

Synthesis, Spectral Studies and Theoretical Treatment of New Au (III) and Cu(II) Complexes of Bidentate Ligands 2-Benzamido Benzothiazole, and 2-Actamido Benzothiazole.

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Abstract

New metal complexes of the ligands 2-Benzamido benzothiazole (B1), and 2-Acetamido benzothiazole (B2) with the metal ions Au (III) and Cu (II) were prepared in alcoholic medium. The prepared complexes were characterized by FT-IR, electronic spectroscopy, Magnetic susceptibility, Flame Atomic Absorption technique as well as elemental analysis and conductivity measurement. From the spectral studies, a square planar as a monomer structure proposed for Au (III) complexes and octahedral dimeric structure for Cu (II) complexes. Semi-empirical methods (ZINDO/1, PM3 and ZINDO/S) were carried out to evaluate heat of formation ΔH_f° , binding energy ΔE_b , dipole moment for copper complexes. While AMBER method was used to calculate energies of Au (III) complexes. Also vibration frequencies, and electronic transitions of prepared ligands were calculated. The electrostatic potential HOMO and LUMO energies were calculated for the ligands to determine the reactive sites for these ligands.

Keywords: Spectral studies, 2-Benzamido benzothiazole, 2-Actamidobenzothiazole.

Introduction

The amide bond $[-C(O)NH-]$ has long attracted much attention since it is an essential building unit in proteins [1]. The high stability of the amide linkage toward hydrolysis is of crucial importance to biological systems [2], since it allows the construction of peptides from relatively simple amino acid precursors. The coordination chemistry of amide ligands is an important part of a number of chemical problems [1,2].

The benzothiazole compounds containing different heteroatom, substituent have a tendency to form a good metal complex. Substituted benzothiazole are antifungal, antibacterial, intramural depressant, anti-tuberculosis agents, showing antitumor activity, anticancer used for treatment of cardiovascular disorder and controlling horticultural viral infection [3]. Activity of the substituted benzothiazole enhances on complex formation with suitable metal [3,4].

The wide range of application of the amide group ligands and its metal complexes aroused our interest to prepare a new series of some metal complexes.

Experimental

A-Material and Methods

1-General Procedure For the Prepared Ligands[4]

In a round bottom flask equipped with magnetic bar stirrer a mixture of (benzyl or ethanyl chloride) (0.06 mole) and (0.06 mole) of 2-amino benzothiazole with 2ml of triethylamine in 25 ml of THF was placed and refluxed for (2-3) hrs. After cooling, the excess of solvent was removed under vacuum and the solid separated was filtered and purified by dissolving in DMF or DMSO and reprecipitating from water or acetone. The steps of the synthesis of these ligands can be illustrated below:-

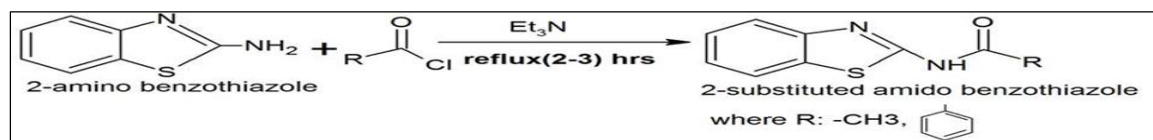


Fig.(1) Synthesis Steps of Ligands (B1 and B2).

2-Preparation of Ligand B1 complexes

The addition of ethanol solution of the suitable metal salt (Chloronic acid monohydrate and Cu nitrate tri hydrate) to an ethanol solution of 2-benzamido benzothiazole (B1) in 1:1 (ligand: metal) molar ratios was carried out. After reflux for 5 hrs, crystalline colored precipitates washed with distilled water, dried and recrystallized from ethanol and dried at 50°C, Table (1) Shows the physical properties of the prepared compounds.

3-Preparation of ligand B2 complexes

These complexes were prepared by the above method except refluxing for 7hrs. Table (1) shows the physical data of the prepared complexes.

