

Synthesis, Spectral Studies, and Theoretical Treatment of New Ni(II), and Co(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-actamido benzothiazole(B2) with metal ions Ni(II), and Co(II) were prepared in alcoholic medium. The prepared complexes were characterized by FT-IR and electronic spectroscopy, Magnetic susceptibility, Flame Atomic Absorption technique as well as elemental analysis and conductivity measurement. From the spectral studies, an octahedral monomer structure proposed for Ni(II) complexes, and a tetrahedral monomer structure for Co(II) complexes. Semi-empirical methods (PM3, and ZINDO/1) were carried out to evaluate the heat formation (ΔH°) binding energy (ΔE_b) and dipole moment (μ) for all metal complexes. Also vibration frequencies, Electrostatic potential, HOMO and LUMO energies for ligands were calculated.

Key words: Benzamidobenzothiazole; Actamidobenzothiazole; Metal complexes.

Introduction:

The interest in coordination chemistry is increasing continuously with the synthesis and characterization of large number of transition complexes with heterocyclic ligands containing nitrogen, oxygen and sulfur donors [1]. The aromatic benzothiazole nucleus is associated with a variety of antihistamine activity pharmacological actions [2] such as fungicidal [3] and leishmanicides activities [4-a]. These activities are probably due to the presence of the -N=C-S group [4-b]. The amide bond [-C(O)NH-] has long attracted much attention since it is an essential building unit in proteins. The high stability of the amide linkage toward hydrolysis is of crucial importance to biological systems, since it allows the construction of peptides from relatively simple amino acid precursors [5]. The coordination chemistry of amide ligands is an

important part of a number of chemical problems [5].

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.

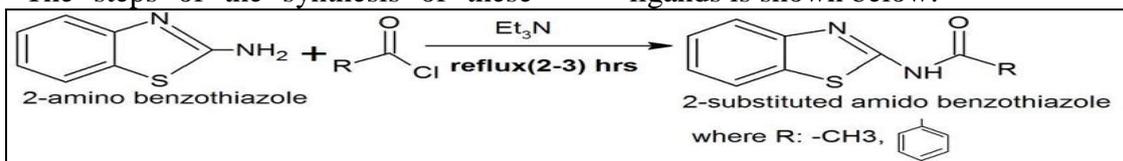
Material and methods:

1-General procedure for prepared ligands [4-a].

In around 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 at DMF or DMSO and reprecipitating from water or acetone.

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The steps of the synthesis of these ligands is shown below:-



Fig(1):Scheme of synthesis for ligands(B1,and B2).

2-Preparation of ligand

B1complexes:-

An ethanolic solution of the suitable metal salt(1mmole nickel nitrate hexahydrate, and cobalt nitrate hexahydrate) was added to an ethanolic solution of 0.25g(1mmole) of 2-benzamido benzothiazole(**B1**) in 1:1(ligand :metal)molar ratios, refluxed for 5hrs, colored precipitates formed washed with distilled water, dried and recrystallized from ethanol and dried at 50°C Table (1) shows the physical properties of the prepared complexes.

3-Preparation of ligand B2 complexes:-These complexes were prepared by the same way as above except refluxing for 7hrs. Table (1) shows the physical data of the prepared complexes.

Instrumentation:-

Elemental C.H.N.S analysis was carried out on a EM-017.mth instrument in laboratories of Chemistry

Department, College of Science, University of Babylon.The FT-IR spectra in the range (4000-400)cm⁻¹were recorded as KBr disc on IR-Prestige-21,Single beam path Laser, Shimadzu Fourier Transform infrared Spectrophotometer .The spectra were recorded in the laboratories of IbnSina State company, 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 Absorptionmeasurements of the prepared complexes were obtained using ShimadzuAtomic Absorption 680 Flame Spectrophotometer .The Conductivity values of the prepared complexes were measured using DMF as solvent, the concentration 10⁻³M using(WTW)Conductometer.

Table(1):Physical data of new ligands(B1 & B2) and their complexes .

