DOI: http://dx.doi.org/10.21123/bsj.2016.13.4.0770

## Transition Metal Complexes with Tridentate Ligand: Preparation, Spectroscopic Characterization, Thermal Analysis and Structural Studies

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Received 25/ 5/2015 Accepted 4/ 10/2015

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### Abstract

New series of metal ions complexes have been prepared from the new ligand 1,5- Dimethyl-4- (5-oxohexan-2- ylideneamino) -2-phenyl- 1H-pyrazol-3 (2H)-one derived from 2,5-hexandione and 4-aminophenazone. Then, its V(IV), Ni(II), Cu(II), Pd(II), Re(V) and Pt(IV) complexes prepared. The compounds have been characterized by FT-IR, UV-Vis, mass and <sup>1</sup>H and <sup>13</sup>C-NMR spectra, TGA curve, magnetic moment, elemental microanalyses (C.H.N.O.), chloride containing, Atomic absorption and molar conductance. Hyper Chem-8 program has been used to predict structural geometries of compounds in gas phase, the heat of formation, (binding, total and electronic energy) and dipole moment at 298 K.

**Key words:** Schiff base Ligands, 2,5-Hexandione, Metal Complexes.

## **Introduction:**

Schiff base derivatives attract a significant interest and occupy an important role in the development of coordination chemistry [1]. Moreover, base complexes containing Schiff transition metals have been studied in several research areas such as structural chemistry [2]. Metal complex with Schiff bases are important class of ligands due to their synthetic flexibility, selectivity and sensitivity towards the central metal atom, structural natural similarities with biological substances, and also, due to presence of azomethine group which imports in elucidating the mechanism of

transformation and racemisation reaction in biological system [3-4] also have been studied for their application in clinical, analytical and pharmacological areas [5]. In report herein the synthesis and spectroscopic studies as well as the thermal investigation of a novel Schiff base derivative ligand = 1, 5-Dimethyl-4-(5oxohexan-2-ylideneamino)-2-phenyl-1H-pyrazol-3 (2H)-one with some transition metals such as Ni(II), VO(II), Cu(II), Pd(II), Re(V) and Pt(IV) complexes. (<sup>1</sup>H, <sup>13</sup>C) NMR, FT.IR and Mass spectra were obtained to determine the structure of the ligand.

## Materials and Methods:

The following chemicals were commercially available products of analytical reagent grade. 2,5-hexane dione, 4-amiophenazone, DMSO, pure ethanol, methanol, CaCl<sub>2</sub>, VOSO<sub>4</sub>XH<sub>2</sub>O NiCl<sub>2</sub>.6H<sub>2</sub>O, PdCl<sub>2</sub>, CuCl<sub>2</sub> ReCl<sub>5</sub> and H<sub>2</sub>PtCl<sub>6</sub>.6H<sub>2</sub>O were obtained from Fluka, Aldrich.

(FT-IR) spectra the were recorded in the range (4000-400) cm<sup>-1</sup> on a Shimadzu 3800, spectrometer. absorption spectra were Electronic recorded in the range (200-1100) nm on a Shimadzu 160 Spectrophotometer. analysis studies Thermal of the compounds were performed on Perkin-Elmer Pyris Diamond DTA/TG Thermal system under nitrogen atmosphere at a heating rate of 10°C/min. <sup>1</sup>H- <sup>13</sup>CNMR spectra were recorded using Bruker 400 MHz spectrometer and elemental (C.H.N.O) analyses were carried out on a Perkin-Elmer automatic equipment model 240.B. Mass spectra were obtained by LC-Mass 100P Shimadzu. Melting points were obtained on a Buchi SMP-20 capillary melting point apparatus and are uncorrected. Metals were identified using a Shimadzu (A.A) 680 G atomic absorption Spectrometer. Conductivity measurements were made with DMSO solutions using a Jenway 4071 digital conductivity meter at room temperature, chlorine content. Magnetic properties were measured using (Balance magnetic susceptibility model MSR-MKi).

