

Synthesis, Characterization, Quantum Chemical Studies, and Biological Activity of an Oxadiazole–Hydrazone Ligand Derived from 3-Ethyl-5-Methylpyridine and Its Metal Complexes

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Abstract: A new 1,2,3-oxadiazole-based hydrazone ligand, (Z)-4-(5-(2-((3-ethyl-5-methylpyridin-2-yl)methylene)hydrazinyl)-1,2,3-oxadiazol-2-yl)benzene-1,2,3-triol (L), and its Cr(III), Fe(III), and Ni(II) complexes were successfully synthesized and characterized by FT-IR, ¹H-NMR, mass spectrometry, magnetic susceptibility, and molar conductivity measurements. The spectral data suggested tetrahedral geometries for the Cr(III) and Fe(III) complexes, while the Ni(II) complex exhibited a square-planar geometry. The electronic properties of the ligand were investigated using density functional theory (DFT). The calculated HOMO-LUMO energy gap (4.60 eV) indicated good molecular stability and moderate chemical reactivity. The antibacterial activity of the ligand and its metal complexes was evaluated against *Serratia* and *Pseudomonas* by the agar well diffusion method. The metal complexes showed higher antibacterial activity than the free ligand, with the Cr(III) complex displaying the strongest inhibitory effect. The combined experimental and theoretical results suggest that coordination with transition metal ions enhances both the electronic properties and the biological activity of the synthesized ligand.

Keywords: oxadiazol, quantum chemistry, antibacterial, molecular orbitals.

1. Introduction

The increasing bacterial resistance to known antibiotics has been a cause of concern in the population, as their therapeutic possibilities have been diminishing. The main cause of the development of bacterial resistance is the indiscriminate use of antibiotics. The growth of bacterial resistance has caused the mortality of a significant number of people worldwide. Even the main commercial antimicrobial compounds (e.g., ampicillin, posaconazole, and ciprofloxacin) may have limited action against resistant strains of microorganisms [1-4]. This has led to intensified research on the synthesis and evaluation of heterocyclic derivatives with antimicrobial properties, such as 1, 3,4-oxadiazoles. Among them, oxadiazole derivatives play an important role in medicinal chemistry [2]. The 1, 3,4-oxadiazole derivatives have been found to exhibit diverse biological activities, including antimicrobial [3, 4], anti HIV (Human immunodeficiency virus (HIV) [5], antitubercular [6], antimalarial [7], anti-inflammatory [8, 9], anticonvulsant [10], and antitumor [11] activities. The choice of 1,3,4-oxadiazole is due to its multiapplicability in the field of medicine[12]. In the present study, new 1, 3, 4-oxadiazoles derivative were synthesized and characterized using different spectral studies and quantum chemical calculations. All new compounds were screened for antibacterial activity.

2. Materials and Methods

All chemicals and solvents used were of chemically pure grade, and commercially available. All metal salts were used as chloride.

2.1 Physical measurement

The melting point or decomposition temperature of all the prepared ligand and metal complexes were observed in an electro thermal melting point apparatus model (Melting SMP31). The FTIR spectra in the range of (250-4000) cm⁻¹ were recorded as KBr discs using a Shimadzu FTIR spectrophotometer (Model: IR- affinity, Shimadzu). Nuclear Magnetic Resonance Spectra were obtained using a Bruker DXR System AL500 (500 MHz). Mass Spectra were obtained using (Network Mass Selective Detector 5973). The purity of the ligand and metal complexes was tested using thin-layer chromatography (TLC).

2.2 Steps preparation of the Ligand

(Z)-4-(5-(2-((3-ethyl-5-methylpyridin-2-yl) methylene) hydrazinyl) -1, 2, 3-oxadiazol-2-yl) benzene-1,2,3-triol was prepared as follows [13]:

2.2.1. Preparation of 2,3,4-trihydroxybenzohydrazide (A)

A mixture of methyl 3,4,5-trihydroxybenzoate (18.4 ml, 0.1 mol) and hydrazine hydrate (10 ml, 0.2 mol) was dissolved in ethanol (100 ml) and refluxed for 8 h. The mixture (A) was evaporated to half, cooled, filtered, and re-crystallized in methanol [7]. The solid (A) was white, with a melting point of 156 °C and a yield of 87%.

2.2.2. Preparation of 4-(5-mercpto-1, 3, 4-oxadiazole-2-yl) benzene-1,2,3-triol (B)

2,3,4-trihydroxybenzohydrazide (A) (18.4gm, 0.1 mol), potassium hydroxide (5.6gm, 0.1 mol) and carbon disulfide (6 ml 0.1 mol) were refluxed in (100 ml) ethanol. The solvent was evaporated and acidified with HCl (25%), then the precipitate was filtered, and the resulting solid was recrystallized from absolute ethanol [8]. The solid (B) was white, with a melting point of 227 °C and a yield of 84%.

