Preparation, spectral characterization, structural study, and evaluation of antibacterial activity of Schiff base complexes for VO^{II}, Cr^{III}, Mn^{II}, Zn^{II},Cd^{II} and Ce^{III}

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Abstract:

A new series of metal ions complexes of VO(II), Cr(III), Mn(II), Zn(II), Cd(II) and Ce(III) have been synthesized from the Schiff bases (4-chlorobenzylidene)-urea amine (L1) and (4-bromobenzylidene)-urea amine (L2). Structural features were obtained from their elemental microanalyses, magnetic susceptibility, molar conductance, FT-IR, UV–Vis, LC-Mass and ^{1}HNMR spectral studies. The UV–Vis, magnetic susceptibility and molar conductance data of the complexes suggest a tetrahedral geometry around the central metal ion except, VO^{II} complexes that has square pyramidal geometry, but Cr^{III} and Ce^{III} octahedral geometry. The biological activity for the ligand (L1) and its Vanadium and Cadmium complexes were studied. Structural geometries of compounds also were suggested in gas phase by using theoretical treatments, using Hyper Chem-6 program for the molecular mechanics and semi-empirical calculations. The heat of formation (ΔH_f^{o}) and binding energy (ΔE_b) in the temperature of 298K for the free ligand (L1) and their metal complexes were calculated by PM3 and ZINDO/I methods. The electrostatic potential of the free ligands were calculated to investigate the reactive sites of the molecules.

Bacteriological evaluation of considerable number of these compounds were maintained using organisms *Escherichia coli and Staphylococcus aureus,* and they were found to exhibit the high effect of activity. This may be attributed to the impact of both the Schiff bases and the metal present in these complexes.

Key words: (4-chlorobenzylidene)-urea amine, Schiff base complexes, Bacteriological activity.

Introduction:

Semicarbazide is a urea derivative in which one amide group of urea is replaced by hydrazine residue. The formula is $H_2NNH(C=O)NH_2$. The hydrochloride salt of semicarbazide is a white; it is used in preparing pharmaceuticals including nitro furan antibacterial (furazolidone, nitrofurazone, and nitrofurantoin) and related compounds. It is used as a derivatization reagent for aldehydes and ketones. It produces crystalline compounds with characteristic melting points with aldehydes and ketones and thus used as a derivation reagent. It is used as a solvent to separate hormones and essential oils. Semicarbazone is a ketone form of semicarbazide which is derived by the condensation reaction between a ketone (or aldehyde) and a semicarbazide, $R_2C=NNHC(=O)NH_2$. A search through literature reveals that there is no work has been done on the transition metal complexes of the Schiff base[1-6]. Keeping this in view, the present paper describes the results of an investigation on Schiff base complexes.

In the present paper, VO^{II}, Cr^{III}, Mn^{II}, Zn^{II}, Cd^{II} and Ce^{III} complexes with

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Schiff bases ligands are reported. These compounds have been characterized in the basis of analysis of the Schiff bases liquid and solid complexes.^{1}HNMR, elemental microanalysis (C.H.N and M), magnetic measurements, UV-Visible, LC-Mass, FT-IR spectra, conductivity measurement and Molar ratio.
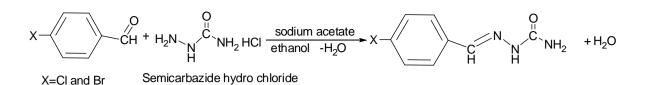
Experimental:
Materials and Methods:

Reagent grade 4-chlorobenzaldehyde, Semicarbazide hydrochloride 4-bromobenzaldehyde DMSO, DMF Vanadyl sulphate monohydrate and ethanol were obtained from Aldrich. Double distilled and used as received while $Ce(NO_3)_3.9H_2O$, $Cr(NO_3)_3.9H_2O$, $Cd(NO_3)_2.4H_2O$, $MnCl_2.4H_2O$ and $ZnCl_2$ were available from BDH chemicals. Solvents were purified by standard methods. The elemental microanalyses C, H and N were carried out on a EUROEA-Elemental analyzer Italia, Fourier Transfer Infrared Rays (FT-IR) the spectra were recorded on a Shimadzu 3800, FTIR spectrophotometer as KBr discs in range (4000-400)cm^{-1} while the solid reflectance, Molar conductivity measurements of the complexes at 25°C in freshly prepared 10^{-3} M solutions in DMF were determined using a PW9526 Digital Conductivity meter. LC-Mass 100P Shimadzu obtained mass spectra. The UV-Vis. spectra of the complexes were recorded in the range (200-1100) nm on a Shimadzu UV-160 spectrophotometer. Magnetic susceptibilities were measured on Johnson Matthey magnetic susceptibility balance and diamagnetic corrections were calculated using(Balance magnetic susceptibility model MSR-MKi), metal contents of the complexes were determined using a Shimadzu A.A680G atomic absorption Spectrophotometer, Nuclear magnetic resonance spectra ^{1}H-NMR for the ligands were recorded using Burker (400MHz) spectrophotometer with a tetramethylsilane (TMS) as an internal standard in DMSO-d^6. Syria. The chloride contents for complexes were determined by potentiometric titration by use platen electrical, the melting points of the prepared compounds were measured using Gallen Kamp apparatus while.

