Synthesis, Spectral Study, Theoretical Treatment and Biological Activity of Some Transition Metal Complexes with 2-Amino Acetic Acid-6-Chloro Benzothiazole

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Abstract:

New metal complexes of the ligand 2-amino acetic acid -6-chloro benzothiazole(L) with the metal ions Au(III),Cu(II),Ni(II),Co(II),and Zn(II) were prepared in alcoholic medium.The prepared compounds were characterized by FT-IR and UV-Visible spectrophotometer, Magnetic susceptibility ,Flame atomic absorption technique as well as elemental analysis and coductivity measurement.From the spectral studies,an square planar monomer structur proposed for Au(III) complex,octahedral diamer structure for Cu(II) complex, octahedral monomer structur proposed for Ni(II),and Co(II) complexes,and tetrahedral structure for Zn(II) complex.Semi-empirical methods (ZINDO/1,PM3 and ZINDO/S) were carried out to evaluate heat of formation ΔH˚f, binding energy ΔEb,dipole moment,for all complexes except Au(III) complex that used AMBER method for this complex, also the vibration frequencies, and electronic transitions was calculated for prepared ligand.Electrostatic potantial,HOMO and LUMO energies for ligand were calculated to determine the reactive sites for this ligand.The bioefficacy of the ligand and its complexes have been examined against the growth of becteria in vitro to evalute their anti-microbial potential.

Key words: amino acetic acid;6-chloro benzothiazole; metal complexes.

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Introduction

A heterocyclic compound is one which possesses a cyclic structure with at least two different kinds of hetro atoms in the ring.Nitrogen,oxygen,and sulfur are the most common hetrocyclic compounds are very widely distributed in nature and are essential to life in various ways(1). 2-aminobenzothiazoles were intensively studied, as the 2- amino benzothiazole scaffold is one of privileged structure in medicinal chemistry(2) and repotedncytotoxic cancer cells.It must be emphasized that combination of 2-aminobenzothiazoles with other hetrocyclic is well known approach to design new drug like molecules,which allows achieving new pharmacological profile action,toxicity lowering(3).

The benzothiazole compounds containing different hetero atom, substituent have a tendency to form a good metal complex.Activity of the substitute benzothiazole enhances on complex formation with suitable metal. These reports encourage the study the metal chelates of substituted benzothiazole with some transition metal(4).

Experimental

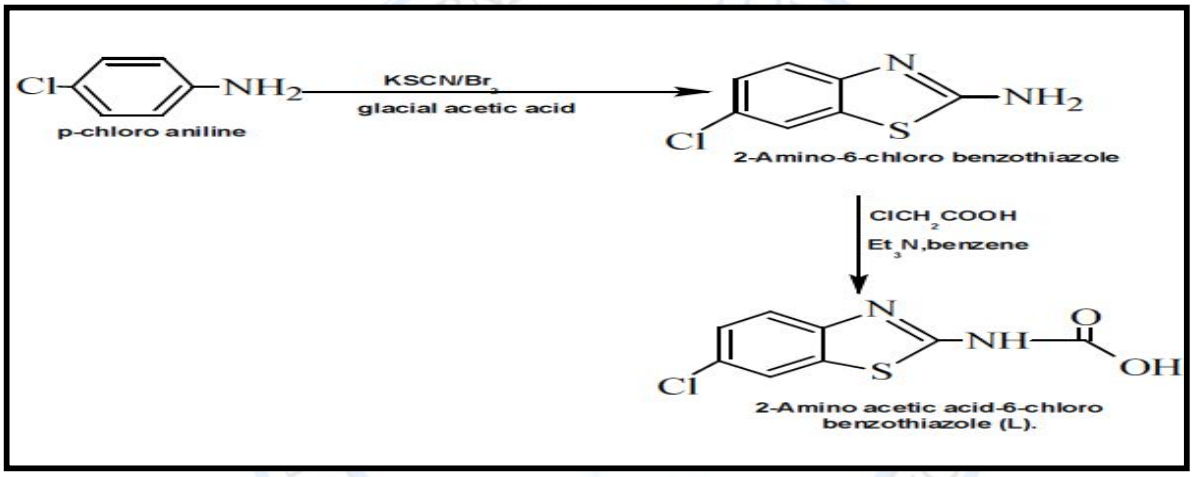
A-Material and methods

1-Preparation of 2-amino-6-chlorobenzothi benzothiazole(C)(5,6).