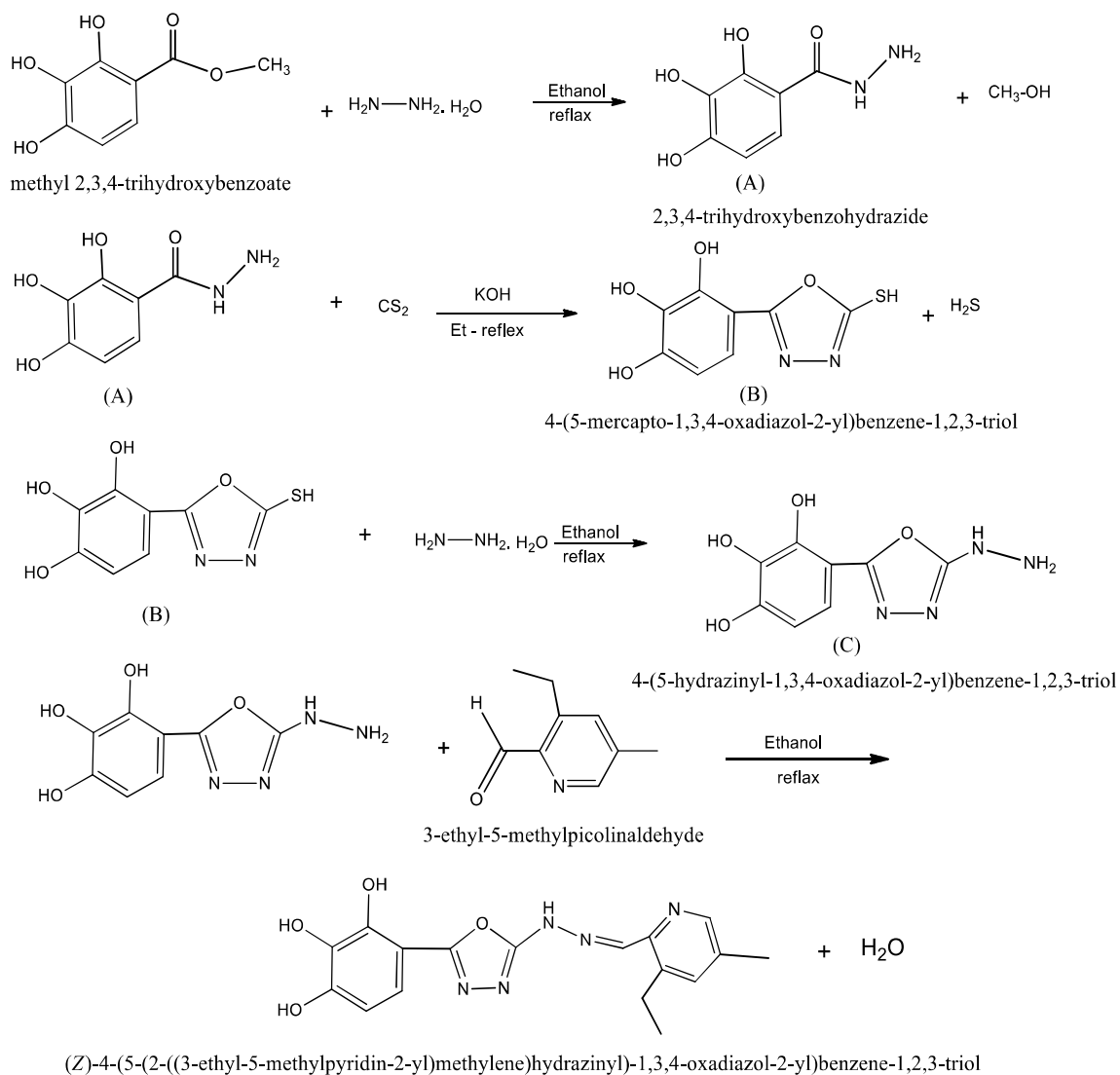
2.2.3. Preparation of 4-(5- hydrazinyl -1,3,4-oxadiazol-2-yl) benzene-1,2,3-triol (C)

4-(5-mercpto-1,3,4-oxadiazole-2-yl)benzene-1,2,3-triol (B) (4gm) (6.33gm, 0.028 mol) and hydrazine hydrate (1.8 ml, 0.057 mol) in ethanol as solvent (50 ml) were refluxed for 20 hours. The mixture was concentrated and then cooled [9]. The white precipitate (C) was filtered and recrystallized from ethanol. The melting point was 226 °C, yield 66.5%.

2.2.4. Preparation of (Z)-4-(5-(2-((3-ethyl-5-methylpyridin-2-yl) methylene) hydrazinyl) -1, 2, 3-oxadiazol-2-yl) benzene-1,2,3-triol (ligand)

The ligand was synthesized by condensation of 4-(5- hydrazinyl -1, 3,4-oxadiazol-2-yl) benzene-1,2,3-triol (C) and 3-ethyl-5-methylpicolinaldehyde (2.52gm, 0.01 mol) (1.52 ml, 0.01 mol) in ethanol (30 ml). The mixture was then refluxed for 4 h. The ligand was precipitated, filtered, and recrystallized from ethanol to obtain a yellow ligand with a

melting point of 289 °C and a yield of 57%.



Scheme1. Preparation Steps of the Ligand

2.3 Preparation of complexes

The metal complexes were obtained by refluxing (1 mmol) of transition metal chloride (1 mmol) Cr (III), Fe (III), and Ni (II) in 50 ml of ethanol with the ligand (1 mmol, 0.22 gm) for 2 h. The resultant solids were filtered, washed with ethanol, and dried in air.

