



Preparation, Characterization and The Biological Activity Study of A New heterocyclic (Azo-Schiff base) Ligand and Their Complexation with {Co,Ni,Cu,Zn(II)}Ions



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A NEW tetra dentate Schiff base ligand has been synthesized from condensation of compound (1): [(4-(1-H-imidazol-2-ylidiazonyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one)] with compound (2) thio semicarbazide. The general formula of complexes are $[M(L)]Cl_2$ Where. M= Co(II), Ni(II) and Cu(II) Zn(II) are reported. The geometry structures of ligand and the complexes were determined through Fourier-transform infrared spectroscopy (FT-IR), Mass spectra, X-ray diffraction analysis, Ultra violet-Visible(UV-Vis), Proton nuclear magnetic resonance (1H NMR) spectral studies, magnetic moment measurement, elemental analysis, and molar conductance. These studies revealed square planar geometries for Ni(II) and Co(II) and Cu(II) complexes, except the Zn(II) complex was a tetrahedral geometry around the central metal ion. Complex formation studies via molar ratio and continuous variation methods were consisted to those found in the solid complexes with a ratio of (M:L) as (1:1). Stability constant of complexes were calculated by spectrophotometric methods. Hyper Chem-8 program has been used to predict geometries structures of compounds in gas phase. The heat of formation (ΔH_f) and binding energy (ΔE_b) at 298 K for the metal complexes were calculated by PM₃ method. Biological activity studies of the ligand and their metal complexes against several organisms, bacteria Gram positive G(+ve) *staphylococcus aureus* and bacteria Gram negative G(-ve) *Escherichia coli*, *klebsiella pneumoniae*, In addition to fungi like *Aspergillus Niger*, *Rhizoclonia bataicola* and *Aspergillus flavus*, are reported. Compounds exhibited the high activity on the growth of all types microorganisms in this study. This may be attributed to the impact of both the chelate effect of Schiff bases ligand and the role of the metal in these complexes.

Keywords: Tetra dentate, Ligand, Azo, Schiff base, Biological, Activity, Complex.

Introduction

A metal surrounded by a cluster of molecule that is used for preparation of complexes named as Schiff's bases, which are produced from condensation of primary amines with aldehydes or ketones[1]. Molecular recognition due to non-covalent interactions between two different molecules has become an important subject in areas of chemistry, biology and physiology. In particular, the selective binding via interactions such as hydrogen bonding and π - π aromatic stacking between the receptor and the neutral guest molecule has been known as the basis of

the main concept in molecular recognition[2]. Heterocyclic phenazone and their derivatives (4-amino antipyrine) are known to act as tri dentate or tetra dentate ligands when coordinated to metal ion. Schiff base of 4-amino antipyrine and their complexes are known for their variety of application[3,4] i.e. in the areas of catalysis clinical application and pharmacology [5-7]. Also the chemistry of antipyrine and their derivatives has been extensively investigated due to their physiological properties [8]. The azo compounds also exhibit their bacteriostatic and other biochemical activities, heterocyclic azo Schiff base and their complexes with transition metal

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ions are also of importance due to complexing, catalytically biological properties[9-10]. The transition metal complexes having oxygen and nitrogen donor Schiff bases possess unusual configuration, structural liability and are sensitive to the molecular environment. The aim of the present study is to synthesize and characterize Co (II), Ni (II), Cu (II) and Zn (II) metal complexes with newly synthesized Schiff base ligand derived from 4-aminoantipyrine, imidazole and thiosemicarbazide.

Experimental

Materials

All the chemicals were supplied by BHD and Fluka and used without further purification.

Measurements: The electro thermal melting point modern 9300 was used to measure the melting point of the ligand and their complexes. Elemental analyses were carried out by means of micro analytical unit of 1180 C. H. N elemental analyzer. Electronic spectra (in ethanol) were recorded on Shimadzu spectrophotometer double beam model 1700 Ultra violet-Visible(Uv-Vis) spectrophotometer, FTIR spectra were recorded in KBr medium on Fourier-transform infrared spectroscopy(FT-IR) Shimadzu spectrophotometer model 8400 in wave number range (4000-400) cm^{-1} . The Proton nuclear magnetic resonance ($^1\text{H-NMR}$) spectra were obtained in Di methyl Sulfoxide(DMSO) solution using (Bruker, Ultra Shield 3000 MKZ, Switzerland). Mass spectra using GC-Mass QP-2010 with energy 70 electron volt, X-ray diffraction were measured using Bestic Germany Aluminium anode model pertpro, wave length of X-ray beam(CUKA)1.54

Angstrom, Anode material-Cu, the voltage=40KV and current=30mA, Magnetic susceptibility measurements were carried out on a balance magnetic MSB-MKI using faraday method. The diamagnetic corrections were made by Pascal's constants. Molar conductivity measurements were determined in Di methyl form amide (DMF) by using an Alpha Digital conductivity meter Model 800 physical characterization of the ligand and their metal chelate complexes was listed in Table (1).

Preparation of the azo- Schiff base ligand:

Preparation of the azo ligand, Scheme(1)

A(2.03gm, 0.01mole) from 4-aminoantipyrine was dissolved in 3ml of conc. HCl and 50ml of water, which is cooled in ice bath. Then added 30ml of (0.7gm, 0.01mole) from Sodium nitrite solution to the above solution with constant stirring. Cooled solution(30ml) of 10% NaOH solution was added to (0.68gm, 0.01mole) imidazole drop wise to the resulting solution with stirring and the mixture was left for 3hr at 0°C . Red precipitate was filtered, recrystallized from hot ethanol and then dried in oven at 60°C for 8 hours., mp (299°C).