Comp.	Color	m.p/° c	Found(Calculated)					M.Wt g.mole ⁻¹	Yield%
			C%	H%	N%	S%	M%		
B1	Pale yellow	167-168	65.28 (66.14)	3.80 (3.93)	12.31 (11.02)	13.22 (12.59)	-----	254.00	70.12
B2	Light yellow	188-190	55.89 (56.25)	4.60 (4.16)	13.55 (14.58)	16.66 (17.43)	-----	192.00	74.88
NiB1	Light yellow	120-122	30.99 (31.89)	3.93 (3.79)	9.95 (10.63)	5.26 (6.07)	10.22 (11.14)	544.69	81.25
CoB1	Greenish blue	128-130	34.48 (35.50)	2.41 (2.90)	10.84 (11.80)	5.93 (6.70)	12.00 (12.46)	472.93	65.33
NiB2	Pale green	118 dec.	22.48 (23.24)	2.73 (3.81)	11.67 (12.05)	6.56 (6.88)	12.13 (12.61)	464.70	93.32
CoB2	Greenish blue	82 dec.	23.57 (24.10)	2.99 (3.79)	11.76 (12.51)	6.31 (7.15)	12.29 (13.16)	447.00	76.21

Where: d=decomposition degree , M=metal

Theoretical calculation

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. Hyper Chem offers ten semi-empirical molecular orbital methods, with options for organic and main group compounds, for transition metal complexes and spectral simulation[6]. PM3 level of semi-empirical method was used for calculation the heat of formation ($\Delta H^{\circ}f$) and binding energy (ΔE_b) for all metal complexes. Electrostatic potential, HOMO, and LUMO for ligands B1, and B2 calculated by using this program.

Results and Discussion:

The elemental analysis showed 1:1(metal:ligand) stoichiometry for the complexes. The analytical data together with some physical properties of the complexes are summarized in Table (1). They agree well with the formula

$ML(NO_3)_2 \cdot nH_2O$ (where M=Ni(II) and Co(II), L=2-

benzamidobenzothiazole(B1), and 2-actamidobenzothiazole (B2)=n=1-2. The complexes were insoluble in common organic solvents, but soluble in DMF and DMSO. The molar conductance values of the complexes indicate their 1:1 electrolytic nature.

1-IR spectra

The IR spectra of the ligands are complicated due to the large

number of the 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 and B2), and their complexes are listed in Table (2). The spectrum of free ligand (B1) shows strong bands at 1674, 1450, 1257, and 1651cm^{-1} assigned to amide (I), amide(II), amide (III), and (C=N) respectively[5], 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 1651cm^{-1} respectively[7], Figures(2,3). The most important difference between the two spectrum is the stretching vibration of amide (I) band appeared at higher frequency in the spectrum of the ligand B2. In the spectra of B1 complexes, the bands due to amide (I) and (C=N) group show shifts to the lower frequencies ($\sim 20\text{-}35$ and $\sim 93\text{cm}^{-1}$) respectively. These changes indicated that the uncharged amide oxygen and C=N groups took part in the coordination. More evidence of the spectra of complexes exhibited new bands assigned to the (M-O), and (M-N) at $466\text{-}594.\text{cm}^{-1}$ for (NiB1), and $466\text{-}582\text{ cm}^{-1}$ for CoB1 respectively [8]. The spectrum of B2 complexes also shows shifting of amide I and C=N bands to the lower frequencies (~ 31 and $27\text{-}47\text{ cm}^{-1}$) respectively, suggesting collapse of these groups of the ligand (B2) in the complexes. More evidence of the spectrum also showed new bands due to M-O, and M-N at $462\text{-}559\text{ cm}^{-1}$ for NiB2, and $424\text{-}543\text{ cm}^{-1}$ for CoB2 respectively[9]. The infrared spectra of all complexes exhibited broad band at ($\sim 3383\text{-}3410$) which supports the presence of lactic held water molecules out of coordination sphere.

Table (2): Infrared spectral bands (cm⁻¹) and their assignments of ligands and their metal complexes

Com.	v(H ₂ O)	v(NH)	Amide (I)	v(C=N)	Amide (II)	Amide (III)	M- v(O)	M- v(N)	δH ₂ O
B1	-----	3294 m	1674 s	1651 s	1450 m	1257 m	-----	-----	-----
B2	-----	3255 m	1697 s	1651 s	1446 s	1269 sh	-----	-----	-----
NiB1	3410.15 b	3375 b	1639 s	1558 m	1450m	1249 w	594 vw	466 m	810 w
CoB1	3390.86 b	3350 b	1654 s	1558 m	1450m	1257w	582 vw	466 w	810 w
NiB2	3383.14 b	3350 b	1666 s	1604 m	1430s	1249 m	559 vw	462 w	825 w
CoB2	3400.00 b	3282 b	1666 m	1624 m	1425 s	1249 m	543 vw	424 w	829 w