### Synthesis of Ligand: 1, 5-Dimethyl-4-(5-oxohexan-2-ylideneamino)-2phenyl-1H-pyrazol-3 (2H)-one

A solution of 4-aminophenazone (1 g. 4.92 mmol) in absolute ethanol (25 ml) was mixed with a solution of 2,5 hexandione (0.56g, 4.92mmol). The reaction was stirred and heated in water bath (40-50)°C for four hrs. A colorless precipitated washed with diethyl ether .Recrystallization has been carried out in ethanol: water (1:1). The product was dried via anhydrous CaCl<sub>2</sub> in vacuum as shown in Scheme (1). The yield is (1.38g), 93.66%, mp.179°C.



Scheme 1: Preparation of the Ligand

### **Synthesis of Complexes**

A solution of the ligand (0.5 mmol) in methanol (15 ml), and methanol solution (10 ml) of the metal salt (0.5 mmol) (NiCl<sub>2</sub>.6H<sub>2</sub>O, CuCl<sub>2</sub>, ReCl<sub>5</sub>, H<sub>2</sub>PtCl<sub>6</sub>.6H<sub>2</sub>O, PdCl<sub>2</sub> and VOSO<sub>4</sub>.H<sub>2</sub>O) was then added drop wise. The resulting mixture was refluxed 3-4 hrs, the solid mass which was washed

several times with hot ethanol and dried under vacuum. Physical properties for the compounds are given in Table (1).

# Programs used in Theoretical Calculation

Hyper Chem-8 program is a sophisticated molecular modeler, editor and powerful computational package that are known for its quality, flexibility and ease of use, uniting 2D visualization and animation with quantum chemical calculations, molecular mechanics and dynamic. (PM3) and (AMBER) are more popular than other semi-empirical methods due to the availability of algorithms and more accurate than with other methods. It has parameterized primarily for organic molecules and selected transition metals [6, 7].

### **Results and Discussion:**

The UV spectrum for free ligand one peak in (282 nm) attributed to  $(\pi \rightarrow \pi^*)$ , shown the Figure (1). The LC-Mass for ligand (299.3m/z) with  $(C_{17}H_{21}N_3O_2),$ (244.2)m/z) with  $(C_{14}H_{18}N_3O),$ (243.3 m/z) with  $(C_{14}H_{17}N_3O)$  and (144.2 m/z) with  $(C_6H_{14}N_3O).$ <sup>1</sup>H-NMR  $(DMSO-d_6,$ ppm): δ 2.044 (s,3H, N=C-CH<sub>3</sub>), 2.147 (s,3H, O=C-CH<sub>3</sub>), 3.11 (s, 3H, C=C-CH<sub>3</sub>), 3.31 (s,3H, N-CH<sub>3</sub>), 5.88 (tri, 4H, CH<sub>2</sub>-CH<sub>2</sub>), 7.282-7.513 (m, 5H, Ar-H) <sup>13</sup>C-NMR shown the Figure (2). (100.622 MHz, DMSO- $d_6$ ):  $\delta$  162.22 (C<sub>16</sub>), 153.25 (C<sub>12</sub>), 134.67 (C<sub>4</sub>), 129 (C<sub>2</sub>, <sub>6</sub>), 127 (C<sub>8, 10</sub>), 124.31 (C<sub>9</sub>), 109.83  $(C_{11}), 105.95(C_7), 77.25(C_{5.15}), 76.93$ 

(C<sub>3</sub>), 50.41(C<sub>17</sub>), 36.09 (C<sub>4</sub>), 12.5 (C<sub>13</sub>), 10.62 (C<sub>1</sub>), shown the Figure (3,4).