Preparation of ligands (4-chlorobenzylidene)-urea amine (L1) and (4-bromobenzylidene)-urea amine (L2)

The ethanolic solution of 4-chlorobenzaldehyde (1.4g, 10 mmol) or 4-bromobenzaldehyde (1.85g, 10 mmol) was refluxed with semicarbazide hydrochloride (1.11g, 10 mmol) add the sodium acetate (1.23g, 15mmol) for 10 hrs, the volume of the solution was reduced to one third. On cooling, a whit solid was separated, filtered and recrystallised from ethanol. After that, the product precipitated (L1) and (L2) yield (78%) and (88%), mp.(214-216) and (210)°C respectively. The LC-Mass for (L1) (197.5m/z) with ($C_8H_8N_3OCl$) and (80 m/z) with (C_5H_6N), (L2) (242 m/z) with ($C_8H_8N_3OBr$) and (110 m/z) with ($C_5H_6N_2O$). The ^{1}HNMR spectrum of ligands L1 and L2, in DMSO–d6 solvent shows a singlet signal at (δ =3.43 ppm) and (δ =3.41 ppm) equivalent to two protons assigned to (N–H$_2$) group and singlet signal at (δ =6.55 ppm) and (δ =6.47 ppm) equivalent to first protons assigned to (N–H) group respectively. First protons of (N=C–H) imine group appears as a singlet signal at (δ =10.35 ppm) and (δ =10.41 ppm) the multiple signals at (δ = 7.346, 7.71, 7.86ppm) and (δ = 7.35, 7.73, 7.89ppm) are due to aromatic hydrogen of carbon respectively of ligands L1 and L2 .

X=Cl and Br   Semicarbazide hydro chloride

Preparation of complexes

The complexes of VO(II), Cr(III), Mn(II), Zn(II) and Cd(II) were prepared by the reaction of ethanolic solution of the ligand L1 and L2 (0.04 mol) and the metal ions (0.02 mol) in 2:1 ratio with vigorous refluxed for 6 hrs, keeping the pH of the solution at 8. The reaction mixture was kept at 0°C for 12 hrs. The solid complexes formed were filtered and washed with ethanol and dried in vacuo. Approximately 80-85% of the yield was obtained for all the complexes.

The Ce(III) complex was also precipitated by a similar procedure in ethanol medium of the ligand L1 and L2 (0.06 mol) and the metal nitrate (0.02 mol) in 3:1 ratio.

Programs used in theoretical calculations

Hyper Chem-6 program is a sophisticated molecular modeler, editor and powerful computational package, that is known for its quality, flexibility and ease of use. uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics and dynamic [7,8]. In the present work, parameterization method 3(PM3) was used for the calculation of heat of formation and binding energy for all metal complexes. PM3 is more popular than other semi-empirical methods due to the availability of algorithms and more accurate than with other methods[8]. PM3/TM is an extension of thePM3 method to include orbital's for use with metal ions. It has parameterized primarily for organic molecules and selected metal ions.

Bacteriological Activity

Bactericidal activity of the ligands and its complexes were evaluated against representative gram-positive and gram-negative bacteria by agar-plate method[9]. All the compounds were prepared freshly by dissolving them in DMF to obtain a final concentration of 5 mM and10 mM. All bacteria were cultivated in nutrient agar. The results obtained are shown in Table (6).