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

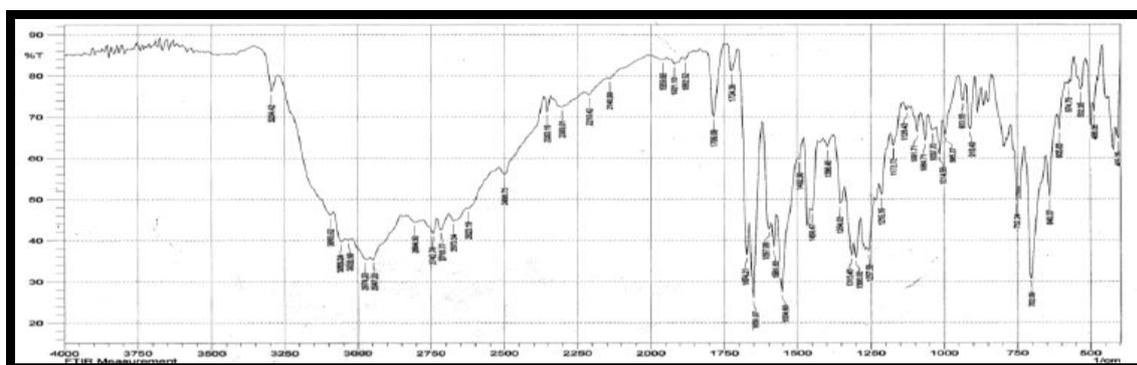


Fig (2): FTIR spectrum of ligand B1

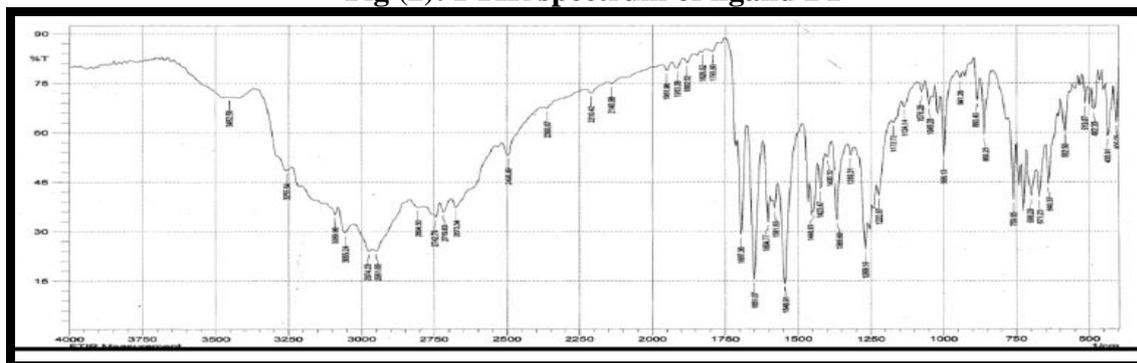


Fig (3): FTIR spectrum of ligand B2

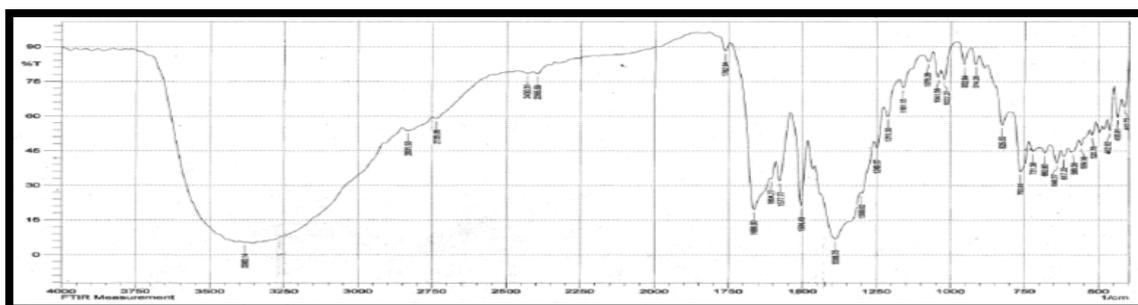


Fig (4): FTIR spectrum of NiB2

Electronic spectral and Magnetic moment studies

The electronic spectra of ligands (B_1 and B_2) exhibits three bands for everyone at 251nm (39840 cm^{-1}), 272nm (36764 cm^{-1}), 301nm (33222 cm^{-1}), and 243nm (41152 cm^{-1}), and 269nm (37147 cm^{-1}), and 298nm (33557 cm^{-1}) for B_1 and B_2 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. The green colour of NiB1 complex is postulated to be distorted octahedral with their respective values. The spectrum of (NiB1) complex exhibits bands in the region 27472, and 18761 cm^{-1} , which are assigned to the ${}^3A_{2g} \rightarrow {}^3T_{1g(P)} v_3$, and ${}^3A_{2g} \rightarrow {}^3T_{1g(F)} v_2$, transitions [5]. The band at 14814 cm^{-1} may be assigned to the spin forbidden transition ${}^3A_{2g} \rightarrow {}^1E_g$. The value of the first transition v_1 was calculated using Tanabe Sugano diagram. The spectrum also exhibits a charge transfer bands at 36900, and 32573 cm^{-1} . The electronic spectrum of pale green NiB2 Complex was identical with the spectrum of NiB1 complex, which shows bands at 26666, and 18691 cm^{-1} , assigned to ${}^3A_{2g} \rightarrow {}^3T_{1g(P)} v_3$ and ${}^3A_{2g} \rightarrow {}^3T_{1g(F)} v_2$, respectively [10]. The band at 14084 cm^{-1} was due to spin forbidden transition ${}^3A_{2g} \rightarrow {}^1E_g$. The value of first transition v_1 was calculated. The spectrum also exhibits a charge transfer band at 34482 cm^{-1} . The octahedral geometry of NiB₁, and NiB₂ complexes is further supported by the value of the v_2/v_1 ratio, which are 1.64 for both complexes [5].

