

SYNTHESIS AND CHARACTERIZATION OF Co⁺², Ni⁺², Cu⁺² and Cd⁺² COMPLEXES WITH (4-(TERT-BUTYL) BENZENETHIOL) ALKANE LIGANDS AND EVALUATION OF ITS BIOLOGICAL ACTIVITY

Shahad A. Qasim, Farah T. Saeed*

Department of Chemistry, College of Science, University of Mosul, Mosul, Iraq.

*e-mail: farah-t-s@uomosul.edu.iq

Received 21.10.2025

Accepted 17.12.2025

Abstract: The research demonstrates that thioether-based coordination complexes obtain their physicochemical properties and biological activity from both the metal ion type and the ligand molecular structure. The synthesized complexes showed tetrahedral coordination geometries, as evidenced by spectroscopic, magnetic, and conductivity measurements, which demonstrated that sulfur atoms function as the main donor sites. The behavior follows the soft donor–soft acceptor interaction framework, which allows the creation of stable metal–sulfur chemical bonds.

The biological properties of metal coordination compounds produced better antibacterial effects than the unbound ligands. The improved results stem from two factors: enhanced lipophilicity after chelation, which enables better cell membrane penetration by bacteria, and decreased metal ion polarity due to electron delocalization within the chelate ring structure. The complexes become more accessible to the cell through these combined effects.

The Ni(II) complex derived from ligand L1 exhibited the most effective antibacterial activity against both bacterial species. The d⁸ electronic configuration of Ni(II) leads to enhanced activity because it produces the best possible match between structural stability and electronic flexibility when the metal center binds to a tetrahedral coordination site. The compound shows better biological performance because its L1 structure contains a short ethylene bond, which produces a compact molecular arrangement that improves metal-sulfur bonding through its optimized metal-ligand electronic interactions.

The research shows that thioether metal complexes exhibit antibacterial properties because their electronic structure interacts with their coordination and ligand structures in a combined manner, leading to the development of biologically active metal-based compounds.

Keywords: Thioether ligands; Disulfide derivatives; Coordination complexes; Tetrahedral geometry; Antimicrobial activity; Transition metals

DOI: 10.65382/2221-8688-2027-1-65-77

Introduction

Thioether ligands have attracted substantial interest over the past several decades, and coordination chemistry has increasingly focused on them due to their ability to form stable metal complexes through highly adaptable binding modes. The soft donor sulfur atoms in thioether groups readily bind to transition metals, forming complexes that exhibit unique electronic properties and often display remarkable structural stability. The stability of these complexes is usually supported by non-covalent interactions, such as hydrogen bonding, which affect their physicochemical properties [1–4].

Bifunctional sulfur-donor ligands create

excellent heterobimetallic structures and multinuclear frameworks because they have adaptable coordination properties. Research indicates that S/P, S/S, and S/N donor systems enable the formation of transition-metal complexes that exhibit diverse structural patterns and chemical properties [5–11].

Gürol and his team developed a dithioglyoxime ligand that forms mono-, tri-, and pentanuclear complexes with Co(II), Ni(II), Pd(II), Cu(II), and Pt(II) to demonstrate sulfur-based framework structural flexibility [12, 13]. Salivon et al. The study showed that diallyl disulfide acts as a tetradentate ligand, forming

distorted tetrahedral complexes with Cu(I) via sulfur and olefinic binding sites [14]. The research indicates that sulfur-rich coordination systems can adopt different structures.

Thioether-based ligands exhibit coordination behavior that produces intricate structures, while their transition-metal binding properties result in improved antimicrobial and anticancer activities [15–17]. The research expands on previous work on sulfur-containing ligands and their coordination properties [15–18] by developing Co(II), Ni(II), Cu(II), and Cd(II) complexes from two newly synthesized thioether ligands, L^1 and L^2 . The sulfur donor sites in these ligands create unique electronic and steric effects, making them useful in medicinal chemistry because their structures can be easily altered through chemical reactions. The research determined both structural elements and physical properties of these complexes to understand their coordination patterns and electronic properties.

The addition of alkyl spacers to thioether ligands provides researchers with an additional tool to control structure, as these spacers allow

them to adjust metal-ligand bonding strength and the overall size of their molecules. The design of metal-based systems with biological value requires understanding how their structural elements affect coordination behavior and functional performance.

The primary aim of this study is to synthesize two thioether ligands with different alkyl spacer lengths and to investigate their coordination behavior toward selected transition metal ions. The research explores how different ligand structures and metal ions affect the structural, electronic, and physical characteristics of the resulting complexes. The study investigates how bacteria interact with these complexes, aiming to determine the chemical bonds between their molecular structures and their ability to fight bacteria. The research unites spectroscopic data with magnetic measurements and conductivity tests to develop a unified system that explains how sulfur-donor metal systems connect their coordination chemistry to their biological functions.

Experimental part

General Remarks. The research used analytical-grade reagents and solvents that did not require additional purification before use. The synthetic procedures were carried out under controlled laboratory conditions to ensure reproducibility and minimize potential sources of contamination. The research team used standard experimental methods to study the synthesis and characterization processes while maintaining identical reaction conditions and sample preparation steps. The research used standard-calibrated equipment to perform spectroscopic and physicochemical tests, with new sample preparations when needed, to obtain dependable measurement results.

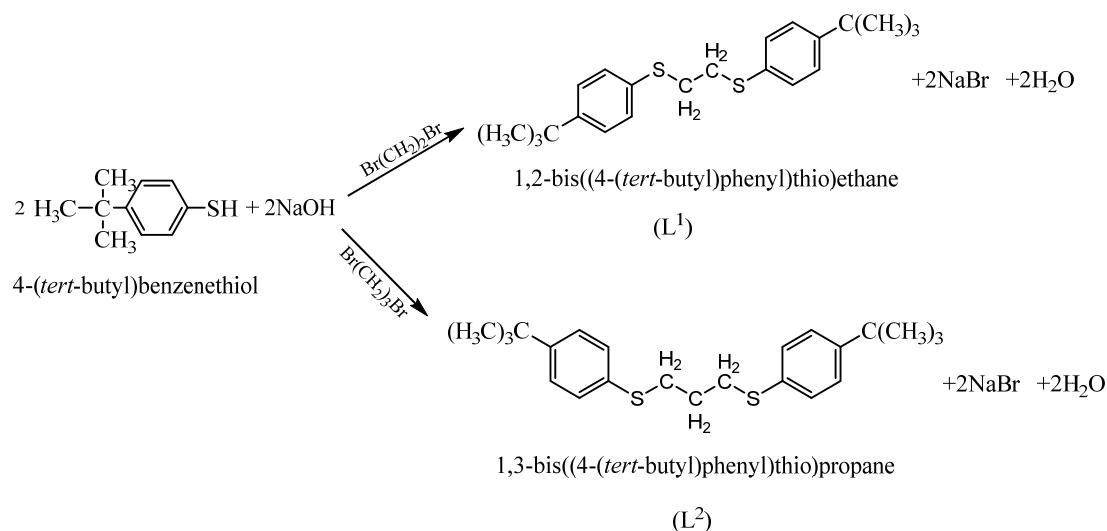
Physical Measurements. The synthesized ligands, together with their metal complexes, were evaluated for physicochemical properties using spectroscopic and analytical methods. Infrared spectroscopy analysis helped scientists detect specific functional group vibrations, enabling them to identify modifications that occurred when metals bound to the compound. The research team used proton nuclear magnetic resonance spectroscopy to study ligand

properties, while electronic absorption spectra helped them examine both electronic transitions and coordination effects. Elemental analyses were performed to verify the proposed stoichiometries of the compounds. The researchers conducted molar conductivity tests in polar solvents to assess the electrolytic behavior of the complexes, and magnetic susceptibility tests to study their electronic properties and molecular structure. The research team conducted all measurements according to established procedures, resulting in dependable, uniform experimental outcomes.

