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Synthesis, Characterization, Antimicrobial activty and Antioxidant Activity of Some Metal Complexes with 4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thiol

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Abstract:

The work describes the synthesis and spectral investigation of Co (II), Ni (II), Cu (II), and Zn (II) complexes with 4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thiol (L). The new ligand was synthesized through three successive steps: first, the preparation of the potassium salt of isoniazid with an alkaline solution of carbon disulfide; second, the ring closure of the potassium salt with an excess of hydrazine hydrate; and finally, the last step involved the condensation of 4-amino-1,2,4-triazole with 4-bromobenzaldehyde in glacial acetic acid as a catalyst to afford a good yield of the new Schiff base, L. The physical and spectroscopic properties of the ligand and its complexes were well studied. The ligand **L** has been used to synthesize new complexes of Co (II), Ni (II), Cu (II), and Zn (II), which have been characterized by using different techniques, such as FT-IR, UV-Vis, 1H-NMR, and 13C-NMR spectrophotometric techniques, as well as elemental analysis C.H.N.S. and flam atomic absorption FAA. The physicochemical properties, such as melting point, magnetic susceptibility, and molar conductivity at room temperature, were determined. The synthesized complexes **C1**, **C2**, and **C3** have taken the octahedral geometry in a mole ratio **(1:1) of M**: **L** and behave as bidentate ligands that attach to metal ions through the N atom of azomethine and the S atom in the thione group. The metal complexes displayed an octahedral geometry around bivalent cobalt, nickel, copper (II), and zinc (II) tetrahedral environments. Moreover, the biological activity of free ligand and its metal complexes solutions (CoL and CuL) was screened against some bacteria and fungi. The free ligand and CuL were more active against bacteria and fungi than CoL. These results can provide an important platform for the design of new compounds with antibacterial and antifungal activity.

As well as this, the study included examining the antioxidant activity of the synthesized metal complexes (ZnL and CuL) using DPPH assay against ascorbic acid as a reference antioxidant agent. The results showed that all the synthesized metal complexes have antioxidant activity but lower than ascorbic acid. As well as the zinc (II) complex, it was found to have higher antioxidant activity than the Cu (II) complex. The highest free radical scavenging capacity of the zinc (II) complex and Cu (II) complex at 500 µg/ml were 75.670 % and 69.409%, respectively.

Key words: Antioxidant activity of triazole, metal complexes of triazole, biological activity of triazole.

1. Introduction

Triazole, which was first coined by Bladin in 1885, is a crystalline solid ranging from white to pale yellow in color. It possesses a weak characteristic odor and is soluble in both water and alcohol. Triazole is classified as a triazine compound and belongs to the class of organic heterocyclic compounds [1]. It is characterized by a five-membered diunsaturated ring and has the molecular formula C2H3N3. Notably, triazole exists in two isomeric forms: 1,2,3-triazole and 1,2,4-triazole, which show tautomers with respect to the hydrogen position [2]. The derivatives of 1,2,4-triazole have been exploring great attention in the recent years due to their unique physical and biological properties [3]. They are an attractive class of chemicals with a wide variety of biological properties, including antifungal, anticancer, anti-inflammatory, antibacterial, and antitumor characteristics,[31].

Phung, H. has studied the synthesis and x-ray crystallography of gold (I) complexes featuring 1,2,4-triazole-derived carbenes with the chemical formula [AuCl(Cy-tazy)]. All the complexes have been characterized by elemental analysis, multinuclear NMR spectroscopy, (ESI) mass spectrometry, single crystal X-ray diffraction, and DFT calculations. In addition, all the prepared gold (I) complexes showed high antiproliferative activities against KB, MCF-7, and HT-29 cancerous cell lines [4, 5]. Zilonakhan C. and co-workers have established the synthesis, spectroscopic, and biological assessment of a novel coordination of zinc (II) chelates. The complexes were prepared using N-(1H-1,2,4-triazol-3-yl)acetamide and hydrated zinc(II) chloride, yielding a product characterized by FT-IR, elemental analysis, thermogravimetric analysis (TGA), and single crystal X-ray diffraction [6].

Antioxidants are an important class of compounds that prevent harmful effects of free radicals in the human body. Antioxidants derived from natural sources are favored over those derived from synthetic sources; however, there are many synthetic compounds reported as efficient antioxidants [9, 10]. 1,2,4-Triazole derivatives have been shown to have antitumor activity toward a number of cancer types. A variety of in vitro investigations have been carried out in recent years for this purpose. It's possible that 1,2,4-triazole derivatives' antioxidant properties are associated with their anticancer properties, [32].

Maddila and Co-workers have recorded the synthesis and antioxidant activity of compounds with phenothiazine bind-substituted benzylideneamino-1,2,4-triazole derivatives and assessed their antioxidant activity in vitro by using nitric oxide, hydrogen peroxide, and DPPH radical scavenger assays [11]. Recently, Sumrra *et al.* [12] have introduced the Schiff base compound 2-{(E)-[(3-{[(Z)-(2-hydroxyphenyl) methylidene] amino}-1H-1,2,4-triazol-5-yl) imino] methyl} phenol. With their complexes with Co (II), Ni (II), Cu (II), and Zn (II), they have been evaluated for their antioxidant activity by DPPH assay. Some of these compounds were found to be important scavengers of free radicals. The results showed that the Ni (II) complex demonstrated potent antioxidant activity, more than the reference butylated hydroxytoluene, while the Cu (II), Co (II), and Zn (II) complexes exhibited good scavenging activity but lower than the Ni (II) complex. On the other hand, the free ligand was found to have very low activity compared to BHT. Thus Drawing from the previous studies, our aim was to synthesize new Schiff base metal complexes and investigate their antimicrobial, antifungal, and antioxidant properties.

2. Experimental

2.1 Materials and methods

The starting materials, 4-bromobenzaldehyde, hydrazine hydrate 80%, carbon disulfide, and isoniazid, were supplied from Merck Chemical Company and Santa Cruz Biotechnology companies with 98-99% purity and used without purification. All the chemicals that were used in this work were commercially available and used without further purification. The hydrated metal chlorides of $CuCl_2.2H_2O$, $CoCl_2. 6H_2O$ and $NiCl_2.6H_2O$ and $ZnCl_2$ were supplied from Merck, Chemistry Department, College of Science, Mustansiriyah University.

2.2. Physical Measurements

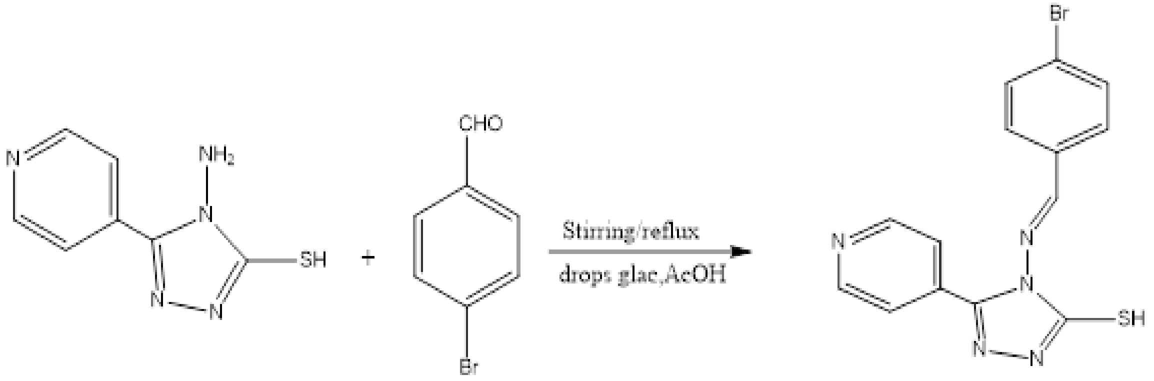
The decomposition points of the prepared triazole precursor, its Schiff base, and its metal complexes were measured by Stuart-SMP30. The vibrational frequencies of the solid-prepared ligands and metal complexes were measured in the region (4000-400) cm^{-1} on the (8400 S-FT-IR SHIMADZU) spectrometer at Mustansiriyah University, College of Science, Iraq. The chemical formula of the prepared compounds was determined by mass spectra technique with the GC-DIMS QP2010 ultra and Orbitrap LTQ XL-Thermo Fisher scientific mass spectrometer at the University of Tehran, Iran. Furthermore, the NMR spectra of the prepared ligand were measured on a 400 MHz Bruker NMR spectrometer at Basra University, College of Education for Pure Sciences.