The nickel complexes have a magnetic moment in the range (3.32-

3.34) B.M, reveals a spin free octahedral configuration. The electronic spectrum of CoB1 complex exhibits three bands at 17857, 16420, and 14947 cm^{-1} due to the third transition v_3 . The value of second transition ${}^4A_2 \rightarrow {}^4T_{1(F)}(v_2)$ was calculated theoretically and found equal to 5147 cm^{-1} using the following equation [5] :-

$$B' = v_3 + v_2 - 3v_1/15$$

The first transition ${}^4A_2 \rightarrow {}^4T_2(v_1)$ could not be observed since it is expected to appear in a range out of instrument scale so it was calculated from infrared spectrum, and found to be 3400 cm^{-1} . The electronic spectrum of greenish blue Co(II) (CoB2) complex was identical with spectrum of CoB1 complex also exhibits three bands at 17699, 16433, and 15015 cm^{-1} due to third transition v_3 . The value of second transition ${}^4A_2 \rightarrow {}^4T_{1(F)}(v_2)$ calculated and found equal to 5033 cm^{-1} using the same equation above. The value of first transition ${}^4A_2 \rightarrow {}^4T_2(v_1)$ was calculated using Infrared spectrum. The magnetic moment in the range of (4.55-4.61) B.M for the Co(II) complexes suggests a high spin arrangement [11,12]. The value of β for all prepared complexes was calculated and found quit low (0.72-0.78) suggests a considerable covalent bonding between the metal ion and ligand atoms. The molar conductivity measurement suggests ionic character for all the complexes. The values of B' , Dq , and $15B'$ for all complexes were calculated, Table (3). According to these data and that obtained from FTIR, C.H.N.S, as well as Atomic absorption and Molar ratio the following structures can be suggested.

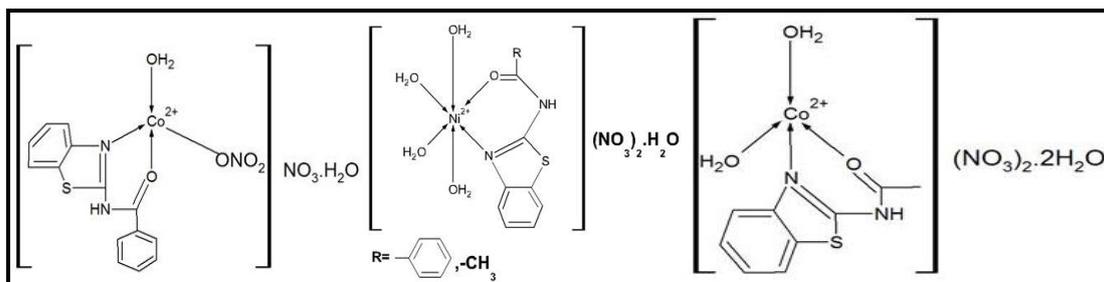


Fig (5): The proposed structure of the prepared complexes.

Table(3): Electronic spectra, magnetic moment, and Molar conductivity for the prepared metal complexes.