Synthesis of Ligands. The thioether ligands L^1 and L^2 were synthesized via a nucleophilic substitution reaction between the corresponding dibromoalkane and 4-(tert-butyl)benzenethiol under basic conditions (Scheme 1). The thiol group becomes a nucleophile upon deprotonation, enabling successful sulfur–carbon bond formation. The reactions needed reflux conditions to achieve full completion before scientists removed inorganic compounds, and then they allowed the target ligands to crystallize under specific conditions.

Both ligands were obtained as stable solids with good yields and purified by standard washing and drying procedures. The researchers verified their chemical compounds through melting-point tests and spectroscopic studies, which demonstrated thioether formation patterns and the absence of thiol proton signals. The

researchers achieved L^1 and L^2 synthesis, producing two compounds with identical structures but differing in alkyl spacer chain length. The researchers studied how different alkyl spacer lengths affect coordination behavior and complex formation using these ligands.



Scheme 1.

Standardized Procedure for the Synthesis of Coordination Complexes. The coordination complexes were prepared using a standardized synthetic approach based on the reaction of the preformed thioether ligands with the corresponding transition metal chlorides in ethanolic media. The ligands were allowed to interact with the metal ions under reflux conditions, promoting efficient coordination through sulfur donor atoms. During the reaction, the formation of solid products indicated successful complexation.

The resulting complexes were isolated by filtration, thoroughly washed to remove unreacted starting materials and residual salts, and then dried under reduced pressure. All complexes were obtained as stable solids with distinct colors characteristic of the coordinated metal ions. This uniform synthetic strategy ensured consistency across the series and enabled a reliable comparison of the structural and physicochemical properties of the complexes derived from ligands L^1 and L^2 .

Results and discussion

Synthesis of Ligands and Complexes. The thioether ligands L^1 and L^2 showed no physical changes, but their spectroscopic data indicated that the sulfur atoms formed bonds to carbon atoms. The absence of thiol-related signals and the presence of characteristic thioether vibrations confirm complete conversion of the starting materials. The following transition metal ions underwent successful coordination under identical reaction conditions, yielding complexes with defined structures and distinct physical properties.

Elemental analysis results are in good agreement with the proposed stoichiometries, supporting the formulation of the complexes as neutral ligand systems associated with ionic chloride species. The synthetic results demonstrate the same patterns for all metal ions because the ligands possess sufficient flexibility and donor strength, enabling them to form stable tetrahedral coordination complexes (Fig. 1). Scientists can study the properties of L^1 - and L^2 -based complexes by leveraging their identical

structural features, including coordination patterns and biological effects.

characteristics of the synthesized ligands and their metal complexes.

Table 1 presents the physical and analytical

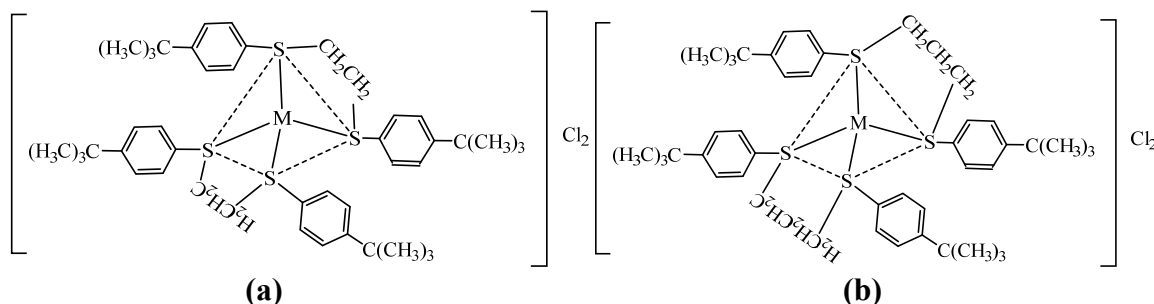


Fig. 1. The hypothesized structure of (a) $[M(L^1)_2]Cl_2$ and (b) $[M(L^2)_2]Cl_2$ complexes. $M = Co(II), Ni(II), Cu(II), \text{ and } Cd(II)$

Table 1. The physical and analytical characteristics of the synthesized ligands and their metal complexes

Seq.	Compound	Color	Molecular Weight	Melting Point (°C)	Yield %	Elemental Analysis – found (calculated) (%)				Molar Conductivity ($\Lambda, cm^2 \cdot ohm^{-1} \cdot mol^{-1}$)
						C	H	S	M	
L ¹	C ₂₂ H ₃₀ S ₂	Pale yellow	385.60	102-105	96	73.69 (73.67)	8.43 (8.70)	17.88 (17.81)	----	---
L ²	C ₂₃ H ₃₂ S ₂	White	372.63	106-108	88	74.14 (74.11)	8.66 (8.65)	17.21 (17.23)	----	---
1	$[Co(L^1)_2]Cl_2$	gray	782.89	125 ^d	89	67.44 (67.49)	7.66 (7.69)	8.50 (7.96)	16.35 (16.41)	167
2	$[Ni(L^1)_2]Cl_2$	yellow	846.79	180 ^d	93	62.35 (62.39)	7.09 (7.03)	8.47 (7.36)	15.12 (15.08)	154
3	$[Cu(L^1)_2]Cl_2$	Pale green	851.65	192 ^d	90	61.99 (61.93)	7.05 (7.09)	8.47 (8.61)	15.03 (15.09)	138
4	$[Cd(L^1)_2]Cl_2$	White	900.51	120 ^d	95	58.63 (58.67)	6.66 (6.61)	8.43 (8.09)	14.21 (14.25)	120
5	$[Co(L^2)_2]Cl_2$	Pale violet	875.08	187 ^d	86	63.08 (63.14)	7.31 (7.37)	8.41 (7.98)	14.63 (14.69)	121
6	$[Ni(L^2)_2]Cl_2$	yellow	874.84	190 ^d	88	63.09 (63.15)	7.32 (7.29)	9.06 (8.54)	14.63 (14.56)	130
7	$[Cu(L^2)_2]Cl_2$	Black	879.70	185 ^d	91	62.75 (62.8)	7.28 (7.33)	9.08 (8.56)	14.55 (14.59)	123
8	$[Cd(L^2)_2]Cl_2$	White	928.56	174 ^d	94	59.45 (59.49)	6.89 (6.96)	9.06 (8.46)	13.78 (13.67)	180

d= decomposition temperature

¹H-NMR Spectral Analysis. The ¹H-NMR spectra of ligands L¹ and L² contain direct evidence that confirms their proposed molecular structures. The observed proton signals match the predicted chemical environments of the aromatic rings, alkyl spacers, and tert-butyl substituents, indicating that thioether formation was successful. The absence of thiol proton signals in the spectrum confirms that the starting thiol compounds have fully transformed into their

coordinated forms, which matches the observed complexation patterns.