3. Result and Discussion

3.1. FT-IR spectra

Figure 1 shows FT-IR spectra of the synthesized ligand and its complexes were obtained using KBr discs for the ligand and CsI for the complexes. The free ligand exhibited six major bands at

(3360) cm^{-1} , (3209) cm^{-1} , (1604) cm^{-1} , (1527) cm^{-1} , (1342) cm^{-1} , (1282) cm^{-1} , (1194) cm^{-1} which are attributable to (ν OH), (ν NH₂), (ν C=N) imine, (ν C=N) oxa, (ν C-O-C) sym, (ν C-O-C) asy and structure movement bands respectively, as shown below (table1). New bands were formed, attributed to the coordinated (M-N), (M-O), and (M-Cl) bonds, and appeared at the region (507) cm^{-1} , (437) cm^{-1} and (304) cm^{-1} , respectively. This indicates that the coordination occurred through the (N), (O) and (Cl) atoms.

Table 1. IR frequencies (cm^{-1}) of the compound and their metal complexes

No.	Compound	$\nu(\text{OH})$	$\frac{(\text{NH})}{\nu}$	$\frac{(\text{C}=\text{N})}{\nu}$ imine	$\frac{(\text{C}=\text{N})\nu}{\nu}$ oxadiazol	$\frac{(\text{C}-\text{O}-\text{C})}{\nu}$	Struc. Movement	$\frac{(\text{M}-\text{N})}{\nu}$	$\frac{(\text{M}-\text{O})}{\nu}$	$\frac{(\text{M}-\text{Cl})}{\nu}$
1	C ₁₇ H ₁₆ N ₄ O ₅	3360	3209	1604	1527	1342(Asy) 1282(sy)	1195	-		
2	[Cr(L ₁) Cl ₃]	3341	3341	1689	1597	1273(Asy) 1242(sy)	1103	503	424	293
3	[Fe(L ₁) Cl ₃]	3410	3410	1697	1620	1303(Asy) 1211(sy)	1103	516	425	240
4	[Co(L ₁)Cl ₂]	3410	3342	1651	1579	1411(Asy) 1234(sy)	1041	370	277	231
5	[Ni(L ₁)Cl ₂]	3466	3259	1637	1512	1373(Asy) 1261(sy)	1192	339	312	275

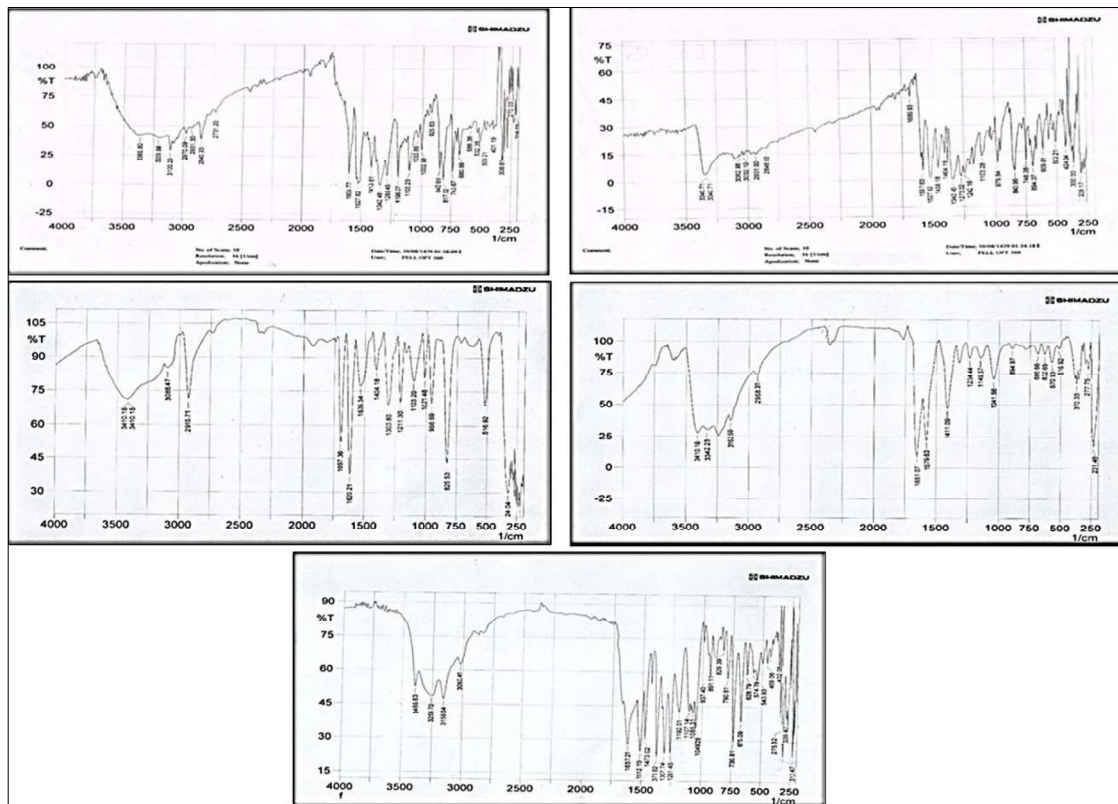


Figure 1. FT-IR spectra of The ligand and complexes.

3.2. Nuclear Magnetic Resonance

The ^1H -NMR spectra of ligand exhibit a 9.59-11ppm(4H,s, OH,NH protons), 6.85-7.96PPM (3H,m,aromatic protons, 1H,m, =CH protons), 3.95 PPM(2H,m, CH₂ protons), 1.35-3.45 PPM(3H,s, CH₃ protons, 3H,m, CH₃ protons) and 2.5(s, DMSO). The proton NMR spectrum of the ligand is shown in figure (1). (^1H -NMR(DMSO- d_6) spectral information was given extra support for the proposition of the structure.