In a 250 ml round bottom flask equipped with a magnetic bar stirrer and dropping funnel, a solution of Br2 (1.2 ml) in a glacial acetic acid (75ml) was allowed to run through the dropping funnel drop wise during 30 min.to amixture of para chloro aniline (0.03mole) and KSCN (0.1mole)in 150 ml glacial acetic acid with stirring.The mixture was stirred for 1hr,than diluted with water and neutralized with solid (NaOH).The precipitated substance was collected triturated and recrystallized from a benzene to obtain 2-amino-6-chloro benzothiazole.

2-Preparation of 2-(amino acetic acid)-6- chloro benzothiazole(7)

A compound (C) (0.003 mole) was added to benzene(35ml) with stirring until solubility complete. To this mixture 2-droup of triethyl amine (TEN) was added and than chloro acetic acid (0.003 mole) was added. The mixture was refluxed for 2hurs then cooled at room temperature. The precipitated solid was filtered and recrystallsied from benzene.The steps of the synthesis of 2-amino-6-chloro benzothiazole can be shown below:-



Figure(1):Steps of synthesis 2-amino acetic acid-6-chloro benzothiazole.

3-Preperation of ligand complexes

Addition of ethanol solution of the suitable metal salt (chloronic acid mono hydrate,copper nitrate tri hydrate,nickel nitrate hexa hydrate,cobalt nitrate hexa hydrate and zinc acetate di hydrate) to an ethanol solution of 2-amino acetic acid-6-chloro benzothiazole in 1:1 (Metal:Ligand) molar ratios was carried out.After reflux for 4hrs.,crystalline colored precipitates washed with distilled water,dried and recrystallized from ethanol and dried at 50˚C,table (1) shows the physical properties of prepared compounds.

B-Instrumentation:-

Elemental C.H.N.S analysis were carried out on a EM-017.mth instrument ,the FT-IR spectra in range(4000-200 cm-1) cut were recorded as CsI disc on IR-Prestige-21,Single beam path Laser,Shimadzu Fourier Transform infrared Spectrophotometer,UV-Visible spectra were measured using UV-1650PC Shimadzu,UV-Visible in the range (200-950) nm.The magnatic Susceptibility values of the prepared complexes were obtained at room temperature using Magnatic Susceptibility Balance of Johanson mattey catalytic system division ,England,Atomic Absorption measurements of the prepared complexes were obtained using Shimadzu Atomic Absorption 680 Flame Spectrophotometer.The Conductivity Values of the prepared Complexes were measured using DMF as solvent,the concentration 0.001M using (WTW) Conductometer.

Table (1):Physical data of the new ligand ,and its metal complexes.

Comp.	Colour	m.p.˚C	Yield%	M.Wt $gmol^{-1}$	Found (calc.)%				
					C	H	N	S	M
L	white	150-152	81.48	242.50	45.37 (44.53)	2.76 (2.88)	10.08 (11.54)	12.34) (13.19)	----
AuL	Orange	206 dec.	90.50	574.46	21.98 (22.97)	1.73 (2.61)	4.29 (4.85)	5.85 (5.57)	33.44 (34.28)
CuL	Pale Green	136-138	54.54%	759.10	29.34 (30.03)	1.34 (2.23)	10.54 (11.06)	8.33 (8.43)	17.02 (16.74)
NiL	green	122 dec.	92.30%	426.19	24.54 (25.34)	3.40 (3.28)	10.19 (9.85)	6.58 (7.50)	13.92 (13.65)
CoL	pink	108 dec.	92.30%	426.43	25.04 (25.32)	3.21 (3.28)	8.84 (9.84)	6.68 (7.50)	13.50 (13.81)
ZnL	white	170-172	64.25%	430.91	36.68 (36.19)	4.82 (4.17)	5.82 (6.49)	6.82 (7.42)	15.52 (15.17)

Results and Discussion

The elemental analysis show 1:1 (metal:ligand) stoichiometry for the complexes.The analytical data together with some physical properties of the complexes are summarized in table (1).The isolated solid complexes are stable at room temperature and insoluble in common organic solvents,but soluble in DMF and DMSO.The molar conductance values of

the complexes indicating that the all complexes are ionic except Cu(II),and Zn(II) complexes which are non ionic.The formation and there geometry were further confirmed by IR,UV-Vis,magnatic spectral studies.