Differences between the spectra of L¹ and L² mainly reflect variations in the alkyl spacer length, which influence the chemical shift positions of the methylene protons without altering the overall spectral pattern. The research results show that the two ligands share similar structures, yet they exhibit sufficient differences

to enable researchers to study how spacer length characteristics [19, 20]. affects their coordination behavior and physical

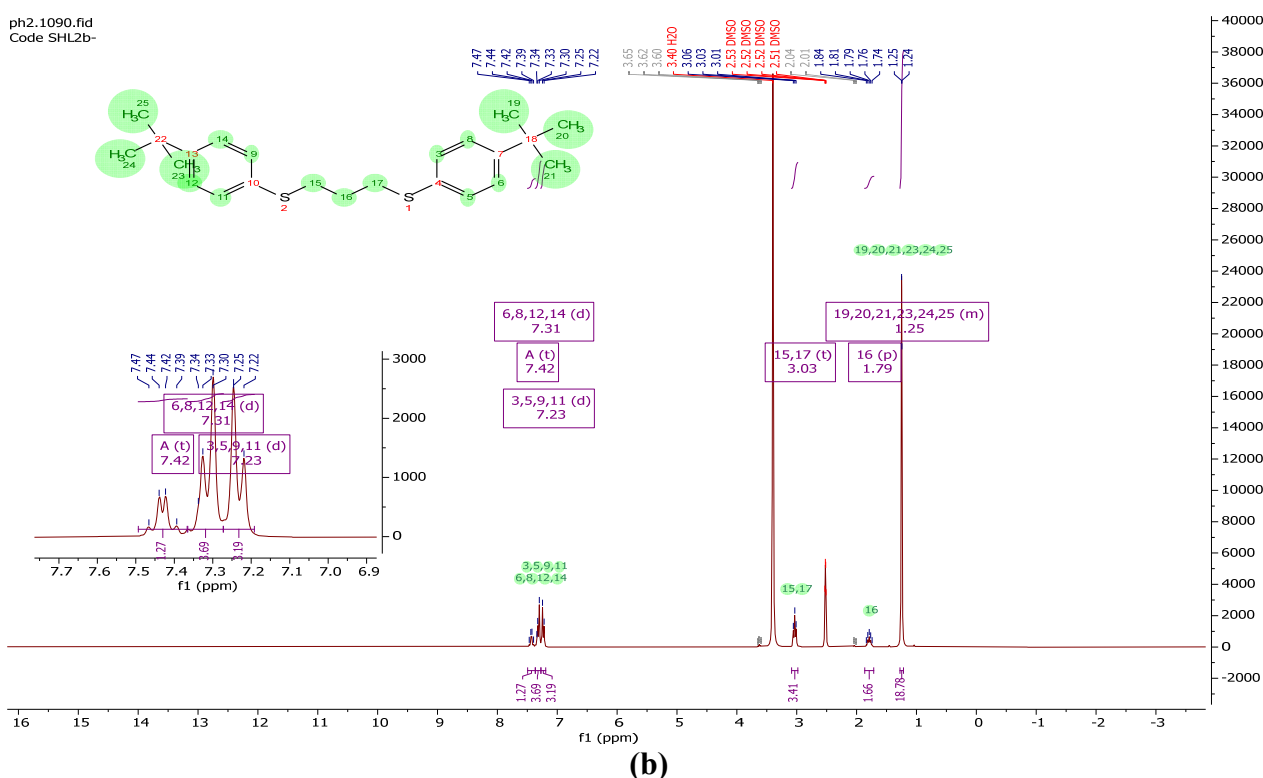
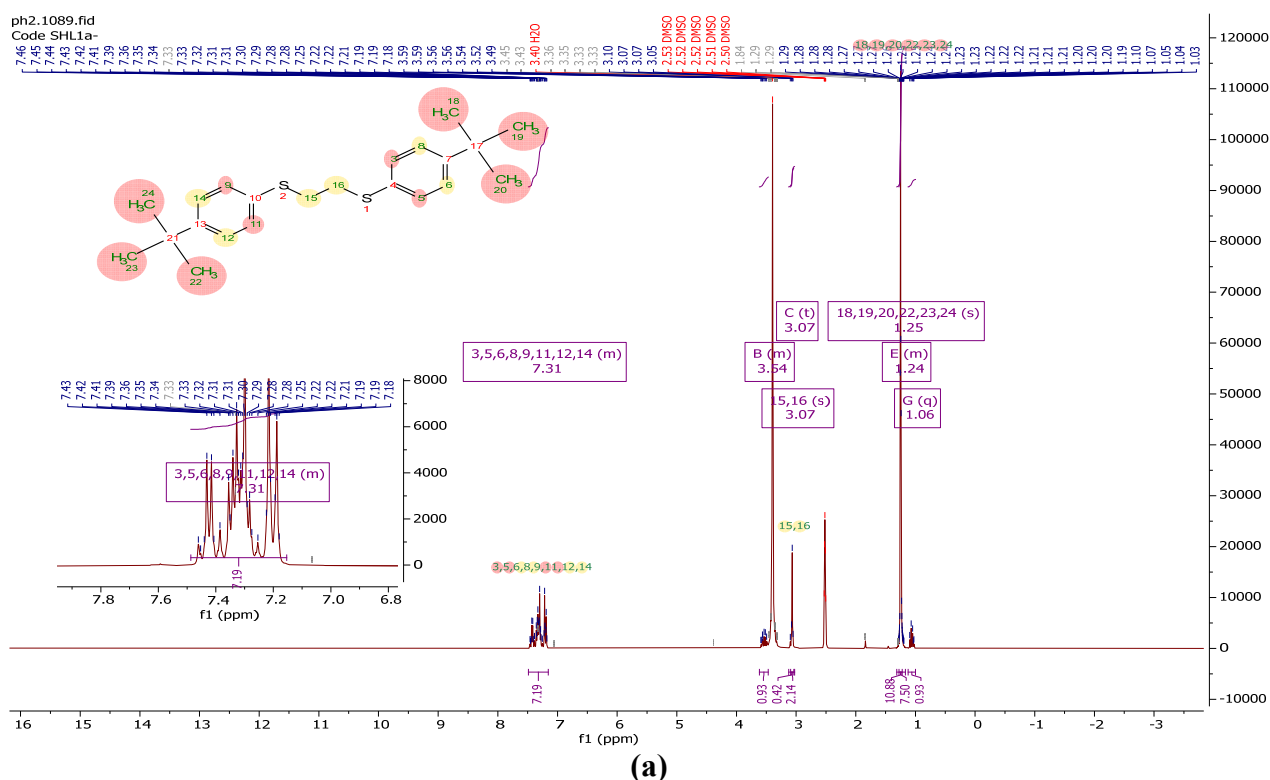


Fig. 2. ^1H NMR for a(L^1); b(L^2)

Conductivity Measurements. Molar conductivity measurements provide useful insight into the ionic nature of the synthesized metal complexes in polar solution. The

conductivity measurements show that the complexes function as electrolytes, confirming that chloride ions exist as free ions rather than being coordinated to the complexes. The research

results match the proposed complex structures, indicating that chloride ions remain beyond the main coordination sphere.