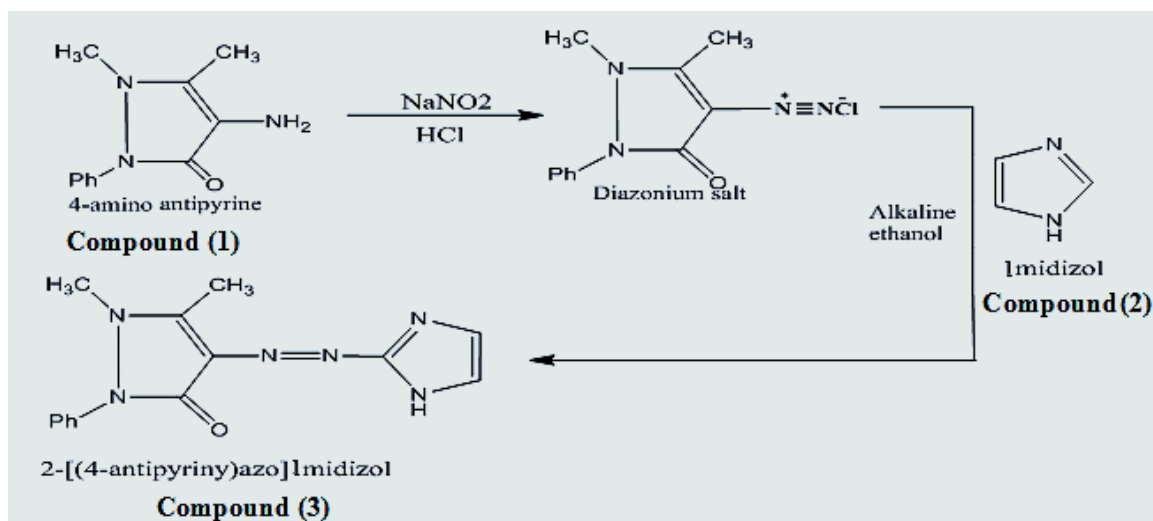
Preparation of The azo- Schiff Base Ligand, Scheme (2)

The new Schiff base ligand was prepared by condensation of compound (4): (4-((1H-imidazol-2-yl)diazenyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one) with compound (5): thiosemicarbazide (0.91gm, 0.02mole) in equimolar(1:1) mole ratio, in absolute alcohol. Few drops of glacial acetic acid were added to the mixture and refluxed for(25h), the product was recrystallized from ethanol and dried over anhydrous CaCl_2 Yield (80 %), mp (122°C).

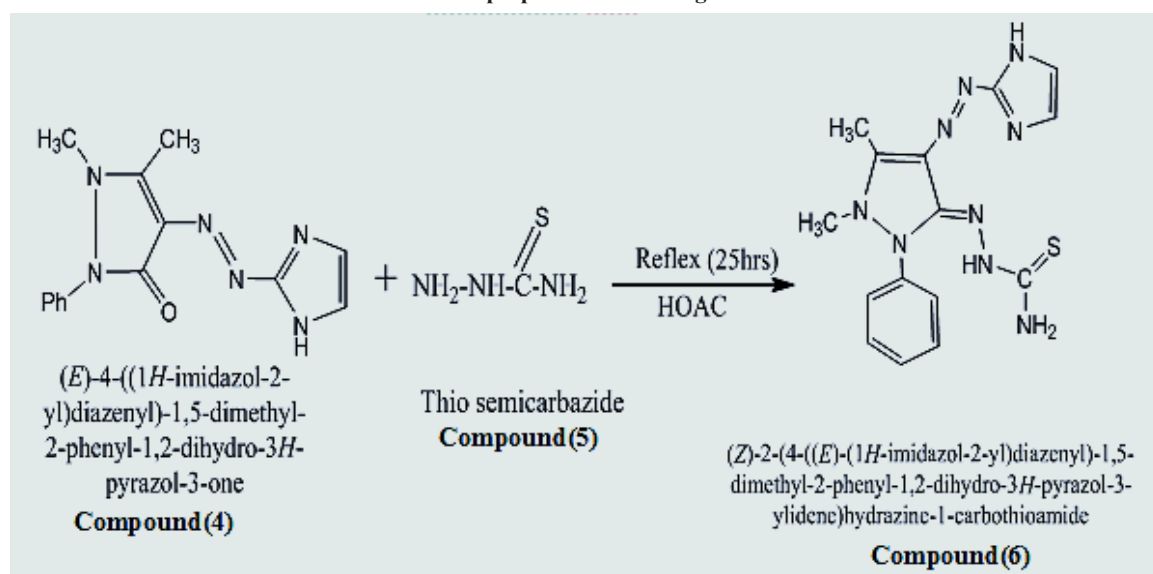
TABLE 1. Some physical data, analysis and molar conductance Data of the ligand and their complexes

Compound.	Color	yield	m.p $^\circ$	Formula	Found(Cal.) %				Ohm $^{-1}\text{cm}^2\text{mol}^{-1}$
					C	H	N	M	
Ligand	Red	80	122	$[\text{C}_{15}\text{H}_{17}\text{N}_9\text{S}]$	(50.70) 51.03	(4.78) 4.99	(35.49) 35.12	-----	-----
$\text{CoL}[\text{Cl}_2]$	Brown	69	180	$\text{Co}(\text{C}_{15}\text{H}_{17}\text{N}_9\text{S})[\text{Cl}_2]$	(37.12) 36.93	(3.50) 3.68	(25.98) 25.72	((12.14) 13.11	73
$\text{NiL}[\text{Cl}_2]$	Brown	60	110	$\text{Ni}(\text{C}_{15}\text{H}_{17}\text{N}_9\text{S})[\text{Cl}_2]$	(37.14) 36.88	(3.50) 3.21	(26.00) 25.72	((12.09) 11.89	79
$\text{CuL}[\text{Cl}_2]$	Violet	70	162	$\text{Cu}(\text{C}_{15}\text{H}_{17}\text{N}_9\text{S})[\text{Cl}_2]$	(36.77) 36.01	(3.47) 4.18	(25.74) 24.99	(12.97) 12.57	78
$\text{ZnL}[\text{Cl}_2]$	Colorless	75	145	$\text{Zn}(\text{C}_{15}\text{H}_{17}\text{N}_9\text{S})[\text{Cl}_2]$	(35.33) 34.10	(3.72) 3.23	(24.73) 25.16	(12.83) 12.42	71

Note: Cal=Calculated; m.p=melting point



Scheme 1. preparation of azo ligand .



