

Synthesis, Characterization and Antimicrobial Activity of Some Transition Complexes with New Schiff Base Derived from Saccharine

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Author's contribution

The sole author designed, analyzed and interpreted and prepared the manuscript.

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ABSTRACT

A new Schiff base Na^+L^- was prepared by condensation of sodium (3E)-3-hydrazinylidene-3H-1,2-benzoxazole-2-ide-1,1-dioxide with 7-methyl-3-oxo-3,4-dihydroquinoxaline-2-carbaldehyde. The transition metal complexes of Cobalt (II), Nickel (II), Copper (II), Zinc (II) and Cadmium(II) with [L] Schiff base were prepared and fully Characterization on the basis of elemental analysis, ¹HMR, Mass spectroscopy, FTIR and electronic spectra, as well as the molar conductivity and magnetic moment measurements were carried out to adopt the Octahedral geometry of $[\text{ML X}_2\text{H}_2\text{O}]$, M= Co(II), Ni(II), Cu(II), X=NO₃⁻ whereas the geometry of Zn(II) and Cd(II) complexes $[\text{MLX}]$, X= Cl⁻ show tetrahedral geometry. The antimicrobial activity of the free Schiff base Na^+L^- and its metal complexes were screened against two gram positive and two gram negative bacterial *Escherichia coli* and *Staphylococcus aureus*. It is obtained that the zinc (II) and Cd(II) complexes exhibited the highest inhibition zone in compared with the free ligand.

Keywords: Quinoxaline schiff bases; transition metal complexes of saccharine; transition metal complexes; quinoxaline-2-carboxaldehyde.

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1. INTRODUCTION

Many biologically important Schiff bases derived from pyrazine, saccharine and quinoxaline-2,3-dione have been reported possessing antibacterial, [1,2] antifungal, [3-5] and antimicrobial [6,7]. Quinoxaline capable of providing sulfur and nitrogen donors has been incorporated at the 2 and 6 position of phenolate ring to construct bio compartmental ligands. The mode of attachment is different in two ligands in order to provide different size and flexibility for the bio compartmental of the type donor S_2N_2O cavity. Transition metal (II) chlorides are employed for the construction of binuclear complexes. The structure as well as electronic, magnetic, and polar graphic studies of the prepared complexes is studied. Several transition metal binuclear complexes with a wide variety of coordination spheres exist [8,9]. Aseel [10] presented new study of novel Schiff bases derived from N-substituted saccharine then screened their biological activity against some micro-organisms. The first report on antimalarial activity related with quinoxaline and phthalazine systems was reported [10]. Taghreed al-Noor et al revealed the significance of Mn(II), Co(II), Ni(II), Fe(II), Zn(II) and Cd(II) complexes with mixed ligands of saccharine and L-histidine [11]. The hypoxic selective cytotoxicity towards V79 cells and the superoxide dismutase-like activity of the complexes were determined and related to physicochemical properties of the compounds [12]. The transition metal complexes derived from Schiff bases of quinoxaline-2,3-dione have reported by Afnan E [13], who investigated the template synthesis of quinoxaline with 4-methyl-1,2 phenylenediamine. Mahmoud N [14,15] have continued in investigation the structures of transition metal complexes with assembly Schiff bases of quinoxaline-2,3-dione with 2,6-diamino pyridine. However, the recent studied approved the biological activity of Schiff bases catalyzed with incorporation heterocyclic moieties like pyrazine and saccharine due to presence of functional groups like $-S=O,C=N-$ and $-C=S$ [15,16]. It has been suggested that the azomethine linkage might be responsible for the biological activities displayed by Schiff bases [17]. Testing of geno toxicity is a mandatory and preliminary step in the safety assessments for the newly synthesized Schiff bases of saccharine including pharmaceuticals, food additives, and industrial substances [18]. The bacterial Ames test, developed in recent years, is a widely used screening test for the possible genotoxic effects

of chemical compounds [19]. The recent study investigation the syntheses, characterization, and biological activity of new Schiff base of saccharine quinoxaline moiety with their complexes of Co(II), Ni(II), Cu(II), Zn(II) and Cd(II).

2. EXPERIMENTAL

2.1 Reagents and Apparatus

Elemental microanalysis (C.H.N) was performed on, a – Eurovector E A 3000 A, Al al -Bayt University (Jordan). IR spectra were recorded on a (SHIMADZU) FTIR-8400S spectrophotometer. Solid samples were run at Al-Mustansiriya University. The 1H -NMR was taken with ultra-shield Bruker 300-MHz, (Jordan). The electronic spectra of the ligands and its complexes in various solvents (0.001 M) were recorded on a Shimadzu UV-Vis spectrophotometer 1650 having wavelength range 200-900 nm. The molar conductance of complexes was measured on Hana conductivity meter in DMF. The metal contents of the complexes were determined by Atomic Absorption measurements were performed by using the instrument Analytik Jena / A Spect LS /FL 1.3.0.0, A bnSina Center, Ministry of Industry. Magnetic moment for a prepared complexes in the solid state at room temperature was measured according to Faraday's method using: Auto Magnetic susceptibility Balance Sherwood Scientific. AL-Mustansiriyah University. The chloride content for complexes was determined by Mohr's method. Mass spectra were performed using the instrument: GC MS –QP 2010 VLTRA, AL-Mustansiriyah University. Purity of products was detected using TLC techniques using a mixture of chloroforms: methanol (4:1 v/v), and ethyl acetate: methanol (3:2 v/v), and Iodine chamber for spot location. Biological activities of some selected samples were performed by agar diffusion methods, Ministry of Science and Technology. The metal nitrates $Co(NO_3)_2 \cdot 6H_2O$, $Ni(NO_3)_2 \cdot 6H_2O$, $Cu(NO_3)_2 \cdot 3H_2O$ and metal chloride $ZnCl_2$, and $CdCl_2 \cdot 2H_2O$, were provided from Sigma-Aldrich company(UAE). The Sodium pyruvate, 5-methyl,1,2-phenylenediamine and solvents were supplied from Fluka company in 99% purity. All other chemicals used were of annular grade.

2.1.1 Calculation method

The quantum chemical calculations were made with using Hyper Chem-8 program [20].