B-Instrumentation

Elemental C.H.N.S analysis were carried out on a EM-017. mthinstrument, the FT-IR

spectra in the range (4000-200) cm^{-1} cut were recorded as KBr 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 Spectrophotometer in range (200-950) nm. The magnetic susceptibility values of the prepared complexes were obtained at room temperature using Magnetic Susceptibility Balance of Johnson 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 10^{-3}M using (WTW) Conductometer.

Table (1)

Physical data of new ligands(B1,B2)and their metal complexes.

Compound	Colour	m.p. °C	Yield %	M.Wt g mol^{-1}	Found (calc.)%				
					C	H	N	S	M
B1	Pale yellow	168-169	70.07	254	65.28 (66.14)	3.80 (3.93)	12.31 (11.02)	13.11 (12.59)	----
AuB1	Dark brown	170 d.	88.88	621.5	29.25 (30.80)	1.78 (2.57)	4.05 (4.50)	4.98 (5.14)	30.81 (31.61)
CuB1	Green	120 d.	60.78	942.1	35.96 (36.93)	3.18 (2.8)	10.90 (11.88)	6.04 (6.79)	13.36 (13.49)
B2	Light yellow	188-190	70.03	192	55.89 (56.25)	4.60 (4.16)	13.55 (14.58)	17.44 (16.66)	----
AuB2	Dark brown	198-200	93.75	536.47	21.38 (22.36)	1.42 (2.42)	6.14 (5.22)	6.27 (5.96)	35.81 (36.71)
CuB2	Green	120dec.	45.33	805.10	30.50 (29.81)	1.58 (1.98)	9.83 (10.43)	8.73 (7.95)	14.83 (15.77)

d=decomposition degree.

C-Theoretical Calculation

HyperChem-8 program is a sophisticated molecular modeler, editor and powerful computational package that are known for its quality, flexibility and easy of use, uniting 3D visualization and animation with quantum chemical calculations, mechanic and dynamic. HyperChem-8 can plot orbital functions resulting from semi-empirical quantum mechanical calculation, as well as the electrostatic potential. The total charge density or the total spin density can also be determined during a semi-empirical calculation. This

information is useful in determining reactivity and correlating calculation results with experimental data. Hyperchem-8 program offers ten semi-empirical molecular orbital methods, with options for organic and main group compounds, for transition metal complexes and spectral simulation [5]. ZINDO/1 level of semi-empirical method was used for calculation the heat of formation (ΔH_f°) and binding energy (ΔE_b) for all Cu (II) complexes, AMBER method used to calculate energies for Au(II) complexes. Electronic transition of the ligands calculated using

ZINDO/S method. Also electrostatic potential, HOMO, and LUMO for prepared ligands calculated by using this program.

Result and Discussion

1-IR Spectra

The IR spectra of the ligands are complicated due to the large number of groups which have overlapping regions. However few bands have been selected in order to observe the effect of complexation. The structurally significant IR bands for the free ligands.

(B1, B2) and their complexes are listed in Table (2). The free ligand (B1) shows strong bands at 1674, 1450, 1257 and 1651 cm^{-1} assigned to amide (I), amide (II), amide (III) and (C=N) respectively [1]. While the spectrum of the free ligand (B2) exhibits the absorption bands for amide (I), amide (II), amide (III) and (C=N) at 1697, 1446, 1269 and 1651 cm^{-1} respectively [6]. The most important different between the two spectra is, the stretching vibration of amide (I) band