The observed behavior supports the conclusion that neutral thioether ligands serve as the main coordination sites because metal-sulfur bonds determine the structure of the inner coordination sphere. The conductivity results therefore agree well with elemental analysis and spectroscopic data, collectively supporting the structural models proposed for the complexes. Results from multiple independent analytical methods are identical, enhancing the reliability of the complete structural identification.

Determination of Magnetic Properties.

Magnetic moment values (μ_{eff}) obtained from measurements for the Co(II) complexes were 5.17 B.M. for $[\text{Co}(\text{L}^1)_2]\text{Cl}_2$ and 5.45 B.M. for $[\text{Co}(\text{L}^2)_2]\text{Cl}_2$, values consistent with high-spin tetrahedral configurations [23]. For the Ni(II) complexes, the μ_{eff} values were 4.63 B.M. for $[\text{Ni}(\text{L}^1)_2]\text{Cl}_2$ and 4.10 B.M. for $[\text{Ni}(\text{L}^2)_2]\text{Cl}_2$, which are within the expected range for high-spin tetrahedral Ni(II) species [23]. The Cu(II) complexes exhibited magnetic moments of 1.75 B.M. for $[\text{Cu}(\text{L}^1)_2]\text{Cl}_2$ and 1.26 B.M. for $[\text{Cu}(\text{L}^2)_2]\text{Cl}_2$. The d-orbital set contains one unpaired electron, leading to a distorted tetrahedral molecular structure. [23]. As expected for a d^{10} system, all Cd(II) complexes were diamagnetic [23].

Magnetic susceptibility measurements offer important insight into the electronic configuration and coordination geometry of the synthesized metal complexes. The magnetic properties of Co(II), Ni(II), and Cu(II) complexes show evidence of unpaired electrons, confirming their high-spin electronic configurations in tetrahedral coordination environments. In contrast, the Cd(II) complexes exhibit diamagnetic behavior, as expected for a closed-shell electronic configuration.

The magnetic properties match all the structural findings that scientists obtained through spectroscopic and conductivity tests. The magnetic data match the electronic spectral features, supporting the assignment of tetrahedral structures and demonstrating that metal-sulfur bonding determines the electronic properties of these complexes. The magnetic results serve as an independent verification system, which confirms the proposed coordination models

through their reliable data.

Electronic Absorption Spectral Analysis. The ultraviolet-visible absorption spectra of the uncoordinated ligands L^1 and L^2 revealed two sharply defined absorption bands, assigned to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, corresponding to the aromatic structure and thioether functional groups. Specifically, L^1 showed bands at 33781 cm^{-1} ($\pi \rightarrow \pi^*$) and 31548 cm^{-1} ($n \rightarrow \pi^*$), while L^2 exhibited bands at 34897 cm^{-1} ($\pi \rightarrow \pi^*$) and 32489 cm^{-1} ($n \rightarrow \pi^*$) [24].

Upon complexation, these ligand-centered bands experienced slight shifts, accompanied by the appearance of charge-transfer (C.T) bands: 28056 cm^{-1} for $[\text{Co}(\text{L}^1)_2]\text{Cl}_2$ and 28902 cm^{-1} for $[\text{Co}(\text{L}^2)_2]\text{Cl}_2$, suggesting ligand-to-metal electron donation through the sulfur atoms [24].

In the Co(II) complexes, weak-intensity d-d bands were observed at 14579 cm^{-1} for $[\text{Co}(\text{L}^1)_2]\text{Cl}_2$ and 14634 cm^{-1} for $[\text{Co}(\text{L}^2)_2]\text{Cl}_2$. The $4\text{A}_2\text{g}(\text{F}) \rightarrow 4\text{T}_2\text{g}(\text{P})$ electronic transition occurs in complexes that have a tetrahedral ligand field environment according to their characteristic spectral features. Supported by their magnetic moments [25]. The Ni(II) complexes exhibited bands at 14679 cm^{-1} for $[\text{Ni}(\text{L}^1)_2]\text{Cl}_2$ and 14289 cm^{-1} for $[\text{Ni}(\text{L}^2)_2]\text{Cl}_2$, assigned to ${}^3\text{T}_1(\text{F}) \rightarrow {}^3\text{T}_1(\text{P})$ transitions [26]. The Cu(II) complexes displayed broad d-d transitions at 13879 cm^{-1} for $[\text{Cu}(\text{L}^1)_2]\text{Cl}_2$ and 14834 cm^{-1} for $[\text{Cu}(\text{L}^2)_2]\text{Cl}_2$, consistent with distorted tetrahedral geometry [27]. As expected for a d_{10} configuration, the Cd(II) complexes showed no d-d transitions and remained diamagnetic [28, 29].

Notably, the variation in charge-transfer band positions between L^1 - and L^2 -based complexes reflects subtle differences in ligand field strength induced by the methylene chain length, which can modulate the electronic environment around the central metal ion [24–31] (Table 2).

The electronic absorption spectra of the synthesized complexes provide evidence of metal-ligand bonding interactions that determine the coordination structure of the complexes. The free thioether ligands exhibit ligand-centered transitions that undergo small but regular shifts upon binding to metal centers, because metal coordination alters their electronic structure. The presence of sulfur donor atoms in coordination results in partial electron transfer to the metal

center, which produces this specific behavior.

The appearance of charge-transfer bands in metal complexes demonstrates that electronic interactions exist between ligands and metal centers, indicating that coordination forms more than just structural bonds because it also creates electronic bonds. The d–d transitions of Co(II), Ni(II), and Cu(II) complexes show characteristic signals, although their intensities remain low, which supports their tetrahedral coordination structures. The agreement between spectroscopic observations and the corresponding magnetic susceptibility data strengthens this interpretation.

The spectral patterns between complexes made from L¹ and L² ligands differ because of their different backbone flexibility rather than their donor types. The L1 compound contains a shorter alkyl spacer, which produces a smaller coordination sphere that should improve metal–ligand orbital overlap and affect the electronic properties of the metal center. The electronic differences between these compounds create a logical framework that explains why their physical and chemical characteristics and biological activities differ.