2.2 Synthesis of 7-methyl-3-Oxo-3,4-dihydroquinoxaline-2-carbaldehyde[A]

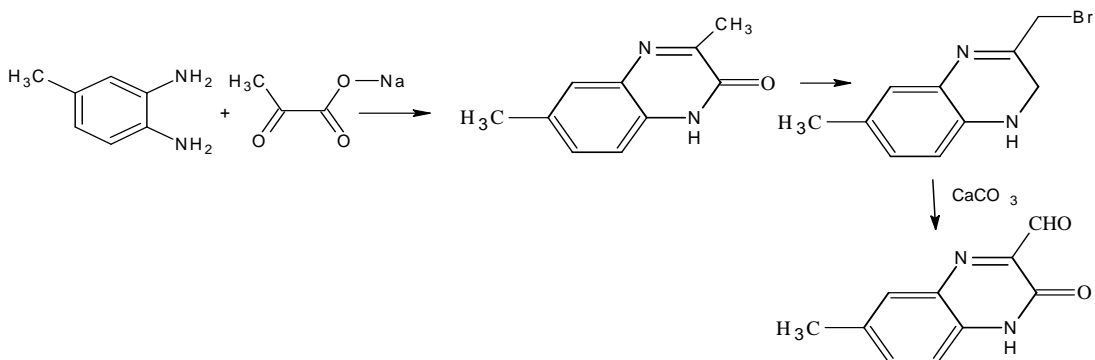
The 3, 7-dimethyl-quinoxaline-2-carboxaldehyde was prepared according to the modification published in literature [12,21] Scheme 1.

Color: orange
Yield: 80%.
M.P.: 168-170°C.

FT-IR (KBr, ν , cm^{-1}): 3300-3100(m,NH), (NH) (quinoxalineamido), 1734, (C=O) (Lactam), 1680 (-C=O-) (Amide pyrazine), 1320(-C-N) (Pyrazine ring). (3020 (m- C-H-Ar), (2980m-C-H-CH₃ aliphatic)

UV/Vis (Méthanol, λ_{max} , nm, (ϵ): 333 ($\epsilon_{\text{max}}=12333 \text{ molar}^{-1}\text{cm}^{-1}$), 244 ($\epsilon_{\text{max}}=1780 \text{ molar}^{-1}\text{cm}^{-1}$).

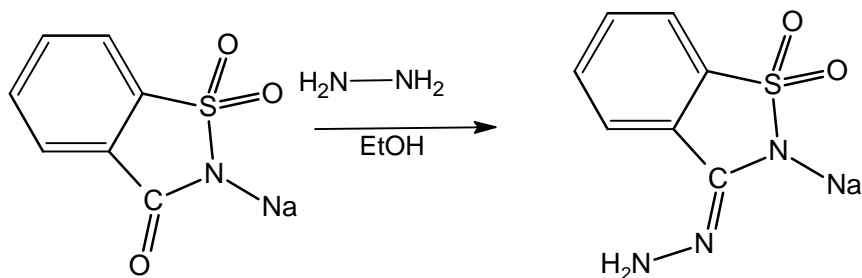
Anal.calcd. for C₁₀H₈N₂O₂: C, 63.82; H, 4.28; N, 14.89. Found: C, 62.67; H, 4.99; N, 14.97.



Scheme 1. Synthesis of precursor [A]

2.3 Preparation of the Compound [sodium (3E)-3-hydrazinylidene-3H-1,2-benzisothiazol-2-ide-1,1-dioxide] [B]

The derivative of sodium salt of saccharine was prepared according method modified in literature [17] Scheme 2.



Scheme 2. Synthesis of sodium(3E)-3-hydrazinylidene-3H-1,2-benzisothiazol-2-ide-1,1-dioxide] [B]

2.4 Synthesis of sodium (3E)-3-((2E)-[(3-hydroxy-6-methyl-3, 4,6,8a-tetrahydroquinoxalin-2-yl)methylidene]hydrazinylidene) -3H-1,2-benziothiazol-2-ide1,1-dioxide

A (0.52 g) of [B] derivative in (50 ml.) ethanol was added gradually to (0.5 g) of 7 methyl-3-oxo-3,4-dihydroquinoxaline-2-carbaldehyde. The reaction mixture was refluxed for 5 hours on water bath and the pale yellow solid separated was filtered, washed several times with ethanol and dried in oven, Scheme 3.

Color: Dark beige

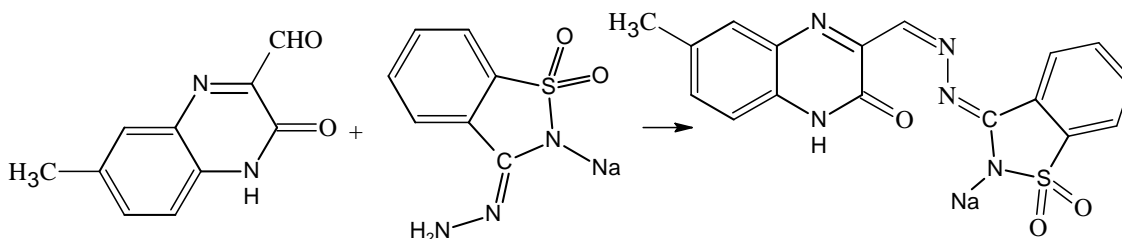
Yield: 80%.

M.P.: 149-151°C.