appeared at higher frequency in the spectrum of the ligand B2 than it in the spectrum of ligand B1. In the spectra of B1 complexes the bands due to amide (I) and (C=N) group show shifts to the lower frequencies by ($\sim 23\text{-}78\text{cm}^{-1}$) respectively. These changes indicate that the uncharged amide oxygen and C=N groups take part in the coordination. More evidence the spectra of complexes exhibit new bands assigned to the (M-N), and (M-O) at 455-582 cm^{-1} for (AuB1), and 466-563 cm^{-1} for CuB1 respectively [7]. The spectra of B2 complexes also shows shifting of amide I and C=N bands to the lower frequencies by ($\sim 58\text{-}66\text{ cm}^{-1}$) respectively, suggesting collapse of these groups of the ligand (B2) in the complexes. More evidence the spectra also show new bands due to M-N, and M-O at 452-559 cm^{-1} for AuB2, and 474-543 cm^{-1} for CuB2 respectively[8]. The infrared spectra of all complexes exhibit a band at ($\sim 3383\text{-}3452$) which supports the presence of lactic held water or ethanol molecule.

Table (2)

Infrared Spectral Bands (cm^{-1}) and Their Assignments of the Ligands and Their Complexes.

Symbol	Amide I	$\nu(\text{NH})$	Amide II	$\nu(\text{C}=\text{N})$	$\nu(\text{C}-\text{S})$	$\nu(\text{M}-\text{O})$	$\nu(\text{M}-\text{N})$	others
B1	1674 s	3294 m	1450 m	1651 s	752 m	-----	-----	-----
AuB1	1639 s	3390 m	1462 sh	1597 w	752 sh	582 m	455 m	$\nu(\text{Au}-\text{Cl}), 327\text{ sh}$ $\nu(\text{EtOH}) 3390$
CuB1	1651 m	3332 m	1462 m	1573m	752 sh	563 vw	466 w	$\nu(\text{H}_2\text{O}) 3448\text{ b}$ $\delta(\text{H}_2\text{O}) 952\text{ w}$
B2	1697 s	3255 m	1446 m	1651 s	759 sh	-----	-----	-----
AuB2	1639 s	3298 m	1465 sh	1585 w	752 s	559 w	459 w	$\nu(\text{Au}-\text{Cl}), 324\text{ sh}$ $\nu(\text{EtOH}) 3383$
CuB2	1639 m	3336 m	1465 sh	1589 w	752 sh	543 w	474 w	$\nu(\text{EtOH}) 3452\text{ m}$

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

2-Electronic Spectral and Magnetic Moment Studies

The electronic absorption spectra are often very helpful in the evaluation of the results furnished by other methods of structural investigation. The electronic spectra of ligands (B1, B2) exhibit three bands at 251nm (39840 cm^{-1}) 272nm (36764cm^{-1}) 301nm (33222cm^{-1}) and 243 nm (41152cm^{-1}), 269 nm (37147cm^{-1}), and 298 nm (33557 cm^{-1}) for B1 and B2 respectively these bands may be due to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ respectively. The electronic spectra of the complexes showed, as

expected, different absorptions from that of the free ligands.

AuB1:- The electronic spectrum of Au(III)B1 complex showed three bands one at 24570 cm^{-1} which refer to $^1\text{A}_{1g} \rightarrow ^1\text{B}_{1g}$ transition, and the other appeared at 32154cm^{-1} which refer to $^1\text{A}_{1g} \rightarrow ^1\text{E}_g$ transition in square planner geometry[9]. The band at 38167 cm^{-1} may be due to charge transfer. Magnetic moment is (0.00 B.M) and the conductivity measurements for the prepared complex in DMF solvent at room temperature showed to be ionic .

CuB1: The electronic spectrum of the CuB1 complex exhibited only one a broad band d-d transition at 13333 cm^{-1} assigned to the ${}^2\text{E}_g \rightarrow {}^2\text{T}_2g$ transition which is in conformity with the octahedral configuration around the copper ion [10]. The spectrum also exhibits a bands at 24875, 33112 and 38167 cm^{-1} , which are assigned to charge transfer band .The value of (μ_{eff}) that measured for this complex is 0.99 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.