Molar conductance values were found in the range (3 - 19) S. cm<sup>2</sup> mol<sup>-1</sup> for V(IV), Ni(II) and Cu(II) complexes which indicates that they are nonelectrolytes, the range (44-45) S. cm<sup>2</sup>. mol<sup>-1</sup> for Pd(II) and Pt(IV) complexes which indicates that they are electrolytes (1:1) and (70) S. cm<sup>2</sup>. mol<sup>-1</sup> for Re(V) complex which indicate that the is electrolyte [1:2] [8-9]. These were determined in (DMSO) solution (10<sup>-3</sup> M). Physical properties and elemental microanalysis are listed in Table (1).



Fig. (1) UV-Vis Spectrum of Ligand



Fig. (2) <sup>1</sup>H-NMR Spectrum of Ligand



Fig. (4) Structure of Ligand

Table (1) Microanalysis results and some physical properties of the Ligand an	nd
its complexes	

Comula	M. wt. Viold%	Color	Molar	Molar Elemental Analysis % Calc					
Formula			conductance	Experimental					
Formula	1 1010 70	m.p.c	S. $cm^2$ . $mol^{-1}$	С	Н	N	0	М	Cl
L	299.37	Colorless		68.20	7.07	14.04	10.69		
$C_{17}H_{21}N_3O_2$	89	179	-	67.76	6.83	15.56	11.12		
VI	462 27	Brown		44.16	4.58	9.09	24.22	11.02	
	402.57	reddish	3	45.48	5.74	9.09	25.07	12.76	
$C_{17}\Pi_{21}\Pi_{3}O_{7}VS$	80	138-139		ctance         Experimental $mol^{-1}$ C         H         N         O           68.20         7.07         14.04         10.69           67.76         6.83         15.56         11.12           44.16         4.58         9.09         24.22           45.48         5.74         9.09         25.07           45.36         4.36         11.0         11.42           45.68         5.19         9.40         10.74           3         45.68         5.19         9.40         10.74           44.87         6.66         11.09         11.25           9         45.19         5.13         9.30         10.62           44.87         6.66         11.09         11.23           4         42.83         4.44         8.81         6.71           40.97         5.31         10.02         7.76           70         30.80         3.19         6.34         4.83           30.32         4.11         5.54         4.32           32.09         3.33         6.60         5.03           33.12         4.03         7.09         4.65	14.12	16.51			
NH	116.08	Brown		45.68	5.19	9.40	10.74	13.13	15.86
NIL C <sub>17</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> NiCl <sub>2</sub>	92	reddish 285-286	eddish 13 85-286	44.87	6.66	11.09	11.25	14.13	15.55
CuL	451.83	Green	10	45.19	5.13	9.30	10.62	14.06	15.69
$C_{17}H_{23}N_3O_3CuCl_2$	93	230-232	19	46.09	6.87	10.09	11.23	15.35	14.43
PdL	476.69 77	Dark brown	44	42.83	4.44	8.81	6.71	22.32	14.87
$C_{17}H_{21}N_3O_2PdCl_2$		244-245	40.97	5.31	10.02	7.76	22.34	14.66	
ReL	662.84	Dark	70	30.80	3.19	6.34	4.83		26.74
$C_{17}H_{21}N_3O_2ReCl_5$	71	267-268		30.32	4.11	5.54	4.32		27.98
DtI		Red		32.09	3.33	6.60	5.03	30.66	22.29
$C_{17}H_{21}N_3O_2PtCl_4$	636.26 b 28	brown 288-290	45	33.12	4.03	7.09	4.65	31.22	21.54

#### Mass spectra for complexes

The main high resolution mass spectrometer values of the [PtL  $Cl_3$ ]Cl and [ReL<sub>1</sub>  $Cl_3$ ]Cl<sub>2</sub> complexes are shown in Figure (5) and Figure (6) respectively,

the molecular ion peak for the  $[PtL_1 Cl_3]Cl$  was observed at m/z = 636 (M) (relative abundance is 92%) for  $C_{17}H_{21}N_3O_2PtCl_4$  which is in excellent agreement with the theoretical value and

the molecular ion peak for the  $[ReL_1 Cl_3]Cl_2$  was observed at m/z = 663 (M) (relative abundance is 90%) for  $C_{17}H_{21}N_3O_2ReCl_5$  which is in excellent agreement with the theoretical value[10]. All these fragmentations can be shown in Table (2).