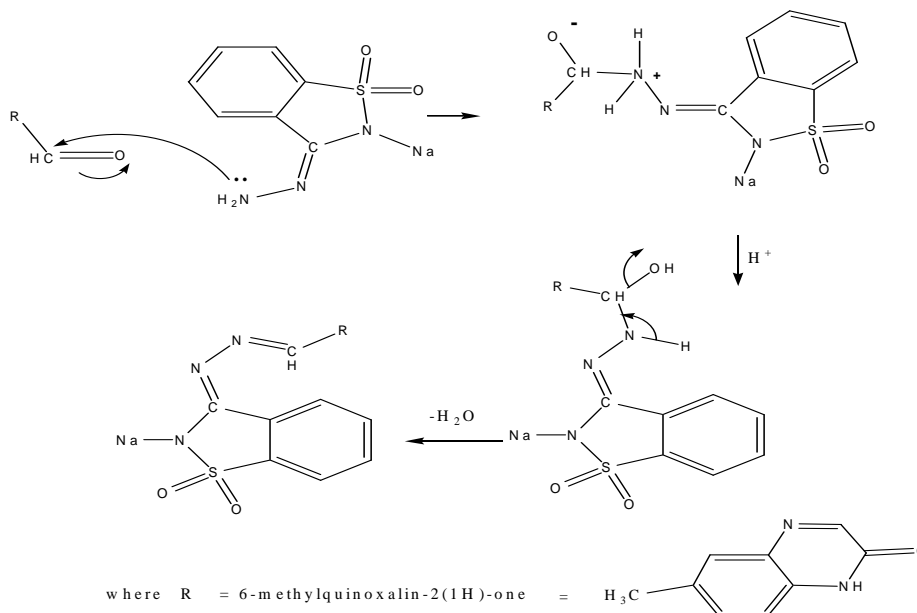
FT-IR (KBr, ν , cm^{-1}): 3562(br,H,OH), 2874-2614(m, C-H,Aliphatic-CH₃),1641(C=O pyrazine ring), 1622(C=N) (NH) (Amide and lactam),1680 (C=O) (Amide), 1610 (C=N) (Imine of pyrazine ring), 2987 (C-H) (Aliphatic-CH₃).

¹H NMR (300 MHz, DMSO-*d*₆, δ , ppm): 3.50 (s, 3H, CH₃), 6.21 (s, 1H, Ar-H), 6.78 (s, 1H, Ar-H) 7.89 (s, 1H, HN), 8.10 (s, 1H, HN), 10.2 (s, 1H, NH),

¹³C NMR (300 MHz, DMSO-*d*₆, δ , ppm): 155.2 (C, C=S thioamide), 131.91 (C,Amide-C=O), 128.9(C, C=N-Imine), 127.7(C,C-N- Pyrazine), 126.7 (C, -C-N-Pyrazine), 123.90 (C,C=C-Ar), 122.04 (C, C=C-Ar), 115.61 (9C, C-Ar), 110.79 (C=C-Ar),51.4 (C, CH₃), 25.2 (C,CH₃).



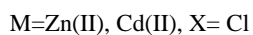
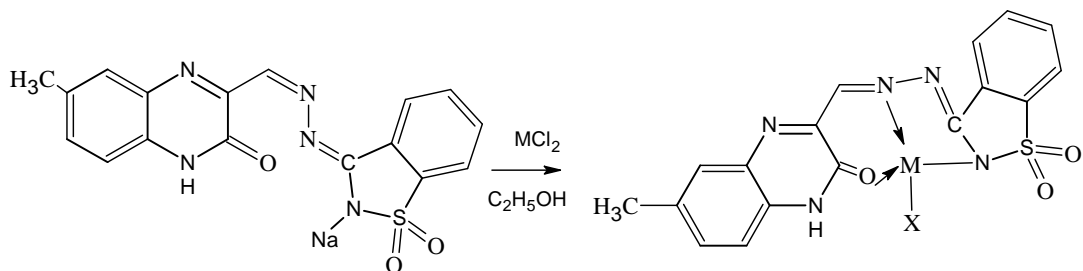
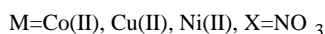
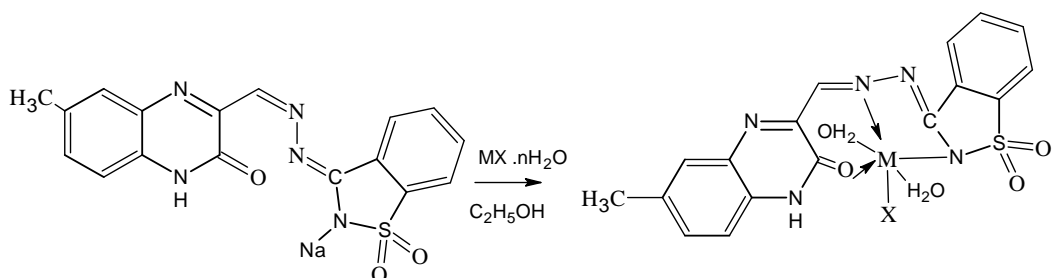
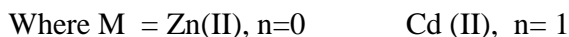
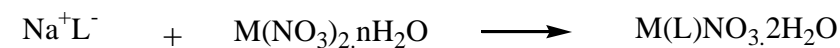
Scheme 3. Synthesis of sodium (3E)-3-((2E)-[3-hydroxy-6-methyl-3, 4,6,8a-tetrahydroquinoxalin-2-yl)methylidene]hydrazinylidene}-3H-1,2-benziothiazol-2-ide1,1-dioxide



Scheme 4. Proposed mechanism for the formation of the Na⁺ Schiff base

2.5 Synthesis of Metal Complexes

A methanolic solution (25 ml.) of [Co(NO₃)₂·6H₂O (0.116 g, 4 mmole), [Ni(NO₃)₂·6H₂O (0.116 g, 4 mmole), [Cu(NO₃)₂·3H₂O (0.096 g, 4 mmole), ZnCl₂ (0.17 g, 4 mmole) and CdCl₂·2H₂O (0.201 g, 4 mmole) was added with constant stirring to methanolic solution of the ligand [Na⁺L⁻] (0.3 g, 0.0008 M) and refluxed at water bath temperature for 2-3 hours. The isolated colored precipitates were washed with hot ethanol and ether dried in vacuum, Scheme 5.



Scheme 5. Synthesis of metal complexes

2.6 Antibacterial Study

The Schiff bases and their metal complexes were evaluated for both their in vitro antibacterial activity against *Escherichia coli* ATCC 8739, *Enterococcus*, *Staphylococcus aureus* and *Klebsiella pneumoniae* FMC 5. The inhibition zone of bacteria in DMSO control solutions were estimated in mm. diameter via agar diffusion method [22]. All the compounds were adsorbed by sterilized antibiotic discs having a diameter of 6 mm [23] in the amount of 50 ppm. The compounds to be tested were dissolved in DMSO to a final concentration of 20 ppm and soaked in filter paper. Discs containing complexes were located on the solid agar medium by pressing slightly. After petri dishes so obtained were placed at 4 C for 2 h, plates inoculated with bacteria were

incubated at 25 ± 0.1 C for 48 hrs. At the end of the period, inhibition zones formed on the food medium were measured in millimeters [19,24]. These tests were performed for two times. Gentamicin's (Bioanalyse) was used as standards.