AuB2:- The electronic spectrum of Au(III)B2 complex was, showed two bands one at 25316 cm^{-1} which refer to ${}^1\text{A}_{1g} \rightarrow {}^1\text{B}_{1g}$ (ν_1) transition and the other

appeared at 29850 cm^{-1} which refer to ${}^1\text{A}_{1g} \rightarrow {}^1\text{E}_g(\nu_2)$ transition in square planer geometry[9]. The bands at 34482, 31746 and 31250 cm^{-1} may be due to charge transfer. Magnetic moment is diamagnetic and the conductivity measurements for the this complex in DMF solvent at room temperature showed to be ionic.

CuB2:- The spectrum of this complex showed a broad band at 12180 cm^{-1} assigned to the spin allowed transition ${}^2\text{E}_g \rightarrow {}^2\text{T}_2g$.The magnetic moment (0.97 B.M) of the diameric complex is in the range of octahedral geometry [11,12]. The spectrum also exhibits charge transfer bands at 25510, 27624 and 31250 cm^{-1} . Conductivity measurement of this complex showed that the complex was to be ionic.

Table (3)

Electronic spectra, magnetic moment, and Molar conductivity for the prepared metal complexes.

Compound	Absorption Bands(cm^{-1})	Assignment	μ_{eff} B.M.	μscm^{-1}	Suggested geometry
B1	33222 36764 39840	$n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	-----	-----	-----
AuB1	24570 32154 38167	${}^1\text{A}_{1g} \rightarrow {}^1\text{B}_{1g}^1$ $\text{A}_{1g} \rightarrow {}^1\text{E}_g$ $\text{L} \rightarrow \text{AuCT}$	0.00	76.0	Square planar
CuB1	13333 24875 33112 38167	${}^2\text{E}_g \rightarrow {}^2\text{T}_2g$ $\text{L} \rightarrow \text{CuCTL}$ $\rightarrow \text{CuCTL} \rightarrow$ CuCT	0.99	38.6	O.h
B2	3557 37174 41152	$n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	-----	-----	-----
AuB2	25319 29850 34482 31746,31250	${}^1\text{A}_{1g} \rightarrow {}^1\text{B}_{1g}$ ${}^1\text{A}_{1g} \rightarrow {}^1\text{E}_g$ $\text{L} \rightarrow \text{AuCT}$ $\text{L} \rightarrow \text{AuCT}$	0.00	80.9	Square planar
CuB2	12180 25510 27624 31250	${}^2\text{E}_g \rightarrow {}^2\text{T}_2g$ $\text{L} \rightarrow \text{CuCTL}$ $\rightarrow \text{CuCTL} \rightarrow$ CuCT	1.02	102.2	O.h

ILCT: Internal ligand charge transfer.