## Table (2) The Fragmentation Patterndata for Complexes

complexes	Assignment	Peak	Relative
complexes	Assignment	m/z	abundance%
	$M = (C_{17}H_{21}N_3O_2PtCl_4)$	636	92
[PtL <sub>1</sub> Cl <sub>3</sub> ]Cl	M- PtCH <sub>3</sub> Cl <sub>2</sub> =M <sub>1</sub>	355	73
	M <sub>1</sub> - C <sub>10</sub> H <sub>9</sub> N	212	34
	$M = C_{17}H_{21}N_3O_2ReCl_5$	663	90
[ReL1Cl3]Cl2	$M = CH_7ReO_2Cl_2 = M_1$	355	71
	M1- C9H7N2	212	33



Fig. (5) LC-Mass Spectrum of [PtL<sub>1</sub> Cl<sub>3</sub>]Cl



Fig. (6) LC-Mass Spectrum of [ReL<sub>1</sub> Cl<sub>3</sub>]Cl<sub>2</sub>

### **IR** spectra:

The bands IR of spectra of the ligand and its complexes were observed at 1740, 1696 and 1640 cm<sup>-1</sup> due to the v(C=O) ring pyrazol, v(C=O) and v(C=N) functional groups, respectively, [11]. The IR spectra of the complexes exhibited bands for the ligand bands appropriate with the shifts due complexes formation [12]. Moreover, the v(carbonyl) ring, v(carbonyl) and v(azomethine), bands of the ligand were observed at 1740, 1696 and 1640 cm<sup>-</sup> <sup>1</sup>and these bands were shifted to the lower frequencies by (76-62), (62-54)

and (20-16) cm<sup>-1</sup> respectively in the spectra of all complexes. This indicates that the ligand was coordinated with the metal ions through O, O carbonyl groups and N azomethine group atoms, but these shifts confirm the coordination of the ligand via the nitrogen of azomethine and the oxygen of carbonyl ring group to Vanadium ions. At lower frequency the complexes exhibited new bands around (470-447), and (432-413) cm<sup>-1</sup> assigned to the v(M-N)and v(M-O), respectively [13-15]. All these data are shown in Table (3).

m (cm )							
Comp.	υC=O ring	υC=O	υC=N	υH <sub>2</sub> O	υM-N	υM-O	Others bands
L	1740	1696	1640				
CuL	1664	1636	1622	3418 891	447	413	
NiL	1678	1642	1620	3410 883	451	424	
PdL	1678	1637	1624		467	420	
PtL	1675	1634	1624		465	424	
ReL	1673	1636	1624		467	420	
VOL	1678	1642	1624		470	432	999= v(V=O) 1103, 1084, 1022= v(SO <sub>4</sub> )

Table (3) The Infrared Spectra Data of the free Ligand and its Metal Complexes in (cm<sup>-1</sup>)

