Synthesis, Characterization and Theoretical Study of Some Mixed-ligand Complexes of 2-Quinoline Carboxylic Acid and 4,4´-dimethyl,2,2´-Bipyridyl with Some Transition Metal Ions

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Abstract

   New mixed ligand complexes have been prepared by the reaction of Quinoline- 2-Carboxylic Acid (HL1) and 4,4´ -dimethyl,2,2´-Bipyridyl (L2) with Co(II),Ni(II) Cu(II), Zn(II), Pd(II) and Au(III) ions. The newly prepared complexes were isolated and characterized by (FT-IR) and (UV-Vis) spectroscopy, elemental analysis, flame atomic absorption technique, thermo gravimetric analysis, in addition to magnetic susceptibility and conductivity measurements. A theoretical treatment of these ligands and prepared complexes in gas phase were studied using Hyper chem.8 program, moreover, ligands in gas phase also have been studied using Gaussian program (GaussView Currently Available Versions (5.0.9) along with Gaussian 09 which is the latest in the Gaussian series of programs).

Keywords: Quinoline-2-Carboxylic Acid, 4,4´-dimethyl,2,2´-Bipyridyl, Hyperchem.8,spectroscopy, Theoretical treatment, Gaussian program.

1.Introduction

   Quinoline carboxylic acids and their analogues show a wide variety of medicinal properties including antitumor [1], antiviral [2], and estrogenic activity [3]. Recent demonstrations reveal that quinoline-2-carboxylic acid can be used as potential anticancer agents [4], and a biological compound involved in the metabolism of tryptophan. It is a strong chelator that provides the donor set similar to that responsible for binding metal ion in pyrroloquinilnequinone cofactor of quinoprotein family [5]. 2,2´-Bipyridine is known to form stable chelate complexes even with low valent transition metal ions [6]. Today, it is even one of the most widely used chelate systems in coordination chemistry and in recent years has also become a very popular ligand in supramolecular and macromolecular chemistry [7]. A quinoline-2-carboxylic acid and co-ligand 4,4´-dimethyl-2,2´-Bipyridyl did not receive any attention in spite of well-defined applications of both molecules. Hence, it was thought to explore the study, synthesis and characterization of some new complexes of quinoline-2-carboxylic acid and co- ligand 4,4´dimethyl-2,2´-Bipyridyl as mixed ligand complexes.

2. Experimental

2.1. Physical Measurements and Analysis

   Melting point apparatus of Gallen Kamp M.F.B-60 was used to measure melting points of all compounds.FT-IR spectra were recorded as CsI discs using FT-IR3800 Shimadzu in the range of (4000-200 cm^{-1}). Electronic spectra were obtained using UV-1650PC Spectrophotometer at room temperature in DMF solvent. Conductivity was measured by capacitor analyzer in DMF solution (10^{-3} M) at room temperature using (WTW) Conductometer. Elemental analysis was performed by using EM-017mth instrument.

   Magnetic susceptibility measurements were obtained at 25 °C Magnetic Susceptibility Balance of Johnson matty catalytic system division, England. The metal percent of all the complexes were determined by using GBS-933 Flam plus Atomic Absorption Spectrophotometer. The thermal analysis of all the prepared complexes have been carried out by 4000 Perkin–Elmer thermal analyzer maintained at a 20.00 °C min^{-1} heating rate.

2.2. Synthesis of Metal complexes

   A solution containing the primary ligand Quinoline-2-Carboxylic acid in 10 ml of absolute ethanol, and the secondary ligand 4,4/-dimethyl-2,2/- Bipyridyl in 5 ml of absolute ethanol were added to a 5 ml warm

absolute ethanol of metal salts $Co(NO_3)_2.6H_2O$, $Ni(NO_3)_2.6H_2O$, $Cu(NO_3)_2.3H_2O$, $(CH_3COO)_2Zn.2H_2O$, $PdCl_2$, and $HAuCl_4.H_2O$ in molar ratio 1:1:1 respectively. The mixture was heated and refluxed with stirring for (3-4) hrs. The colored precipitates were filtered, washed several times with ethanol, and finally recrystalized by ether-ethanol mixture then dried using desiccators.

3. Results and Discussion

Some physical properties and data of the ligands (HL1) and (L2) with their metal complexes are given in Table (1). The molar conductivity in DMF solvent indicates the electrolyte behavior of all complexes except Zn (II) complex [8].