Scheme 2 . Preparation Azo-Schiff base ligand.

Preparation of metal complexes

The metal complexes were prepared by mixing of 20ml ethanol solution of ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$, ZnCl_2) with the 20ml ethanol solution of Schiff base in (1:1) (metal: ligand) ratio. The resulting mixture was refluxed for 1h, then isolated after reduction of volume by evaporation. It was filtered off, washed with ethanol and dried under vacuum to yield complexes, all data are listed in Table(1)

Theoretical calculations

Electronic structure calculation provide useful estimate of the energetic properties of chemical systems including molecular structure. All theoretical calculations in this work were performed using the computational implemented

in the Hyperchime package 8.02. Program. The optimized structural parameters of Schiff base ligand were calculated by the semi-empirical calculation at PM3 method.

Determination of Antimicrobial Activity [10]

The purpose of the screening program is to provide antimicrobial efficiencies of the investigated compounds. The prepared compounds were tested against some Fungi and bacteria to provide the minimum inhibitory concentration (MIC) for each compound. The antimicrobial activities of the investigated compound were tested against the bacterial species *staphylococcus aureus*(+ve), *Escherichia coli*(-ve), *klebsiella pneumonic* (-ve), and fungal species *Aspergillus Niger*, *Rhizoctonia bataticola* and *Aspergillus*

flavus by the well diffusion method for preparation of plates and inoculation, 1.0 ml of inoculum were added to 50 ml of agar media (50°C) and mixed. The agar was poured into (120 mm) petri dishes and allowed to cool to room temperature. Wells (6mm in diameter) were cut in the agar plates using proper sterile tubes. Then, wells were filled up to the surface of agar with 0.1ml of the test compounds dissolved in ethanol. The plates were left, on leveled surface, incubated for 24 hours at 30°C for bacteria and 48h for fungi and the diameter of the inhibition zones were read. The results were compared with a similar run of standards of antibacterial and anti-fungal drugs. The MIC (as the lowest concentration of drug in the medium) that showed no microbial growth by visual observation of the complexes was determined by serial dilution technique.

Results and Discussion

All the complexes are stable in air and freely soluble in DMSO, DMF, sparingly soluble in methanol with ethanol. The metal complexes were characterized by elemental analysis, molar conductivities, IR, UV-Vis and ¹H NMR spectra, which gave agreement in calculated data with the experimental data. The value reveals that the metal to ligand ratio is (1:1) in Table (1). The magnetic susceptibilities of the complexes at room temperature were consistent with square planer geometry for Co(II), Ni(II) and Cu(II) expected the Zn(II) complex is tetrahedral and the higher conductivity values of the chelates support the electrolytic nature of the metal complexes.

Micro analysis

The elemental analysis data of the complexes as shown in table (1) the formation 1:1 [M:L] ratio it was found that the theoretical values are in good agreement with the found data. The purity of the

Schiff base ligand were tested by TLC technique and C, H and N elemental analysis.

Infrared Spectra

The IR provides valuable information regarding the nature of the functional group attached to the metal atom. The most important infrared spectral bands that provide conclusive structural evidence for the coordination of the ligand to the central metal ions are given in table 2. In principle, the ligand can exhibit thione-thiol tautomer's since it contains a thioamido -NH-C=S functional group. The ν (S-H) band at 2560 cm⁻¹ is absent in the IR spectrum of ligand but ν (N-H) band at 3260 cm⁻¹ and 3160 cm⁻¹ are present, indicating that in the solid state, the ligand remains as the thione tautomer [11-12]. The infrared spectrum of the ligand indicated the presence of primary amine ν (NH₂) group due to appearance of absorption of frequency at 3383 cm⁻¹ [13].

A strong absorption band at 1645 cm⁻¹ due to ν (C=N) present in the pyrazole and imidazole ring in the free ligand has shifted to lower side by 15-19 cm⁻¹ in all four complexes, this indicates the involvement of (C=N) azomethane group in coordination [14]. The bands near (1170, 806) cm⁻¹ in the free Schiff base ligand may be assigned to ν (NH-C=S) and ν (C=S). This has shifted to lower wave number in complexes indicates that sulphur is coordinating to the metal ion [15]. Also, the ligand exhibits a band at (1500, 1425) cm⁻¹ assignable to (N=N) group and shifted to lower frequency in metal complexes (10-23 nm). This indicates the participation of the nitrogen atom of azo group in coordination [16]. The far IR spectra of the metal chelates show some new bands at 520 ± 10 cm⁻¹ and 443 ± 10 cm⁻¹ have been assigned to ν (M-N) and ν (M-S) modes respectively [17]. Representative example for their spectra is given in Fig. (1).

TABLE 2. Some characteristic IR absorption bands of the ligand and its complexes in cm⁻¹.