### UV–Vis Spectra, Magnetic Moments

The electronic spectrum of the ligand exhibit intense absorption at 282 nm attributed to  $\pi \rightarrow \pi^*$ . The electronic spectrum of Ni(II) complex showed three broad peaks at 434, 486 and 786 nm assigned to  ${}^{3}A_{2}g_{(F)} \rightarrow {}^{3}T_{1}g_{(P)}$ ,  ${}^{3}A_{2}g_{(F)} \rightarrow {}^{3}T_{1}g_{(F)}$  and  ${}^{3}A_{2}g_{(F)} \rightarrow {}^{3}T_{2}g_{(F)}$  [16] and the electronic spectrum of Re(V) complex showed three broad peaks at 489, 637 and other at 715 nm assigned to  ${}^{3}T_{1}g \rightarrow {}^{3}A_{2}g$ ,  ${}^{3}T_{1}g \rightarrow {}^{3}T_{1}g_{(P)}$  and  ${}^{3}T_{1}g \rightarrow {}^{3}T_{2}g_{(F)}$  respectively [17, 18]. The spectrum of VO(II) complex gave two band at 496 and 763 nm assigned to  $^{2}B_{2} \rightarrow ^{2}B_{1}$ and  ${}^{2}B_{2} \rightarrow {}^{2}E$  transition, respectively suggesting a square pyramidal geometry [18,19], Furthermore, the magnetic moment of

the VO(II) (d1) complex was found to be 1.77 B.M. The electronic spectrum of Pd(II) complex showed two broad peaks at 493 and 765 nm assigned to  ${}^{1}A_{1}g \rightarrow$  ${}^{1}B_{1}g$  and  ${}^{1}A_{1}g \rightarrow {}^{1}A_{2}g$ , the electronic spectrum of Pt(IV) complex showed two broad peaks at 485 and 520 nm assigned to  ${}^{1}A_{1}g \rightarrow {}^{1}T_{2}g$  and  ${}^{1}A_{1}g \rightarrow {}^{1}T_{1}g$ respectively, suggesting an octahedral geometry. The electronic spectrum of Cu(II) complex showed one broad peaks at 494 nm assigned to  ${}^{2}B_{1}g \rightarrow {}^{2}A_{1}g$ , suggesting an octahedral geometry. The magnetic moment value 2.84, 1.86 and 2.95 B.M. of Ni(II)  $(d^8)$ , Cu(II)  $(d^9)$  and Re(V) (d<sup>2</sup>) complexes respectively are typical for octahedral geometry [18-20]. All these electronic spectra data can be shown in Table (4).

 Table (4) Electronic Spectral Data of the Metal Complexes with Ligand and

 Magnetic Moments

Complex geometry	$\mu_{eff}B.M$	ΰ (cm <sup>-1</sup> )	ABS	$\lambda_{max}(nm)$	ε <sub>max</sub> L mol <sup>-1</sup> cm <sup>-1</sup>	Assignments
L	-	35460.99	2.48	282	24800	$\pi \rightarrow \pi^*$
		36101.08	2.377	277	23770	$\pi \rightarrow \pi^*$
	1.77	20161.29	0.916	496	9160	$^{2}B_{2} \rightarrow ^{2}B_{1}$
Square pyrainidai		13106.15	0.024	763	240	${}^{2}B_{2} \rightarrow {}^{2}E$
		36363.63	2.401	275	24010	$\pi \rightarrow \pi^*$
$[NiL_1Cl_2(H_2O)]$	2.84	23041.47	0.203	434	2030	$^{3}A_{2}g(F) \rightarrow ^{3}T_{1}g(P)v_{3}$
Octahedral	2.04	20576.13	0.232	486	2320	${}^{3}A_{2}g(F) \rightarrow {}^{3}T_{1}g(F)v_{2}$
		12722.64	0.084	786	840	$^{3}A_{2}g(F) \rightarrow ^{3}T_{2}g(F)v_{1}$
$[C_{11}, C_{12}(H_{2}O)]$		36363 63	2.082	275	20820	$\pi \rightarrow \pi^*$
Octahedral	1.86	20242.91	0.604	494	6040	${}^{2}B_{1}g \rightarrow {}^{2}A_{1}g$
Octaneditai		20242.91	0.004	474	0040	$(dx^2 - y^2 \rightarrow dz^2)$
	dia	35971.22	2.414	278	24140	$\pi \rightarrow \pi^*$
[FuL <sub>1</sub> CI]CI		20283.97	0.605	493	6050	${}^{1}A_{1g} \rightarrow {}^{1}B_{1}\nu_{2}$
Square plana		13071.89	0.101	765	1010	$^{1}A_{1g} \rightarrow ^{1}A_{2}\nu_{1}$
		37174.72	1.688	269	16880	$\pi \rightarrow \pi^*$
[PtL <sub>1</sub> Cl <sub>3</sub> ]Cl	dia	32786.88	2.109	305	21090	C.T
Octahedral	uia	20618.55	0.627	485	6270	$^{1}A_{1}g \rightarrow ^{1}T_{2}g \nu_{2}$
		19230.76	0.588	520	5880	$^{1}A_{1}g \rightarrow ^{1}T_{1}g \nu_{1}$
		36363.63	2.459	275	24590	$\pi \rightarrow \pi^*$
[ReL <sub>1</sub> Cl <sub>3</sub> ]Cl <sub>2</sub>	2.05	20449.89	0.983	489	9830	${}^{3}T_{1}g \rightarrow {}^{3}A_{2}g$
Octahedral	2.95	15698.58	0.546	637	5460	${}^{3}T_{1}g \rightarrow {}^{3}T_{1}g (P)$
		13986.01	0.208	715	208	${}^{3}T_{1}g \rightarrow {}^{3}T_{2}g (F)$