Table (1)
Some physical and analytical data for the ligands and their metal complexes.

Comp.	Color	M.P ^{O}C	Yield%	M.Wt g.mol^{-1}	Elemental analysis% Found (Calc.)			
					C	H	N	M
$C_{10}H_7NO_2$ (HL1)	White	154-156	----	173.17	----	----	----	----
$C_{12}H_{12}N_2$ (L2)	White	172-174	----	184.64	----	----	----	----
[CoL1L2] NO$_3$.2H$_2$O	Greenish blue	96-98	70.96	513.67	51.963 (51.40)	5.075 (4.28)	10.131 (10.90)	12.06 (11.46)
[NiHL1L2(H$_2$O)$_2$](NO$_3$)$_2$.H$_2$O	Pale green	144-146	77.41	594.46	45.246 (44.41)	3.469 (4.21)	10.911 (11.77)	10.54 (9.87)
[CuHL1L2(H$_2$O)$_2$] (NO$_3$)$_2$	Olive	182-184	86.75	581.34	44.630 (45.41)	3.967 (3.95)	11.530 (12.04)	11.13 (10.93)
[ZnL1L2(OAC)H$_2$O]	Off White	116-118	70.37	499.13	56.983 (57.70)	5.183 (4.60)	7.974 (8.41)	12.51 (13.10)
[PdL1L2] Cl.1/2 H$_2$O	Pale brown	186-188	90.26	507.63	53.000 (52.00)	3.180 (3.54)	7.943 (8.27)	21.07 (20.98)
[AuL1L2] Cl$_2$.H$_2$O	Brown	104-106	84.68	642.57	40.514 (41.08)	2.828 (3.11)	6.210 (6.53)	30.26 (30.66)

3.1. Infrared Spectra Studies

Table (2) shows tentative assignments of the IR peaks for the free quinoline -2-carboxylic acid and some metals together with the co-ligand 4,4$^{/}$-dimethyl-2,2$^{/}$ Bipyridyl. The (HL1) may coordinate with metal ions through monodentate, bidentate chelating and bridging according to Nakamoto and Deacon & Phillips [9].The infrared spectrum of the solid state 2-quinaldic acid indicates that it's exists in two tautomeric forms at the same time, as a neutral molecule (quinoline-2-carboxylic acid) and as a zwitter ion (quinolinium-2-carboxylate) [10].IR spectrum of the ligand shows a typical broad band in the range (3417-2534) cm^{-1} with its maximum at (2939) cm^{-1} which refers to stretching frequency of ν (O-H) of carboxylic acid [9^{b}].This can still be observed in the IR spectrum of nickel and copper complexes, this confirmed the incomplete deprotonation of ligand in these complexes [11].On the other hand, the absence of absorption bands in this region in IR spectra for all complexes confirmed the complete deprotonation of the ligand in these complexes [12]. Further confirmation comes from the absence of C-O-H bending peak for COOH group at 908 cm^{-1} [13]. The difference of the value between the asymmetric and symmetric stretching of COO^{-} frequencies ($\Delta v = v_{sym}COO^{-} - v_{asym} COO^{-}$) of all complexes have been compared in order to predict the coordination mode of metal ions with quinoline-2-carboxylic acid as shown in Table (2). The Δv values, for each prepared complexes, indicates the monodentate coordination of the carboxylate group. The bending of δ (C=N) in all complexes shifted

and appeared at the range (408-393) cm^{-1} with its maximum at (405) cm^{-1} [14].indicates that the nitrogen atom of quinoline-2-carboxylic acid also had coordinated with metal ions. Furthermore, new bands attributed to ν (M-O) and ν (M-N) which appeared at (570-520) cm^{-1} and (420-489)cm^{-1} respectively in all complexes also confirmed L1 had coordinated with the metal ions through oxygen atom of carboxylate group and nitrogen atom [9^b]. The coordination of 4,4$^/$-dimethyl-2,2$^/$ Bipyridyl is indicated by the positive shift of ν(C=C) and ν(C=N) ring streching frequencies and the presence of their deformation modes at 1168 and 1936cm^{-1}. The position of the bands which was found in the spectrum of 4,4$^/$-dimethyl-2,2$^/$ Bipyridyl has been completely changed in the spectra of the complexes where it is used

as co-ligand and new bands appeared at ~1560-1590 cm^{-1} confirming the coordination nature of this ligand, the 424 cm^{-1} band of 4,4$^/$-dimethyl-2,2$^/$ Bipyridyl (C-C out of plane bending) shifts to higher frequency and splits into two components in the complexes which again confirms the coordination of this ligand through two nitrogen atoms [10]. An additional band in the range (260-270) cm^{-1} which has been observed in all complexes indicates that the nitrogen atoms of the co-ligand coordinates with metal ion [15]. The presence of water molecules causes the appearance of broad O-H stretching bands in the region of 3473-3417 cm^{-1} in most IR spectra of the complexes [16].