Results and Discussion:

All the complexes are air stable, and insoluble in water DMSO, DMF, $CHC1_3$ and CH_2C1_2. They were identified by their physical and analytical data. The analytical data, Table (1) are in good agreement with the general formula $[M(L)_2](X)_n$. with M= Zn(II), Mn(II),VO(II) and Cd(II); and L=L1 and L2 and X= Cl, SO_4 and NO_3; and n= 1 for (VO), 2 for (Mn, Zn and Cd), $[Cr(L)_2(NO_3)_2]NO_3$ and $[Ce(L)_3](NO_3)_3$ The monomeric nature of the complexes were evidenced from their magnetic susceptibility values. Study of magnetic and electronic spectral data is quite informative in characterizing the geometry of the complexes. These complexes were electrolytic[10-12] (1:1) for Cr and VO complexes and (1:2) for Mn, Zn and Cd complexes and (1:3) for Ce complex due to the low conductivity values.

Table 1: Physical Characteristics and analytical data for (L1), (L2) and its metal complexes

Mol. Formula Mol. Weight	Color	Yield%	m.p (^{O}C)	C% Calc	H% Calc	N%Calc	M% Calc	Cl% Calc
				C% Expt	H% Expt	N% Expt	M% Expt	Cl% Expt
$(C_8H_8N_3OCl)$ L1=197.62	White	78	214-216	48.62	4.08	21.26	-	17.96
				48.01	5.01	21.05		16.87
$(C_8H_8N_3OBr)$ L2=242.02	Yellow	88	210	39.69	3.33	17.36	-	-
				38.43	4.12	17.34		-
$[Cr(NO_3)_2(L1)_2]NO_3$ =633.25	Violet	81	110-112	30.35	2.55	19.91	8.21	11.2
				31.11	2.11	20.13	7.87	12.11
$[Cr(NO_3)_2(L2)_2]NO_3$ =722.16	Violet	80	118-120	26.61	2.23	17.46	7.2	
				25.87	3.24	16.89	8.08	
$[Cd(L1)_2](NO_3)_2$ =631.66	Light yellow	84	116-118	30.42	2.55	17.74	17.80	11.23
				31.15	2.21	16.87	17.88	11.76
$[Cd(L2)_2](NO_3)_2$ =720.57	Dark yellow	85	123-125	26.67	2.24	15.55	15.60	
				26.06	2.13	15.44	15.88	
$[Ce(L1)_3](NO_3)_3$ =919.00	Light brown	83	160-162	31.37	2.63	18.29	15.25	11.57
				30.82	2.31	18.15	17.35	11.85
$[Ce(L2)_3](NO_3)_3$ =1052.35	Dark brown	82	168-170	27.39	2.30	15.97	13.31	
				28.27	3.02	16.01	13.14	
$[Mn(L1)_2]Cl_2$ =521.09	Light yellow	82	198-200	36.88	3.09	16.13	10.54	27.21
				37.11	3.76	15.72	11.11	26.88
$[Mn(L2)_2]2Cl$ =609.99	Light yellow	80	211-213	31.50	2.64	13.78	9.01	11.62
				30.46	2.96	13.72	9.26	12.01
$[Zn(L1)_2] Cl_2$ =531.54	Light yellow	81	183-185	36.15	3.03	15.81	12.30	26.68
				35.87	2.88	16.25	13.03	26.87
$[Zn(L2)_2] Cl_2$ =620.44	Bright yellow	82	188-190	30.97	2.60	13.55	10.54	11.43
				31.31	2.16	12.75	11.01	12.64
$[VO(L1)_2]SO_4$ =558.25	Yellow greenish	82	230-232	34.42	2.89	15.05	9.13	12.70
				34.98	3.07	15.75	10.01	13.03
$[VO(L2)_2]SO_4$ =647.15	Yellow greenish	83	238-240	29.70	2.49	12.99	7.87	-
				30.36	3.12	13.34	8.11	-

Infrared spectra

The IR spectra provide valuable information regarding the nature of functional group attached to the metal atom. The IR spectra of the ligands L1 and L2 showed strong bands in the 3286, 3190 cm^{-1} and 3294, 3201 cm^{-1} respectively assignable attributed to the −NH$_2$ group and the strong bands in the 3460 cm^{-1} and 3449 cm^{-1} respectively assignable attributed to the −NH group The appearance of this peaks in all the spectra of the complexes indicates that the –NH$_2$ and −NH groups is free from complexation[13]. The two bands observed in the range 1689-1692 cm^{-1} and 1590-1597 cm^{-1} can be assigned to ν(C=O) and ν(C=N) respectively for ligands L1 and L2[14]. In spectra of all the metal complexes, these bands show red shifts indicating the coordination of metal ions through carbonyl oxygen as well as imine nitrogen of semicarbazone moiety the assignments of the characteristic bands are summarized in Table (2). The metal complexes show new bands around 524-570 cm^{-1} and 489-540 cm^{-1} which are due to formation of M-N and M-O bands respectively[15,16]. In addition, the Vanadyl complexes shows a band at 940 cm^{-1} attributed to V=O frequency[17].