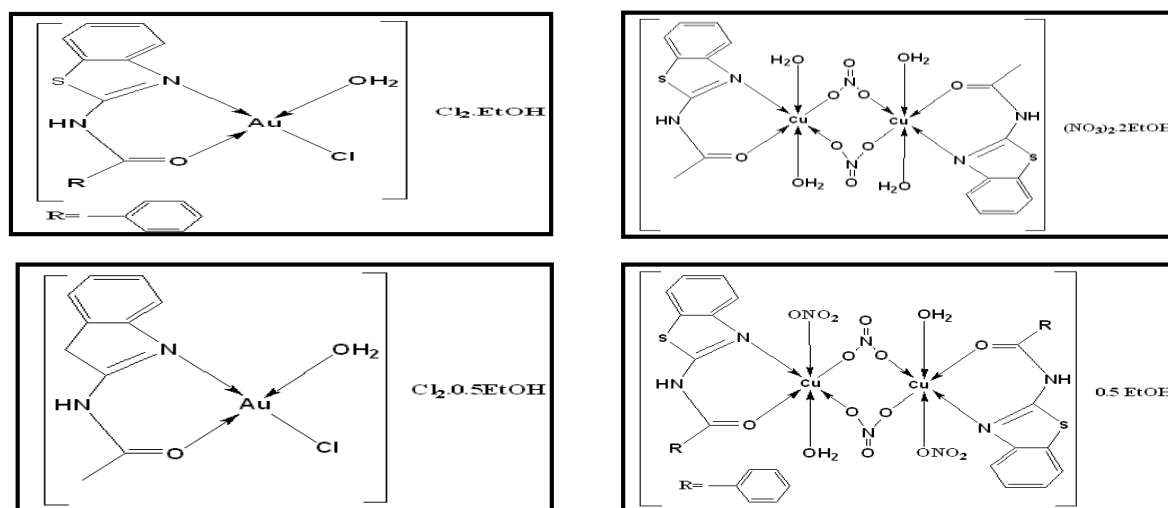


Fig.(2) Proposed Structure of Prepared Complexes.

3-Study of complexes formation in solution

Complexes of ligands B1, and B2 with metal ions were studied in solution using ethanol as a solvent, in order to determine [M/L] ratio in the complexes follow molar ratio method [13]. A series of solutions were prepared having a constant concentration (10^{-3} M) of metal ion and ligand. The [M/L] ratio determined from the relationship between the absorption of the 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 treatment

The program Hyper chem-8 was used for semi-empirical molecular mechanic calculation. The heat of formation (ΔH_f°), binding energy (ΔE_b) and dipole moment (μ) for free ligands and complexes were calculated using ZINDO/1 and AMBER methods, Table(4). Also PM3 was used for evaluating the vibrations of new ligands (B1 and B2), Table (5) compares the theoretically calculated wave numbers with experimental values.

Table (4)
Conformation Energetic (in $K.J.mol^{-1}$) and Dipole Moment (in Debye) for Ligand L2 and its Metal Complexes.

Compound	ZINDO/1				AMBER
	ΔH_f°	ΔH_f°	ΔE_b	μ	$\Delta H_f^\circ = \Delta E_b$
B1	208.81	-26628.05	-40290.65	3.85	-----
AuB1	-----	-----	-----	-----	355.57
CuB1	491.64	-59041.48	-89482.73	6.09	-----
B2	59.90	-18526.911	-28178.50	3.66	-----
AuB2	-----	-----	-----	-----	111.67
CuB2	3623.85	-47205.88	-70498.29	8.33	-----

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

a-Optimization Geometry Energies and Vibrational for Free Ligands B1 and B2.

The result of ZINDO/1 method of calculations in gas phase for the heat of formation, binding energy and dipole moment of new benzothiazole derivatives were tabulated in Table (4).

The vibration spectra of free ligands have been calculated. As shown in Table (5). The theoretically calculated wave number for the ligands (B1, B2) shows the same deviations

from the experimental values. These deviations are generally acceptable in theoretical calculations.

Table (5)
Comparison of experimental and theoretical vibration frequencies for free ligands.

Symbol	$\nu(N-H)$	$\nu Amide(I)$	$\nu C=N$	$\nu AmideII$
B1	3294.42*	1674.21*	1651.07*	1450.47*
	3314.98**	1903.14**	1649.17**	1439.19**
	(0.6)***	(13)***	(-0.1)***	(-0.7)***
B2	3255.84*	1697.36*	1651.07*	1446.77*
	3345.87**	1941.85**	1638.88**	1401.64**
	(2.6)***	(14)***	(-0.7)***	(-3.1)***

Where*:Experimental frequenc, **:Theoretical frequency,***: Error% due to main different in the experimental measurements and theoretical treatment of vibrational spectra.

b-Electronic Transition

The theoretical UV-spectra of the ligands were calculated using ZINDO/S method and showed some deviations from the experimental values. These deviations are generally acceptable in theoretical calculations [14]. The serial number of atoms was plotted in the structure of ligands in order to determine the type of orbitals than type of transition. Theoretical UV-spectrum of Ligand B1 showed two bands at 249.9 and 295.7 nm which related to $\pi \rightarrow \pi^*$ (O18 \rightarrow C11) and $n \rightarrow \pi^*$

(N7 \rightarrow C8) transitions respectively, while the experimental spectrum showed three bands at 251.00, 272.50, and 301.50 nm assigned to $\pi \rightarrow \pi^*$, and $n \rightarrow \pi^*$ respectively. Theoretical spectrum of B2 showed two peaks at 256.9 and 273.7 nm the quantum data indicate these peaks are generated from $\pi \rightarrow \pi^*$ (O13 \rightarrow C11) and $n \rightarrow \pi^*$ (N7 \rightarrow C8) transitions respectively. The experimental spectrum of this ligand showed three absorption bands at 243, 269, and 298 which assigned to $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ respectively.