Table (2)
Main FTIR bands in (cm^{-1}) observed in the spectra of metal ions mixed ligands complexes.

Comp.	*ν$_{asy.}$ COO$^-$*	*ν$_{sym.}$ COO$^-$*	*νC=O*	*νC=N+νC=C*	*ν M-N*	*ν M-O*	*ν M-N (Bipy)*	*Others*
C$_{10}$H$_7$NO$_2$ (HL1)	**1580**	**1390**	**1697**	**1604,1535, 1508, 1473**	----	----	----	----
C$_{12}$H$_{12}$N$_2$ (L2)	----	----	----	**1604,1519, 1481, 1450**	----	----	----	----
[CoL1L2] NO$_3$.2H$_2$O	**1592**	**1384**	----	**1612,1562, 1512, 1462**	**443**	**570**	**262**	**νOH=3441 δH2O=848.6 NO3=1384,1176, 964**
[NiHL1L2(H$_2$O)$_2$](NO$_3$)$_2$.H$_2$O	**1595**	**1394**	**1693**	**1612,1560, 1512, 1465**	**489**	**528**	**270**	**νOH=3402 δH2O=856 NO3=1394,1176, 968**
[CuHL1L2(H$_2$O)$_2$] (NO$_3$)$_2$	**1598**	**1381**	**1693**	**1612,1562, 1512, 1465**	**489**	**524**	**262**	**νOH=3348.7 δH2O=856.3 NO3=1381,1172, 948**
[ZnL1L2(OAC)H$_2$O]	**1594**	**1388**	**1697**	**1612,1566, 1516, 1465**	**420**	**528**	**266**	**δH2O=852 OAC=1728**
[PdL1L2] Cl.1/2 H$_2$O	**1572**	**1365**	----	**1600,1528, 1516,1465**	**455**	**528**	**262**	**νOH=3348.4**
[AuL1L2] Cl$_2$.H$_2$O	**1575**	**1365**	----	**1604,1527, 1506, 1454**	**455**	**536**	**262**	**νOH=3448**

3.2. Magnetic Moment Study

The magnetic moment (μeff) for the cobalt (II) complex (d^7) has been estimated to be (4.56) B.M. This higher value of (μeff) in this complex may be due to the contribution of spin orbital coupling [17]. In nickel (II) complex, it was recorded at (3.11) B.M. [18], while the (μeff) of the cupper (II) complex is (2.11) B.M [19]. This value lies within the expected value for one electron. On the other

hand, zinc (II), palladium (II), and gold (III) complexes are diamagnetic Table (3).

3.3. The Electronic Spectra
3.3.1. Electronic Spectra of Ligands

The electronic spectrum of H L1 exhibits four main bands appeared at 45045 cm^{-1} , 41666 cm^{-1}, 34843 cm^{-1}, and a shoulder band at 30487 cm^{-1} due to (π→π*), (n→π*), (n→π*) and (n→π*) transitions respectively

[20]. While the Electronic spectrum of L2 exhibits two main bands: the first one appeared at 41152 cm^{-1} due to interaligand ($\pi \rightarrow \pi^*$) transition, the second absorption appeared at 33670 cm^{-1} arises from (n$\rightarrow \pi^*$) transition that may be located on nitrogen atom of –N=C-. A comparative look of electronic absorption spectral data of the ligands and their complexes indicates that n$\rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transitions of the ligands has shifted to higher frequencies [20], Table (3).