Table 2. UV spectra and magnetic moments of synthesised compounds

No.	Compound	Absorption bands	Transition	Band maxima λ cm ⁻¹	μ_{eff} (B.M.)
L ¹	C ₂₂ H ₃₀ S ₂	33781 31548	(n- π^*) (π - π^*)	38490	--
L ²	C ₂₃ H ₃₂ S ₂	34897 32489	(n- π^*) (π - π^*)	37692	--
1	[Co(L ¹) ₂]Cl ₂	14579 28056	⁴ A _{2g} (F) → ⁴ T ₁ (P) C.T	37693	5.17
2	[Ni(L ¹) ₂]Cl ₂	36902 41457 14679 35890	π $\xrightarrow{\pi^*}$ n $\xrightarrow{\pi^*}$ ³ T ₁ (F) → ³ T ₁ (p) C.T	35791	4.63
3	[Cu(L ¹) ₂]Cl ₂	13879	² T ₂ → ² E	36578	1.75
4	[Cd(L ¹) ₂]Cl ₂	---	---	37456	Dia
5	[Co(L ²) ₂]Cl ₂	14634 28902	⁴ A _{2g} (F) → ⁴ T ₁ (P) C.T	37612	5.45
6	[Ni(L ²) ₂]Cl ₂	37341 41908 14289 36812	π $\xrightarrow{\pi^*}$ n $\xrightarrow{\pi^*}$ ³ T ₁ (F) → ³ T ₁ (p) C.T	35845	4.10
7	[Cu(L ²) ₂]Cl ₂	14834	² T ₂ → ² E	35612	1.26
8	[Cd(L ²) ₂]Cl ₂	---	---	32768	Dia

Infrared Spectral Analysis (Fig. 3). The infrared spectral data confirm the proposed coordination mode used to synthesize the metal complexes. The free ligand spectra show no sign of the ν (S–H) stretching band because their thiol groups exist in a non-protonated state before they form complexes. This observation suggests that sulfur atoms are readily available for metal binding, which is consistent with the formation of stable thioether–metal interactions (Table 3).

Upon complexation, the ν (C–S) stretching vibrations exhibit systematic shifts compared with those of the uncoordinated ligands. The

observed changes in bond strength and electron density distribution patterns occur because sulfur atoms take part in coordination bonds. The appearance of new absorption bands in the low-frequency region, arising from ν (M–S) vibrations, indicates that metal atoms form direct bonds with sulfur atoms. The spectral features show identical patterns in all complexes, demonstrating that sulfur atoms in the complexes donate electrons to the metals through similar bonding mechanisms.

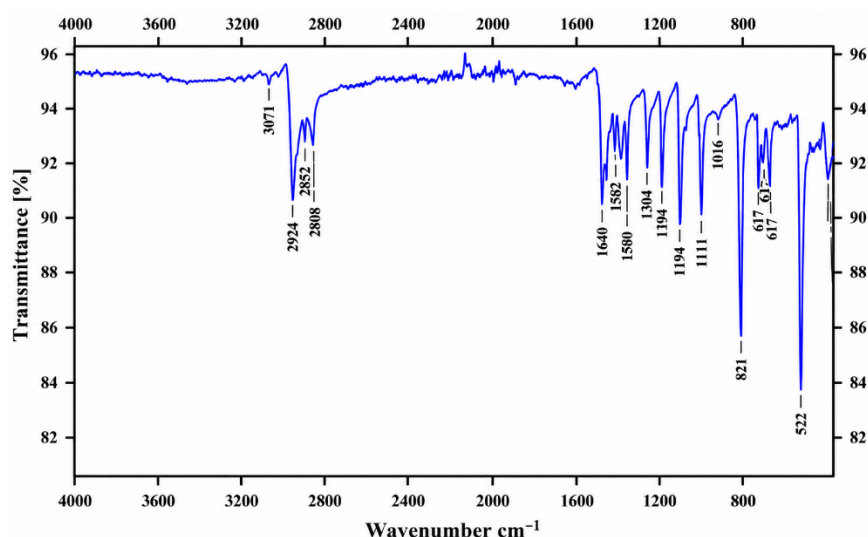
The measured infrared spectral patterns match the data from magnetic susceptibility and

conductivity tests and from electronic spectral tests. The independent analytical methods that converged on the same conclusion proved that the proposed bidentate coordination pattern exists and confirmed the tetrahedral molecular

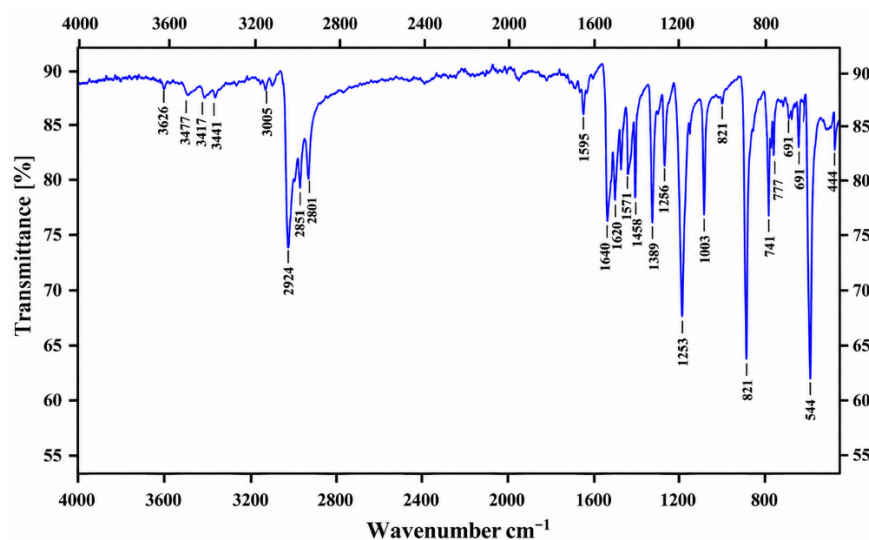
structure. The FT-IR data serve as vital evidence of the structural arrangement of complexes and confirm results from other physical assessment methods.

Table 3. FT-IR Spectroscopic Characterization of the Prepared Ligands and Their Corresponding Metal Complexes

No.	Compound	$\nu(\text{C-H})$	$\nu(\text{C-S})$	$\nu(\text{M-S})$
L ¹	C ₂₂ H ₃₀ S ₂	2958	552	--
L ²	C ₂₃ H ₃₂ S ₂	2959	544	--
1	[Co(L ¹) ₂]Cl ₂	2959	630	465
2	[Ni(L ¹) ₂]Cl ₂	2960	633	459
3	[Cu(L ¹) ₂]Cl ₂	2956	629	455
4	[Cd(L ¹) ₂]Cl ₂	2961	666	469
5	[Co(L ²) ₂]Cl ₂	2959	636	450
6	[Ni(L ²) ₂]Cl ₂	2960	635	459
7	[Cu(L ²) ₂]Cl ₂	2958	623	475
8	[Cd(L ²) ₂]Cl ₂	2959	594	467



(a)



(b)