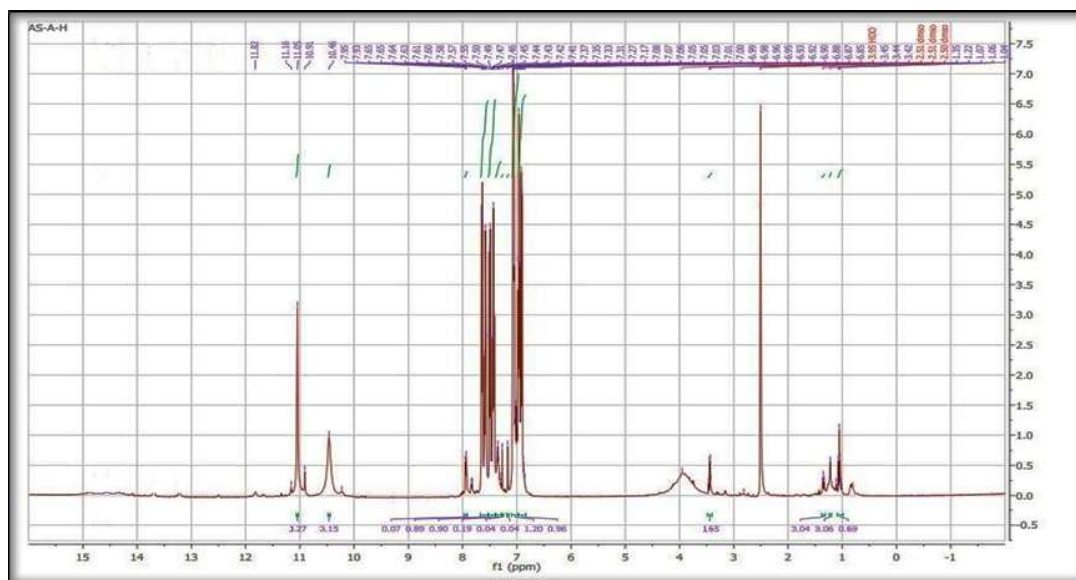


Figure 2. ^1H -NMR spectra of The ligand.

3.3. Mass spectra

The mass spectrum of the ligand exhibits a molecular ion peak $[M]^+$. At 354 m/z, the ligand spectra show fragments at (43, 57, 83, 97, 109, 125, 152, 236, 264) m/z, as shown in figure (3). The mass spectrum of complex $[Ni(L)Cl_2]$ shows a molecular ion peak $[M]^+$ (483) m/z, which is equivalent to the molecular mass of the complex. This complex shows another fragment ion peak with the loss of a chlorine atom at (448, 413) due to $[Ni(L)Cl]^+$ and $[Ni(L)]^+$, respectively (Figure (4)). The mass spectrum of complex $[Cr(L)Cl_3]$ shows a molecular ion peak, $[M]^+$ (514) m/z, which is equivalent to the molecular mass of the complex. This complex shows another fragment ion peak with the loss of a chlorine atom at (479, 444, 409) due to $[Cr(L)Cl_2]^+$, $[Cr(L)Cl]^+$, and $[Cr(L)]^+$ respectively. The mass spectrum of complex $[Fe(L)Cl_3]$ shows a molecular ion peak, $[M]^+$ (509) m/z, which is equivalent to the molecular mass of the complex. This complex shows another fragment ion peak with the loss of a chlorine atom at (474, 439, 404) due to $[Fe(L)Cl_2]^+$, $[Fe(L)Cl]^+$, and $[Fe(L)]^+$, respectively. The mass spectrum of complex $[Co(L)Cl_3]$ shows a molecular ion peak, $[M]^+$ (518) m/z, which is equivalent to the molecular mass of the complex. This complex shows another fragment ion peak with loss of chlorine atom at (483, 449, 414) due to $[Co(L)Cl_2]^+$, $[Co(L)Cl]^+$, and $[Co(L)]^+$ respectively. The mass spectra of the complexes shown in figures (5), (6), (7).