3.3.2 Electronic Spectra of [CoL1L2] NO$_3$.2H$_2$O Complex

The greenish-blue complex showed three bands at 16583, 16447, and 14947 cm^{-1} which assigned to $^4A_2 \rightarrow ^4T_{1p}$ ν_3 transition. This transition is known to be triplet in the divalent cobalt of tetrahedral geometry. This splitting is due to spin orbital coupling [21]; therefore, ν_3 has been calculated as the average of these three bands. While ν_1 ($^4A_2 \rightarrow ^4T_2$) and ν_2 ($^4A_2 \rightarrow ^4T_1$) could not be seen since which expected to appear in the range out of scale, so the second transition (ν_2) calculated theoretically and it has been estimated to be (5393) cm^{-1}, while first transition (ν_1) calculated from infrared spectrum and found to be (3441) cm^{-1}; moreover, B$^/$, Dq, and β were calculated and the low value of β indicates that the bond is covalent. These parameters are accepted for cobalt (II) tetrahedral complexes [21], Table (3).

3.3.3 Electronic Spectra of [NiHL1L2(H$_2$O)$_2$](NO$_3$)$_2$.H$_2$O Complex

The electronic spectrum of nickel (II) complex showed three bands at 9803, 14662, and 30211 cm^{-1} which corresponding to $^3A_2g \rightarrow ^3T_2g$, $^3A_2g \rightarrow ^3T_1g$, and $^3A_2g \rightarrow ^3T_{1g(p)}$ respectively. The spectrum also shows a band at 13333 cm^{-1} corresponds to $^3A_2g \rightarrow ^1Eg$ which refers to forbidden transition. These bands indicate an octahedral geometry around Ni (II) ion [22]. The absence of the frequency at (20000) cm^{-1} proves that the prepared complex is not square planer [23^a]. Nephelauxetic factor β and Racah parameter B$^/$ were calculated by fitting the ratio ν_3/ν_2 from Tanabe-Sugano diagram for d^8 system Table (3).

By fitting the ratio of frequencies (ν_2/ν_1) which equals to 1.5 indicates that the complex has distorted octahedral geometry [23^b], comparable with the value of a regular geometry which equals to 1.6[24]. The formula is further confirmed to be ionic by conductivity measurements. From these results and other analyses, an octahedral geometry around Ni (II) ion can be proposed

3.3.4. Electronic Spectra of [CuHL1L2(H$_2$O)$_2$] (NO$_3$)$_2$Complex

Electronic spectrum of Cu (II) complex shows a broad absorption band at 11695 cm^{-1} which refers to electronic transition $^2B_1g \rightarrow ^2A_1$g. The second band at 26666 cm^{-1} which assigned to $^2B1g \rightarrow ^2Eg$ transition [25], as well as another band at 28653cm^{-1} which corresponds to charge transfer from the donor atoms of ligands to cupper (II) ion, Table (3).

3.3.5. Electronic Spectra of [ZnL1L2(OAC)H$_2$O]Complex

Since the UV–Visible spectra of d^{10} ion do not furnish a lot of information, therefore, some shifting and change in the shape of the bands were compared with those of ligands [26]. The prepared off white Zn(II) complex shows two bands at 41841 and 33444 cm^{-1}, as well as a shoulder at 30864 cm^{-1}.

3.3.6 Electronic Spectra of [PdL1L2] Cl.1/2 H$_2$O Complex

The spectrum of Pd(II) complex shows band at 21645 and 28011 cm^{-1} which are assigned to $^1A_1g \rightarrow ^1B_1g$ and $^1A_1g \rightarrow ^1E_1g$ transitions [27], while the band appearing at 31250 cm^{-1} is correspond to L$\rightarrow$PdCT transition [23b], Table (3), the results are in fairly good agreement with literatures which suggest that Pd(II) complex has square planer environments of ligands [28].

3.3.7 Electronic Spectra of [AuL1L2] Cl$_2$.H$_2$O Complex

The electronic spectrum of this complex Table (3) shows three bands at 26666, 29850 cm^{-1} which refers to $^1A_1g \rightarrow ^1B_1g$ and $^1A_1g \rightarrow ^1Eg$ transition respectively, and the third band appeared at 30769 cm^{-1} due to charge transfer in square planner geometry [29].