A-Chemistry

1-FT-IR Spectra

The IR spectrum of benzothiazole derevative ligand shows a typical broad band in the range (2400-3450 cm^{-1}) with its maximum at (3302 cm^{-1}) refers to stretching frequency of ν(OH) band of carboxylic acid [8] . The spectrum also displayed a strong band at (1643 cm^{-1}) due to the stretching frequency of carbonyl group[7] .The sharp band at 1462 cm^{-1} may be assigned to (δN-H+νC-N)[9].The absorption bands at (1249,810,and775 cm^{-1}) related to stretching frequency of ν(C-O) ,ν(C-Cl),and ν(C-S) bonds respectively.

In the spectra of complexes ,the bands due to stretching frequency of ν(C=O), and ν(C-O) shifted to the lower frequency by (~8-23,3-49) respectively , except in Zn(II) complex this bands shifted to the higher frequency. These changes indicate that the carboxylate group take part in the coordination. More evidence a new weak bands appeared at (~505-524 cm^{-1}) assigned to stretching frequency of ν(M-O)[8]. For Au (III),Cu (II),and Zn(II) complexes, the ligand behaves as a bidenitate ligand through the carboxylate group ,furthermore there is no appreciable change in the other groups, while the spectra of Ni(II), and Co(II) complexes exhibited shifting the stretching frequency of the band ν(C=N) to the lower frequency by (50,and 54 cm^{-1}) respectively in addition to change in carboxylate group, this indicate that this ligand here behaves as a tridentate through (N,N,O) atoms in these complexes, more evidence a new weak bands appeared at 489 and 462,cm^{-1} assigned to stretching frequency of νNi-N,and νCo-N respectively. Furthermore there is no appreciable change in the (C-S) band ,we exclude the possibility of sulfur atom to participation in coordination .The spectra of all complexes observied bands around (3545-3387 cm^{-1}) assigned to the presence of the water or ethanol molecules [10].The bands appeared at (1384, 1141, 1094) and (1384, 1138, 1072) cm^{-1} in Ni(II), and Co(II) complexes may be assigned to nitrate ionic group, While Cu(II) complex

exhibited bands at (1373, 1350, and 900 cm^{-1}) related according to notes of nakamoto[11] to bridge nitrate group as bidentate in this complex, table(**2**).

Table (2) :most diagnostic FTIR bands of the Ligand and its complxes .

Symb.	ν(NH)	ν(C=O)	ν(C=N)	ν(C-O)	δNH+νCN	ν(C-S)	ν(M-O)	Others
C	3456 s 3271m	--------	1631 s	-------	----------	763 sh	--------	δNH_2 1531s 1492 w
L	3300 b	1643 s	1577 m	1249 m	1462 sh	775 sh	-------	ν(OH)3302 b
AuL	3305 m	1635 S	1570 m	1246 w	1465 sh	767 M	513 m	νEtOH 3394 sh AuCl 324
CuL	3400 b	1620 M	1577 m	1200 w	1469 m	767 M	513 w	νEtOH 3545 sh $\nu ONO_2$1373.s, 1350 s,1050 w.
NiL	-------	1620 M	1527 w	1265 w	1465 m	775 W	524 w	νH2O 3387b ν(M-N)489 w $\nu NO_3$1384s,1141 m,1094
CoL	-------	1620 M	1523 w	1296 w	1465 m	775 W	505 w	νH_2O3414 b (M-N)462w $\nu NO_3$1384 s,1138 m,1072w
ZnL	3313 m	1651 S	1577 s	1276 m 1249 m	1462 sh	783 Sh	516 w	νEtOH 3394 sh νOAC,1728m, 1535 s