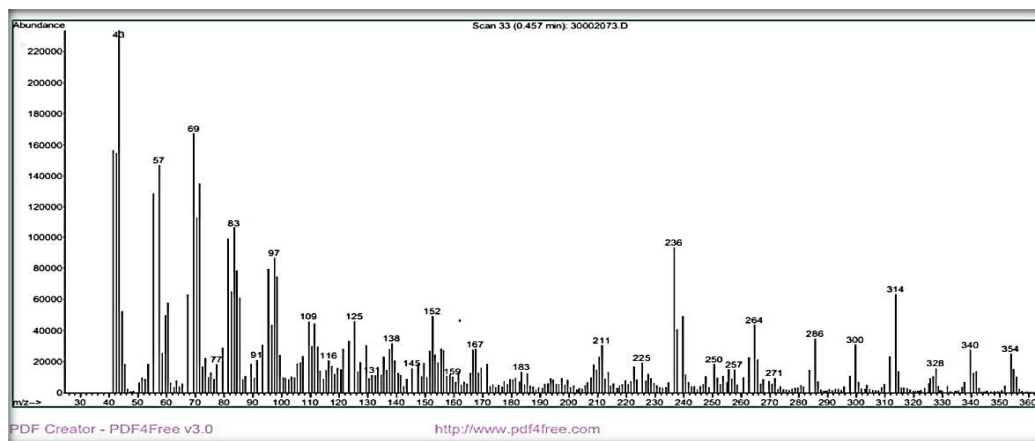


Figure 3. Mass spectra of the ligand

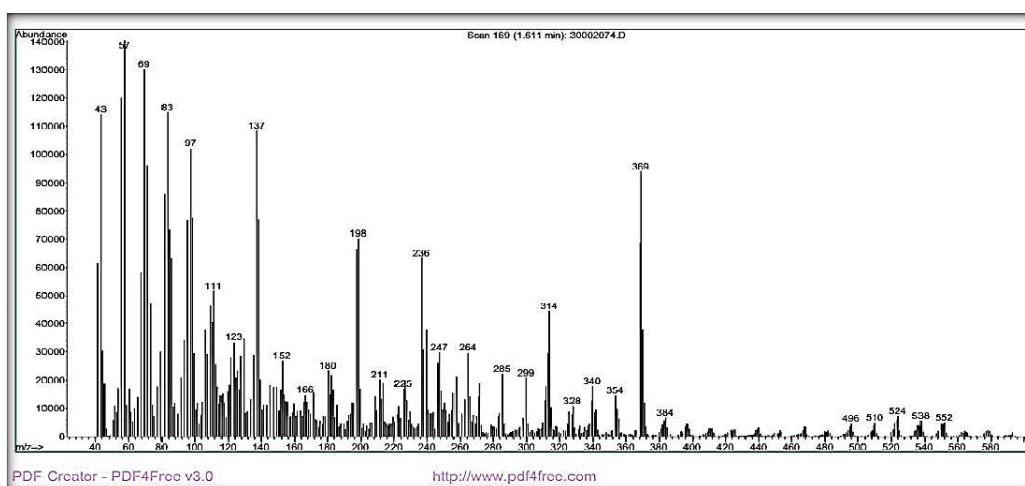


Figure 4. Mass spectra of $[\text{Ni}(\text{L})\text{Cl}_2]$

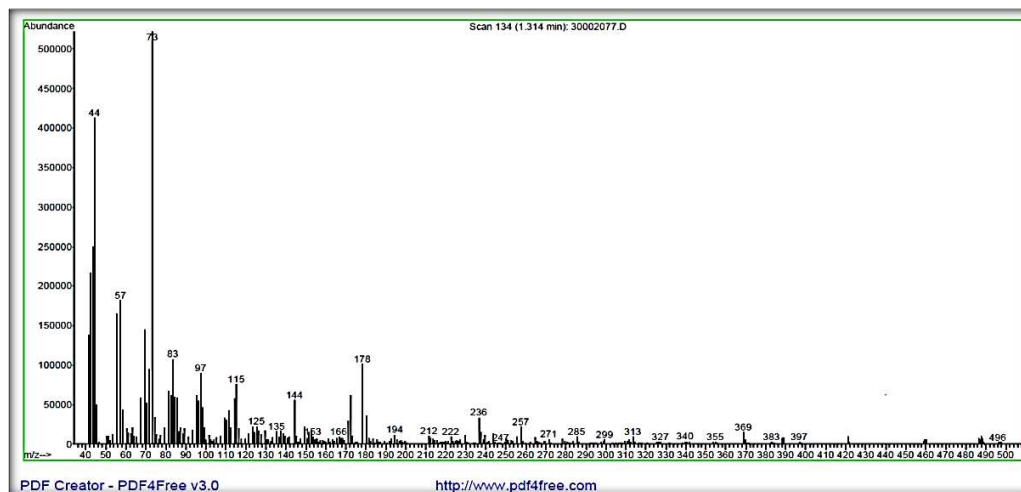


Figure 5. Mass spectra of $[Cr(L)Cl_3]$

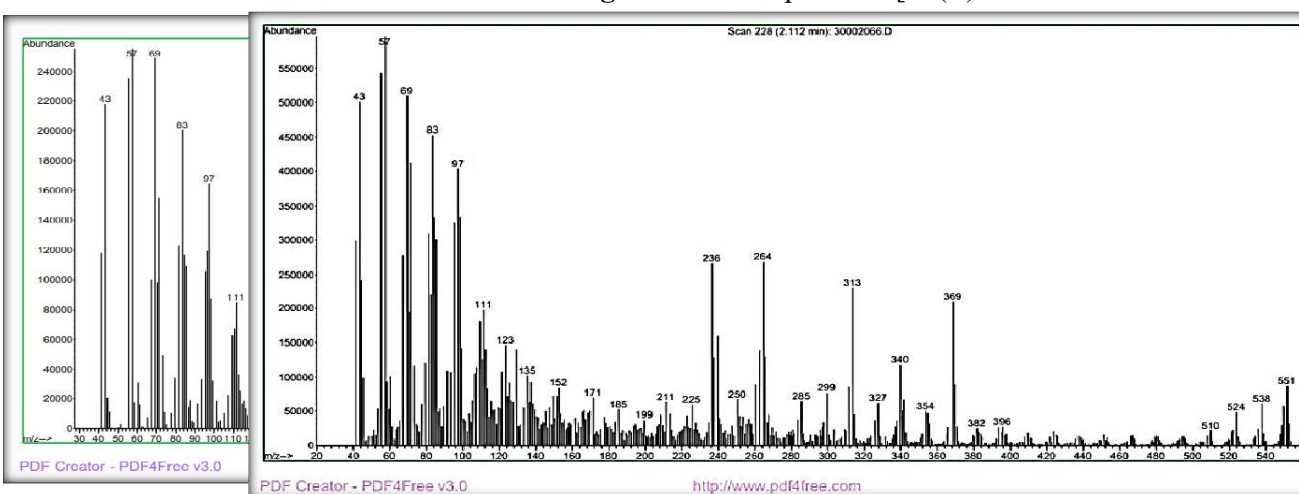
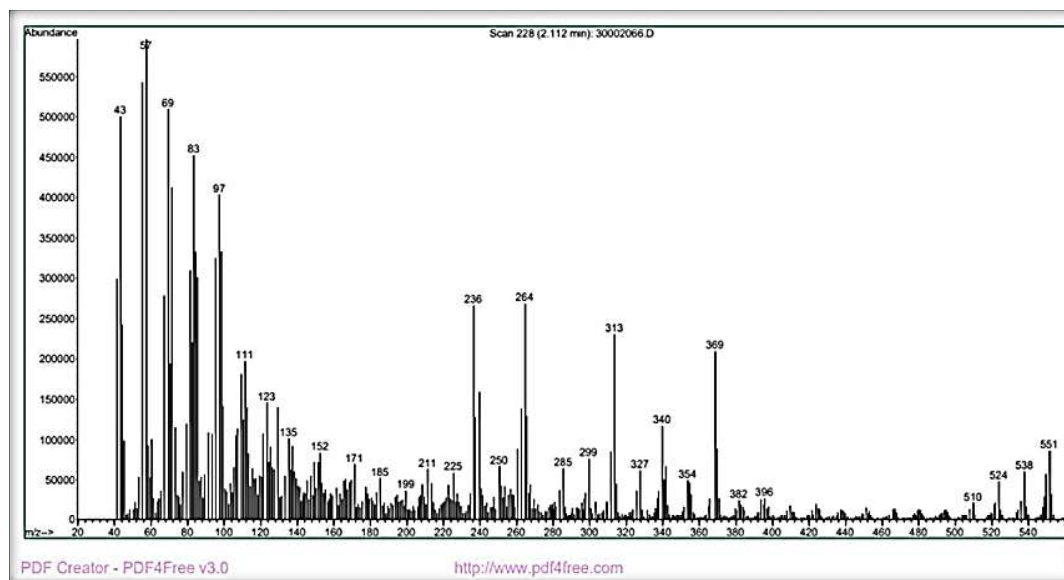


Figure 6. Mass spectra of $[\text{Fe}(\text{L})\text{Cl}_3]$ **Figure 7.** Mass spectra of $[\text{Co}(\text{L})\text{Cl}_3]$

3.4. Magnetic susceptibility

The magnetic susceptibility data (μ_{eff} B.M) for metal complexes provide information about the electronic state of the central ion (transition metal ion) of the complexes. The (μ_{eff} B.M) values of Cr,Co (III)complex 3.74,3.87BM. The (μ_{eff} B.M) value of Fe(III)complex 2.05BM is likely to be octahedral geometry. The (μ_{eff} B.M) value of Ni(II)complex is 0.14 BM, which is likely to have a square planar geometry.

3.5. Quantum chemical calculations

Quantum chemical methods and molecular modeling techniques enable the definition of a large number of molecular quantities that characterize the reactivity, shape, and binding properties of a complete molecule, as well as of molecular fragments and substituents. The use of theoretical parameters presents two main advantages: first, the compounds and their various fragments and substituents can be directly characterized based on their molecular structure only, and second, the proposed mechanism of action can be directly accounted for in terms of the chemical reactivity of the compounds under study. The calculated quantum chemical parameters, As illustrated in Table (2).

Table 2. Quantum chemical Parameter of ligand

Quantum Parameter	Equation	Values with (ev)
ELUMO	-	-5.905