Comp.	Bands cm^{-1}	Assignment	$^{\circ}\text{B}$	B'	β	Dq	$15\text{B}'$	μ effect B.M	Molar cond. μscm^{-1}	Suggested structure
NiB1	11433(cal) 18761 27472 36900 32573	$^3\text{A}_{2g} \rightarrow ^3\text{T}_{2g}$ $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g(\text{F})}$ $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g(\text{P})}$ ILCT ILCT	1035	772.4	0.74	1143	795	3.32	119	Octahedral
CoB1	3400 5147(calc.) 16408(av.)	$^4\text{A}_2 \rightarrow ^4\text{T}_2$ $^4\text{A}_2 \rightarrow ^4\text{T}_{1(\text{F})}$ $^4\text{A}_2 \rightarrow ^4\text{T}_{1(\text{P})}$	970	757.0	0.78	378.5	11100	4.55	87.1	Tetrahedral
NiB2	11190(cal) 18691 26666 34482	$^3\text{A}_{2g} \rightarrow ^3\text{T}_{2g}$ $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g(\text{F})}$ $^3\text{A}_{2g} \rightarrow ^3\text{T}_{1g(\text{P})}$ ILCT	1035	746.6	0.72	1119	11190	3.34	107	Octahedral
CoB2	3420 5033(calc.) 16387(av.)	$^4\text{A}_2 \rightarrow ^4\text{T}_2$ $^4\text{A}_2 \rightarrow ^4\text{T}_{1(\text{F})}$ $^4\text{A}_2 \rightarrow ^4\text{T}_{1(\text{P})}$	970	744.1	0.76	364.5	11160	4.61	115.5	Tetrahedral

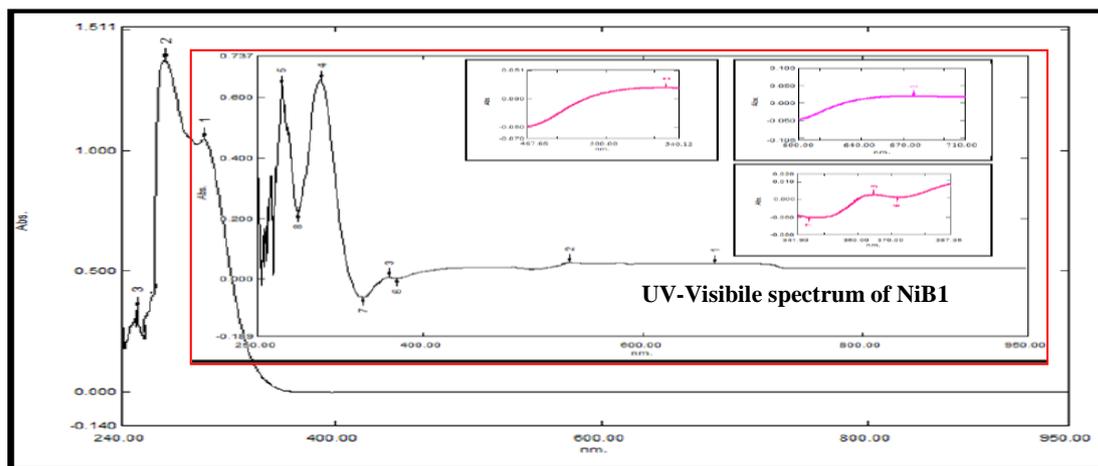


Fig (6):Electronic spectrum of B1and NiB1

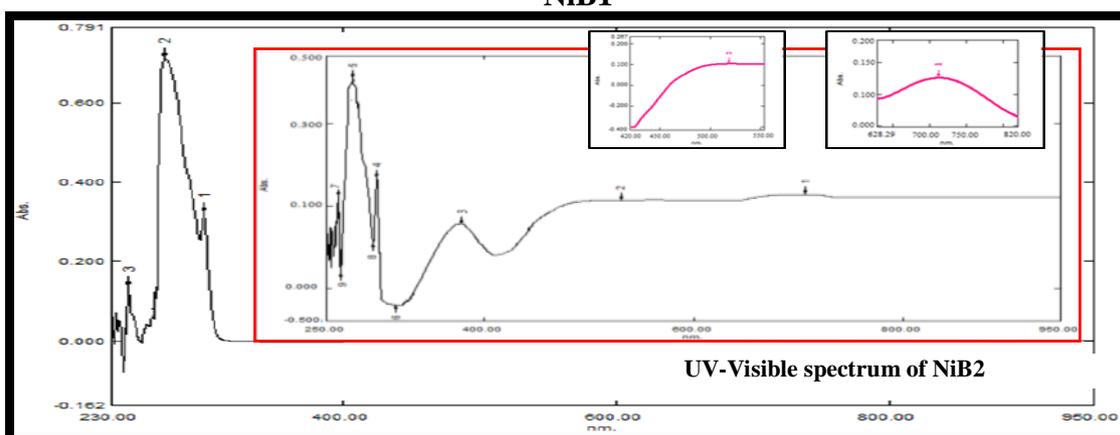


Fig (7):Electronic spectrum of B2 and NiB2

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 following molar ratio method[13]. A series of solutions were prepared having a constant concentration (10⁻³M) 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.