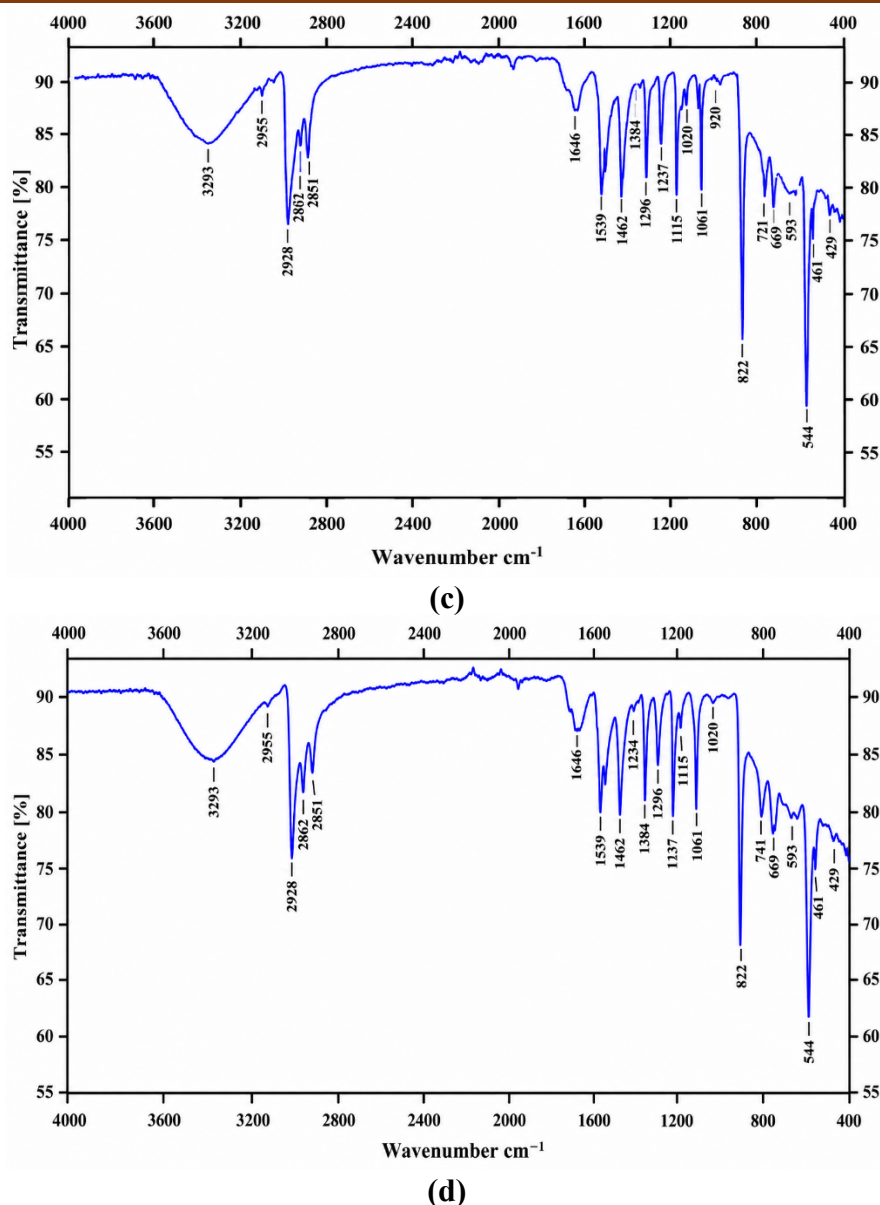


Fig. 3. IR-Spectra of (a) L^1 , (b) L^2 , (c) $[\text{Ni}(\text{L}^1)_2]\text{Cl}_2$, (d) $[\text{Ni}(\text{L}^2)_2]\text{Cl}_2$

The physicochemical characterization data show that the synthesized metal complexes have structural features that match one another. The spectroscopic data, along with magnetic measurements and conductivity results, are identical, confirming that thioether ligands in their neutral state bind to sulfur atoms to form tetrahedral metal complexes with chloride ions positioned outside the main coordination shell. The series contains similar structures, which enable researchers to study their operational characteristics, as the main differences stem from metal ions and flexible ligands rather than new coordination patterns. The integrated structural analysis allows researchers to determine why different compounds exhibit different antibacterial properties, which will help them

evaluate structure-activity relationships in the following section.

Antimicrobial Activity. The researchers tested the antimicrobial properties of their synthesized compounds against *Staphylococcus aureus* (Gram-positive) and *Escherichia coli* (Gram-negative), as these bacteria are standard organisms for testing broad-spectrum antibacterial compounds. The agar well diffusion test at 10 $\mu\text{g/mL}$ concentration showed that all complexes displayed antibacterial properties, but complex (2) generated the largest inhibition zones, which measured 18 mm for *S. aureus* and 17 mm for *E. coli*. The free ligands showed limited antibacterial activity, as indicated by zone sizes of 11-16 mm, but metal coordination with transition metals improved their

antibacterial performance by helping them enter lipophilic (Fig. 4, Table 4).
bacterial membranes and making them more

Table 4. Assessment of the Antibacterial Activity of the Ligands and Their Corresponding Metal Complexes

No.	Symbol	Compounds	<i>Staphylococcus aureus</i> (mm)	<i>E. coli</i> (mm)
L ¹	L1	C ₂₂ H ₃₀ S ₂	0	0
1	Co1	[Co(L ¹) ₂]Cl ₂	16	14
2	Ni1	[Ni(L ¹) ₂]Cl ₂	18	17
L ²	L2	C ₂₃ H ₃₂ S ₂	0	0
5	Co2	[Co(L ²) ₂]Cl ₂	16	11
6	Ni2	[Ni(L ²) ₂]Cl ₂	16	11
	CIP	ciproflo	24	15

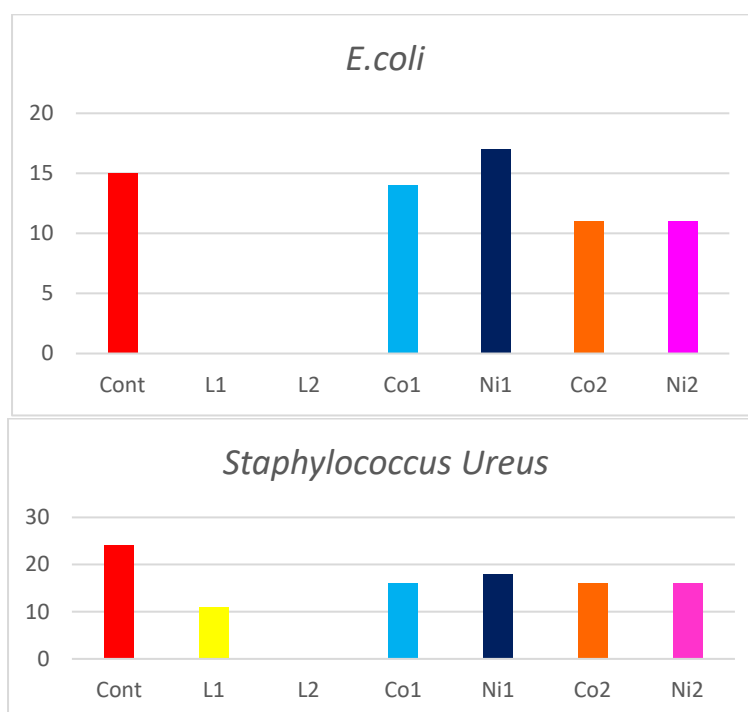


Fig. 4. Antibacterial activity of compound against (a) *Staphylococcus aureus* (b) *E. coli*

Antibacterial tests of the synthesized ligands and their metal complexes show that transition-metal ions enhance the biological activity of these compounds. The free thioether ligands exhibit no antibacterial activity, whereas their metal complexes exhibit significant activity against Gram-positive and Gram-negative bacterial strains. The observation supports current scientific knowledge, which shows that metal coordination leads to major alterations in the interactions of organic compounds with biological systems.

The increased antibacterial activity of the complexes may be attributed to chelation effects,

which reduce the overall polarity of the metal ion by partially sharing its charge with the sulfur donor atoms. The process makes the complexes more lipophilic, enabling them to pass through bacterial cell membranes and interact more effectively with cellular targets. The metal center in the compound could block vital enzymatic processes and cellular functions, thereby helping to stop bacterial cell multiplication.