2.3. Preparation of 4-amino-5-(pyridin-4-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione, A2

The precursor 1,2,4-triazole was prepared according to the mentioned method in the literature [16] with minor modification. A mixture of potassium isonicotinic hydrazide salt, A1 (2.53 g, 0.012 mole), with 10 ml (0.015 mole) of hydrazine hydrate, was heated under reflux for 5 hours. The color of the mixture was turned from black-green into light yellow with the evolution of hydrogen sulfide gas. A white precipitate was isolated by pouring the reaction mixture into 10 ml of ice water with acidification by 10 drops of concentrated hydrochloric acid. Recrystallization of the crude from hot ethanol afforded yellow crystals of a derivative. Yield 88%, M.p 248-250 C°, M.wt 193.1 g/mol, R_f = 0.66 (ethyl acetate: acetonitrile, 1:2). FT-IR (KBr, cm^{-1}): υ (NH_2) *asym*. and sym. (3400 and 3380), υ (NH) (3170), υ(S-H) (2580), υ(C=S) (1075).

2.4. Synthesis of (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione,L

Dissolving of A2 (1.293 gm., 0.01 mole) in 15 mL hot ethanol was gradually added to a (1.50 gm., 0.010 mole) of 4-bromobenzaldehyde in 10 drops of glacial acetic acid; the mixture was refluxed for 6 hours, and then the reaction



was controlled using TLC. After keeping the mixture to settle overnight at room temperature. The precipitate was filtered and washed with hot ethanol, dried to obtain the ligand L. M.p. 300-302 C°, M.wt. 359.90 g/mol, Rf = 0.77 (ethyl acetate: acetonitrile, 1:2), Scheme 1.

Scheme 1. Preparation of 1,2,4-triazole ligand, L.

2. 5. Synthesis of the metal complexes C1-C4

2. 5.1. Cobalt (II) Complex C1

Complex C1 was synthesized by dissolving L (0.359 gm., 1 m mole) in a hot mixture of ethanol (20 mL) and mixing it with a solution of metal ion $CoCl_2.6H_2O$ (0.238 g, 1 m mole) in 20 mL ethanol in a 1:1 ratio of metal to ligand. The mixture was heated in a water bath with stirring for 60 minutes; the green solid complex was formed after cooling and the addition of 10 mL of diethyl ether. The filtered complex was washed several times with cold water and ethanol and dried in air and the oven for 3 hours. Color: pale green; Yield: 61%; M.P.: 344-346°C; FT-IR υ (cm-1): 3500 (OH_2), 3230 (N-H), 1580 (C=N), 1220 (C=S), 510 (M-N), 470 (M-O), 403 (M-OH_2).

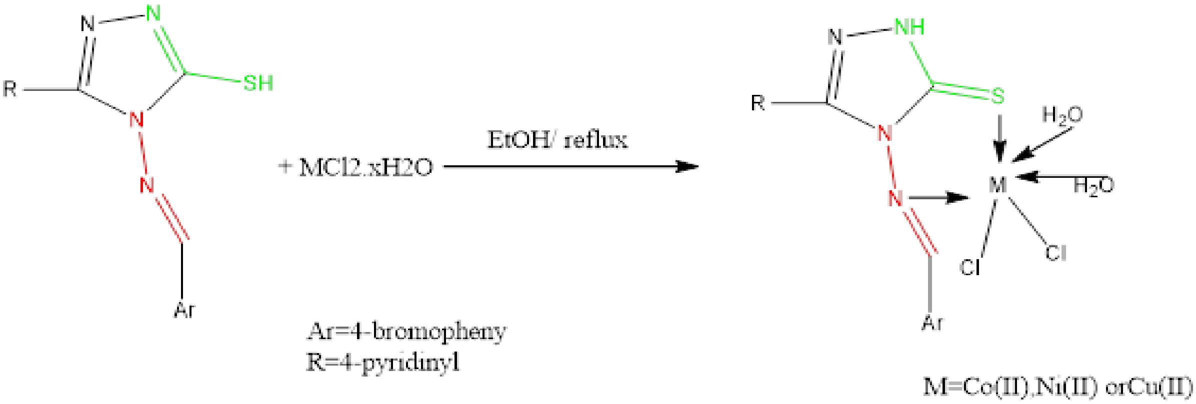
2.5.2. Nickel (II) Complex C2

Complex C2 was synthesized by dissolving L (0.359 gm., 1 mmole) in a hot mixture of 10 mL and mixing with a solution of metal ion $NiCl_2.6H_2O$ (0.237 gm., 1 mmole) in 10 mL ethanol in a 1:1 ratio of metal to ligand. The mixture refluxed for 2 hours, and the dark green complex was formed after cooling and addition of 10 mL of diethyl ether. The filtered complex was washed several times with cold water and ethanol and dried in air and the oven for 4 hours. Color: green; Yield: 90%; M.P.: 194-198°C; FT-IR υ (cm-

1): 3550 (O-H, H_2O), 1615 (C=N-Py), 1590 (C=N-), 1230 (C=S), 490 (M-N), 433 (M-O), 400 (M-OH_2).

2.5.3. Copper (II) Complex C3

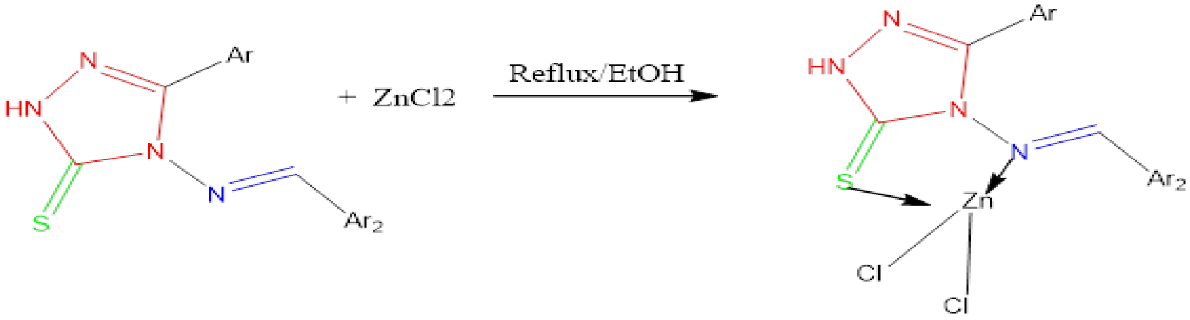
Complex C3 was synthesized by dissolving L (0.359 gm., 1 m mole) in hot mixture of (20 mL) and mixing with solution of metal ion $CuCl_2.2H_2O$ (0.171 g., 1 mmole) in 10 mL ethanol in 1:1 ratio of metal to ligand. The mixture heated on water bath for 45 minutes, the solid complex was formed after cooling and addition of 10 mL of diethyl ether. The filtered complex was washed several times with cold water, ethanol and dried in air and oven for 4 hours, Color Olive; Yield 95 %; M.P 255-258 C^o, FT-IR υ (cm^{-1}): 3300(br) (O-H) , 1588 (C=N), 1218(m) ,1075 (m) (C=S), 560 (M-N), 460 (M-OH_2), Scheme 2.



Scheme 2 Synthesis of $[MLCl_2(H_2O)].H_2O$ complexes

2.5.4. Zinc (II) Complex C4

The zinc(II) complex was synthesized by dissolving L (0.285 gm., 1 m mole) in hot mixture of (15 mL) and mixing with solution of metal ion $ZnCl_2$ (0.143 g., 1 mmole) in 10 mL ethanol in 1:1 ratio of metal to ligand. The mixture heated under reflux for 2 hours, the solid complex was formed after cooling and addition of 10mL of diethyl ether. The filtered complex was washed several times with cold water, ethanol and dried in air and oven for 4 hours, Color Off white; Yield 75 %; melting point 217-219 C^0, FT-IR υ (cm^{-}



1): 3200 (O-H), 3080 (OH_2), 1588 (C=N), 1210 (C=S), 445(Zn-N), 440 (Zn-O),Scheme 3.

Scheme 3 Synthesis of [$ZnCl_2$] complexes

2.6. Biological activity

The agar well diffusion method was used to detect the antibacterial activity of the prepared Schiff base, (E)-4-((4-bromobenzylidene) amino). -5-(pyridin-4-yl)-2, 4-dihydro-3H-1, 2, 4-triazole-3-thione and its metal complexes (CuL and CoL) against various pathogens, including two strains of gram-positive bacteria (*Staphylococcus aureus* and *Staphylococcus epidermidis*), two strains of gram-negative bacteria (*Escherichia coli* and *Klebsiella sp.)*, as well as against fungus such as *Candida albicans,* at the concentrations of 10^{-2} and 10^{-4} M according to Lewus et al. (1991) and Mahdi (2017). All of the bacterial isolates used in this study were grown in nutrient broth and incubated at 37C° for 18 to 24 hours. After the incubation period, 0.1 ml of each bacterial solution was applied to the nutrient agar surface and left for 24 hours at 37C°. A bacterial suspension with a moderate turbidity, which is approximately equivalent to 1.5x108 CFU/mL when compared to the standard turbidity solution, was obtained by adding a single colony to a test tube containing 5 mL of normal saline. A portion of the bacterial suspension was carefully transferred and evenly distributed on Mueller-Hinton agar medium using a sterile cotton swab, and it was then allowed to sit for ten minutes. In the prior agar layer, three wells per plate with a diameter of five millimeters were created. After detaching the agar discs, a micropipette was used to add 50 µl of the synthesized compounds to each well. After an 18-hour period of incubation at 37C°, the diameter of the inhibitory zones on the plates was determined. The results were compared with those of common medications, such as fluconazole for Candida albicans, vancomycin hydrochloride for gram-negative bacteria, and exigent for gram-positive bacteria. As a control, DMSO was employed.