Theoretical treatment

The program Hyper chem-8 was used for semi –empirical molecular mechanic calculation .The heat of formation $\Delta H^{\circ}f$, binding energy(ΔE_b)and dipole moment (μ) for free ligands and complexes were calculated by PM3,and ZINDO/1 methods, Tables (4), and(5). Also PM3 was used for evaluating the vibrations of new ligands (B₁ and B₂), Table (6) compares the theoretically calculated wave numbers with experimental values.

Table(4):The calculated energies(in KJmol^{-1}) and dipole moment (in Debye) for ligand B1 and its complexes

Comp.	PM3			ZINDO/1		
	$\Delta\text{H}^\circ\text{f}$	ΔE_b	μ	$\Delta\text{H}^\circ\text{f}$	ΔE_b	μ
B₁	208.81	-13447.79	3.21	-26628.05	-40290.65	4.12
NiB1	-239.35	-17072.81	6.17	-31132.73	-47966.18	7.65
CoB1	-537.96	-14923.44	2.61	-28372.56	-43833.98	8.42

Table(5):The calculated energies(in KJmol^{-1}) and dipole moment (in Debye) for ligand B₂ and its complexes.

Comp.	PM3			ZINDO/1		
	$\Delta\text{H}^\circ\text{f}$	ΔE_b	μ	$\Delta\text{H}^\circ\text{f}$	ΔE_b	μ
B₂	59.90	-9591.69	3.61	-18526.91	-28178.50	3.66
NiB2	-287.99	-13110.44	6.24	-22875.76	-35698.20	4.54
CoB2	-363.84	-11086.54	2.97	-20909.49	-32359.89	8.48

As shown in Tables 4 and 5, the binding energy and energy required for formation of the compounds can be arranged as follows:

$$1-\Delta\text{H}^\circ\text{f}(\text{NiB}_1) < \Delta\text{H}^\circ\text{f}(\text{B}_1), \Delta\text{H}^\circ\text{f}(\text{CoB}_1) < \Delta\text{H}^\circ\text{f}(\text{B}_1)$$

$$2-\Delta\text{E}_\text{b}(\text{NiB}_2) < \Delta\text{E}_\text{b}(\text{B}_2), \Delta\text{E}_\text{b}(\text{CoB}_2) < \Delta\text{E}_\text{b}(\text{B}_2)$$

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

Optimization geometry energies and vibrational for free ligands B₁, and B₂

The result of PM3 method of calculations in gas phase for the heat of formation, binding energy, and dipole moment of new benzothiazole derivatives were tabulated in Tables (4), and(5). The vibration spectra of free ligands have been calculated, as shown in Table (6). 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. The most diagnostic calculated vibrational frequencies were chosen for the assignment of ligands which are included in Table (6), Figures (9), and(10).

Table (6): Comparison of experimental and theoretical vibration frequencies for free ligands(B₁ and B₂).

Symb.	$\nu(\text{N-H})$	$\nu\text{Amide(I)}$	$\nu(\text{C=N})$	$\nu\text{AmideII}$
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)**8	(-0.7)***	(-3.1)***

Where *: Experimental frequency, **: Theoretical frequency

***: Error% due to main different in the experimental measurements and theoretical treatment of vibrational spectra

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 and LUMO).Overlap between the HOMO and LUMO is a governing factor in many reactions. The HOMO and LUMO values were plotted in three dimension counters to get more information about these molecules Figure (8). The results showed that the LUMO of transition metal ion prefers to react with HOMO of donor atoms of ligands.