Compound	ν (C=N)	ν (NH-C=S)	(C=S)	ν (N=N)	ν (M-N)	ν (M-S)
Ligand	1645	1170	806	1500,1425	-----	-----
CoL]Cl ₂]	1631	1154	770	1492,1400	515	445
NiL]Cl ₂]	1630	1149	761	1490,1403	530	432
CuL]Cl ₂]	1629	1147	767	1490,1402	515	453
ZnL]Cl ₂]	1626	1145	760	1491,1406	520	443

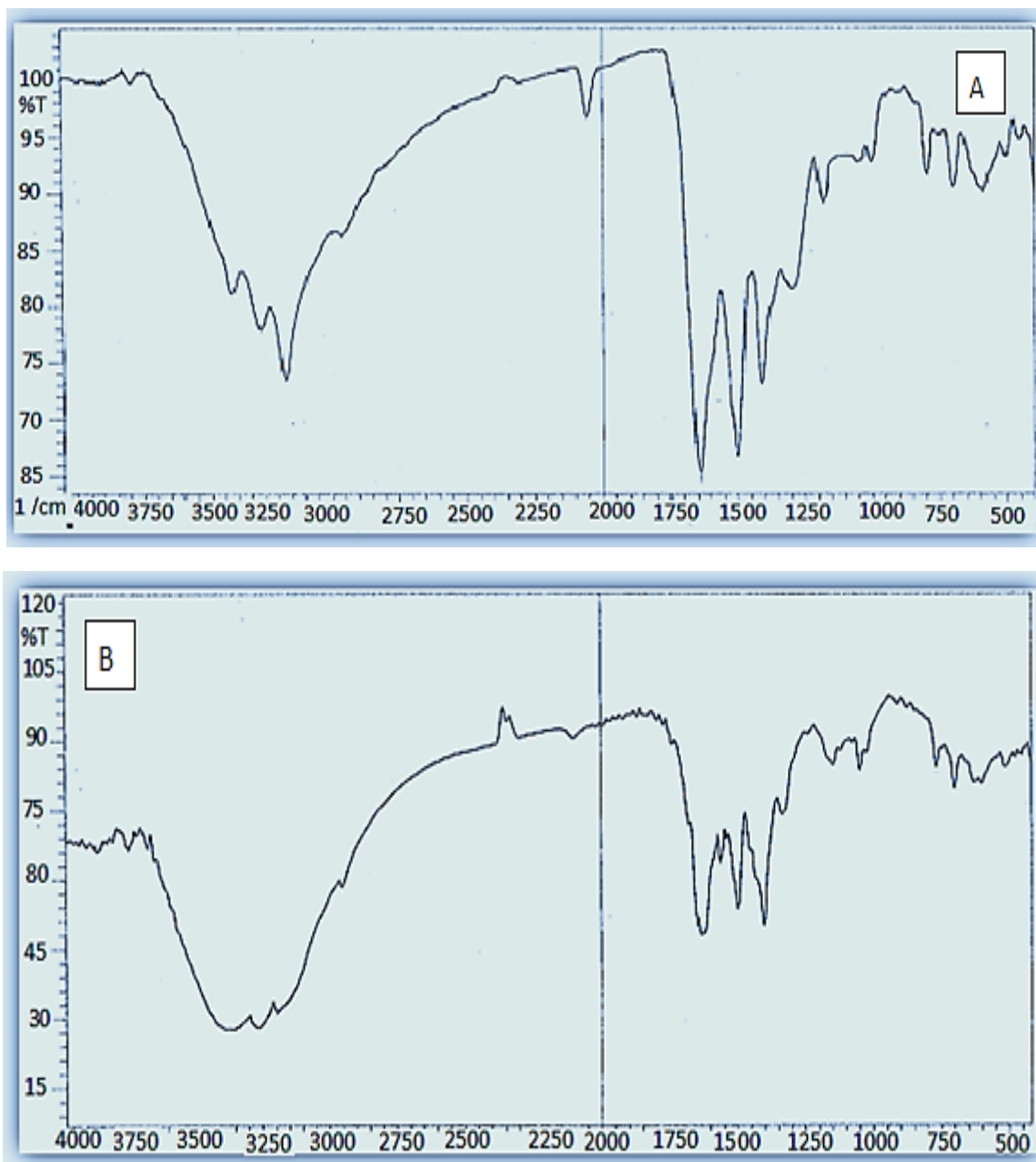


Fig.1. IR spectra of :(a) the ligand & (b)[CuL]Cl₂.

Mass spectra

The mass spectrum of synthesized ligand is recorded at room temperature. The obtained molecular ion peaks confirm the proposed formulae for the synthesized compound. The mass spectrum of ligand showed the molecular ion peak at m/z 355 that confirms the proposed formulae for the synthesized compound (which are in good agreement with their formula as expressed from micro analytical data. The mass spectral data fragmentation of the ligand was shown in (Fig.2).

X-ray diffraction Analysis

The X-ray diffraction, XRD, patterns of the ligand and its metal complex [CuL]Cl₂ are in figure (5). The XRD Patterns of the ligand and Cu(II) complex has sharp diffraction peaks at around $2\theta = 30-80$. This indicates that ligand with complex are a mixture of crystalline and amorphous phases. Calculate d -spacing or ' d ' values of reflections were obtained by using Bragg's equation [$n\lambda = 2d \sin \theta$]. The average size of the particle and their size distribution were evaluated by the Scherrer equation: $D = K \lambda / \beta \cos \theta$, The values in Table.(3).

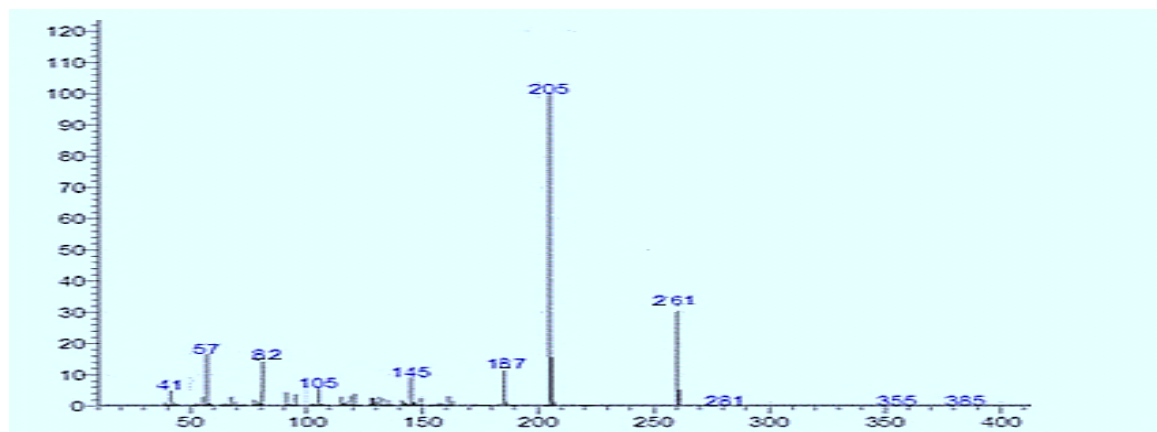


Fig.2. Mass spectra of the ligand Azo Schiff Base .