Table 2: FT-IR spectral data (wave number) cm^{-1} for the ligands (L1 and L2)and its complexes

Compound	υNH_2	υNH	$\upsilon C=O$	$\upsilon C=N$	$\upsilon M-O, \upsilon M-N$	Additional Bands
$(C_8H_8N_3OCl)$ L1	3286, 3190	3460	1689	1597	-	
$(C_8H_8N_3OBr)$ L2	3294, 3201	3449	1692	1590	-	-
$[Cr(NO_3)_2(L1)_2]NO_3$	3285, 3199	3361	1669	1553	489, 524	1319,1027 $\upsilon M-NO_3$
$[Cr(NO_3)_2(L2)_2]NO_3$	3268, 3195	3351	1659	1554	498, 566	1311,1011 $\upsilon M-NO_3$
$[Cd(L1)_2](NO_3)_2$	3269, 3187	3354	1665	1564	491, 567	
$[Cd(L2)_2](NO_3)_2$	3293, 3193	3351	1663	1549	504, 559	
$[Ce(L1)_3](NO_3)_3$	3278, 3201	3340	1662	1554	524, 560	
$[Ce(L2)_3](NO_3)_3$	3274, 3198	3346	1657	1550	521, 567	
$[Mn(L1)_2] Cl_2$	3287, 3206	3352	1662	1554	520, 570	
$[Mn(L2)_2] Cl_2$	3275, 3196	3349	1658	1554	526, 556	
$[Zn(L1)_2] Cl_2$	3277, 3200	3350	1661	1553	522, 566	
$[Zn(L2)_2] Cl_2$	3290, 3199	3348	1664	1555	521, 568	
$[VO(L1)_2]SO_4$	3288, 3198	3350	1663	1556	523, 570	940 υ V=O
$[VO(L2)_2]SO_4$	3289, 3185	3351	1663	1550	522, 566	940 υ V=O

Magnetic susceptibilities and electronic spectral studies:

The spectra of the ligands L1, L2 and their metal complexes were recorded in DMSO solution at room temperature. From the data Table (3), it's observed that all the complexes exhibit octahedral, tetrahedral and square pyramidal geometry around the metal ions.

Vanadium complexes:

Vanadium complexes showed two bands related to square pyramid Vanadium complexes[17] they were observed at 795, 565 nm and 783,563 nm respectively for Vanadium complexes with L1 and L2 Table (3) for the first and second transition and were assigned to $^2B_2g \rightarrow {}^2Eg$ and $^2B_2g \rightarrow {}^2B_1g$ transition respectively[18-19] the magnetic moment (1.7 B.M) is lower than spin only value, this is due to spin coupling[19]. Conductivity in DMSO showed that the complexes were ionic (1:2) electrolytic nature.

Zinc and Cadmium complexes:

The prepared complexes are Light yellow and diamagnetic which are expected d^{10} ions. The UV-Vis spectrum of the compound shows a relative change in the band position compared to that of the free. The conductivity measurement for this complexes in DMSO at 25 $^\circ$C showed to be (1:2) electrolytic nature[16,17]. The most propable structural of that complexes are tetrahedral geometry.

Cerium (III) complexes:

The magnetic moments values, μ_{eff} of the Ce^{III} complexes are the 2.34 and 2.57 B.M. respectively, being consistent with mononuclear complexes and free from ant ferromagnetism. All Ce^{III} complexes show a new absorption bands at 314 and 333 nm respectively for cerium with L1 and L2, which may be related to metal ligands charge transfer excitations[10]. The complexes have a coordination number 6 and may exist in octahedral geometries.

Manganese (II) complexes:

Manganese (II) complexes for ligands L1 and L2 showed peaks at 760nm and 706 nm respectively ,the peaks ware attributed to the (d-d) transition of the type ($^6A_1 \rightarrow {}^4A_1$) .the magnetic moment are 5.55 and 5.42 B.M respectively and conductivity in DMSO showed that the complexes were ionic (1:2) electrolytic nature. The most propable structural of that

complexes are tetrahedral geometry [20].