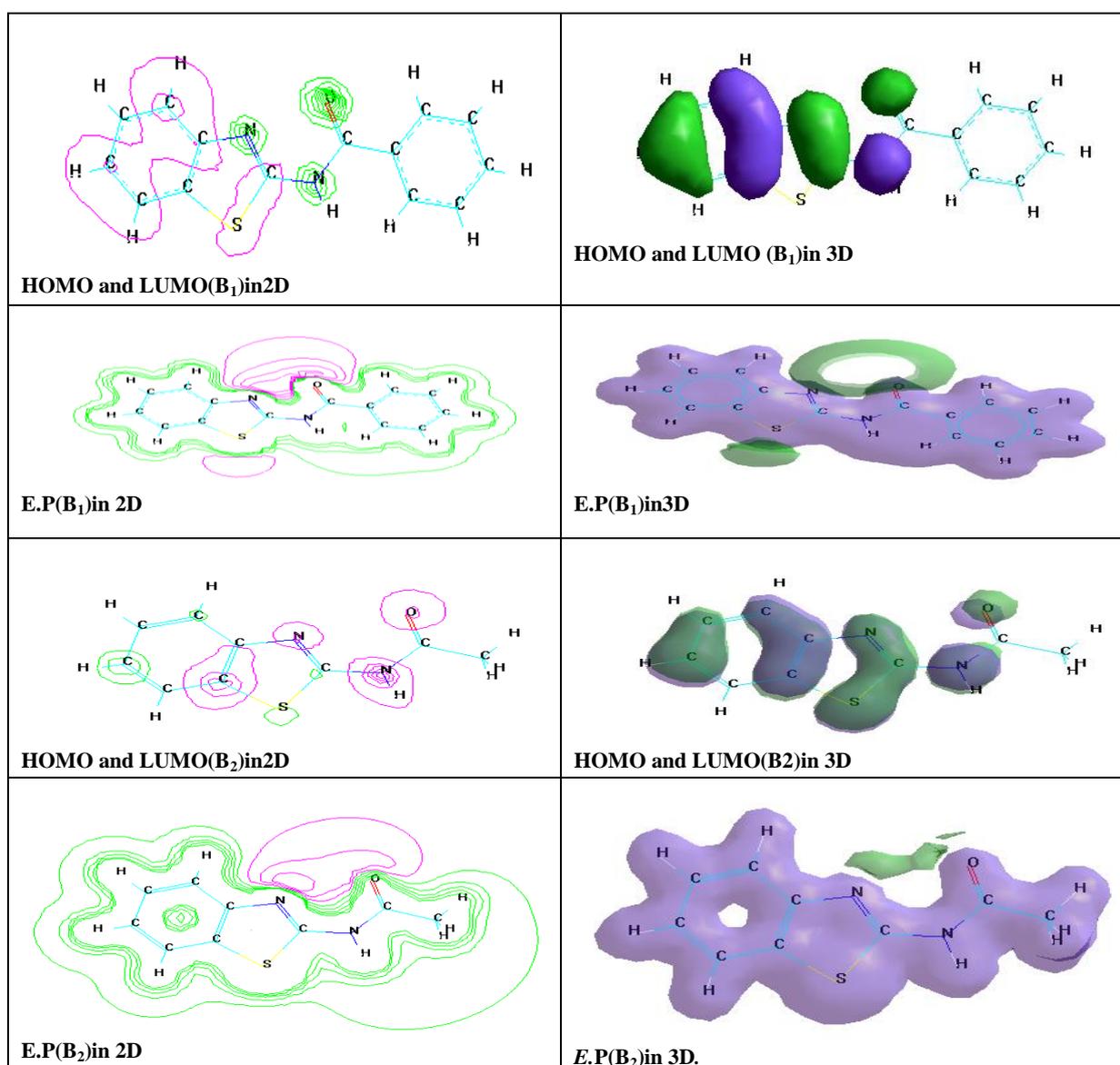


Fig (8):HOMO , LUMO and Electrostatic potential as 2Dand 3D counters for free ligands.