The Ni(II) complex derived from ligand L¹ showed the strongest antibacterial activity among all tested compounds. The observed behavior results from the simultaneous effects that metal ions and ligands produce in the system. The

electronic properties of Ni(II), along with its small coordination space from the short ligand chain, enable better metal–ligand bonding and better cell penetration. The research shows that antibacterial activity results from the combined effects of coordination geometry, electronic configuration, and ligand framework structure, rather than from a single structural element.

The current research failed to identify

which molecular targets or cellular pathways were involved, so the proposed explanations require additional experimental verification.

Research shows that sulfur-donor metal complexes behave similarly to other substances because their biological effects stem from changes in their physical and chemical properties instead of depending on a specific essential component.

Conclusion

The research demonstrates that thioether ligands serve as an efficient system for transition-metal ion coordination, producing structurally identical complexes as evidenced by spectroscopic, magnetic, and conductivity testing. The research data show that sulfur atoms serve as the primary donor sites, forming enduring metal–sulfur bonds due to their tetrahedral molecular structure. The biological tests show that metal coordination makes the compounds more effective against bacteria than the unbound ligands are, demonstrating that

chelation affects the biological properties of these molecules. The different activity levels among complexes demonstrate that metal ion types, together with ligand structures, determine how these complexes function. The Ni(II) complex shows that biological function requires two essential factors: electronic flexibility and coordination site stability. The research results help scientists better understand how thioether-based metal complexes relate their structures to their properties while demonstrating their value for bioinorganic chemistry applications.

Conflict of interest

The authors announced that there are no conflicts of interest regarding this current work.

References

1. Wu A., Lucas C.R. Stereochemical nonrigidity in thioether complexes. *Inorg. Chem.*, 1992, **Vol. 31(12)**, p. 2354-2358. DOI: [10.1021/ic00038a012](https://doi.org/10.1021/ic00038a012)
2. Adhikary B., Liu S., Lucas C.R. Complexes of cobalt, nickel, palladium and silver with N_2S_x ($x=3$ or 4) ligands involving aromatic nitrogen and thioether donors. *Inorg. Chim. Acta*, 1997, **Vol. 261(1)**, p. 15-21. DOI: [10.1016/S0020-1693\(96\)05572-7](https://doi.org/10.1016/S0020-1693(96)05572-7)
3. Ahsen V., Gürek A., Gül A., Bekaroglu Ö. Synthesis of a 13-membered macrocyclic tetrathiadioxime and its mono- and tri-nuclear complexes with tetrahedrally coordinated palladium (II). *J. Chem. Soc. DaltonTrans.*, 1990, **No. 1**, p. 5-8. DOI: [10.1039/DT9900000005](https://doi.org/10.1039/DT9900000005)
4. Musluoglu E., Ahsen V. Synthesis and Characterization of 1,2-Bis(aziridin-*N*-yl) glyoxime and its Nickel(II), Palladium(II) and Cobalt(II) Complexes. *J. Chem. Res. (S)*, 1999, **No. 2**, p. 142-143. DOI: [10.1039/A807944G](https://doi.org/10.1039/A807944G)
5. Dilworth J.R., Wheatley N. The preparation and coordination chemistry of phosphorusulfur donor ligands, *Coordination Chemistry Reviews*, 2000, **Vol. 199(1)**, p. 89-158. DOI: [10.1016/S0010-8545\(99\)00185-X](https://doi.org/10.1016/S0010-8545(99)00185-X)
6. Buttrus N.H., Saied F.T., Zeedan S.W. Mono, di and trinuclear complexes Co^{+2} , Ni^{+2} , Cu^{+2} , Bi^{+3} and Sb^{+3} with bis-(*n*-butylthio)ethane. *J. Edu. Sci.*, 2007, **Vol. 19(4)**, p. 14-22
7. Chaudhury S., Blaurock S., Hey-Hawkins E. P–H-Functionalized 2-(Phosphanyl)ethanethiols, Their Titanocene Derivatives $[Cp_2Ti(SCH_2CH_2PHR)_2]$ ($R = Ph, 2,4,6-Me_3C_6H_2, 2,4,6-iPr_3C_6H_2$) and Reaction of $[Cp_2Ti(SCH_2CH_2PPh)_2]$ with $[Cu(CH_3CN)_4]BF_4$. *J. Inorg. Chem.*, 2001, **Vol. 2001**, p. 2587-2596. DOI: [10.1002/1099-](https://doi.org/10.1002/1099-)