Where:w=weak,s=strong,sh=sharp,m=medium,b=broad

2-Electronic spectral and Magnatic moment studies

The electronic spectrum of ligand generally exhibited two main bands .The first absorption band appeared at 256 nm(39062 cm^{-1}) due to interaligand ($\pi \rightarrow \pi^*$) transition located on the C=O group. The second absorption band appeared at 273nm(36630 cm^{-1}) arises from ($n \rightarrow \pi^*$) transition,located on the on the oxygen atom on the C=O group or on the nitrogen atom of –N=C- group[7].

AuL:The electronic spectrum of orange AuL complex showed four bands one at 26881 cm^{-1} which refer to $^1A_1g \rightarrow {}^1B_1g$ transition ,and the other appeared at 30769 cm^{-1} which refer to $^1A_1g \rightarrow {}^1Eg$ transition [12].The bands at 32154 cm^{-1} may be due to charge transfer. The conductivity measurements for the prepared complex in DMF solvent at room temperature

showed to be ionic .The complex is diamagnetic moment in solid state is found to be zero Bohr magneton.So the propble geometry for this complex is sqare planar.

CuL: The electronic spectrum of the CuL complex exhibited only one broad band at 12531 cm^{-1} assigned to the $^2Eg \rightarrow {}^2T_2g$ transition ,which is in conformity with the octahedral configuration around the copper ion .Though three transitions are expected in this case ,they are very close in energy and often appear in the form of one broad band envelop[13]**.** The spectrum also exhibits a band at 23980 ,34482 and 38610 cm^{-1} ,which are assigned to charge transfer band.The value of ($\mu_{eff.}$) that measured for this complex is 0.97 B.M.,this lower value of magnetic moment for Cu suggested dimeric structure of complex leading to spin–spin coupling.Conductivity measurement show the complex to be non ionic .

NiL: The electronic spectrum of Ni(II)L complex exhibits two bands in the region 15105, and 23809 cm^{-1} which assigned to the $^3A_2g \rightarrow {}^3T_1g_{(F)}(\nu_2)$,and $^3A_2g \rightarrow {}^3T_1g_{(p)}$ (ν_3) transitions. respectively.These bands indicated an octahedral geometry around the Ni(II) ion[14]**.**More evidence for the suggesting octahedral geometry of the present complex ,is supported by the absences of band in the range (20000 cm^{-1}) which is characteristic for squar Ni(II)complex[15]**.**The spectrum also exhibits a charge transfer bands at 34482 and 46948 cm^{-1}.The values of 10Dq, B/and the nephelauxetic factor β were calculated by using Tanaba-Sugano diagram for octahedral d^8system,table(**3**). The.The obtained β value for Ni(II) complex is less than unity ,suggesting the metal ligand bonds have a considerable amount of covalent character[10].The.ratio ν_2/ν_1 will be calculated and seen which is equal 1.46 that refers to distortion octahedral.Megnatic moment is (3.12) B.M is additional evidence for an 3e unpaired in octahedral geometry,and the conductivity measurement show that the complex is to be ionic.