3. RESULTS AND DISCUSSION

The new ligand and its metal complexes were stable kinetically and thermodynamically on the basis of their solubility in DMF, DMSO and elevation of melting points. However the condensation of quinoxaline-2-carboxaldehyde with the 2-hydrazino-saccharine involves nucleophilic attack as shown in the following mechanism, Scheme 4. The Table 1 shows the elemental analyses and some physical properties of the prepared complexes.

3.1 Mass Spectra

The gas chromatography-mass spectra of the free ligand were presented in Fig. 1 and Scheme 6. The molecular ion of relative intensity 33% at 367 m/z is constituent with the proposed formula of the Schiff base. However the other fragments at 354, 224, 174 and 147 could be attributed to cleavages of CH₃, PhCHN₂O, CH₇O₂, CHN respectively that would remarkably agree well with the proposed mechanisms of fragmentations of saccharine derivatives.

3.2 Molar Conductivity Measurements

The molar conductance values of the complexes measured at room temperature in DMF were in the range 22-40 S. cm² mol⁻¹ indicating their non-electrolyte nature behavior of the complexes [25] described in Table 3.

3.3 F.T.I.R Spectra

The most important IR spectral bands of the ligand and its metal complexes are listed in Table 2. The $\nu(\text{C}=\text{N})$ band at 1622 cm⁻¹ of the free ligand was subjected to lower wave number in the regions 1534-1599 cm⁻¹ shifts to lower frequencies in complexes indicating weakening of the azomethine bond due to coordination to the metal [16,18]. The IR spectrum of the ligand Na⁺ L⁻ exhibits a strong band due to $\nu(\text{C}=\text{N})$ at 1649 cm⁻¹ and broad band at 3292 cm⁻¹ due to $\nu(\text{C}-\text{OH})$ which is consistent with the literature [13-15]. As well as the presence of medium

bands in the 2960-2926 cm⁻¹ may be attributed to aliphatic C-H bonds related to 6-substituted aromatic ring that has been Annulated to pyrazine ring. Furthermore the medium absorptions in the region 1239-1244 cm⁻¹ that belongs to -S=O of saccharine would entirely support the completion of Schiff base formation [9,26]. The assignment of vibration modes in IR spectra of metal complexes showed the absence of O-H and N-H since the tautomer's forms were present of lactim and lactam forms, thus agrees well with data obtained from NMR spectra for the 7-methyl-3-oxo-3,4-dihydroquinoxaline-carbaldhyde[A₂]. The data obtained from IR spectra proved the coordination behavior of ONN donor tri dentate ligand through -NH, -C=N- and -C=O functional groups related to N₁ of saccharine, terminal imine -C=N- and carbonyl of pyrazine moiety respectively. The observed N-H stretching frequencies of the saccharine starting material was disappeared in the spectrum of the sodium salt Lewis base Na⁺L⁻ which indicated the deprotonation of acidic -NH moiety. The band located at approximately 1480 cm⁻¹ corresponded to the $\nu(\text{O}-\text{H})$ deformation mode, which further confirmed that the bond between the metal and ligand occurred through the oxygen of the lactim form [12,13]. The bands due to the metal-ligand stretching modes are expected to be present in the low frequency region between 442-599 and 424-489 cm⁻¹ [14,15]. The measured frequencies are often difficult to assign with confidence due to the relatively poor quality of the spectra in this region. In addition, the range of the spectra covered in this study (KBr pellets) was between 4000 and 400 cm⁻¹.