2.7. Spectrophotometric (DPPH) assay

This assay was confirmed according to the modified procedure in the reported reference (29-30). A mixture of synthesized metal complexes (CuL and ZnL) and ascorbic acid (as a standard) at concentrations of (62.5, 125, 250, and 500 µg/mL) were taken separately and added up to 0.25 mL of DPPH solution (0.13 mg DPPH/mL methanol); then the volume was completed to 1.5 mL with methanol. The last mixture was left to stand for 30 min in a tenebrous place. A control contained all reagents without a sample. The measurement of the absorbance at 517 nm against a blank was used to determine the DPPH radical scavenging activity. The following equation: DPPH scavenging effect = $[(Ac - As) / Ac] \times 100$, where Ac refers to control reaction absorbance (0 µg/ml) and as refers to test specimen absorbance.

3. Results and discussion:

The new Schiff base, (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione, was synthesized with a high yield of 88% through the condensation of 4-amino-5-(4-pyridyl)-1,2,4-triazole-3-thiol with a solution of 4-bromobenzaldehyde in the presence of drops of glacial acetic acid as a catalyst, which accelerates the nucleophilic attack of the –NH_2 group on the carbon atom of 4-bromobenzaldehyde. The new Schiff base and its complexes were fully characterized using elemental analysis and various spectroscopic techniques. The metal content in the solid complexes (C1-C4) was determined using flame atomic absorption (FAAS). Solubility tests revealed that all complexes were insoluble in common organic solvents but fully soluble in DMF and DMSO. In contrast, the ligand was found to be soluble in most common organic solvents except (Et_2O) and insoluble in H_2O. Molar conductivity measurements of the complexes' solutions in DMSO indicated that they do not exhibit electrolytic properties, with values ranging between (14.79-22.5 $\Omega^{-1}.cm^2.mol^{-1}$), confirming the proposed chemical formulas of the C1-C4 complexes. These results suggest that the synthesized metal complexes possess good thermal stability, non-electrolytic behavior, and a spatial structure consistent with theoretical expectations. Additionally, differences in physical and spectroscopic properties reflect the influence of chemical coordination on the behavior of these complexes, opening avenues for future studies on their potential applications in biological and pharmaceutical fields.

Table 1- Analytical data of the ligand, L and its metal complexes C1-C4

No .	General formula	M.wt (g/mol)	Color	Melting Point C°	Ω^{-1} $Ohm^{-1}.cm^{2}.mol^{-1}$
A	$C_7H_7N_5S$	193.1	Yellow	248-250	-
L	$C_{14}H_{10}BrN_5S$	359.90	Yellow	300-302	
C1	$[Co(L)(H_2O)_2Cl_2]$	544-90	Green	344-346	15.8
C2	$[Ni(L)(H_2O)_2Cl_2Cl_2].H_2O$	598.75	Orange	194-198	22.50
C3	$[Cu(L)(H_2O)_2Cl_2]$	610.54	Green	255-258	17.20
C4	$[ZnLCl_2]$	422.27	Off white	217-219	14.79

Table 2: Symbols, molecular formulas and names of the synthesized Ligand (L) and its complexes C1-C4

Sym.	Molecular formula	Name
A	$C_7H_7N_5S$	4-amino-5-(pyridine-4-yl)-4H-1,2,4-triazole-3-thione
L	$C_{14}H_{10}BrN_5S$	(E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thiol
C1	$[Co(L)(H_2O)_2Cl_2]$	[di chloro (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thioldiaqua cobalt (II)]
C2	$[Ni(L)(H_2O)_2Cl_2].H_2O$	[di chloro (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thiolnickel(II)] mono hydrate
C3	$[Cu(L)(H_2O)_2Cl_2].H_2O$	[di chloro (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thioldiaqua copper (II)] di hydrate
C4	$[Zn(L)Cl_2]$	[di chloro (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-4H-1,2,4-triazole-3-thiolzinc(II)]

3.1. Mass Spectra:

The potassium salt of dithiocarbamate (A1) resulted from addition carbon disulfide to isoniazid in KOH solution leads to appear good indication of MS spectrum at M/e=352 indicating the right structure of the salt structure, Figure 1.

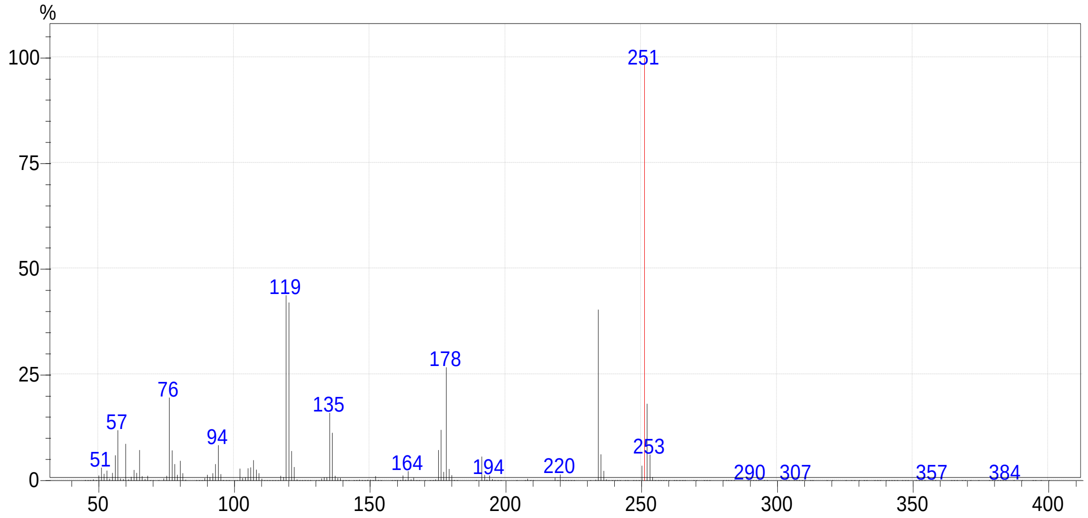
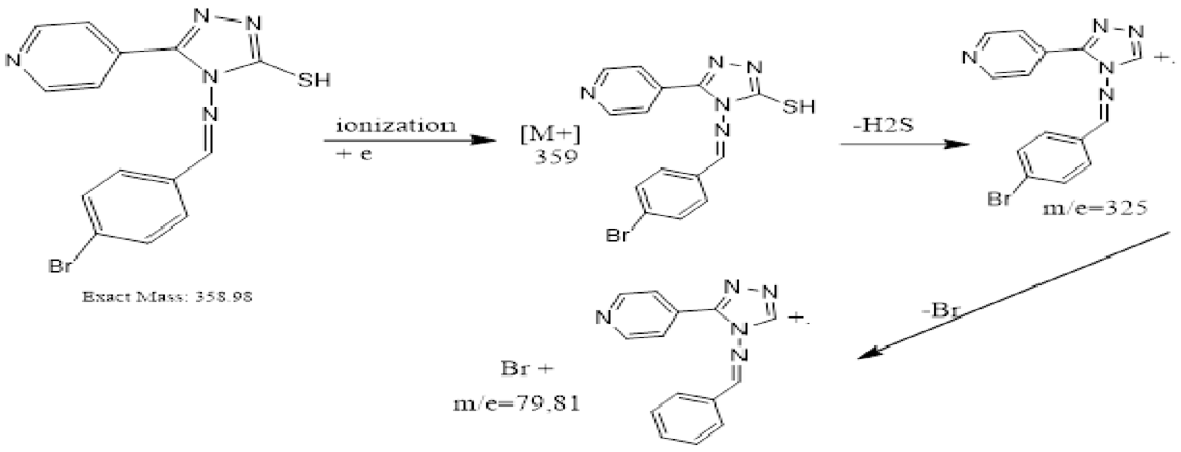


Figure 1. MS spectrum of potassium-isonictontinhydrazine-1-carbonyldithiolate

The mass spectrum of the free ligand L displayed a parent ion peak at M/z = 359.1 and 361 due to the ionization the gas phase of the bromo derivative at high temperature with the effect of Br-79 and Br-81 isotopes which corresponds to (M^+) confirming the molecular weight of the prepared ligand and confirms the condensation of 4-bromobenzaldehyde with 4-amino-1, 2, 4-triazole, A derivative in acidic medium of glacial acetic acid. As well as the base peak observed at M/z = 79 and m/z = 81 revealed the chemical structure of the prepared Schiff base. The summarized fragmentation pattern mechanism in MS spectrum is shown in scheme 4.