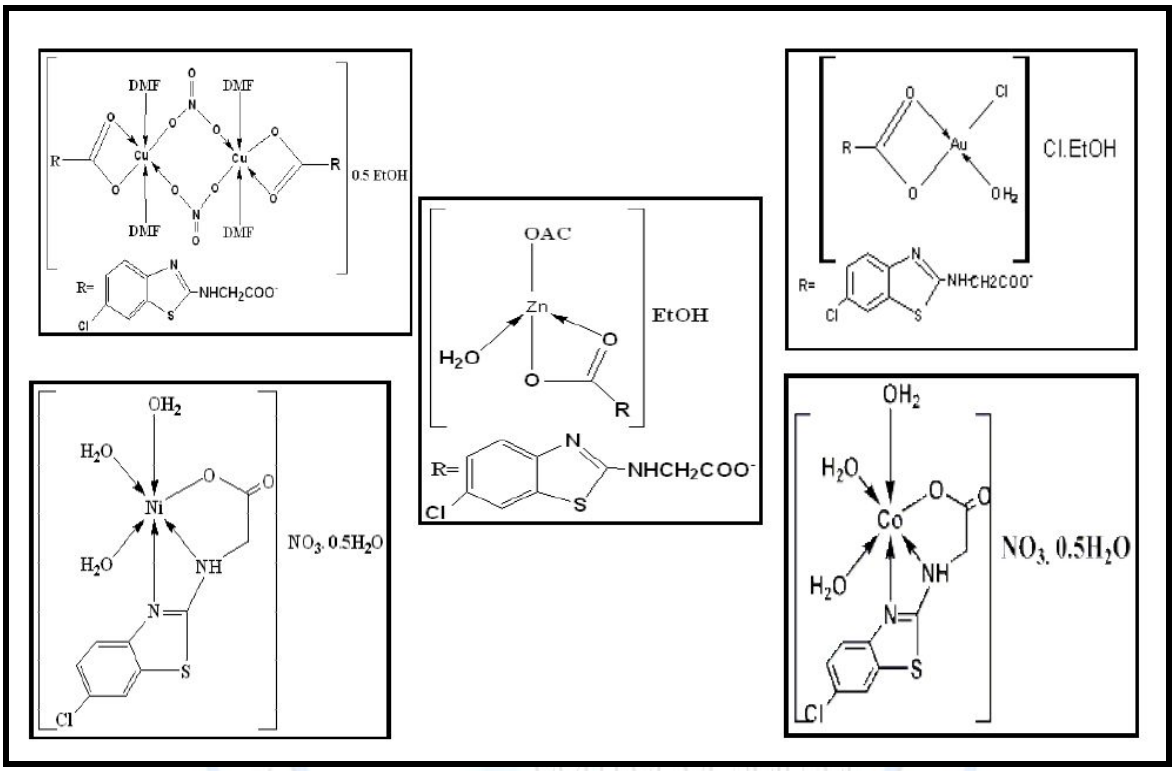
CoL:The electronic spectrum of pink CoLcomplex showed three absorption bands at10868,18969,and 23057 cm^{-1}, these bands have been assigned to the transitions $^4T_1g \rightarrow {}^4T_2g(\nu_1)$,$^4T_1g \rightarrow {}^4A_2g(\nu_2)$,and$^4T_1g \rightarrow {}^4T_1g(\nu_3)$,respectively , on the basis of these assignment it was possible to calculate the ligand field parameters 10Dq , B/and β by usingTanaba-Sugano diagram for d^7 system [16,17],the results are found in table (**3**).The value

of the calculated β is (0.623),this value refers to the covalent character of the bonding between the cobalt ion and the donor atom of ligand [18].The assigned values of ν_2,10Dq and others electronic values calculated are all in good agreement with cobalt (II) octahedral complexes [19].The molar conductivity measurements indicate that the complex was ionic .

ZnL:Since the UV-Visible spectra of d^{10}ion do not furnished a lot of information ,so some shifiting and change in the shape of the bands were compared with those of the ligand[20] .The prepared white complex was diamagnetic that which is expected for d^{10} ion .The spectrum of the complex shows relative change in the bands position compared to that of the free ligand.The conductivity measurements in DMF solvent at 25˚C showed to be non ionic .

Table (3):-Electronic spectra,Conductance in DMF solvent,and magnetic moment(B.M)for the prepared ligand L1 and its metal complexes.