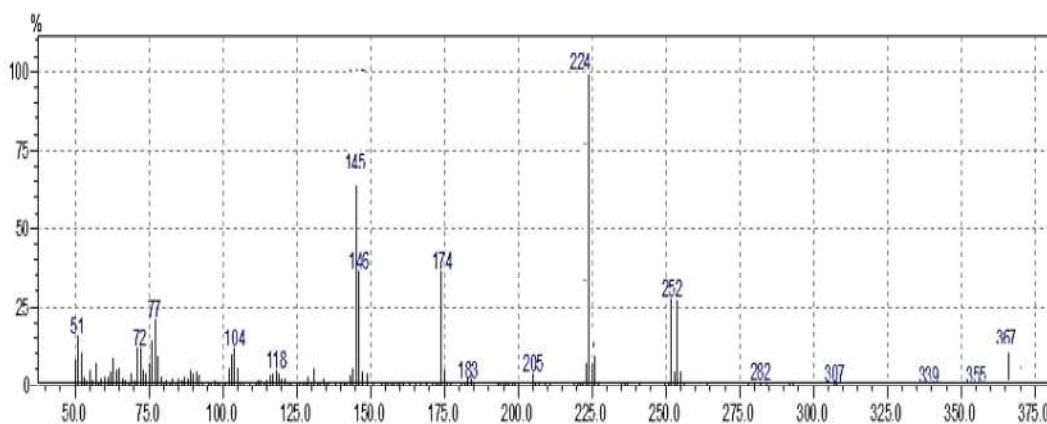


Fig. 1. GC-mass spectrum of Na⁺L⁻ Schiff bases in gas phase

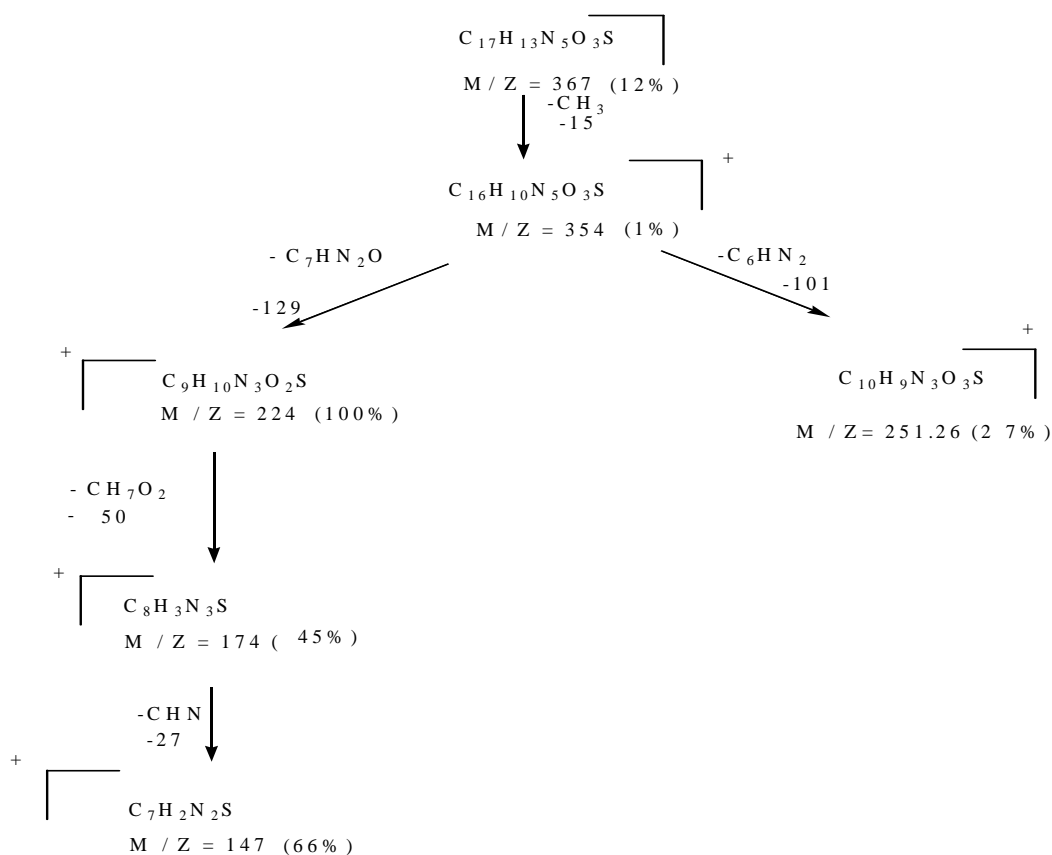
Table 1. The physical properties and elemental analysis of the prepared ligand [Na+L-] and metal complexes

Compound	Color	Molucule weight	M.p. (°C) ^{a d=decompose.tempture}	% element analysis ^{found (Calculated)}					
				C	H	N	S	Metal	Chloride
C ₁₇ H ₁₂ O ₃ N ₅ N _a S	pale yellow	390	149-151	55.58 (52.44)	3.57 (3.11)	19.06 (17.99)	8.73 (8.24)	-	
C ₁₇ H ₁₆ O ₈ N ₆ SCo	Dark-green	523.34	236d	36.11 (39.01)	2.48 (3.08)	17.25 (16.06)	6.58 (6.13)	12.09 (11.26)	-
C ₁₇ H ₁₆ O ₈ N ₆ SNi	pigie	523.10	201d	41.92 (39.03)	2.48 (3.08)	17.25 (16.07)	6.58 (6.13)	12.05 (11.22)	
C ₁₇ H ₁₆ O ₈ N ₆ SCu	dark-Green	528	248d	41.51 (38.67)	2.46 (3.05)	17.08 (15.92)	6.52 (6.07)	12.92 (11.04)	
C ₁₇ H ₁₂ O ₃ N ₅ SZnCl	Yellow	467	192d	41.35 (43.70)	2.45 (2.59)	17.02 (14.99)	6.49 (6.86)	13.25 (14.00)	6.43 (7.59)
C ₁₇ H ₁₂ O ₃ N ₅ SCdCl	pale Yellow	514	200d	39.71 (39.71)	2.16 (2.35)	13.65 (13.62)	6.21 (6.24)	21.90 (21.86)	5.7 (6.89)

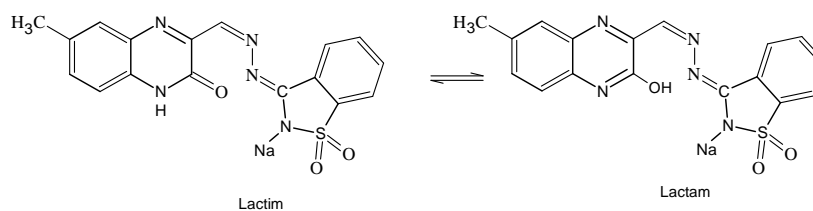
Table 2.FT-IR absorptions of the Schiff base [Na⁺L⁻] and its metal complexes in cm⁻¹

Compound	V _{NH, OH}	V _{C=O}	V _{C=N}	V _{C=C}	V _{S=O}	V _{M-N}	V _{M-O}	Aromatic _{C-H} aliph _{C-H}
Na ⁺ L ⁻	3292,3562	1680	1622 1580	1554	1245			3088-CHAr 2987-CH alpa
CoLX(H ₂ O) ₂	-	1649	1593-1559	1556-1545	1244	424-472	542	3023 2960
NiLX(H ₂ O) ₂	-	1664-1651	1580	1554	1243	455	542	3088 2987
CoLX(H ₂ O) ₂	-	1645	1585	1566-1533	1241	434-489	511-599	3012 2901
ZnLCl	-	1654	1634	1568	1240	445	523	
CdLCl	-	1656	1611-1599	1579	1239	434	546	3043 2926

*s: strong, m: medium, br: Broad, w: Weak, sh :shoulder, X=NO₃ and Y=CH₃CO₂ anions