Scheme 4. Fragmentation mechanism of ligand in gas phase of MS spectrum



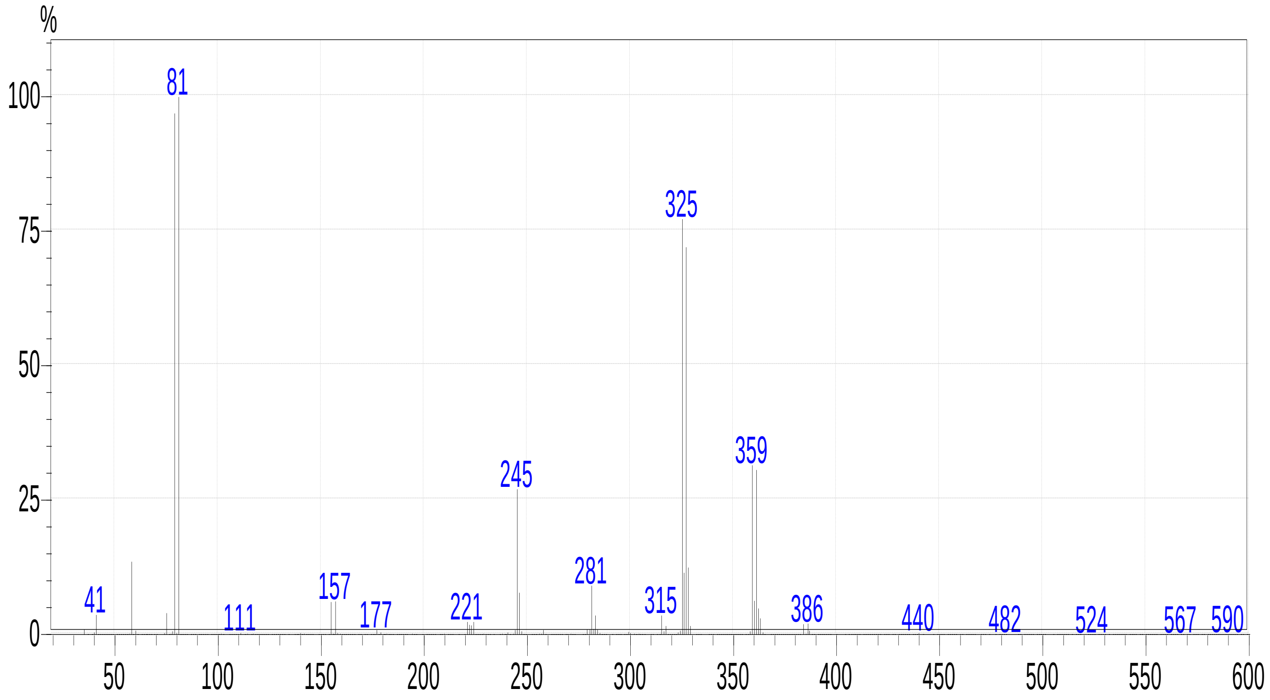


Figure 2. MS spectrum of Schiff base, L

3.2. NMR spectra:

The ^{1}H-NMR spectrum of the synthesized Schiff base ligand (L) recorded in DMSO-d6 exhibited a characteristic singlet at 12.25 ppm, corresponding to the thiol (-SH) proton of the triazole ring, and a signal at 8.98 ppm attributed to the imine (-CH=N-) proton. Additionally, multiplet peaks observed in the range of 7.5-8.5 ppm were assigned to the aromatic protons of the pyridine and 4-bromophenyl rings, Figure (3).

The ^{13}C-NMR spectrum, also recorded in DMSO-d6, confirmed the structural integrity of the ligand, displaying a significant peak at 168 ppm corresponding to the thiocarbonyl (-C=S) carbon and another at 150 ppm associated with the imine (-CH=N-) carbon. A peak at 23 ppm was attributed to the aliphatic methyl group attached to the pyrrole ring, while aromatic carbon signals appeared within the 120-135 ppm range, confirming the presence of the pyridine and 4-bromophenyl rings, Figure (4).

Upon complexation, noticeable shifts in the chemical shifts of thiol (-SH) and imine (-CH=N-) groups were observed, indicating coordination through nitrogen and sulfur atoms. These findings support the proposed chelation mechanism of the ligand with metal ions, reinforcing its bidentate binding nature.

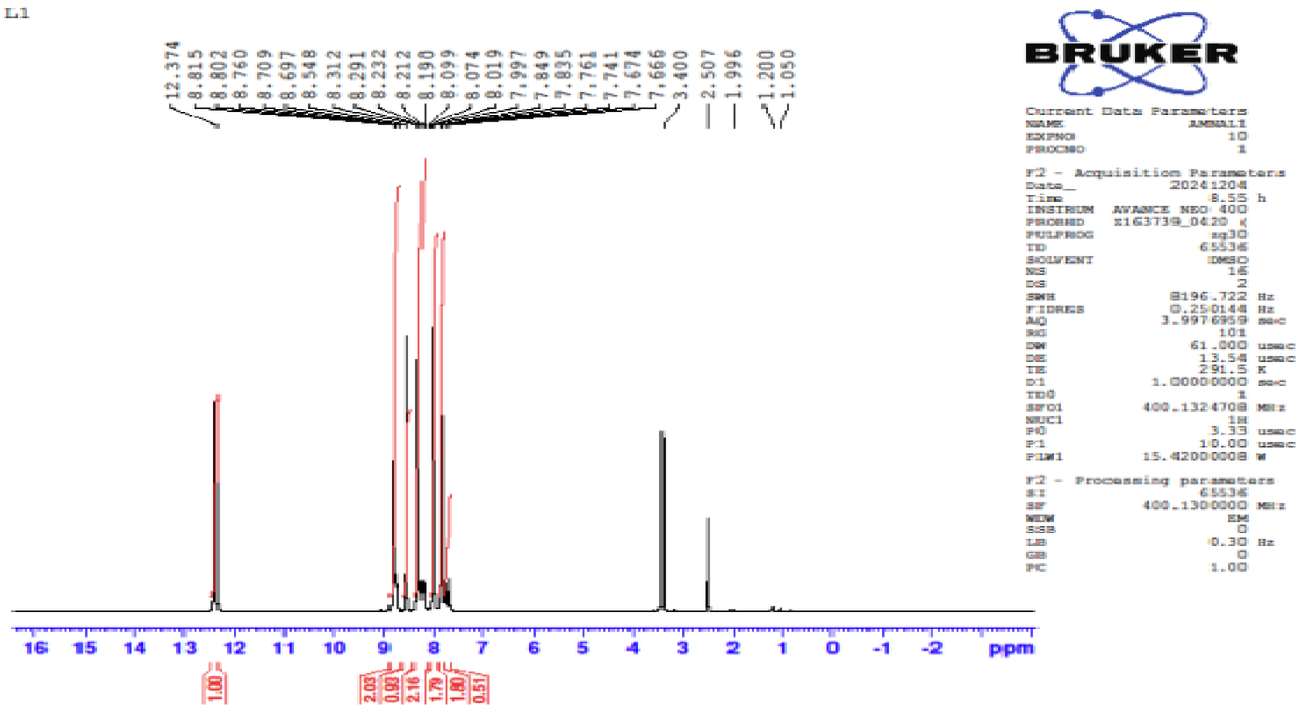


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Figure 3. H NMR spectrum of (L) in DMSO- d^{6}