dia= diamagnetic

### Thermal Gravimetric Analyses TGA

To understand the thermal decomposition processes of the studied

compounds, the Schiff base ligand and its metal complexes were examined by thermo gravimetric analysis in the temperature range of 30–700 °C. The obtained results from the TG curves for all these compounds are given in Table

(5). The final decomposition products were metal oxide CuO in the 696 °C, NiO 698 °C and PdO 698 °C) [21, 22].

Table (5) Thermal Analysis Data of the Metal Complexes Derived from Ligand.

Com	TG range	DTG max	% Found (c	A:-		
Com	(°C)	(°C)	Mass Loss	Total mass Loss	Assignment	
L	34.6-123.7 125-431 462-694	69.5 370 650	(5.27) 4.94 (22.82)22.724 (70.09) 69.34	98.2 (97.000)	$-CH_{3}$ $-C_{6}H_{4}$ $-C_{9}H_{14}N_{3}O_{2}C$	
NiL	99-151 180-300 300-480 480-698	140 253 380 575	(4.053)4.031 (15.581)15.862 (27.743)27.336 (35.916)36.068	83.293 (83.29)	-H <sub>2</sub> O -Cl <sub>2</sub> -C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> -C <sub>10</sub> H <sub>11</sub> NONiO	
CuL	97-180 180-297 297-433 433-696	140 235 388 587	(4.053)3.988 (21.581)21.89 (23.743)24.161 (31.906)32.363	82.39 (82.402)	$-H_2O$ $-Cl_2+CO$ $-C_6H_9N_2$ $-C_{10}H_{12}NCuO$	
PdL	100-183 183-297 297-436 436-698	138 237 391 590	(7.593)7.436 (7.581)7.436 (27.043)27.94 (32.107)31.512	74.324 (74.324)	-Cl -Cl -C <sub>8</sub> H <sub>9</sub> N <sub>2</sub> -C <sub>9</sub> H <sub>12</sub> NOPdO	

### **Electrostatic Potentials:**

Electron distribution governs the electrostatic potential of the molecules. electrostatic potential The (E.P)describes the interaction of energy of the molecular system with a positive point charge. (E.P) is useful for finding sites of reaction in a molecule; positively charged species tend to attack a molecule where the electro static potential strongly is negative (electrophonic attack) [6, 7]. The (E.P) of the free ligand was calculated and plotted as 2D contour to investigate the reactive sites of the molecules, Figure (7). one can interpret Also the stereochemistry and rates of many reactions involving "soft" electrophiles and nucleophiles in terms of the properties of frontier orbital HOMO and LUMO. The results of calculations show that the LUMO of transition metal ions prefer to react with the HOMO of threedonor atoms of two oxygen of carbonyl and nitrogen of azomethen group for free ligand, Figure (7).