TABLE 3. Inter planar distances, 2θ value and FWHM relative intensity for Ligand and complex .

Compound	2θ Obs. (degree)	d calc. spacing(\AA°)	FWHM [$^\circ 2\theta$]
Ligand=L	30.693	2.910	0.132
	38.091	2.360	0.143
	51.840	1.762	0.114
	56.697	1.622	0.102
	38.016	2.365	0.219
	51.765	1.764	0.213
	30.170	2.959	0.297
Cu(II)-complex	37.792	2.378	0.241
	51.615	1.769	0.176
	56.174	1.636	0.127
	56.547	1.626	0.218
	74.630	1.270	0.101

Electronic Spectra and magnetic moments

The electronic absorption spectra of ligand and their metal complexes were recorded at 300K using Suitable the solvent absorption region assignment of the absorption bands and the proposed geometry of the complexes are given in Table (4). The electronic spectral data of the ligand and metal complexes in ethanol field around the metal ion has been deduced from the electronic spectra. The electronic absorption spectrum of the ligand shows three bands at 302 nanometer (nm) (33112cm^{-1}), $382\text{nm}(26178\text{cm}^{-1})$ and $440\text{nm}(22727\text{cm}^{-1})$ which assigned to $\pi-\pi^*$ and $n-\pi^*$ respectively.

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Cobalt (II) Complex

The spectrum of the Co(II) complex shows three bands at, $322\text{nm}(31055\text{cm}^{-1})$, $374\text{nm}(26737\text{cm}^{-1})$ and $638\text{nm}(15673\text{cm}^{-1})$ there are assigned to charge transfer and ${}^1A_{1g} \rightarrow {}^1B_{1g}$ respectively[18]. The magnetic moment value of this complex is (3.52)B.M. Thus the square planar geometry has been suggested for this Co(II) complex[19].

Nickel (II) Complex

The electronic spectrum of Ni(II) complex shows three bands at $274\text{nm}(36496\text{cm}^{-1})$, $626\text{nm}(15974\text{cm}^{-1})$ and $762\text{nm}(13123\text{cm}^{-1})$ these are assignable to charge transfer and ${}^1A_{1g} \rightarrow {}^1A_{2g}$ and

$^1A_{1g} \rightarrow ^1B_{1g}$ respectively [20]. This complex is diamagnetic in nature. Therefore a square planar geometry has been suggested [21].

Copper (II) Complex

The electronic spectrum of the Cu(II) complex exhibit bands at 266nm (37593cm^{-1}), 318nm (31446cm^{-1}) and 638nm (15673cm^{-1}) which have been assigned to charge transfer and $^2B_{1g} \rightarrow ^2A_{1g}$ transitions respectively [22]. The magnetic moment of the complex is (1.82 B.M). The reforea square planar stereochemistry has been suggested [23].

Zinc(II) Complex

No transitions were observed in the visible region for Zn(II) complex consistent with the d^{10} configuration of the Zn(II) ion. This complex is also found to be diamagnetic [24] As expected for d^{10} configuration. Fig. (4) shows the spectra of ligand and copper complex.

$^1\text{H-NMR}$ Spectra

The spectrum of newly synthesized ligand gave a satisfactory data and the molecular structure was assigned on the basic of ^1H NMR chemical shift by using DMSO with tetra methyl saline as an internal reference. The $^1\text{H-NMR}$ spectrum of the ligand showed clear signals involved singlet at δ (2.5) (part per million) ppm belong to the proton of solvent (DMSO) and multiples signals at δ (7.3-7.9) ppm which were assigned to aromatic protons of phenyl ring of antipyrine. Multiple signals at δ (8.2-8.3) ppm which belong to amine

groups. Singlet at δ (3.3) ppm belong to the proton of methyl (N-CH_3). Singlet at δ (11.2) ppm belong to the proton of ($-\text{C-NH}$), Singlet at δ (12.1) ppm belong to the proton of $-\text{C-NH}$ imidazole ring, as shown in Fig.(3).

Conductivity Measurement

The molar conductance of the synthesized ligand complexes were measured using 10^{-3}M DMSO solvent at room temperature. The complexes (Co(II), Ni(II) Cu(II) and Zn(II) are 1 : 2 electrolytes in nature and may be formulated $[\text{ML}]\text{Cl}_2$, implying the non-coordination of chloride anion to the central metal ion. All chelate complexes prepared in this work showed values ranged between (71-79) $\text{S.mol}^{-1}.\text{cm}^2$, these values indicating that higher conductivity of the complexes [25-26]. According to these results the structural formulas of these ligand and complexes may be proposed in Fig.(6).

Calculation of the Metal Complexes Stability Constant

Stability constant of complexes are determined by measuring the absorbance of mixture solution of both metal and ligand, at fixed wave length λ_{max} . The degree of formation of the complexes are calculated based on the relationship $\beta = (1-\alpha)/(\alpha^2c)$ for 1:1 metal complexes and $\alpha = A_m - A_s/A_m$. Where A_m as are the absorbance of the fully and partially formed chelate complexes respectively. The calculated ($\log \beta$) values of these complexes are listed in Table (5).