EHOMO	-	-1.297
Energy bandgap	EHOMO - ELUMO	4.624

Ionization potential	$I = -E_{\text{HOMO}}$	-5.907
Electron affinity	$A = -E_{\text{LUMO}}$	-1.298
Electronegativity	$\chi = \left(\frac{1+A}{2} \right)$ $= - \left(\frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2} \right)$	-3.601
Chemical hardness	$\eta = \left(\frac{1-A}{2} \right)$	-2.300
Chemical potential	$\mu = - \left(\frac{1+A}{2} \right)$	3.601
Electrophilicity index	$\omega = \frac{\mu^2}{2\eta}$	-2.817
Chemical softness	$\sigma = \frac{1}{\eta} = \frac{1}{(E_{\text{HOMO}} - E_{\text{LUMO}})}$	-0.217
Electronic Energy	-	-1248.981
Dipole Moment (Debye)	-	5.068

The energy gap between the HOMO and LUMO (ΔE) was calculated to be 4.604 eV (Table 2). This large gap between the HOMO and LUMO indicates good stability, high excitation energies, and large chemical hardness of this molecule. Two energetic parameters correlated with the frontier orbitals were calculated: the ionization potential (I) and electron affinity (A). The high ionization potential of the ligand indicates that it is a good electron donor, and the relatively low electron affinity indicates that it is not highly reactive. The dipole moment (μ in Debye) is another important electronic parameter used to describe the polarity of a molecule [39]. Molecules with high dipole moments tend to interact with other molecules through electrostatic interactions, electronic chemical potential (μ), absolute electronegativity (χ), global hardness (η), chemical softness (σ), and global electrophilicity index (ω). The results show that this compound has good stability, high excitation energy, and high electrophilicity [18], comparison with another compound, as illustrated in Table (3 and 4) and Figures (8, 9 and 10).