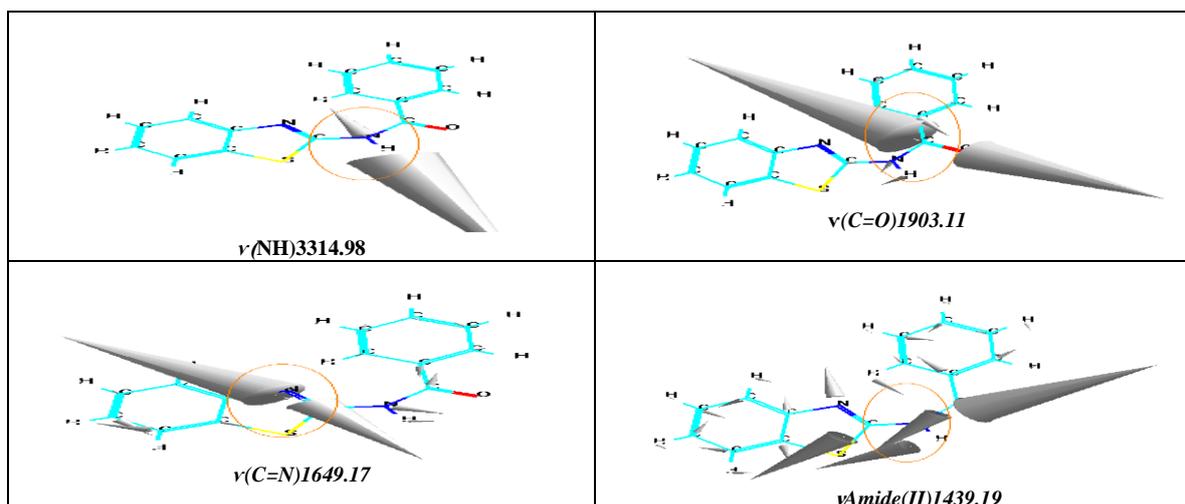


Fig (9): Calculated vibrational frequencies of 2-(benzamido) benzothiazole(B1)

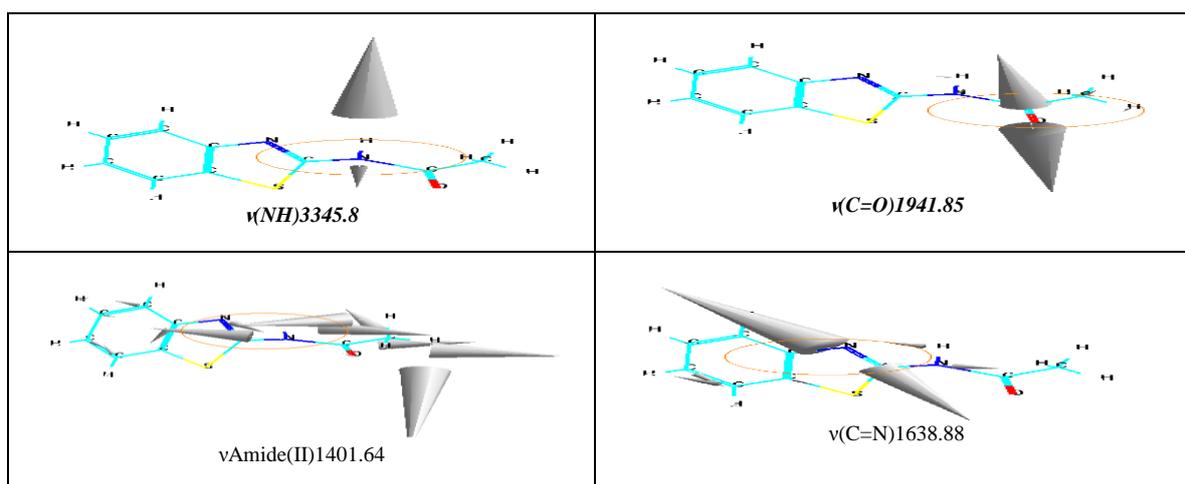


Fig (10): Calculated vibrational frequencies of 2-(actamido) benzothiazole(B2)

Conclusion

The ligands behave as a bidentate chelating with oxygen and nitrogen atoms, to form an octahedral geometry for the nickel complexes and a tetrahedral geometry for the cobalt complexes. The theoretical calculation data of the frequencies for the ligands and their complexes agreed and help to assign an ambiguously the most diagnostic bands.

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تحضير ودراسة طيفية ومعالجة نظرية لمعقدات النيكل الثنائي والكوبلت
الثنائي لليكاندات ثنائية السن (2-بنزومايدوبنزوثايزول و 2-
استمايدوبنزوثايزول)

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الخلاصة:

جرى تحضير معقدات جديدة لليكاند 2-بنزومايدوبنزوثايزول والليكاند 2-استمايدوبنزوثايزول مع ايونات العناصر النيكل الثنائي والكوبلت الثنائي في وسط كحولي. شخصت 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 الثماني السطوح لمعقدات النيكل والشكل الرباعي السطوح لمعقدات الكوبلت. اجريت المعالجة النظرية باستخدام الطرق شبة التجريبية لحساب حرارة التكوين وطاقة الترابط والعزم ثنائي القطب للمعقدات المحضرة. كذلك تم حساب الترددات الاهتزازية والجهد الالكتروستاتيكي والمواقع الفعالة للاوربتال الواقع في اعلى مستوى طاقة والذي يحتوي الكترون واحد او اكثر والاوربتال في اوطأ مستوى طاقة والذي لا يحتوي الكترونات لليكاندات المحضرة.