TABLE 4. Electronic absorption spectral and magnetic susceptibility data of the ligand and the complexes .

Comp.	Solvent	Absorption (nm, cm^{-1})	Band assign- ment	Geometry	Mef.B.M
Ligand	EtOH	(302nm(33112cm^{-1}) (382nm(26178cm^{-1}) (440nm(22727cm^{-1})	n	—	—
CoL]Cl ₂]	EtOH	(322nm(31055cm^{-1}) (374nm(26737cm^{-1}) (638nm(15673cm^{-1})	I NCT INCT $^1A_{1g} \rightarrow ^1B_{1g}$	Square planar	3.52
NiL]Cl ₂]	EtOH	(nm(36496cm^{-1}) 274 (626nm(15974cm^{-1}) (762nm(13123cm^{-1})	I NCT $^1A_{1g} \rightarrow ^1A_{2g}$ $^1A_{1g} \rightarrow ^1B_{1g}$	Square planar	Dia
CuL]Cl ₂]	EtOH	(266nm(37593cm^{-1}) (318nm(31446cm^{-1}) (634nm(15673cm^{-1})	INCT INCT $^2B_{1g} \rightarrow ^2A_{1g}$	Square planar	1.82
ZnL]Cl ₂]	EtOH	(372nm(26881cm^{-1})	I NCT	Tetrahdral	Dia

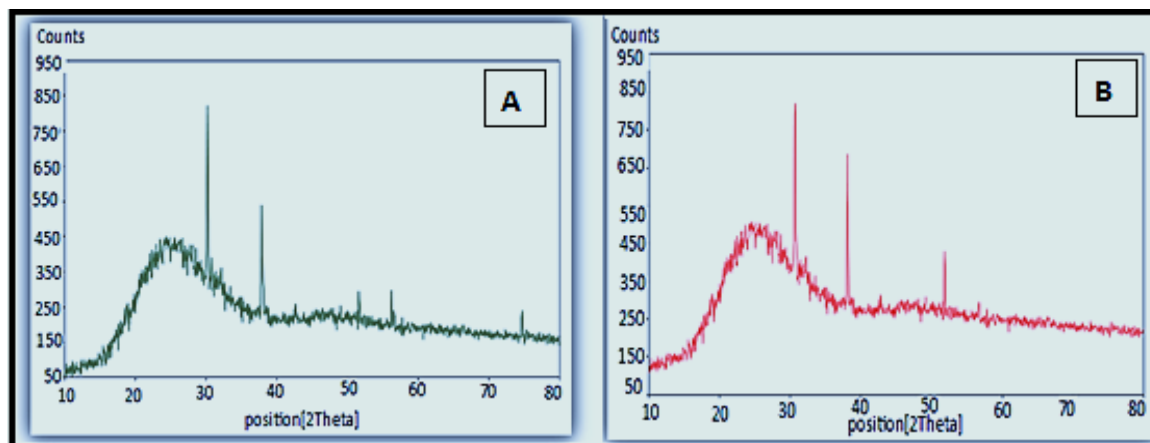


Fig.3 . X-ray diffraction patterns for (A): Ligand,(B): Cu(II) .

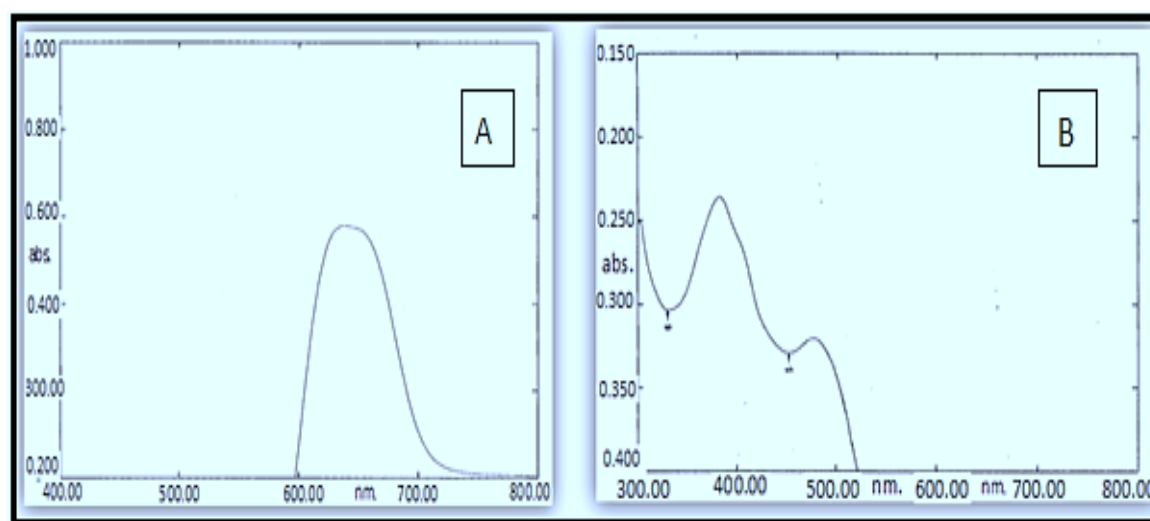


Fig. 4. Electronic spectrum of: (a) the ligand & (b)[CuL]Cl₂ .