Table (3)
Electronic spectra, conductance in DMF solvent and magnetic moment (B.M) for ligands and their metal complex.

| *Comp.*	$C_{10}H_7NO_2$ (HL1)	$C_{12}H_{12}N_2$ (L2)	[CoL1L2] $NO_3.2H_2O$	[NiHL1L2(H_2O)_2] (NO_3)_2.H_2O	[CuHL1L2 H_2O)_2] (NO_3)_2	[ZnL1L2 (OAC)H_2O]	[PdL1L2] Cl.1/2 H_2O	[AuL1L2] $Cl_2.H_2O$
Absorption	30487(sh) 34843 41666 45045	33670 41152	3441 5393(cal.) 15992(av.)	13333 9803 14602 30211	11695 26666 28653	30846 (sh) 33444 41841	21645 28011 31250	26666 29850 30769
Assignment	n→π* n→π* n→π* π→π*	n→π* π→π*	$^4A_2$→$^4T_2$ $^4A_2$→$^4T_1$ $^4A_2$→$^4T_{1(P)}$	$^3A_{2}g$→^1Eg $^3A_{2}g$→$^3T_{2}g$ $^3A_{2}g$→$^3T_{1}g$ $^3A_{2}g$→$^3T_{1}g$	$^2B_{1}g$→$^2A_{1}g$ $^2B_{1}g$ →^2Eg L→CuCT	ILCT ILCT ILCT	$^1A_{1}g$→$^1B_{1}g$ $^1A_{1}g$→^1Eg L→PdCT	$^1A_{2}g$→$^1B_{1}g$ $^1A_{2}g$→^1Eg L→AuCT
B°	----	----	971	1035	----	----	----	----
B$^/$	----	----	737.5	917.6	----	----	----	----
β	-----	----	0.75	0.88	----	----	----	----
Dq/B$^/$	-----	----	0.47	1.1	----	----	----	----
10Dq	----	----	3460	9900	----	----	----	----
15 B$^/$	----	----	11062	989.9	----	----	----	----
μ_{eff}	----	----	4.56	3.11	2.11	0.00	0.00	0.00
μ_{scm}^{-1}	----	----	76.6	72.7	72.2	16.6	73.4	52.6
Suggested Structure	----	----	T.d	O.h	O.h	O.h	Sq. Planer	Sq. Planer

ILCT: Internal ligand charge transfer.

3.4 Thermal Analysis

Thermal analyses were done to confirm the presence of water molecules as suggested in the new prepared complexes by following the degradation steps in TG curves and the obtained results has been listed in Table (4).

Table (4)
Thermal analytical data of the water molecule for the newly prepared complexes.

Comp	*Weight loss found (Calc.)%*	*Temp range in TG (ºC)*
[CoL1L2] NO₃.2H₂O	**6.51(7.00)**	**118.93-220.71**
[NiHL1L2(H₂O)₂](NO₃)₂.H₂O	**8.58(9.08)**	**129.65-170.22**
[CuHL1L2(H₂O)₂] (NO₃)₂	**4.71(5.19)**	**122.15-192.62**
[ZnL1L2(OAC)H₂O]	**2.93(3.63)**	**282.33**
[PdL1L2] Cl.1/2 H₂O	**0.98(1.07)**	**72.60-225.86**
[AuL1L2] Cl₂.H₂O	**2.92(2.80)**	**74.90—220.10**