Scheme 6. The proposed mechanism of Na^+L^- fragmentation in mass spectra



Scheme 7. Lactam-lactim forms of NaL ligand

3.4 Electronic Spectra and Magnetic Moment

The electronic spectroscopy is a valuable tool for coordination chemists to obtain important information regarding structure of complexes. Ligand usually being organic compounds show absorption in UV region, which may extend to longer wavelengths in case of extended conjugation. The appearance of new weak bands in the visible region might give proof for coordination the active site of the ligand toward the central metal ion [27,28,21]. The UV-Visible

spectra of ligand solution in methanol displayed two distinct absorptions at 250 and 310 nm which are due to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ of chromophores isomethine $-C=N$, $-C=C-$, $S=O$ and $-C=O$ [16,26]. The data of electronic spectra for all prepared compounds are presented in Table 3. The cobalt (II) complex shows two spin-allowed transitions at 355 and 510 nm which ascribed to $T_1^4g \rightarrow T_2g^4$ and $T_1^4g \rightarrow T_1^4(p)$ respectively. The copper(II) complex solution exhibits three low energy resolute bands in the regions 249, 420 and 860 nm that may be assigned to LMCT $^2A_1g \rightarrow ^2B_1g$ and $A_1g^2 \rightarrow B_1g^2$

transitions respectively [14], this supports square planar geometry [26]. The Complexes are dark solids and their DMF solutions showed intense absorption bands ($\Lambda_m = 103-104 \text{ M}^{-1} \text{ cm}^{-1}$) around 300–370 nm due to the presence of the coordinated quinoxaline derivatives [15,21]. However, the nickel(II) complex in DMF exhibits weak and sharp bands in the regions 428 nm and 366 nm transitions that are attributed to ${}^3A_{2g} \rightarrow {}^3T_{2g}$ and ${}^3A_{2g} \rightarrow {}^3T_{1g}$ respectively thus confirm the octahedral symmetry around nickel(II) ion [27,28]. On contrast the cadmium(II) complex showed two high intensity absorptions in the 290-385 nm region that are assigned to ligand field of ligand and LMCT transitions respectively. The strong absorption at 330 nm in the spectra of Cd(II) complex suggest the presence of acetate acetato anion in the coordination sphere of its structure [27,28]. The cobalt (II) and copper(II) complexes were paramagnetic due to their electronic configurations of $3d^7$ and $3d^9$ that magnetic moments values were 4.1 and 1.70 BM. Respectively with presence of orbital contribution of cobalt(II) complex [28-30]. The UV spectra contain intense bands corresponding to CT bands in the 280–240 nm range. The metal complexes of Quinoxaline-2,3-dione Schiff bases have been assigned similar bands to metal \rightarrow ligand transitions [28-30]. These bands are much more intense ($\log \epsilon_{\text{max}}: 3.71-3.03$) than the d-d bands ($\log \epsilon_{\text{max}}: 2.82-1.04$).

3.5 ${}^1\text{H}$ NMR Study

The Fig. 2 shows the absorptions of 12.2 ppm of -NH deshielded imidazole moiety and other at 10.2 ppm that was regarded to pyrazine [26]. However the peaks at 2.0- 3.5 and 7.6-7.9 ppm

were assigned to methylene -CH- protons and aromatic Ar-H ones as multiple peak [26,29].

3.6 Antimicrobial Activity

The antibacterial Gram negative species (-ve) activities and Gram positive species (+Ve) of the ligand [Na^+L^-] and their metal scanned complexes were tested by using agar diffusion method. The antibacterial activities of the prepared compounds against bacteria, *Escherichia coli*, *Klebsiella pneumoniae*, *Enterococcus* and *Staphylococcus*. Standard Gentamicin 10 $\mu\text{g}/\text{ml}$, Nitro Furamtoin 9 100 MC, Azithromycin 15 μg and Trimethprime were taken as the standard reference for antibacterial are presented in Table 4. The higher inhibition zone of metal complexes than those of the ligand can be explained on the basis of Overton's concept and Chelation theory. 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 p-electrons over the whole chelating ring and enhances the penetration of the complexes into lipid membranes and blocking of the metal binding sites in the enzymes of microorganisms. There are other factors which also increase the activity is solubility, conductivity and bond length between the metal and ligand [22,23,31-33].

3.7 Theoretical Study of the Predictive Complexes

The Electron distribution governs the electrostatic potential of molecule, and it is used to predict the nucleophilic attack of metal ion to the reactive sites in the ligand. The Electrostatic

Table 3. The theoretical vibrational modes of the prepared compounds

Compound	νNH	$\nu\text{C=O}$	$\nu\text{C=N}$	$\nu\text{C=C}$	$\nu\text{S=O}$	$\nu\text{M-N}$	$\nu\text{M-O}$	Other band
Na^+L^-	3238	1645	1614 1578	1558	1215			3060-CHAR 2987-CH alpha
$[\text{CoLX}(\text{H}_2\text{O})_2]$	-	1651	1580-1560	1556-1545	1242	424-472	543	3013 3006
$[\text{NiLX}(\text{H}_2\text{O})_2]$	-	1655	1619	1512	1235	452	552	3080
$[\text{CuLX}(\text{H}_2\text{O})_2]$	-	1665	1624-1585	1565-1532	1237	430-490	599-509	3012 2922
ZnLCl	-	1670	1630	1567	1260	443	523	
CdLCl	-	1666	1622-1587	1553	1223	425	543	3041 2970

Table 4. The electronic spectra and molar conductance of the prepared complexes

Complex	UV-visible, λ (nm)	Tentative assignment	μ (B.M.)	Λ_m (S.mol ⁻¹ .cm ²)	Geometry
Na ⁺ L ⁻	310 255	n \rightarrow π^* $\pi \rightarrow \pi^*$	-	10	-
[CoLX(H ₂ O) ₂]	340 600 800	LMCT ⁴ T _{1g} \rightarrow ⁴ T _{1g} (p) ⁴ T _{1g} \rightarrow ⁴ T _{2g}	4.1	22	Octahedral
[NiLX(H ₂ O) ₂]	300 422 410	LMCT ³ A _{2g} \rightarrow ³ T _{2g} ³ A _{2g} \rightarrow ³ T _{1g}	2.7	27	Octahedral
[CuLX(H ₂ O) ₂]	249 550 760	$\pi \rightarrow \pi^*$ ² A _{1g} \rightarrow ² B _{1g} ² A _{1g} \rightarrow ² B _{2g}	1.70	28	Octahedral
ZnLCl	319 350 389	n \rightarrow π^* LMCT MLCT	0.0	30	Tetrahedral
CdLCl	366 330	n \rightarrow π^* LMCT	0.0	40	Tetrahedral

* Λ_m = Molar conductances were measured in DMF solutions and CT: Charge transfer