Comp.	L	AuL	CuL	NiL	CoL	ZnL
Absorption Bands(cm^{-1})	31446 36630 39062	26881 28735 32154 37037	12531 23980 34482 38610	10310 (calc.) 15105 23809 34482,46948	10868 18969 23057	30769 35587 38314
Assignments	n→π* π→π* π→π*	$^1A_1g\rightarrow{}^1B_1g$ $^1A_1g\rightarrow{}^1Eg$ L→AuCT L→AuCT	$^2Eg\rightarrow{}^2T_2g$ L→CuCT L→CuCT L→CuCT	$^3A_2g\rightarrow3T_2g$ $^3A_2g\rightarrow3T_1g_{(f)}$ $^3A_2g\rightarrow3T_1g_{(P)}$ L→NiCT	$^4T_1g\rightarrow{}^4T_2g$ $^4T_1g\rightarrow{}^4A_2g$ $^4T_1g\rightarrow{}^4T_1g_{(P)}$	ILCT ILCT ILCT
B˚	-----	----	----	1035	971	----
B/	----	----	----	636.42	605.23	----
B	----	---	----	0.61	0.62	----
Dq/B/	----	----	----	1.62	1.81	----
10Dq	----	----	----	10310	10890	----
15B/ Separationterm	-----	-----	----	7983.64	18075	----
$\mu_{eff.}$ B.M	--------	0.00	0.97	3.12	4.51	0.00
μscm^{-1}	--------	80.20	62.50	86.10	82.30	7.00
Suggestedgeometry	---------	Square planar	O.h	O.h	O.h	T.d



Figure(2):-Suggested structure of the prepared complexes .

3-Study of complexes formation in solution:

Complexes of benzothiazole derevative ligand with metal ions were studied in solution using ethanol as a solvent ,in order to detrmine [M/L] ratio in the complexes follow molar ratio method[21].

A series of solutions were prepared having a constant concentration (10^{-3}) of metal ion and ligand .The [M/L] ratio determined from the relationship between the absorption of absorbed light and the mole ratio of [M/L].The results of complexes in ethanol suggest that the metal to ligand ratio was [1:1] for all complexes which were similar to that obtained from solid state study.

4-Theoretical Study:

The program Hyper Chem-8 was used for the semi-empirical and molecular mechanical calculation at optimized energies, the result of ZINDO/1 method of calculation in gas phase for heat of formation ($\Delta H^{\circ}f$),binding energy (ΔE_b) and dipole moment (μ) for free ligand and its complexes of Cu(II),Ni(II),Co(II),and Zn(II) while Amber method was using for Au(III) complex,table(**4**). PM3 was used for evaluating the wave number for the ligand and compared with the experimental frequencies to predict the deviation,table (**5**).ZINDO/S method was used to calculate electronic transitions for the ligands and compared with experemintal transition to explain the transitions.

Table (4): Conformation energetic (in K.J.mol^{-1}) and dipole moment (in Debye) for ligand(L) and its metal complexes.

Comp.	ZINDO/1			AMBER
	$\Delta H^{\circ}f$	ΔE_b	μ	$\Delta H^{\circ}f = \Delta E_b$
C	-14364.26	-21803.95	5.23	----------
L	-19067 .57	-28968.36	2.04	----------
AuL	----------	----------	----------	315.32
CuL	-44415.23	-66703.46	19.04	----------
NiL	-21757.75	-33829.51	14.17	----------
CoL	-21877.05	-33947.14	17.33	----------
ZnL	-26835.74	-39819.81	7.56	----------

The table above explained that the heat of formation of complexes is smaller than it for ligand,and the binding energy also smaller than it for ligand thus,we expected that the complexes are to be thermodynamically more stable than ligand.

Table (5): Comparison of experimental and theoretical vibrational frequencies for benzothiazole derevatives ligand(L).

Symb.	νC=O	νC=N	νAmideII	νCH aromatic	νC-S	ν C-H eliphatic	ν OH
L	1643.35 * 1971.77** (19)***	1577.77* 1641.12** (4.0)***	1462.04* 1331.56** (-8.9)***	3024.38* 3000.11** (-0.8)	775.38* 708.29** (-8.6)***	2885.51* 2899.6** (0.4)***	3302.13* 3850.48** (16) ***

Where:*Experimental frquency,theoretical frequency,***Error% due to main different measurements and theoretical treatment of vibrational spectra.**

The theoretical UV-spectrum of ligands was calculated using ZINDO/S method and showed some deviations from the experimental values .These deviations are generally acceptable in theoretical calculations[22]. The serial number of atoms was plotted in the structure of ligands in order to determine the type orbitals than type of transition figure (3).The theoretical UV-spectrum of ligand L showed two absorption peaks at 276.9 and 279.4 nm.The quantum data indicate that these peaks are generated mainly from π→π* transition (O15→C13) and n→π* transition (N8→C9).The experimental spectrum also showed two peaks at 256.00 and 273.00 nm.