3.5 Suggested Structures of new Complexes
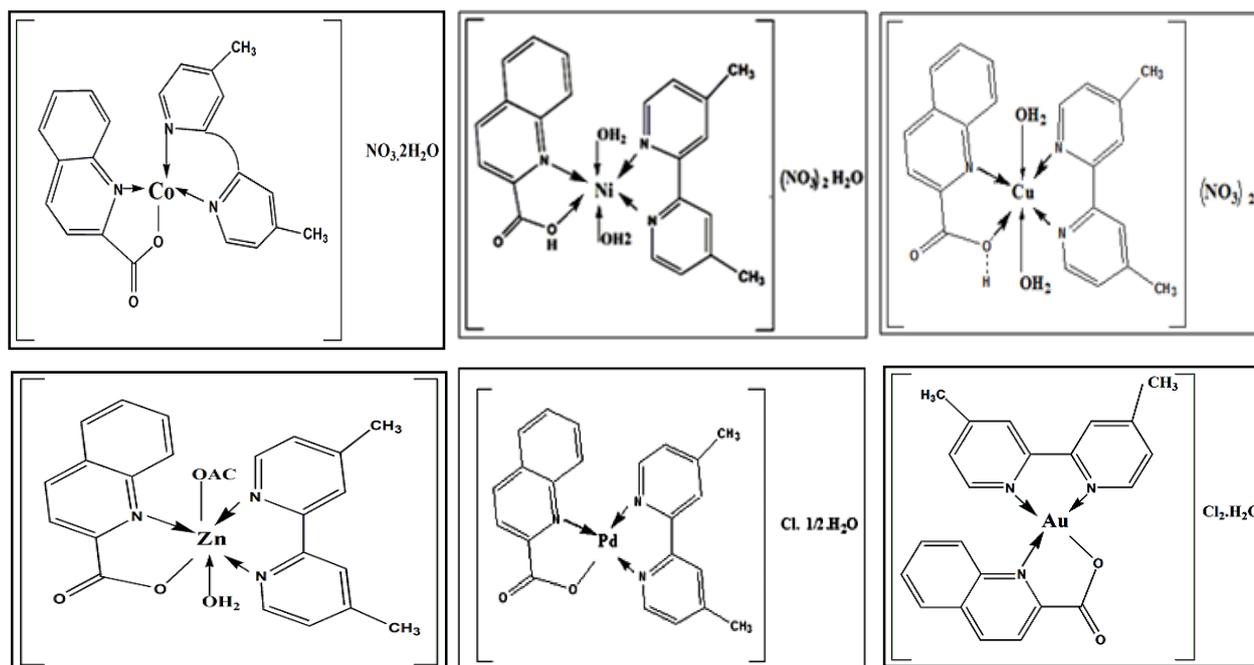
4. Theoretical Studies

In this work, Hyperchem.8 program has been used to calculate The heat of formation (ΔH^o_f), binding energy (ΔE_b) and dipole moment (μ) for the free ligands and their metal complexes using semi-empirical (ZINDO/I, PM3) and molecular mechanics (AMBER) methods at 298 K. It was found that the complexes are more stable than their ligands Table (5); Furthermore, the electrostatic potential for free ligands was calculated to investigate the reactive site of the molecules, PM3 was used to evaluate the vibrational spectra of free ligands. It has been found that these obtained frequencies agree well with experimental results; in addition, the calculation helped to assign unambiguously the most diagnostic bands Table (6). Electronic spectra measurements for the ligands were calculated theoretically by using ZINDO/S method and comparing it with the experimental results. It was found that there was a close agreement between the theoretical calculations and experimental results Table (7). While Gaussian program semi-empirical (PM3) method was used to calculate the geometry optimization, dipole moment (μ) and total energy as shown in Table (8). Electrostatic potential, E_{LUMO} and E_{HOMO} was obtained also; evaluate the vibrational spectra

of free ligands, and these obtained frequencies agree well with experimental results as shown in Table (9). Electronic spectra measurements for the ligands were calculated theoretically by using the job type: Single point energy (SP) along with ZINDO method and also the job type Frequency (Freq) used along with CIS method (3-21G) and compared both methods with the experimental results as shown in Table (10). It was found that there was a close agreement between the theoretical and experimental results.

Table (5)
Conformation energetic in (Kcal.mol⁻¹) and dipole moment (in Debye) for ligands and their metal complexes using hyperchem-8 program.

Compound	PM3			ZINDO/1			AMBER
	ΔH^o_f	ΔE_b	μ	ΔH^o_f	ΔE_b	μ	$\Delta H^o_f=\Delta E_b$
$C_{10}H_7NO_2$ (HL1)	-39.8326	-2345.56	3.027	-4515.74	-6821.47	3.324	----
$C_{12}H_{12}N_2$ (L2)	329.69	-2259.59	4.589	-4860.72	-7450.01	5.209	----
{CoL1L2]NO₃.2H₂O	----	----	----	-10216.87	-15474.80	13.84	----
[NiHL1L2(H₂O)₂](NO₃)₂. H₂O	----	----	----	-10993.76	-16631.72	8.291	----
[CuHL1L2(H₂O)₂](NO₃)₂	----	----	----	-11412.33	-17028.19	12.13	----
[ZnL1L2(OAC)H₂O]	----	----	----	-12836.02	-18803.69	10.78	----
PdL1L2] Cl.1/2 H₂O	----	----	----	----	----	----	44.01
AuL1L2] Cl₂.H₂O	----	----	----	----	----	----	48.47

Table (6)
Comparison of experimental and theoretical main vibration frequencies for Qinoline-2-carboxylic acid (HL1) and 4,4′-dimethyl -2,2′-bipyridyl(L2)using hyperchem-8program

Symb.	$v(C=O)$	$v(C=N+C=C)$	$\delta(C-O)$	$v(O-H)$
HL1	1980.78 1697.36* (16.69)	1631.59 1604* (1.68)	1394.36 1261.45 * (10.54)	3852.17 2939 * (4.47)
Symb.	$v(C=N+C=C)$	$v(C-H)$aliph.	$v(C-H)$arom.	$\delta(C-N)$
L2	1780.43 1604.77* (10.94)	3170.58 2981.95* (2.99)	3035.50 3078.39* (0.033)	1233.03 1273.02* (-3.14)

(*) Experimental Frequency Error %.