Table 5. The antimicrobial activity ligand and its metal complexes

Comp. no	Susceptible microorganisms			
	Inhibition zone 50 mg/mole			
	Gram negative species(-ve)		Gram positive species (+Ve)	
	<i>Escherichia coli</i>	<i>Klebsiella pneumonia</i>	<i>Enterococci</i>	<i>Staphylococcus aureus</i>
[Na+L-]	8	8	6	8
[NiLX(H ₂ O) ₂]	8	7	10	16
[CoLX(H ₂ O) ₂]	16	10	8	22
[CuLX(H ₂ O) ₂]	10	12	20	12
ZnLCl	12	10	16	12
CdLCl	7	7	10	16
Gentamicin 10 μ g	18	24	18	15
Nitro Furantoin 9 100 MC	14	-	-	8
Tri meth prim	-	-	14	30
Azithromycin 15 Mcg	20	35	20	-

Potential of free ligands was calculated and plotted as 2D as shown in Figs. 3,4. This used to investigate the interactions between ligands and metals. Hyper Chem can show the forms of the highest occupied (HOMO) and the lowest unoccupied molecular orbital (LUMO) (also known as Frontier orbital's) by a plot through the molecule Overlap between the HOMO and LUMO is a governing factor in the reaction, Fig. 3 show Semi-empirical calculations could give an understandable picture about the intermolecular interactions. It is a tool for the determination of stability of molecule by incorporating quantum mechanical parameters

into the calculation. In the present study used PM3 method for the semi empirical calculation. All theoretically probable structures of complexes have been optimized with the method for the semi empirical calculation that implemented in the program package HyperChem.8 as shown in Fig. 4, The complexes studied theoretically using semi-empirical method of hyper chem. 8.0 program (PM3) to: Optimized the structural geometries. The vibration spectra and electronic spectra for complexes were estimated and then compared with the experimental values. The theoretical results agreed with those found experimentally [20,34].

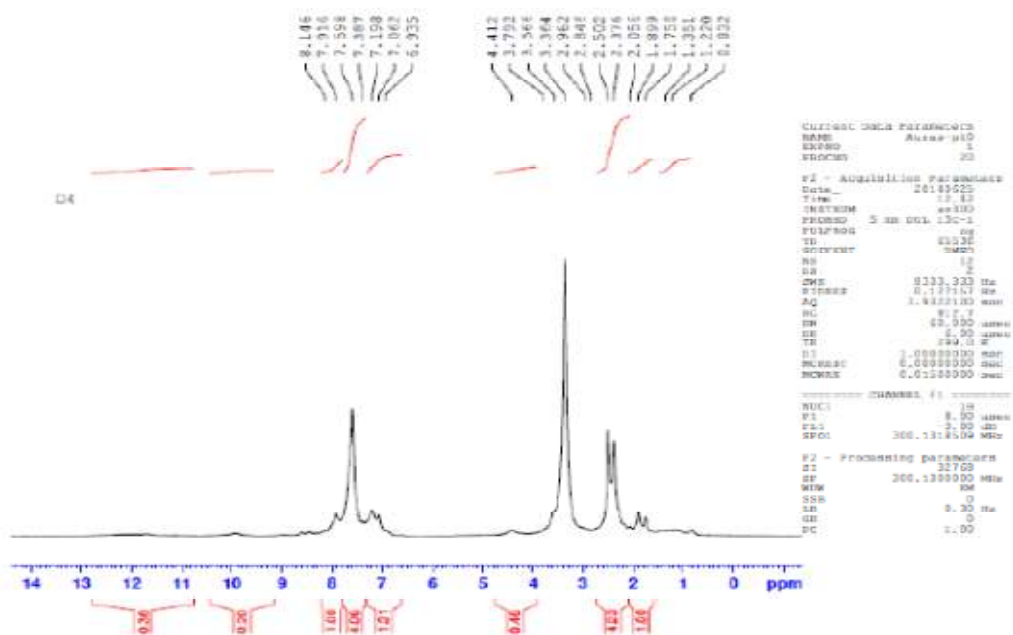


Fig. 2. ^1H NMR spectra of Schiff base Na^+L^- in DMSO-d_6 solution

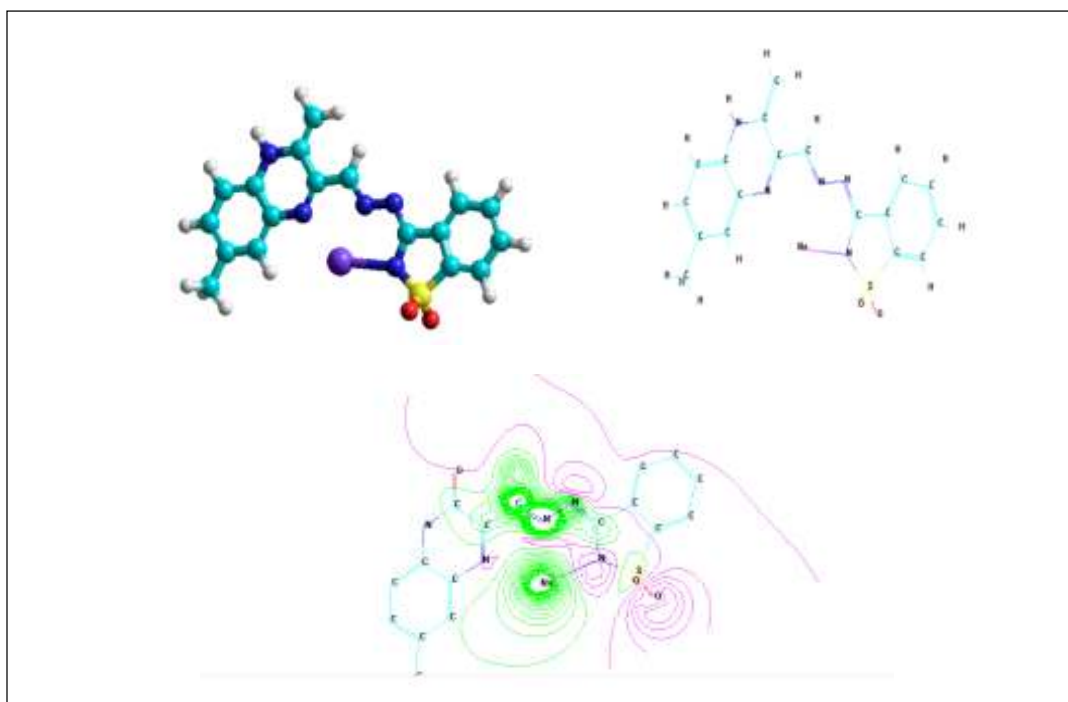


Fig. 3. Electrostatic potential as 2D contours for ligand Na^+L^- . The HOMO and LUMO as 2D