The electrostatic potential (E.P.) describes the interaction of energy of the molecular system with a positive point charge.(E.P) of the ligand were plotted as two and three dimension contours to investigate the reactive sites of the molecule. Also, one can interpret the stereochemistry and rates of many reactions involving soft electrophiles and nuclephiles in terms of the properties of frontier orbital's (HOMO & LUMO). Overlap between the HOMO and LUMO is a governing factor in many reactions. The HOMO and LUMO value were plotted in three dimension counter to get more information about these molecules Fig **(2)**. The results shows that the LUMO of transition metal ion prefers to react with HOMO of donor atoms of ligand.

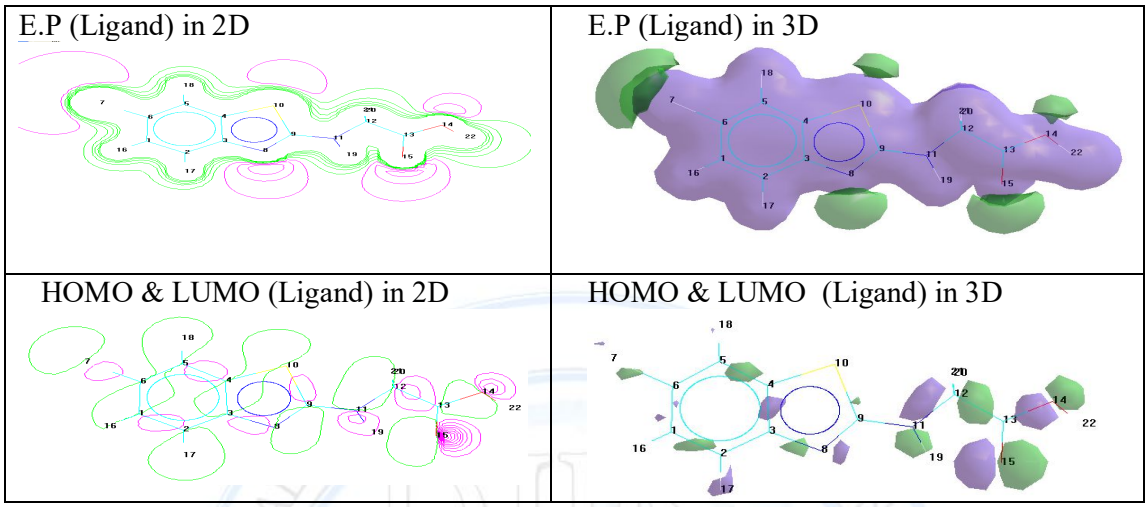
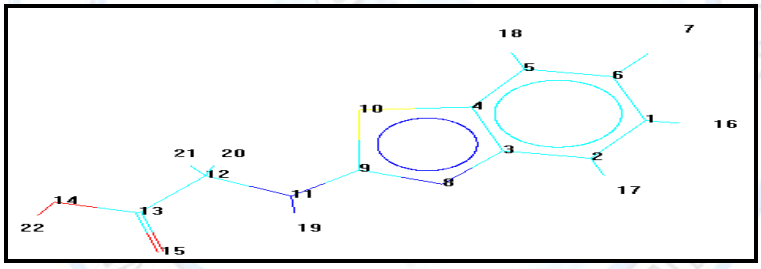


Fig (2): HOMO, LOMO and Electrostatic potential as 2&3D counters for Ligand(L)



Figure(3):Serial number of atoms view of ligand(L).

B-Biological studies

The free ligand and its metal complexes were screened against Escerchia coli as gram negative and Staphococcus aureus as gram psative becteria to assess their potential antimicrobial activity.The results are quite promising.The becteria screening results ,table **(6)**.The antimicrobial data reveal that the complexes are more bioactive than the free ligand agensit E.coli bacteria.The enhanced activity of the metal complexes may be ascribed to the increased lipophilic nature of the complexes arising due to chelation .It is probably due to faster diffusion of the chelates as a whole through the cell membrane or due to chelation theory.