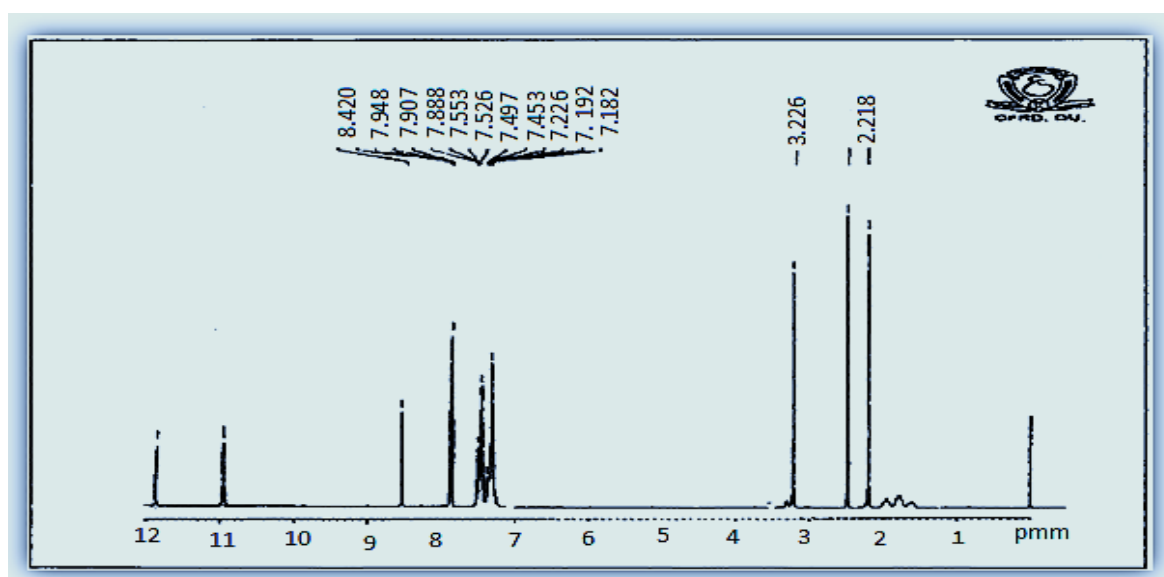


Fig.5 . ¹H NMR spectrum of the ligand .

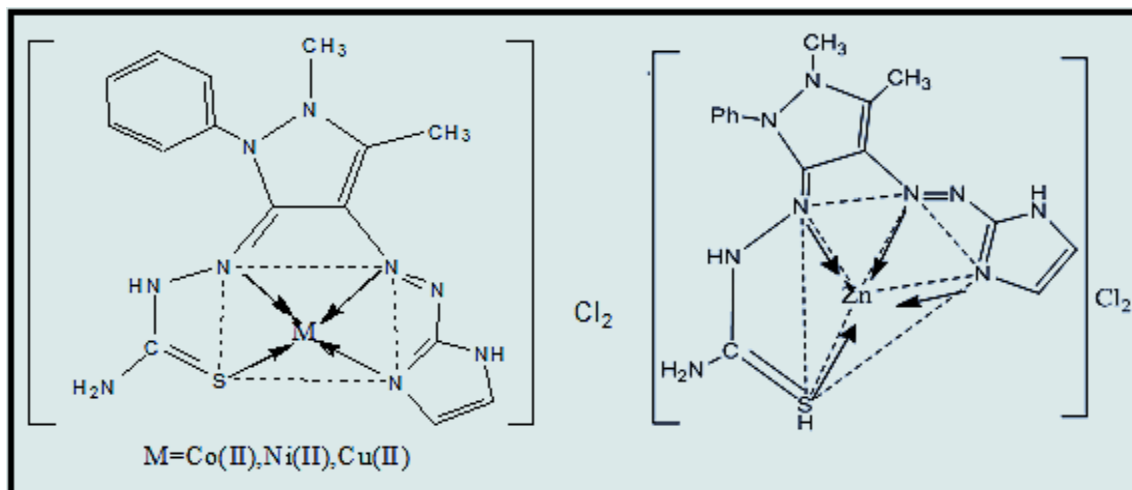


Fig.6. The proposed structural formula of the metal chelate complexes .

TABLE 5. Some energetic properties of Schiff base complexes in units of (k Cal/mol) .

Compound	Total energy	Binding energy	Electronic energy	Zero point energy	Heat of formation	Log β
Ni complex	-108620.59	-4278.52	-839084.14	204.62	356.76	6.6233
Co complex	-102207.89	-4499.45	-842608.89	210.34	245.41	6.5564
Zn complex	-71047.54	-4124.35	-814671.19	182.77	106.25	6.4592
Cu complex	-112953.71	-4598.308	-885157.97	200.17	119.079	6.9182

Note: KCal=Kilo Calories

Optimized Geometries Energy for Schiff base

The result of semi-empirical PM3 for structure optimization are shown in figure7. This figure illustrates the geometry of molecule in the balls, cylinders model, stick with density charges model and electrostatic potential model. Also surface of the electrostatic potential is useful for finding sites of reaction in a molecule, the green colors indicate to positive ESP regions and the red colors indicate to negative ESP regions[27]. The optimized total energies and some semi-empirical energetic properties are given in table 5. The more stable geometry of a molecule has a minimal total energy[28]. From PM3 calculation, it is obtained that the smallest value of total energy to complex Cu(II) which is mean the Schiff base complex Cu(II) more stable than other azo- Schiff base complexes, these resulting good agreement with experiment result[29].

Antimicrobial Activity

The result showed that most of the complexes have more toxicity against the bacterial from the

fungi species. Also exhibited the complexes toxicity against the bacterial and fungi more form ligand. Then the free ligand such increased activity of the metal chelates can be explained on the basis of chelation theory[30]. On chelation, the polarity of the metal ion will be reduced to a greater extent due to the overlap of the ligand orbital and partial sharing of the positive charge of the metal ion with donor groups. Further, it increases the delocalization of the complexes into lipid membranes and blocking of the metal Binding sites in the enzymes of microorganisms. These complexes also disturb the respiration process of the cell and thus block the synthesis of proteins, which restricts further growth of the organism[31]. Furthermore, the mode of action of compounds may involve the (C=N), (N=N) and (NH-C=S) groups with active centers of cell constituents resulting in the inter ferrous with normal cell process. The data of antimicrobial activates of the prepared ligand and it's complexes are given in (Table 6 and 7).