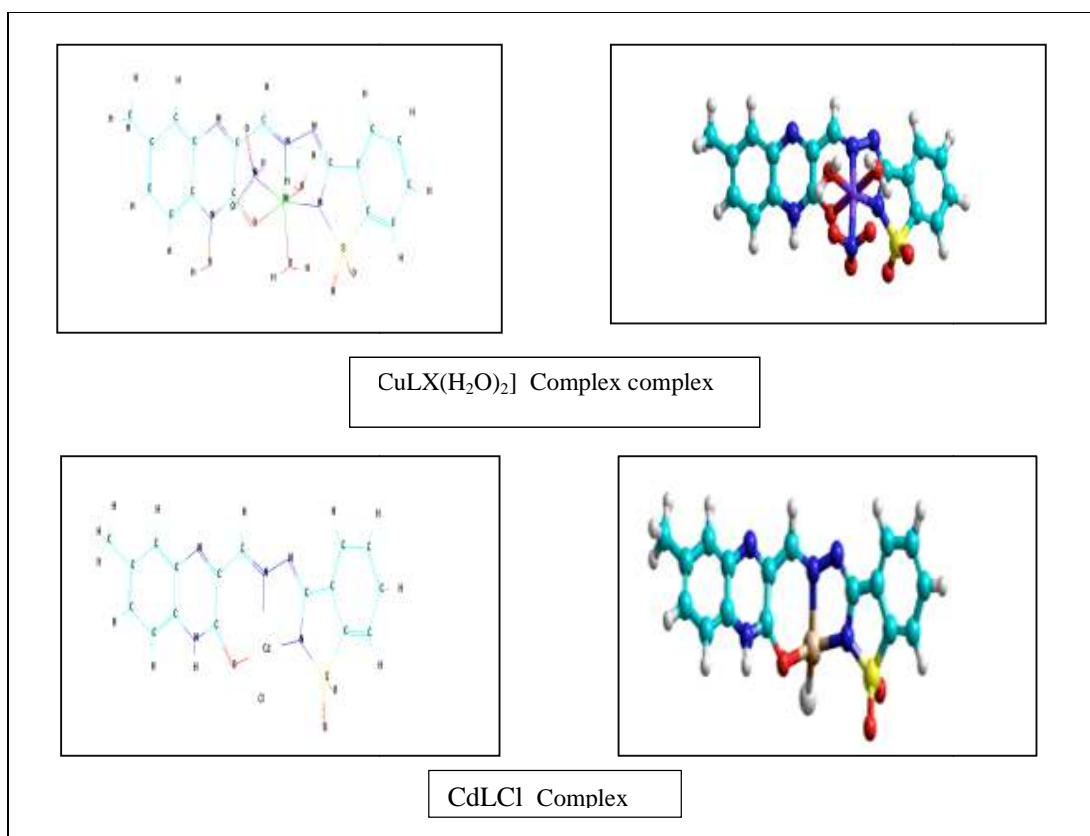


Fig. 4. Conformational structure of complex CuLX, CdLCl

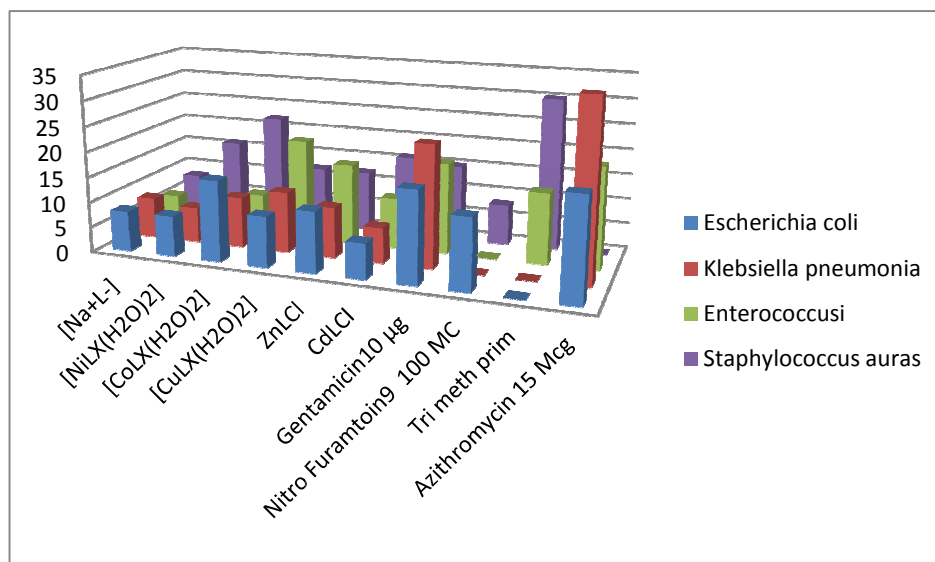


Fig. 5. The Antimicrobial activity ligand Na⁺L⁻ and its metal complexes against Gram negative species (-ve) *Escherichia coli*, *Klebsiella pneumonia* and Gram positive species (+Ve) *Enterococcus*, *Staphylococcus aureus*

4. CONCLUSIONS

According to the results obtained from elemental analyses and spectral studies, it is obtained that all complexes were octahedral except zinc (II) and cadmium (II) complexes were tetrahedral. The new Schiff base behaved as tridentate monobasic via ONN system that possess oxygen atom of carbonyl in 2-position, nitrogen of imine and acidic Na of saccharine ring. The IR spectra adopted the participation of nitrate – NO₃ ions in coordination with Co(II), Ni(II), Cu(II) whereas the chloride ions were content in structure of Zn(II) and Cd(II) complexes. Also, the synthesized of a ligand Na+L- and a series of Co(II), Ni(II), Mn(II), Cu(II), Zn(II), Cd(II) complexes were tested the Antimicrobial activity against Gram negative species (-ve) *Escherichia coli*, *Klebsiella pneumonia* and Gram positive species (+ve) *Enterococcus*, *Staphylococcus aureus*.

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COMPETING INTERESTS

Author has declared that no competing interests exist.

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