Table(6):-Antibecterial activities for ligand and its complexes.

Comp.No.	Comp.	Staphlococcus aureus				Escherchia coli			
		1mM	2mM	3mM	4mM	1mM	2mM	3mM	4mM
1	Ligand	++++	++++	++++	++++	+	+	+	+
2	AuL	+++	++++	++++	++++	+++	++++	++++	++++
3	CuL	+++	++++	++++	++++	+++	+++	++++	++++
4	NiL	++++	++++	++++	++++	++	+++	+++	+++
5	CoL	+++	++++	++++	++++	+++	++++	++++	++++
6	ZnL	+++	++++	++++	++++	++++	++++	++++	++++

(+)=(1-4) mm=slightly active

(++)=(4-8) mm=modratly active

(+++)=(8-12) =active

(++++) = >12 =highly active.

Conclusion

The ligand 2-amino acetic acid -6-chloro benzothiazole was successfully synthesized by condensation reaction. The ligand behaves as bidenetate ligand through carboxylate group in Au(III),Cu(II),and Zn(II) complexes,while in Ni(II),and Co(II) Complexes behaves as a tridenetate ligand through (O,N,N)atoms.The theoretical calculation data of the frequencies for the ligand agreed and help to assign unambiguously the most diagnognostic bands.Theoretical ectronic transition helped to assign type of transition,and the calculation of energies give information about the most stable structure.

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Synthesis, Spectral Study, Theoretical Treatment and Biological Activity of Some Transition Metal Complexes with 2-Amino Acetic Acid-6-Chloro Benzothiazole

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تحضير والتشخيص الطيفي والمعالجة النظرية والفعالية البايولوجية لبعض معقدات العناصر الانتقالية مع 2- امينو اسيتك اسيد-6- كلورو بنزوثايزول

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الخلاصة

جرى تحضير معقدات جديدة لليكاند 2-امينو اسيتك اسيد-6-كلورو بنزوثايزول مع ايونات العناصر الذهب الثلاثي والنحساس الثنائي والنيكل الثنائي والكوبلت الثنائي والزنك الثنائي في وسط كحولي.شخصت المركبات المحضرة بواسطة تقنيات الاشعة تحت الحمراء والاشعة فوق البنفسجية-المرئية والحساسية المغناطيسية والامتصاص الذري اللهبي وكذلك التحليل الدقيق للعناصر والتوصيلية الكهربائية.من خلال الدراسة الطيفية اقترح الشكل المربع المستوي لمعقد الذهب والشكل الثماني السطوح بهيئة دايمر لمعقد النحاس والشكل ثماني السطوح لكل من معقدات النيكل والكوبلت والشكل الرباعي السطوح لمعقد الزنك.

أجريت معالجة تكون المعقدات نظرياً في الطور الغازي باستخدام برنامج (Hyperchem-8) باستخدام الطرق شبه التجريبية ZINDO/1 , PM3,ZINDO/S لحساب حرارة التكوين وطاقة الترابط والعزم ثنائي القطب عند درجة حرارة 298 كلفن لليكاند ومعقداته المحضرة ماعدى معقد الذهب حيث استخدمت طريقة AMBER لحساب الطاقة لهذا المعقد. كذلك تم حساب الترددات الاهتزازية والانتقالات الالكترونية لليكاند المحضر و تم حساب الجهد الاليكتروستاتيكي لبيان المواقع الفعالة للأوربيتال الواقع في أعلى مستوى طاقة والذي يحتوي إلكترون واحد أو أكثر (HOMO) والأوربيتال الواقع في أوطأ مستوى طاقة والذي لا يحتوي الكترونات (LUMO) لليكاند. تم اختبار الليكاند ومعقداته ضد البكتريا النامية لبيان الفعالية البايولوجية لتلك المركبات.

الكلمات المفتاحية: امينو اسيتك اسيد, 6- كلورو بنزوثايزول, معقدات الفلز