Table 3. Comparison of Energy band-gap of prepared ligand with some other compound

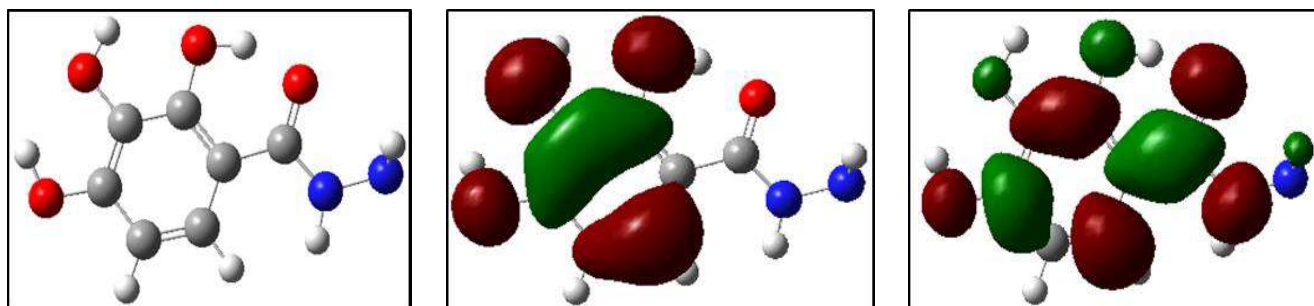
Compound	Energy band-gap(ev)	Reference
1,4-Benzothiazine derivatives	6.618-6.658	19
Sulfamethoxazole	5.091	20
Olmesartan	7.026	21
2-thiophene carboxylic acid	7.0073	22
2-thiophene carboxylic acid hydrazide	6.9464	22
Prepared ligand	4.604	In this study

The results of calculating the global parameters of the chemical reaction from the energies of LUMO and HOMO, as shown in the table, indicate that a large energy gap (LUMO–HOMO) corresponds to a low chemical reaction and high kinetic stability and lower reactivity. B (4.90) > A (4.65) > C (4.60), Compound B has the largest band gap, making it the most stable and least

reactive. Compound C has the smallest gap, suggesting higher reactivity. Ionization Potential (IP) Energy required to remove an electron ($IP = -HOMO$). A higher IP indicates greater resistance to electron loss. The order of stability against oxidation was $B (5.983) > A (5.636) > C (5.609)$. Electron Affinity (EA) Energy released when an electron is added ($EA = -LUMO$). A higher EA indicates a stronger electron-accepting ability. $B (1.080) > C (1.005) > A (0.981)$, compound B is the best electron acceptor. Electronegativity (χ) Average of IP and EA ($\chi = (IP + EA)/2$). A higher χ indicates a stronger electron attraction. $B (3.531) > A (3.308) \approx C (3.307)$, compound B is the most electronegative. Hardness (η): Resistance to electron distribution changes ($\eta = (IP - EA)/2$). $B (2.451) > A (2.327) > C (2.302)$, indicating that compound B is the hardest (most stable). Softness (S): Inverse of hardness ($S = 1/\eta$). $C (0.217) > A (0.215) > B (0.204)$; compound C was the softest (most reactive). Electrophilicity Index (ω): A higher ω indicates a stronger electrophilic character. The order of decreasing electrophilicity is as follows: $B (2.544) > C (2.376) > A (2.351)$, indicating that compound B is the strongest.

Table 4. Selected quantum chemical parameters for compounds

system	HOMO	LUMO	Eg	IP	EA	Electron egativity	Hardness	Softness	electroph ilicity
A	-5.636	-0.981	4.655	5.636	0.981	3.308	2.327	0.215	2.351
B	-5.983	-1.080	4.903	5.983	1.080	3.531	2.451	0.204	2.544
C	-5.609	-1.005	4.603	5.609	1.005	3.307	2.302	0.217	2.376

**Figure 8:** Optimized structure of compound A, HOMO molecular orbital of A, LUMO molecular orbital of A

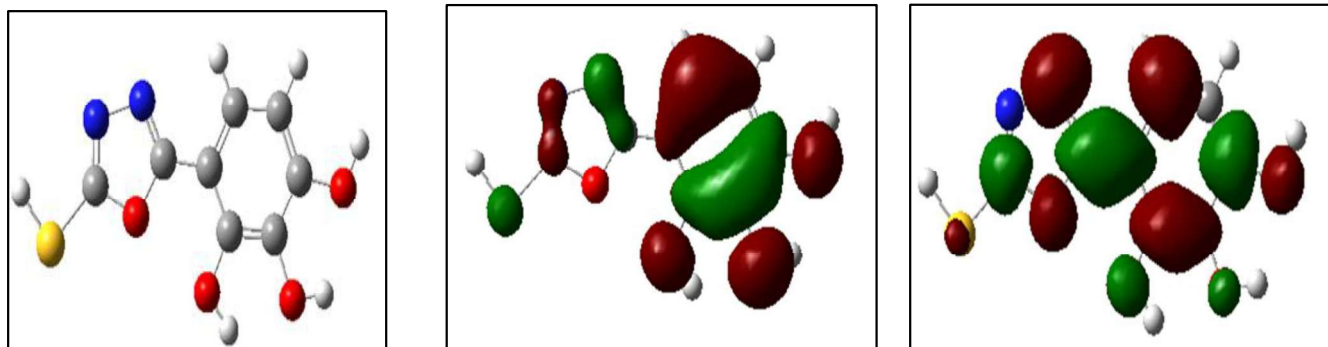


Figure 9: Optimized structure of compound B, HOMO molecular orbital of B, LUMO molecular orbital of B.