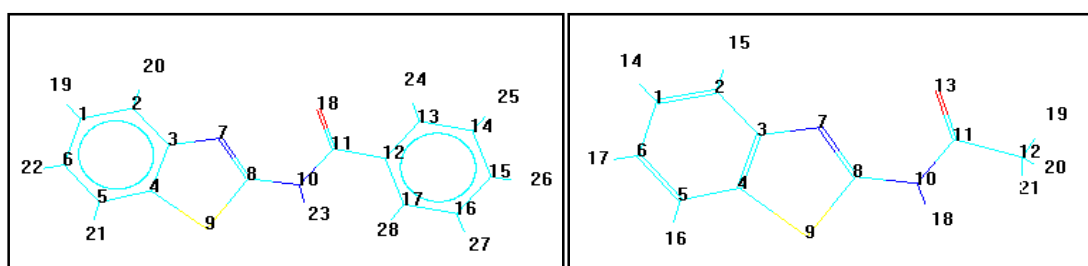


Fig.(3) Serial Number of Atoms View of Ligands.

c-Electronic Potential (E.P)

The electrostatic potential (E.P.) describes the interaction of energy of the molecular system with a positive point charge (E.P) of the ligands were plotted as two and three dimension contours to investigate the reactive sites of the molecules. Also, one can interpret the stereochemistry and rates of many reactions involving soft electrophiles and nucleophiles 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. (4). The results shows that the LUMO of transition metal ion prefers to react with HOMO of donor atoms of ligand.