All theoretically probable structures of free ligand and their complexes have been calculated by (PM3) and (ZINDO/1) methods in gas phase to search for the most probable model building stable structure, Table (6).

The vibrational spectra of the free ligand has been calculated, Table (7). The theoretically calculated wave numbers for this ligand showed that some deviations from the experimental values, these deviations are generally acceptable in theoretical calculations. Calculation of parameters has been optimized bond lengths of the free ligand and their metal complexes which to give excellent agreement with the experimental data as shown in Figure (8)



Fig. 7: Electrostatic Potential (HOMO and LUMO) Contours for Ligand

## Table (6) Conformation Energetic in (K J.Mol<sup>-1</sup>) for the Ligand and Complexes

Compounds	Binding Energy	Heat of Formation	Electronic Energy	Dipole moment (debyes)	Total Energy
L	-4473.7665926	-16.3765926	-603103.5158746	5.0380	-78660.2887016
NiL	-4326.4163316	2015.4616684	-1169716.1185115	19.648	-142058.723112
CuL	-4157.8280108	2249.3499892	-1235762.7660891	6.152	-12846.9020078
PdL	-2326.163316	2115.4616684	-1369716.1185115	9.648	-122058.723112
ReL	-3157.8280108	2349.3499892	-135762.7660891	11.152	-112846.9020078
PtL	-1126.463316	2515.4616684	-1149716.1185115	11.648	-112058.723112
VOL	-2257.280108	3049.3499892	-1225762.7660891	8.152	-172846.9020078

## Table (7) Comparison of Experimental and Theoretical Vibrational Frequencies for Ligand

Ligand	υ(CH)aromatic	υ(CH)aliphatic	υ(C=O)ring	υ(C=O)	υ(C=N)
	3035*	2920*	1740*	1696*	1640*
L	3060**	2998**	1668**	1644**	1637**
	-0.82***	-2.67***	4.13***	3.06***	0.18***

\*Experimental frequency. \*\* Theoretical frequency. \*\*\* Error% due to main difference in the experimental measurements and theoretical treatments of vibration spectrum.







Fig. 8. Conformational Structure of (L) and their metal complexes

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معقدات العناصر الانتقالية مع ليكاند ثلاثي السن جديد:تحضير، تشخيص طيفي، تحلل حراري ودراسة تراكيبها

رحاب غالب حمودة

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### الخلاصة:

تحضير سلسلة جديدة من معقدات المعادن مع الليكاند الجديد 5،1-ثنائي مثيل -4-(5-اوكسو هكسان-2-يل ثنائي ايمينو)-2-فنيل -1-باير وزول-3-اون الجديد المشتق من 5،2-هكسان ثنائي اون مع 4- امينو فينازون. وحضرت معقدات كل من الفناديوم الرباعي ، النيكل الثنائي، النحاس الثنائي، البلاديوم الثنائي، الرينيوم الخماسي والبلاتين الرباعي. شخصت المركبات المحضرة بوساطة أطياف الاشعة تحت الحمراء، فوق البنفسجية – المرئية، الكتلة والرنين النووي المغناطيسي لنظيري البروتون والكاربون، ومنحنى التحلل الحراري الوزني والعزم المغناطيسي والتحليل الدقيق للعناصر ومحتوى الكلور الامتصاص الذري والتوصيلية المولارية. باستخدام برنامج الهايير كيم -8 حددت تراكيب المركبات بالطور الغازي لايجاد حرارة التكوين وطاقة الترابط والحرارة الكلية وطاقة الالكترونات وعزم ثنائي القطب بدرجة 200 كلفن.

الكلمات المفتاحية : ليكاندات قواعد شف ، 2,2 هكسان ثائى اون ،معقدات العناصر .