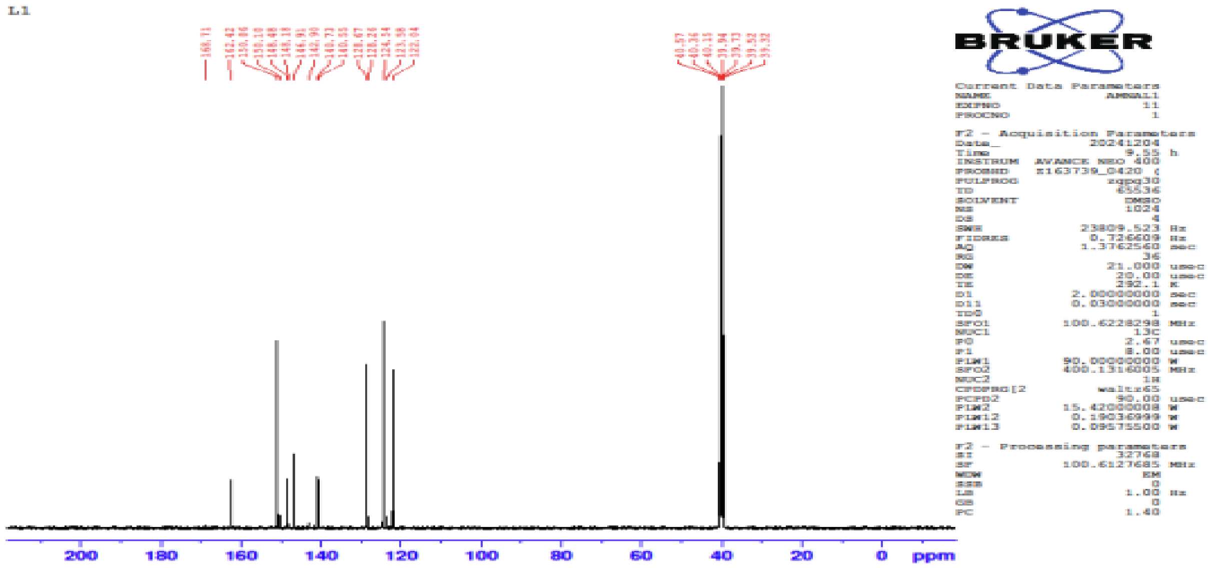

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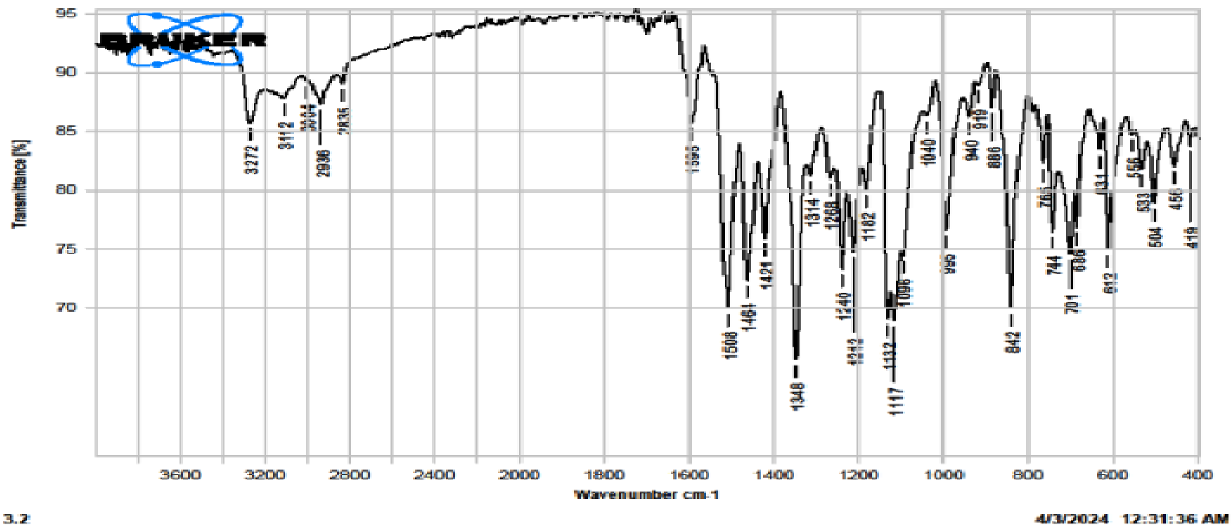
Figure 4.^{13}C NMR spectrum of (L) in DMSO- d^{6}

3.3. FT-IR spectra of ligand, L and its metal complexes:

The FT-IR spectrum is good spectral technique for characterization the functional groups in the 1, 2,4-triazole ligand and its complexes with cobalt(II), nickel(II) ,copper(II) and zinc(II). The main vibrational modes of IR spectrum of (L) ligand shows strong band at 1645 cm^{-1} and absorptions at (1223-1200 cm^{-1}) and 1070 cm^{-1} assigning to ʋ-C=N- and thioamide –C=S respectively, this new band is strong evidence for condensation of 2-acetylpyrrole with the amino group –NH2 of 4-amino-1,2,4-triazole precursor [3,19].. However, the medium absorptions at around (1610-1575 cm^{-1}) are belonged to the stretching of ʋ-C=N- pyridine ring attached directly to triazole at C-5 atom, Figure 5. The comparison of IR spectra of (C1-C4) complexes with the spectrum of L ligand is good proof for appearance of new bands at lower frequencies of (400-600 cm^{-1}) which are assigned to the coordination bonds of (Cu-N, Co-N, Ni-N) and (Cu-S, Co-S Ni-S and Zn-S) respectively. As well as the lowering in the vibrational modes of ʋ-C=N- immine group to the region (1550-1595 cm^{-1}) reveals the coordination bonding of metal ions to nitrogen atoms of immine moiety [6, 18]. Besides that, the shifting of frequencies of ʋ-C=S to less values at (1080-175 cm^{-1}) in all spectra of complexes revealed the participation of sulfur atom in linkage with the metal ions via (M-S) bonding, Figure (6).

Figure 5. FT-IR spectrum of ligand (L)