Chromium (III) Complexes:

The magnetic moments values, μ_{eff} of the Cr(III) complexes are the 3.9 and 3.9 B.M. respectively, being consistent with mononuclear complexes and free from ant ferromagnetism. Chromium (III) complexes show a new absorption bands at 318, 455, 631nm and 327, 452, 631 nm respectively for chromium with L1and L2, for the first, second and third transition and were assigned to $^4A_2g \rightarrow {}^4T_1g$ (P), $^4A_2g \rightarrow {}^4T_1g$ (F) and $^4A_2g \rightarrow {}^4T_2g$ (F) transition respectively. The complexes have a coordination number 6 and may exist in octahedral geometries[18,19].

Table 3: U.V-Visible spectra of free ligands and their complexes in 10^{-3} M in DMSO, Magnetic Moments and Molar Conductance in DMSO.

Compound	λ_{max} nm	Wave Number cm^{-1}	(d-d) Transitions	Molar Conduct-ance Am(Ω^{-1} cm^2 mol^{-1})	μeff (BM)	Suggested Structure
($C_8H_8N_3OCl$) L1	300	33333.3	$n \rightarrow \pi^*$	-	-	
($C_8H_8N_3OBr$) L2	316	31645.5	$n \rightarrow \pi^*$	-	-	
[Cr(NO$_3$)$_2$(L1)$_2$]NO$_3$	318 455 631	31446.5 21978 15847	$^4A_2g \rightarrow {}^4T_1g$ (P) $^4A_2g \rightarrow {}^4T_1g$ (F) $^4A_2g \rightarrow {}^4T_2g$ (F)	25	3.9	Octahedral
[Cr(NO$_3$)$_2$(L2)$_2$]NO$_3$	327 452 631	30581 22123 15847	$^4A_2g \rightarrow {}^4T_1g$ (P) $^4A_2g \rightarrow {}^4T_1g$ (F) $^4A_2g \rightarrow {}^4T_2g$ (F)	31	3.9	Octahedral
[Cd(L1)$_2$](NO$_3$)$_2$	-	-	-	43	diam	Tetrahedral
[Cd(L2)$_2$](NO$_3$)$_2$	-	-	-	47	diam	Tetrahedral
[Ce(L1)$_3$](NO$_3$)$_3$	-	-	-	157	2.34	Octahedral
[Ce(L2)$_3$](NO$_3$)$_3$	-	-	-	154	2.57	Octahedral
[Mn(L1)$_2$] Cl$_2$	760	13157	$^6A_1 \rightarrow {}^4A_1$	51	5.55	Tetrahedral
[Mn(L2)$_2$] Cl$_2$	706	14164	$^6A_1 \rightarrow {}^4A_1$	47	5.42	Tetrahedral
[Zn(L1)$_2$] Cl$_2$	-	-	-	48	diam	Tetrahedral
[Zn(L2)$_2$] Cl$_2$	-	-	-	49	diam	Tetrahedral
[VO(L1)$_2$]SO$_4$	795 565	12577 17699	$^2B_2g \rightarrow {}^2Eg$ $^2B_2g \rightarrow {}^2B_1g$	55	1.7	Square pyramidal
[VO(L2)$_2$]SO$_4$	783 563	12769 17679	$^2B_2g \rightarrow {}^2Eg$ $^2B_2g \rightarrow {}^2B_1g$	59	1.7	Square pyramidal

Theoretical study

The vibration spectra of the Schiff base (L1) were calculated by using a semi-empirical (PM3) and (ZINDO/I) method. The results obtained for wave numbers are presented in Table (5) Fig (2), and the comparison with the experimental values indicates a some deviation. These deviation may be due to the harmonic oscillator approximation and lack of electron correlation. It was reported [21] that frequencies coupled with Hartree- Fock Theory (HFT) approximation and a quantum harmonic oscillator approximation tends to be 10% too high.

(ZINDO/I) Zerners INDO method: Is the most suitable semi- empirical method for determining structures and energies of molecules with the first or second transition row metal[22].

Parameterization model, Version 3 (PM3): It a recently developed semi-empirical method that may contain as yet undiscovered defect[22] the parameters for PM3 were derived by comparing a much large number and wider variety of experimental versus computed molecular properties. PM3 which is primarily used for organic molecules, is also parameterized for many main groups and transition metal elements

Optimized geometries energy of metal complexes for Schiff base

A theoretically probable structures of metal complexes with Schiff base have been calculated to search the most probable model building stable structure Fig (1), the calculated optima geometries for ligands and it's metal complexes. The result of PM3 method of calculation in gas phase for the binding energies and heat of formation of Cr(III), Mn(II), Cd(II) ,Zn(II) and V(IV) these are describe in Table (4).