Table (7)
Comparison of experimental and theoretical electronic transition for ligands from ZINDO/S calculation and Experiment method using hyper chem-8 program.

Symbols	Transition	Experimental	Theoretical(ZINDO/S)
HL1	n→π	328sh	306
	n→π*	287	279.4
	n→π*	240	229
	π→π*	222	214
L2	n→π*	297	274.55
	π→π*	243	--------
	n→π*	-------	237.02
	π →π*	-------	195.0

Table (8)
Conformation energetic in (Kcal.mol⁻¹) and dipole moment (in Debye) for ligands
(HL1,L2) using Gaussian program.

Compound	Total energy	μ
HL1	-32.44762449	3.3846
L2	45.4167809	3.4377

Table (9)
Comparison of experimental and theoretical vibration frequencies for Qinoline-2-carboxylic acid
(HL1) 4,4ʹ-dimethyl-2,2ʹ-bipyridyl (L2)using Gaussian programs.

Symb.	v(C=O)	v(C=N+C=C)	δ(C-O)	v(O-H)
HL1	2065.71 1697.36* (17.83)	1628.07 1604* (1.47)	1282.41 1261.45 * (1.63)	3239.37 2939 * (9.27)
Symb.	v(C=N+C=C)	v(C-H)aliph.	v(C-H)arom.	δ(C-N)
L2	1745.74 1604.77* (8.07)	3170.22 2981.95* (5.93)	3031.92 2981.95* (1.63)	1228.28 1273.02* (-3.64)

(*) Experimental Frequency Error %.

Table (10)
Comparison of experimental and theoretical electronic transition for ligands from CIS and
ZINDO calculation and Experiment method using Gaussian program.

Symbols	Transition	Experimental	Theoretical	
			CIS	ZINDO
HL1	n→π n→π* n→π* π→π*	328sh 287 240 222	(222)max	(311.59)max
			CIS	ZINDO
L2	n→π* π→π* π→π*	297 243 -------	(185)max	(279.77)max

5. Conclusion

In this paper, we succeeded to prepare mixed ligands of (Quinoline-2–carboxylic acid and 4,4ʹ-dimethyl-2,2ʹ-bipyridyl) with some heavy and light transition metal ions. The new solid metal complexes were isolated and characterized using the available conventional techniques. The results indicate that the primary ligand Quinoline-2–carboxylic acid behaves as bidentate through the nitrogen and oxygen atoms, while the co-ligand 4,4ʹ -dimethyl-2,2ʹ-bipyridyl behaves as bidentate ligand but through the two nitrogen atoms with metal ions. Moreover, the results obtained for the ligands and their complexes which were isolated in solid state were compared with the results obtained from the gas phase study using Hyper Chem-8 and Gaussian programs exhibited almost identical results between these states.

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الخلاصـة

تم تحضير معقدات جديدة من مفاعلة كوانلين –2–حامض الكربوكسيلي و 4,4'–داي مثيل,2,2'–باي بريديال مع ايونات الفلزات:الكوبلت (II)، نيكل (II)، النحاس (II)، الخارصين (II) البلاديوم (II)، والذهب (III). تم عزل وتشخيص المعقدات الجديدة المحضرة بالطرق الطيفية والفيزيائية كطيف الاشعة تحت الحمراء والاشعة فوق البنفسجية–المرئية والتحليل الدقيق للعناصر وتعيين نسبة الفلز والتحليل الحراري فضلا عن القياسيات الحساسية المغناطيسية والتوصيلية. وجد ان المعقدات المحضرة مونمرية وذات شكل هندسي ثماني السطوح في نيكل (II)، النحاس (II)، الخارصين (II) اما معقدات البلاديوم (II)، والذهب (III) وجدت على شكل مربع مستو، في حين ان الكوبلت (II) رباعي السطوح. تم اجراء معالجة نظرية لهذه الليكندات المحضرة في الطور الغازي باستخدام برنامجي

(Hyper chem.8 and Gaussian program (GaussView Currently Available Versions (5.0.9) along with Gaussian 09 which is the latest in the Gaussian series of programs).