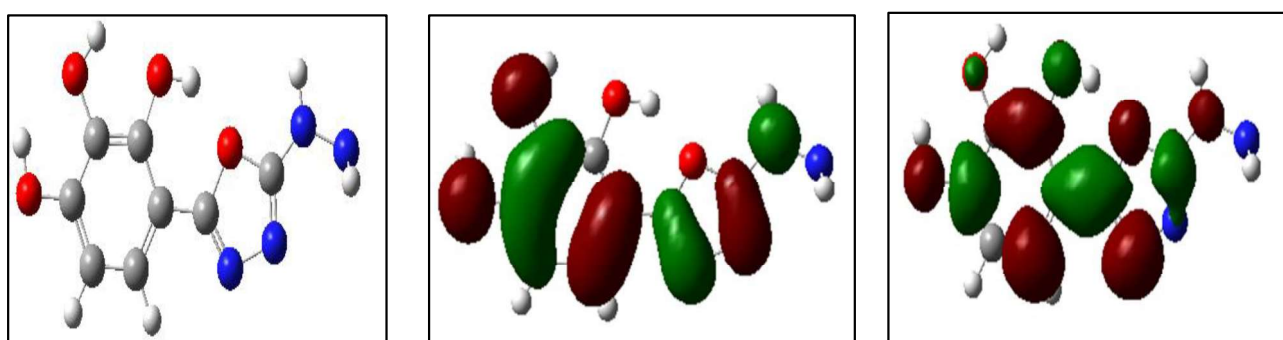


Figure 10: Optimized structure of compound C, HOMO molecular orbital of C, LUMO molecular orbital of C

3.6 Biological activity

The ligand and its transition metal ion complexes were evaluated for antimicrobial activity against gram-negative bacteria, such as *Serratia* and *Pseudomonas*, using the agar well diffusion method. All microbial cultures were adjusted to the 0.5 McFarland standard, and dimethyl sulfoxide (DMSO) was used to prepare all test solutions. Nutrient agar was used as the culture medium for the experiments. The observed results showed that the transition metal complexes exhibited enhanced antimicrobial activity compared to the free ligand. This result can be attributed to the greater lipophilic nature of the complexes, which favors their permeation through the lipid layers of the bacterial membranes. The activity of transition metal complexes can be explained based on Overton's concept and chelation theory [15] (Table 5 and Figures 11 and 12).

Table 5: Anti-bacterial data of ligand and its complexes

Compound	<i>Pseudomonas</i> Inhibition zone(mm)	<i>Serratia</i> Inhibition zone(mm)
L	5	10
[Cr(L) Cl ₃]	15	20

[Ni(L)Cl ₂]	13	14.5
[Fe(L)Cl ₃]	14	15.6



Figure 11. Biological activity of ligand against gram negative bacteria *Serratia* and *Pseudomonas*

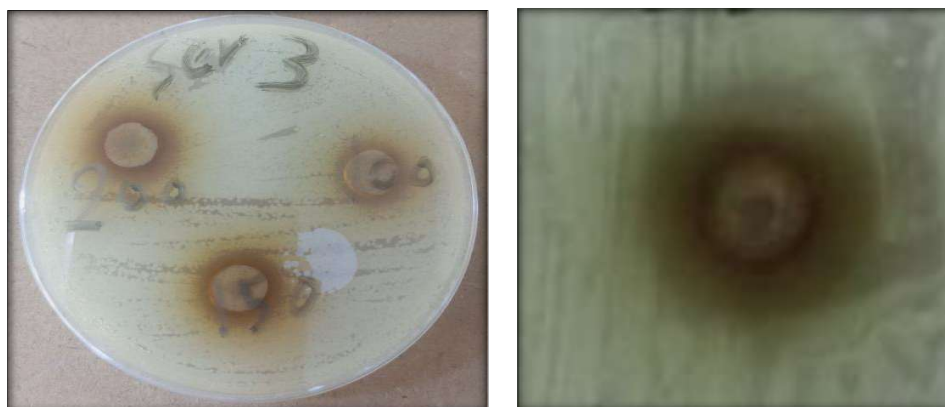


Figure 12. Biological activity of the complexes against gram negative bacteria *Serratia* and *Pseudomonas*

4. Conclusion

A new 1,2,3-oxadiazole-based hydrazone ligand and its Cr(III), Fe(III), and Ni(II) complexes were successfully synthesized and characterized using different spectroscopic and physicochemical techniques. The obtained data confirmed the proposed structures and suggested tetrahedral geometries for the Cr(III) and Fe(III) complexes, while the Ni(II) complex exhibited a square-planar geometry. DFT calculations supported the experimental findings and indicated that the ligand possesses good kinetic stability with moderate chemical reactivity. The biological evaluation demonstrated that coordination with transition metal ions enhanced the antibacterial activity of the ligand against *Serratia* and *Pseudomonas*, with the Cr(III) complex showing the highest activity. Overall, the results suggest that metal complexation improves both the electronic properties and biological performance of the synthesized ligand, making these compounds promising candidates for further biological investigations and the development of new bioactive coordination

compounds.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.”

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