- 0682(200109)2001:10<2587::AID-EJIC2587>3.0.CO;2-B
8. Hiroshi O., Keiichi T., Yoshiyuki M., Nobuyuki T. Syntheses and characterizations of μ -dicarboxylato-bis(pentaamminecobalt(III)) complexes. *Bull. Chem. Soc. Jpn.* 1981, **Vol. 54(6)**, p. 1736-1739. DOI: [10.1246/bcsj.54.1736](https://doi.org/10.1246/bcsj.54.1736)
 9. Bairagi S., Pradhan A.N., Cordier M., Roisnel T., Ghosh S. Syntheses, structures, and electronic properties of mono- and bimetallic thiolato complexes containing unusual coordination modes of thiolato ligands. *Eur. J. Inorg. Chem.* 2023, **Vol. 26(16)**, e202300060. DOI: [10.1002/ejic.202300060](https://doi.org/10.1002/ejic.202300060)
 10. Raman N., Ravichandran N.S., Thangaraja C., Copper(II), cobalt(II), nickel(II) and zinc(II) complexes of Schiff base derived from benzil-2,4-dinitrophenyl hydrazone with aniline. *J. Chem. Sci.* 2004, **Vol. 116**, p. 215-219. DOI: [10.1007/BF02708270](https://doi.org/10.1007/BF02708270)
 11. Trifunovic S., Markovic Z., Sladic D., Andjelkovic K., Sabo T., Mini D. The synthesis and characterization of nickel(II) and copper(II) complexes with the polydentate dialkyl dithiocarbamic acid ligand 3-dithiocarboxy-3-aza-5-aminopentanoate. *J. Serb. Chem. Soc.*, 2002, **Vol. 67**, p. 115-122. DOI: [10.2298/JSC0202115T](https://doi.org/10.2298/JSC0202115T)
 12. Gürol I., Ahsen V., Bekaroglu Ö. Synthesis of soluble complexes from a tetradentate dithioglyoxime ligand. *J. Chem. Soc. Dalton Trans.*, 1992, **No. 14**, p. 2283-2286. DOI: [10.1039/DT9920002283](https://doi.org/10.1039/DT9920002283)
 13. Saied F. Synthesis and characterization of Zn(II), Cd(II) and Hg(II) complexes with thioether ligands and their adducts with 1,10 phenanthroline. *Journal of Education And Science*, 2007, **Vol. 19(1)**, p. 1-8. DOI: [10.33899/edusj.2019.162869](https://doi.org/10.33899/edusj.2019.162869)
 14. Salivon N.F., Oliinik V.V. Synthesis and crystal structures of π complexes of copper(I) halides with diallyl disulfide $2\text{CuX} \cdot \text{DADS}$ ($\text{X} = \text{Cl, Br}$; $\text{DADS} = \text{CH}_2=\text{CH}-\text{CH}_2-\text{S}-\text{S}-\text{CH}_2-\text{CH}=\text{CH}_2$). *Russian J. Chem.*, 2006, **Vol. 32**, p. 208-213. DOI: [10.1134/S1070328406030079](https://doi.org/10.1134/S1070328406030079)
 15. Aziz K.A., Saeed F.T. Synthesis and Characterization of a number of Complexes of Pt(I), Pd(I), Cd(I) And Zn(I) With New Ligands Containing Oxygen. *Bull. Chem. Soc. Ethiop.* 2025, **Vol. 39(7)**, p. 1349-1361. DOI: [10.4314/bcse.v39i7.9](https://doi.org/10.4314/bcse.v39i7.9)
 16. Tabatabaee M., Mohamadinasab R., Ghaini K., Khavasi H.R. Hydrothermal synthesis and characterization of a binuclear complex and a coordination polymer of copper(II). *Bull. Chem. Soc. Ethiop.* 2010, **Vol. 24(3)**, p. 401-409. DOI: [10.4314/bcse.v24i3.60687](https://doi.org/10.4314/bcse.v24i3.60687)
 17. Shabaa A.A., Sariya W.Z. Synthesis, characterization, molecular docking, and in vitro screening of new metal complexes derived from acyclovir Schiff base with ciprofloxacin ligand. *Iraqi J. Sci.* 2023, **Vol. 64(12)**, p. 6072-6092. DOI: [10.24996/ijsc.2023.64.12.1](https://doi.org/10.24996/ijsc.2023.64.12.1)
 18. Marinho M.V., Yoshida M.I., Guedes K.J., Krambrock K., Bortoluzzi A., Hörner M., Machado F.C., Teles W.M. Synthesis, crystal structure, and spectroscopic characterization of trans-bis[(μ -1,3-bis(4-pyridyl)propane)(μ -(3-thiopheneacetate-O)) (3-thiopheneacetate-O)] dicopper(II), {[Cu₂(O₂CCH₂C₄H₃S)₄ μ -(BPP)₂]}_n: From a dinuclear paddle-wheel copper(II) unit to a 2-D coordination polymer involving monatomic carboxylate bridges. *Inorg. Chem.* 2004, **Vol. 43(4)**, p. 1539-1544. DOI: [10.1021/ic035251y](https://doi.org/10.1021/ic035251y)
 19. Khaleel N., Jaafar M. Preparation, characterization and biological study of new boron compound and Schiff base derived from 2-aminophenol with their Cu (II) and Pt (IV) complexes. *IOSR Journal of Applied Chemistry*, 2016, **Vol. 9(8)**, p. 4-11.
 20. Chetana P.R., Srinatha B.S., Somashekar M.N., Policegoudra R.S. Synthesis, spectroscopic characterisation, thermal analysis, DNA interaction and antibacterial activity of copper(I) complexes with N, N'-disubstituted thiourea. *Journal of Molecular Structure*, 2016, **Vol. 1106**, p. 352-365. DOI: [10.1016/j.molstruc.2015.10.010](https://doi.org/10.1016/j.molstruc.2015.10.010)
 21. Israa A.S. Synthesis and characterization of ligating properties of organic disulfides complexes with Co⁺², Ni⁺² and Cu⁺² metal ions. *Tikrit Journal of Pure Science*, 2012, **Vol. 17(2)**, p. 95-98.
 22. Neves A.I.S., Santos I.C., Belo D., Almeida M. Cation and ligand roles in the coordination of Fe(III) bisdithiolene complexes; the crystal structures of

- (BrBzPy)₂[Fe(qdt)₂]₂ and [Fe(a-tpdt)₂]₂ salts. *CrystEngComm*. 2009, **Vol. 11**, p. 1046–1053. DOI:10.1039/B813242A
23. Cotton F.A., Wilkinson G. *Advanced Inorganic Chemistry*. 4th ed. Interscience. New York. 1988. p. 772-789.
24. Turan N., Sekerci M. Synthesis and characterization of Co(II), Ni(II), Cd(II) and Cu(II) complexes of bis-Schiff base obtained from 1,8 diamino-naphthalene. *J. Chem. Soc. Pak.*, 2009, **Vol. 31**, p. 564-568.
25. Bharty M.K., Bharti A., Dani R.K., Kushawaha S.K., Dulare R., Singh N.K. Studies on novel Cu(II) complexes of 5-(4-hydroxy-phenyl)-1,3,4-thiadiazole-2-thiol and 5-thiophen-2-yl-3H-1,3,4-oxadiazole-2-thione: Synthesis, spectral and structural characterization. *Polyhedron*, 2012, **Vol. 41(1)**, p. 52-60. DOI: [10.1016/j.poly.2012.04.025](https://doi.org/10.1016/j.poly.2012.04.025)
26. Chohan Z.H., Khan K.M., Supuran C.T. Synthesis of antibacterial and antifungal cobalt(II), copper(II), nickel(II) and zinc(II) complexes with bis-(1,1'-disubstituted ferrocenyl) thiocarbohydrazone and bis-(1,1'-disubstituted ferrocenyl) carbohydrazone. *Appl. Organomet. Chem.*, 2004, **Vol. 18(7)**, p. 305-310. DOI: [10.1002/aoc.620](https://doi.org/10.1002/aoc.620)
27. Abbas A.S., Susan D.A., Shaima H.S., Zainab Abd A.H. Synthesis and Spectroscopic Characterization for Some Metal ion Complexes with 2-Hydroxy-3-((5-Mercapto-1,3,4-Thiadiazol-2-yl) Diazenyl)-1-Naphthaldehyde. *Baghdad Sci. J.*, 2016, **Vol. 13(2)**, p. 105-113. DOI: [10.21123/bsj.2016.13.2.2NCC.0105](https://doi.org/10.21123/bsj.2016.13.2.2NCC.0105)
28. Saeed I.A., Al-Asalli S.M., Saeed F.T. Synthesis and Characterization Of New Complex Salts Of Some Transition Metals With Carbazolium And Phosphonium Salts. *Chemical Problems*, 2025, **Vol. 23(4)**, p. 563-572. DOI: 10.32737/2221-8688-2025-4-563-572
29. Buttrus N.H., Tariq F.S. Bis(N-methyl benzimidazolium-2-thio) ethane, Propane or Butane Diiodide and Its Co(Ii),Ni(Ii),Cu(Ii) And Zn(Ii) Ionic Salts. *International J. Chem.* 2012, **Vol. 22(2)**, p. 117-122
30. Abdljabar R.R., Saeed F.T. Synthesis and Characterization of Mn⁺², Co⁺², Ni⁺², Cu⁺² And Zn⁺² Complexes With 4-(2-(Benzo-1,3-Dioxol-5-yl)-4,5-Diphenyl-2,5-Dihydro-1h-Imidazol-1-yl)aniline and Evaluation of their Biological Activity. *Chemical Problems*, 2024, **Vol. 22(2)**, p. 197–210. DOI: 10.32737/2221-8688-2024-2-197-210.
31. Chaudhary R., Shelly. Synthesis spectral and pharmacological study of Cu(II), Ni(II) and Co(II) coordination complexes. *Res. J. Chem. Sci.*, 2011, **Vol. 15(1)**, p. 1-5.