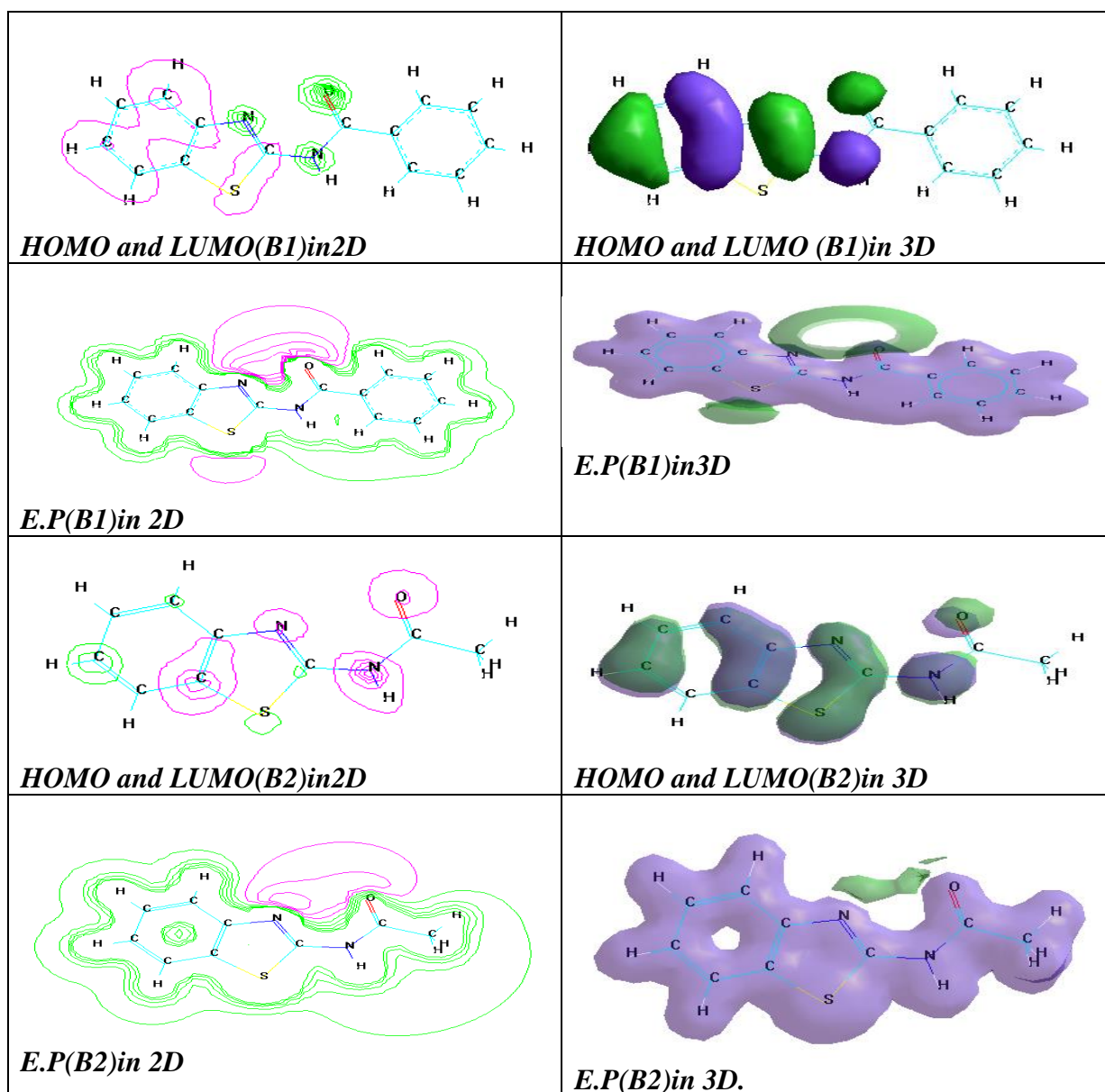


Fig. (4) HOMO, LUMO and Electrostatic potential as 2D and 3D counters for free ligands.

Conclusion

The ligands behave as a bidentate chelating with oxygen and nitrogen atoms, to form an octahedral geometry for the copper complexes and a square planar geometry for the Gold complexes. The theoretical calculation data of the frequencies for the ligands and their complexes agreed and help to assign unambiguously the most diagnostic bands. Theoretical electronic transitions helped to assign type of transition. Calculation of energies give information about the most stable structure.

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الخلاصة

جرى تحضير معقدات جديدة لليكاند ٢- بنزمايدوبينزو ثايزول والليكاند ٢- استمايدوبينزو ثايزول مع ايونات العناصر الذهب الثلاثي والنحاس الثنائي في وسط كحولي. شخّصت المركبات المحضرة بواسطة تقنية الاشعة تحت الحمراء والاشعة فوق البنفسجية-المرئية والحساسية المغناطيسية والامتصاص الذري اللهي وكذلك التحليل الدقيق للعناصر والتوصيلية الكهربائية. من خلال الدراسة الطيفية اقترح الشكل المربع المستوي على هيئة مونمر لمعقدات الذهب بينما اقترح الشكل الثماني السطوح على هيئة دايمر لمعقدات النحاس اجريت المعالجة النظرية باستخدام الطرق شبة التجريبية لحساب حرارة التكوين وطاقة الترابط والعزم ثنائي القطب لمعقدات النحاس بينما استخدمت طريقة AMBER لمعقدات الذهب. كذلك تم حساب الترددات الاهتزازية والجهد الالكتروستاتيكي والمواقع الفعالة للاوربييتال الواقع في اعلى مستوى طاقة والذي يحتوي الكترون واحد واكثر والاوربييتال في اوطأ مستوى طاقة والذي لا يحتوي الكترونات لليكاندات المحضرة.