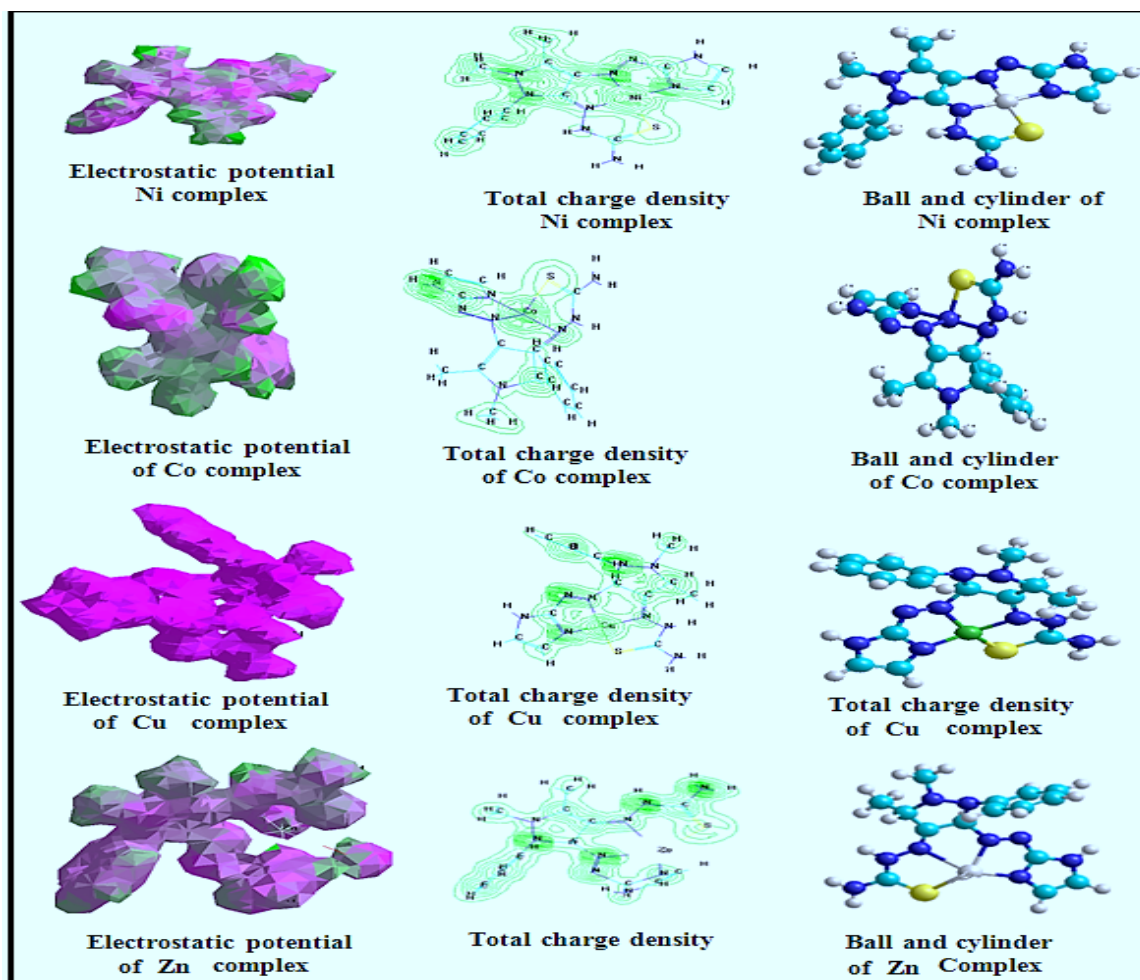


Fig.7. Energetic properties of Schiff base complex calculated at PM3 calculation method.

TABLE 6. (MIC) of the ligand free and complexes against growth of fungi (Mg/ml).

Compound	<i>A. niger</i>	<i>A. flavus</i>	<i>R. bataicola</i>
Ligand	66	70	75
NiL]Cl ₂]]	42	45	36
CoL]Cl ₂]]	48	40	46
CuL]Cl ₂]]	44	38	42
ZnL]Cl ₂]]	42	38	38
Nystatin	15	18	10

TABLE 7. (MIC)of the ligand free and complexes against growth of bacteria (Mg/ml).

Compound	<i>E. coli</i>	<i>K. pneumoniae</i>	<i>S. aureus</i>
Ligand	55	50	52
CoL]cl ₂]]	30	38	44
NiL]cl ₂]]	34	44	56
CuL]cl ₂]]	26	32	20
ZnL]Cl ₂]]	32	30	20
Ampicillin	8	20	20
Penicillin	10	10	6

Conclusion

In this paper, we have explored the synthesis and coordination chemistry of some complexes obtained from the reaction of the tetra dentate ligand with some metal ions. The isolated products were characterization by available techniques. The proposed geometry of the Zn(II) complex is tetrahedral but the Co(II), Ni(II) and Cu(II) complex are a square-planar. Complexes formation study via molar ratio has been investigated and results were consistent to those found in the solid complexes with a ratio of (M:L) as (1:1). Hyper Chem-8 program has been used to predict structural geometries of compounds in gas phase. The heat of formation (ΔH_f) and binding energy (ΔE_b) at 298 K for the metal complexes was calculated by PM₃ method, and Biological activity studies of the ligand and their metal complexes against the bacterial species *staphylococcus aureus*, *Escherichia coli*, *klebsiella pneumoniae*, and fungal species *Aspergillus niger*, *Rhizoctonia bataticola* and *Aspergillus flavus* are reported. Compounds exhibited the high activity on the growth of all types Microorganisms in this study. According to these results the structural formulas of these complexes may be proposed in Fig.(6).

Conflict of Interests

The authors declare that no competing interest exists.

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