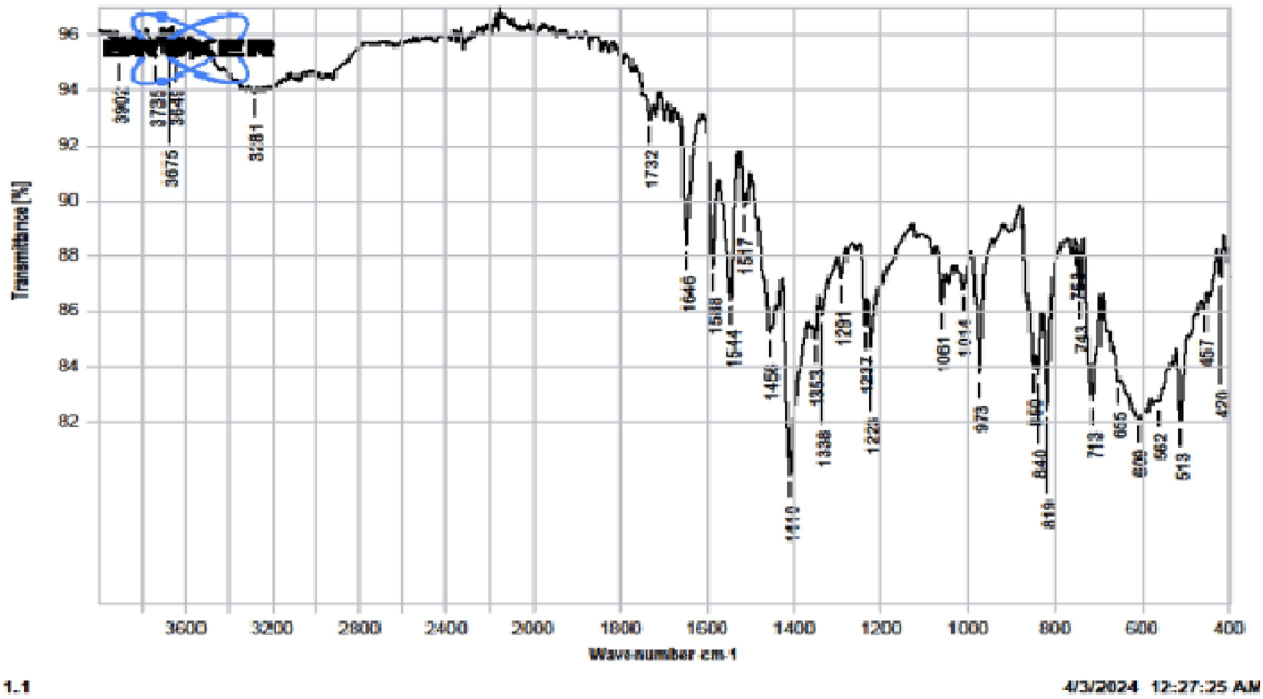


Figure 6. FT-IR spectrum of [CuL $(H_2O)_2Cl_2$] complex

3.4. Electronic Spectra and Magnetic Susceptibility of Metal Complexes:

The electronic spectra of ligand and its complexes are summarized in Table 3. The electronic spectrum of (E)-4-((4-bromobenzylidene)amino)-5-(pyridin-4-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione in absolute ethanol recorded two intense bands at 250 and 375 nm respectively, these are assigned to ligand spectra of the chromophore groups of –C=N and –C=S, Figure 7. The green solution of cobalt (II) complex in ethanol displayed weak intense bands in the regions 650 nm, 560nm and 400 nm which are attributed to the transition $^4T_{1g}\rightarrow{}^4T_{2g}(F)$ (ν_1), $^4T_{1g}\rightarrow{}^4A_{2g}(F)$ (ν_2), and $^4T_{1g}\rightarrow{}^4T_{1g}(P)$ (ν_3), respectively. The three spin-allowed transitions in the visible region for Co (II) complex investigate the high-spin octahedral cobalt (II) complexes with ground term ^4F [17, 22]. which mainly splits to three microstates from the stable ground $^4T_{1g}$ (F), therefore the application of T-S (Tanabe-Sugano) diagram leads to intercepts y_1, y_2 at E_1/B', E_2/B' to provide Racah parameter (B′) which was found to be 600 cm^{-1} and the crystal field splitting energy 10Dq found to be 14880 cm^{-1}, indicating the high spin octahedral environment around Co (II) ion, Figure 8. The covalence parameter (β) was calculated and found to be 0.80 indicating the high degree of interaction between *s*, *p* and *d*-orbitals of ligand and metal ions with synergetic effect, hence inter electronic repulsion has been decreased during the process of chelation. The green solution of nickel(II) complex in DMF showed three spin-allowed transitions at around 725 nm, 610 nm and 440 nm which are associated with $^3A_{2g}\rightarrow{}^3T_{2g}(F)$ (ν_1), $^3A_{2g}\rightarrow{}^3T_{1g}(F)$ (ν_2), and $^3A_{2g}\rightarrow{}^3T_{1g}(P)$ (ν_3) transitions, respectively. The application of T-S diagram on UV-Visible spectrum through the ratio ν_2/ν_1 found to be 1.45 which results in the values of y_1, y_2, x_1 intercepts at E_1/B', E_2/B' and Dq/B' was found to be 28, 13, and 21, respectively. The calculation refer B′ equal to 695 cm^{-1} and 10Dq equal to 16430 cm^{-1} indicating octahedral environment around nickel(II) ion [17,18]. As well as electron-electron repletion in d^8 configuration was decreased through overlapping with thione (–C=S) and immine (–C=N–) groups, this was confirmed from nephelauxetic effect found to be 0.70. The solid nickel(II) complex recorded effective magnetic moment of 2.85 BM which is associated with the two unpaired electrons (t_{2g}^6, e_g^2) being greater than the spin-only value (2.05 BM) and in well agreement of its octahedral geometry with orbital contribution to the magnetic moment. The greenish-yellow solution copper (II) in spectrosol methanol (0.001 M) displayed one weak shoulder band at 590 nm which is ascribed with $^2Eg\rightarrow{}^2T_2g$ transition, Figure 5. As well as the high intense peaks at 390 nm is mainly assigned to MLCT band, respectively. The copper (II) ion with the electronic configuration d^9 has one unpaired electron in the 3*d*-orbital. Therefore, its spin-only magnetic moment value should be 1.75 B.M. However, the CuL complex at room temperature recorded an effective magnetic moment value of 1.78 BM, indicating the z-out elongation with octahedral geometry [20-22]. The zinc (II) complex having a d^{10} configuration favors the formation of complexes with tetrahedral geometry. The electronic spectrum of C4 displayed three high intensity bands at 375 and 290 nm are also assigned to $Cl\rightarrow Zn^{2+}$ and π-π* transitions, respectively [20, 25].

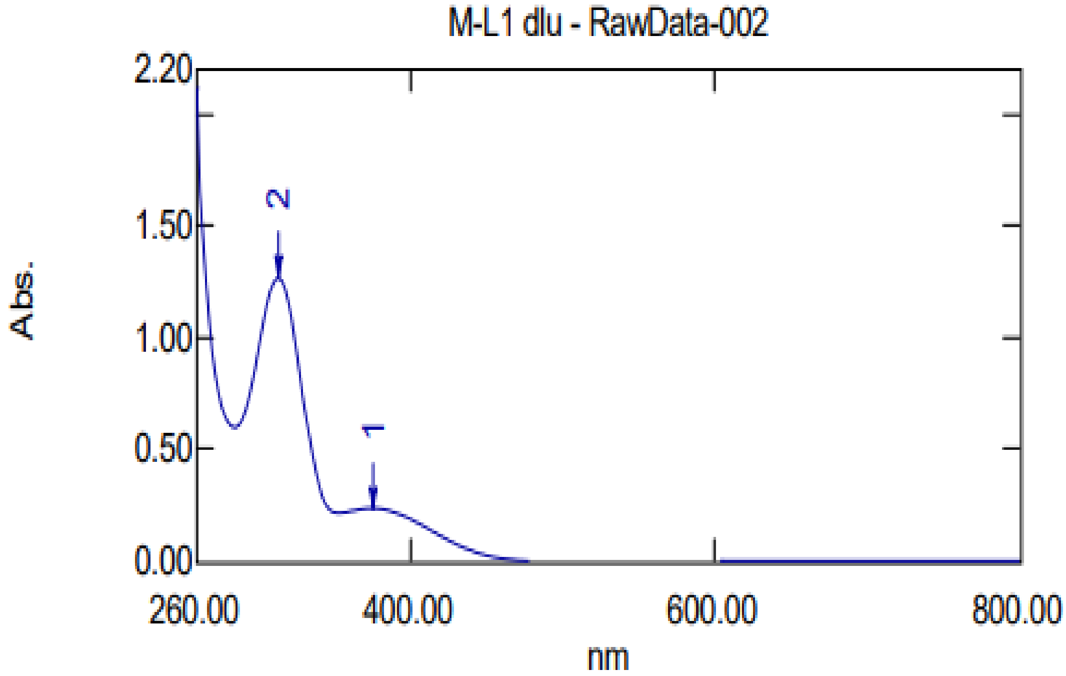


Figure 7. UV-Visible spectrum of ligand in ethanol (0.001 M).

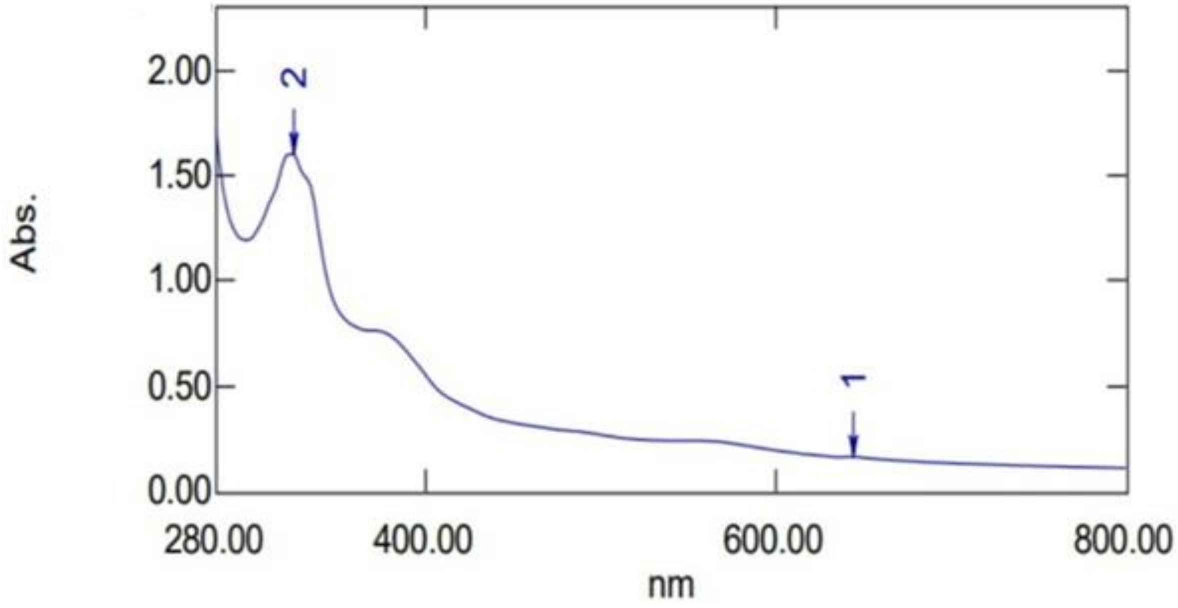


Figure 8. UV- Visible spectrum of C1 complex in DMF (0.001 M).

Table 3. Electronic spectra of ligand and its complexes

Symbol	Bands, λ nm (cm^{-1})	Band assignment	Geometry	Molar conductivity (S/mol)	Magnetic moment, μ (BM)
L	250 (40000) 375 (26666)	$\pi\rightarrow\pi^*$ $n\rightarrow\pi^*$	-	-	-
C1	650 (15385) 560(17858) 400 (25000) 380 (26316)	$^4T_1g\rightarrow{}^4T_2g$(F) $^4T_1g\rightarrow{}^4A_2g$ (F) $^4T_1g\rightarrow{}^4T_1g$ (P) CT	Octahedral	[40]	4.36
C2	725, (13793) 610 (16393) 445(22472)	$^3A_2g\rightarrow{}^3T_2g$ (F) $^3A_2g\rightarrow{}^3T_1g$ (F) $^3A_2g\rightarrow{}^3T_1g$(P)	Octahedral	[33]	2.90
C3	590 (16950) 390 (25642) 260 (38462)	$^2Eg\rightarrow{}^2T_2g$ CT $\pi\rightarrow\pi^*$	Distorted octahedral	[39]	1.78
C4	355(28170) 310(32258)	$Cl\rightarrow Zn^{2+}$ $\pi\rightarrow\pi^*$	Tetrahedral	[15]	0.0

