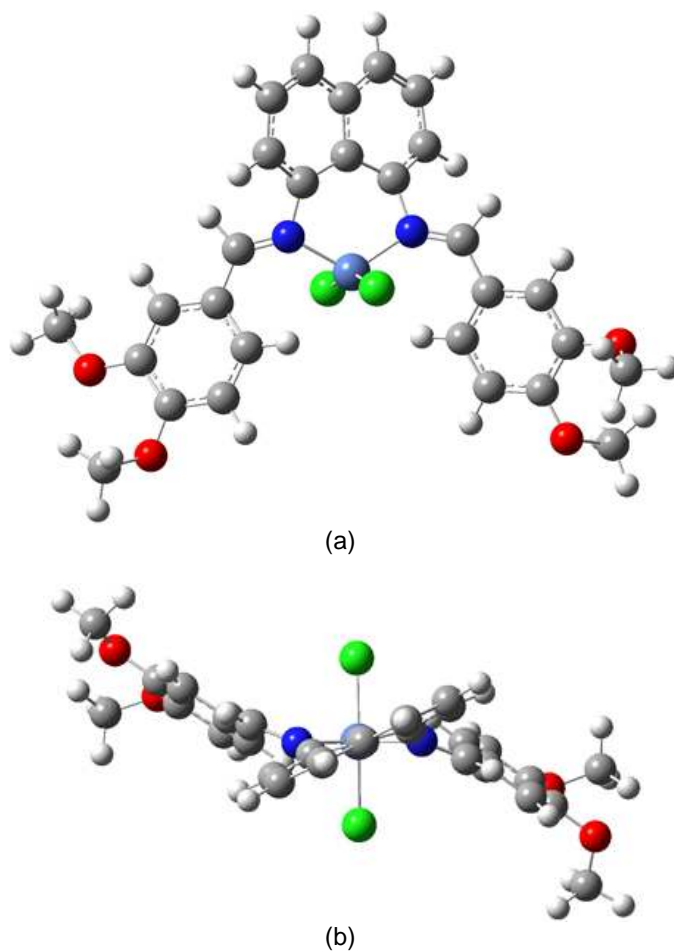
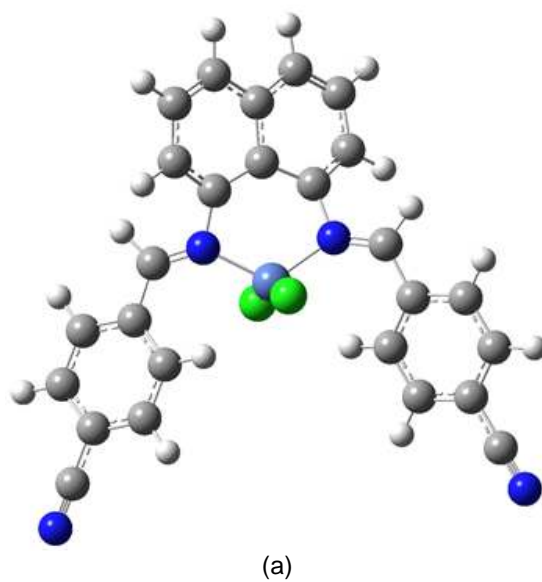


Fig. 2. The optimized ground state geometry for the L2H2-Ni complex at B3LYP/631G(d) level of theory. (a) and (b) correspond to the side- and top-view for the same structure



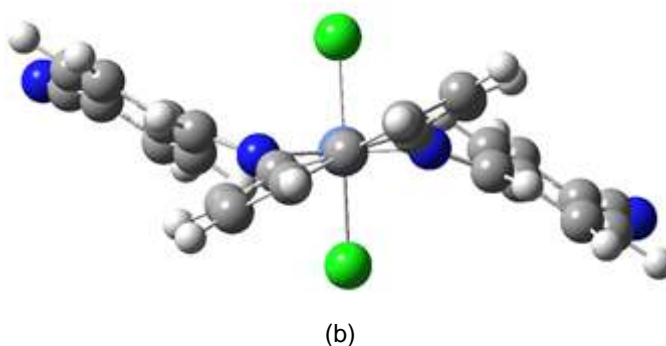


Fig. 3. The optimized ground state geometry for the L3H2-Ni Complex at B3LYP/631G(d) level of theory. (a) and (b) correspond to the side- and top-view for the same structure

4. CONCLUSION

We reported the preparation and characterization of Ni(II) complexes of the Schiff bases derived from the condensation of 1,8-diaminonaphthalene with substituted benzaldehydes at different positions in the benzene ring. Structural characterization was performed using several techniques such as $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, elemental analysis and FT-IR spectroscopy. The optimized ground state geometries for all the prepared complexes were reported at B3LYP level of theory using 6-31G(d) and 6-31+G(d,p) basis sets. The optimized ground state geometries for all the prepared complexes at both levels of theory are in excellent agreement with each other.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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