3.5. Biological Activity

The antimicrobial activity of the prepared Schiff base, (E)-4-((4-bromobenzylidene) amino)-5-(pyridin-4-yl)-2, 4-dihydro-3H-1, 2, 4-triazole-3-thione (L) and its metal complexes (CuL and CoL) were tested against various pathogens, including gram-positive bacteria (*Staphylococcus aureus* and *Staphylococcus epidermidis*), gram-negative bacteria (*Escherichia coli* and *Klebsiella sp.)*, and fungus (*Candida albicans)*. Exigent, vancomycin hydrochloride, and fluconazole were used as standard drugs. The diameter of the inhibitory zone was measured to reveal the ability of the prepared compounds to inhibit the growth of microorganisms. It was observed that the 1, 2, 4-triazole ligand, copper (II) complex, and cobalt (II) complex have highly effective inhibitory activity against positive and negative bacteria and fungi, with the highest inhibitory activity for the copper (II) complex at concentrations of 10^{-2} M and 10^{-4} M; the diameter of the inhibition zone ranges between 21 and 27 mm (Table 4), (Figure 9), (Figure 10). This result probably has to do with the complexes' increased lipophilicity, which slowed the microbes' regular cellular functions and enhanced their antimicrobial activity or chelating powers. (1).The biological activity of Schiff base solution in DMSO with multiple coordination centers primarily stems from their ability to bind to essential metal ions utilized by pathogenic bacteria in their metabolism, thereby disrupting their biological processes. This mechanism is well-established in the literature [27, 28]. For copper (II) and zinc (II) complexes, their biological activity is primarily attributed to the impact of the metal ion on the cell membranes of bacterial strains and the fungus. Metal complexes have a preference for penetrating the lipid layer of cell membranes based on the Tweedy chelation theory. This mode of action allows the complexes to exert their antimicrobial effects,[33].

Table (4) The inhibition zones (mm) of anti-bacterial and anti-fungal activity for ligands and its metal complexes

Compounds / microorganisms	**Conc.**	**Fungus**	**Gram negative bacteria**		**Gram positive bacteria**	
		Candida albicans	Escherichia coli	Klebsiella sp.	Staphylococcus aureus	Staphylococcus epidermidis
L(5)	10^{-2}	24	24	20	25	26
	10^{-4}	18	20	24	19	24
CoL(6)	10^{-2}	20	23	10	20	24
	10^{-4}	17	21	10	18	13
CuL(7)	10^{-2}	21	26	24	27	27
	10^{-4}	26	23	21	25	24

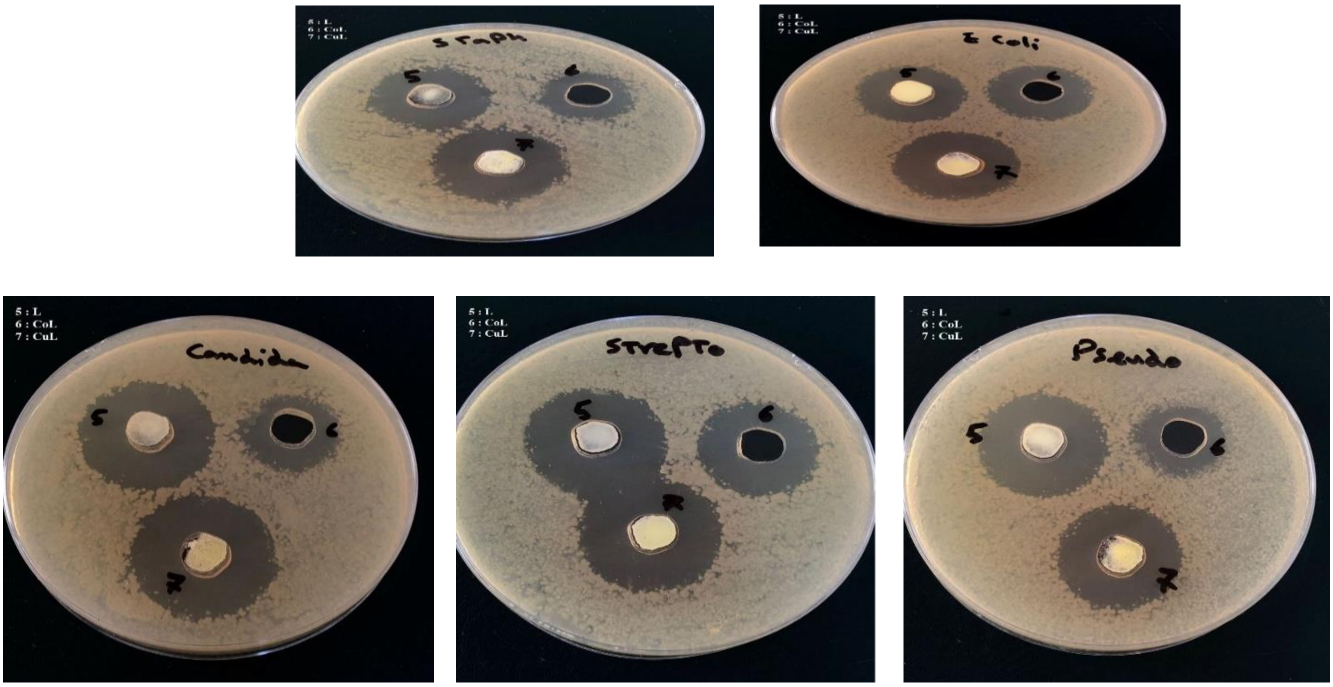


Figure (9) Inhibition zone of gram- positive and gram-negative bacteria with different concentration of L, CoL and CuL. Conc. (10^{-2})

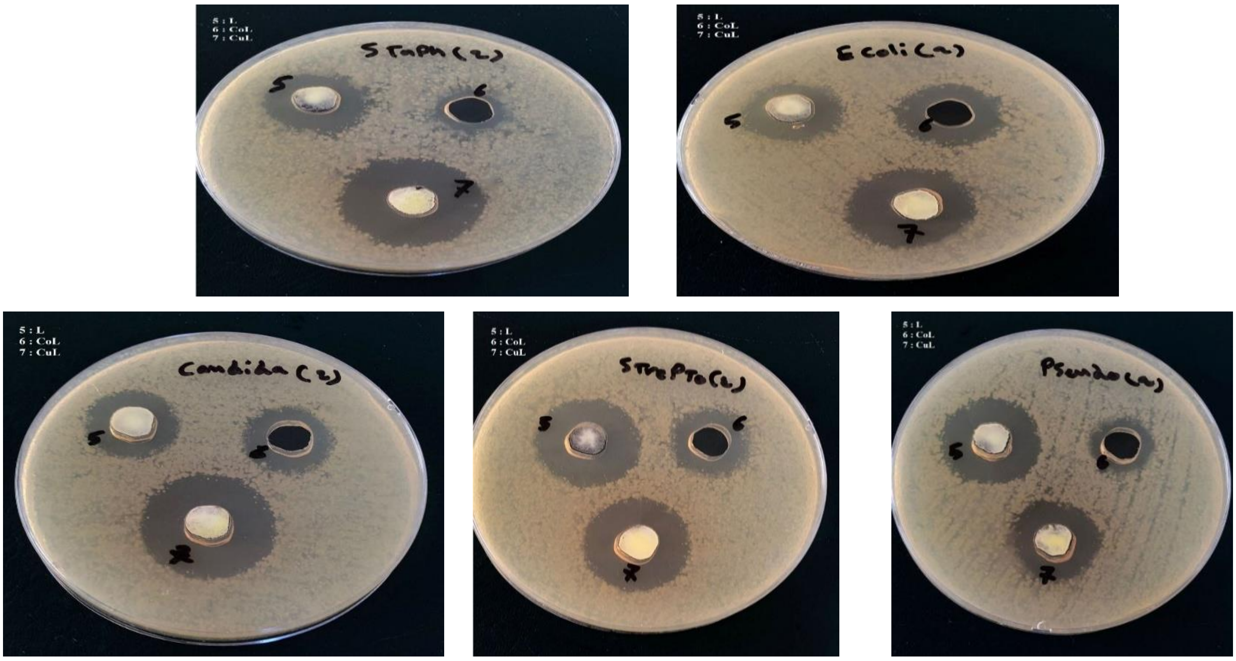


Figure (10) Inhibition zone of gram- positive and gram-negative bacteria with different concentration of L, CoL and CuL. Conc. (10^{-4})

3.6. Spectrophotometric (DPPH) assay

The antioxidant activities of some of the prepared complexes (CuL and ZnL) were listed in Table (5) and Figure (11) by measuring their abilities to donate hydrogen or scavenge DPPH radicals. The results also showed that the higher the concentration of the complex, the greater its antioxidant activity, as the maximum effectiveness of the complexes (75.670 for ZnL and 69.409 for CuL) versus 93.406 for ascorbic acid at 500 µg/mL, while the least antioxidant activity appeared at a concentration of 62.5 µg/mL (63.685 for ZnL, 65.831 for CuL, and 85.787). The antioxidant activity of CuL and ZnL can be explained by their possession of donor groups (NH2, NH, and SH), which can act as scavengers of free radicals and are able to resist oxidation. While the presence of electron-withdrawing groups, including the phenyl ring, and Br decreases antioxidant activity, [34].

Table 5: The activity of antioxidant of the prepared compounds

Compounds	**DPPH Assay**			
Con.	62.5 µg/mL	125 µg/mL	250 µg/mL	500 µg/mL
Sample CuL	65.831	66.726	67.084	69.409
Sample ZnL	63.685	67.084	74.239	75.670
Ascorbic acid	85.787	90.974	91.690	93.406

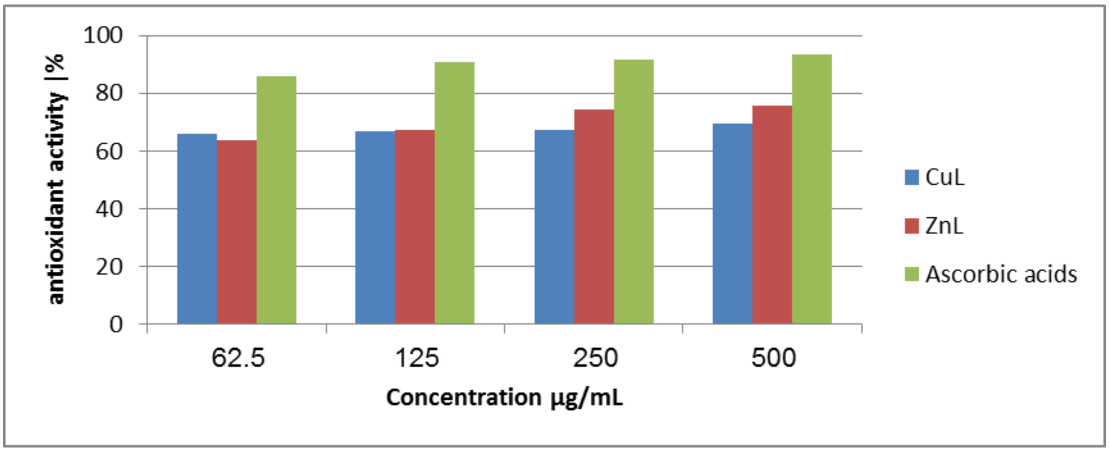


Figure (11) Antioxidant activity of some synthesized compounds

4. Conclusions:

According to the results obtained from elemental analyses, NMR,FT-IR, EIS-MS spectra and magnetic moments , the complexes of cobalt(II),nickel(II) and copper(II) with the new ligand, were octahedral in 1:1 mole ratio and chemical formula, $[ML(H_2O)_2Cl_2]$,L=(E)-4-((4-bromobenzylidene)amino)-5-

(pyridin-4-yl)-2,4-dihydro-3H-1,2,4-triazole-3-thione. However, the zinc(II) complex was adopted tetrahedral geoemtry in [$ZnLCl_2$] chemical formula. As well as the tautomerism of thioamide with thiol could be characterized on the basis of FT-IR spectra and H-NMR spectra which assign the presence of absorptions of acidic protons of –SH and absorption of C-13 NMR of C-S at chemical shifts at a round (175-185 ppm). The new ligand was formed up on heating under reflux with good yield as mentioned in the practical part. As well as the metal complexes of cobalt(II), nickel(II), copper(II) and zinc(II) were isolated in good yield up on direct reactions of their metal chlorides with the free Schiff base in hot ethanol. The analytical data and spectroscopic results of FT-IR,NMR and MS spectra revealed the agreement of empirical data with the observed data. The octahedral geometry around Co(II), Ni(II) and Cu(II) was investigated on the basis of UV-Visible spectra and magnetic moments measurements, Figure (12).

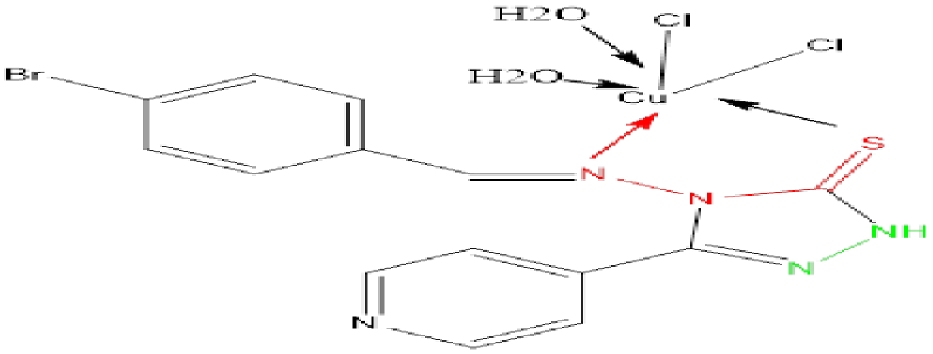


Figure 12. Octahedral geometry of Cu (II) complexes

In vitro assays revealed that CuL has the highest antibacterial and antifungal activity against pathogens. As well as ZnL, it has the highest antioxidant activity against the DPPH radical. These findings may aid in the development of new antioxidant, antifungal, and antibacterial compounds.

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تحضير، توصيف، ونشاط مضاد للأكسدة لبعض معقدات الفلزات مع 4-((4-بروموبنزيليدين)أمينو)-5-(بيريدين-4-يل) - 4 H -4,2,1- ترايازول-3-ثيول

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مستخلص البحث:

يصف هذا البحث تحضير والتوصيف الطيفي لمعقدات الكوبالت (II)، والنيكل (II)، والنحاس (II)، والزنك (II) مع الليكاند 4-((4-بروموبنزيليدين)أمينو)-5-(بيريدين-4-يل) - 4 H -4,2,1- ترايازول-3-ثيول (L) . تم تحضير الليكاند الجديد من خلال ثلاث خطوات متتالية: الاول تحضير ملح البوتاسيوم من الإيزونيازيد باستخدام محلول قلوي من ثاني كبريتيد الكربون. يتبعه إغلاق الحلقة لملح البوتاسيوم باستخدام كمية زائدة من هيدرات الهيدرازين. بالخطوة الاخيرة يتضمن تكثيف 4-أمينو-1,2,4-تريازول مع 4-بروموبنزالديهيد في حمض الأسيتيك الجليدي كمحفز، مما أدى إلى الحصول على كمية جيدة من قاعدة شيف الجديدة (L). تمت دراسة الخصائص الفيزيائية والطيفية لليكاند ومعقداته بشكل دقيق. كما تم توصيف المعقدات الجديدة باستخدام تقنيات تحليلية متعددة، منها: مطيافية الأشعة تحت الحمراء (FT-IR) و الأشعة فوق البنفسجية-المرئية (UV-Vis) و مطيافية الرنين النووي المغناطيسي للبروتون (^{1}H-NMR) والكربون (^{13}C-NMR) والتحليل العنصري (CHNS) و مطيافية الامتصاص الذري اللهبي (FAA) . كما تم تحديد بعض الخصائص الفيزيائية والكيميائية، مثل درجة الانصهار، القابلية المغناطيسية، والتوصيلية المولارية عند درجة حرارة الغرفة. أظهرت النتائج أن المعقدات C1 وC2 وC3 تتخذ بنية ثمانية السطوح بنسبة مولية (1:1) بين الفلز والليكاند، حيث يتصرف الليكاند كربيطة ثنائية السن ترتبط بأيون الفلز من خلال ذرة النيتروجين في مجموعة الأزوميثين وذرة الكبريت في مجموعة الثيون. بينما أظهرت معقدات الفلزات الثنائية التكافؤ بنية ثمانية السطوح للكوبالت (II)، والنيكل (II)، والنحاس (II)، في حين كان معقد الزنك (II) ذا بنية رباعية السطوح. علاوة على ذلك، تم فحص النشاط البيولوجي لمحاليل الليكند والمعقدات المعدنية (CoL and CuL) ضد بعض البكتيريا والفطريات .اضهرت النتائج ان كل من الليكند الحر ومعقد النحاس كانوا اكثر فعالية تثبيطية ضد البكتيريا والفطريات مقارنة بمعقد الكوبلت. يمكن أن توفر هذه النتائج منصة مهمة لتصميم مركبات جديدة ذات نشاط مضاد للبكتيريا ومضاد للفطريات . كما تضمنت هذه الدراسة دراسة النشاط المضاد للأكسدة للمعقدات المعدنية المحضرة (ZnL و CuL) باستخدام اختبار DPPH ضد حامض الأسكوربيك كعامل مرجعي مضاد للأكسدة. أظهرت النتائج أن جميع المعقدات المعدنية المحضرة لها نشاط مضاد للأكسدة اقل مقارنة بحمض الاسكوربيك. وكذلك وجد أن معقد الزنك (II) له أعلى نشاط مضاد للأكسدة مقارنة بمعقد النحاس (II). كما اضهرت الدراسة ان أعلى قدرة كسح لمعقد الزنك (II) ومعقد Cu II ، كانت 75.670% و69.409% على التوالي عند تركيز 500 ميكروغرام / مل .