The results reflected that the complexes of imine exhibited to be more stable than the donor chelating ligand, this difference in stability of complexes might be related to the chelating effect Fig (3).

Table (4): Conformation energetic in (KJ.mol^{-1}) for ligands and its metal complexes

compounds	PM3		ZINDO/I	
	$\Delta H_f°$	ΔE_b	$\Delta H_f°$	ΔE_b
L1	12.378933	-2198.8560667		
MnL1	-65.0953082	-4280.6713082		
VL1	---	---	-8312.7773127	-12695.2143127
ZnL1	-94.3439130	-4359.3330870		
CdL1	-9238.608342	-13388.2383428		
CrL1	-163.4977939	-284.507529544		
L2	11.3758933	-2338.8560667		
MnL2	-67.0053082	-4330.6713082		
VL2	---	---	-8333.7773127	-12445.2143127
ZnL2	-93.3339130	-4359.3969870		
CdL2	-9738.778342	-13688.8883428		
CrL2	-166.4976639	-246.507669544		

Table (5): Comparison of experimental and theoretical vibration Frequencies for the ligands

ligand	NH$_2$		NH	C=O	C=N	
L1	(3286)* (3292)** (-0.18)***	(3190)* (3178)** (0.37)***	(3460)* (3225)** (3.9)***	(1689)* (1698)** (-0.53)***	(1597)* (1599)** (-0.12)***	(1597)* (1602)** (-0.31)***
L2	(3294)* (3288)** (-0.18)***	(3201)* (3189)** (0.37)***	(3449)* (3443)** (-0.18)***	(1692)* (1690)** (-0.12)***	(1590)* (1588)** (-0.12)***	

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

Bacteriological activity:

The bacteriological activity of the ligand L1 and it is metal complexes was studied by using inhibition method for two types of pathogenic bacteria. One type of bacteria was gram positive, which is *Staphylococcus*. The second one was gram negative, which is *Escherichia coli*. The biological effect of the chemical complexes was studied for the (2) types of bacteria as shown in Table (6).The rate of inhibition diameter was varied according to the variation in the complex type and Bacterial, the complexes high effective on the ligand.

Table (6): Antibacterial activities for Schiff base and its complexes

Compounds	*Staphylococcus aureus* (+)		*Escherichia coli* (-)	
	5mM	**10mM**	**5mM**	**10mM**
L1	-	-	+	-
VOL1	-	-	++++	-
CrL1	+	-	+	++
MnL1	+	+	+	++
ZnL1	++	+++	+++	++++
CdL1	++	+++	+++	-
CeL1	++	++	++++	++++

(-) = No inhibition = inactive, (+) = (3-5)mm = slightly active, (++) = (5-7)mm = moderately active, (+++) = (7-10) mm = active, (++++)= (10-12) highly active
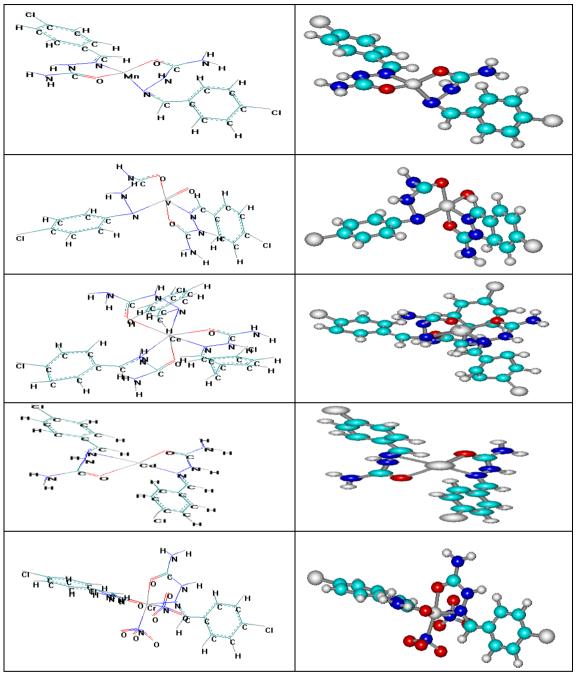
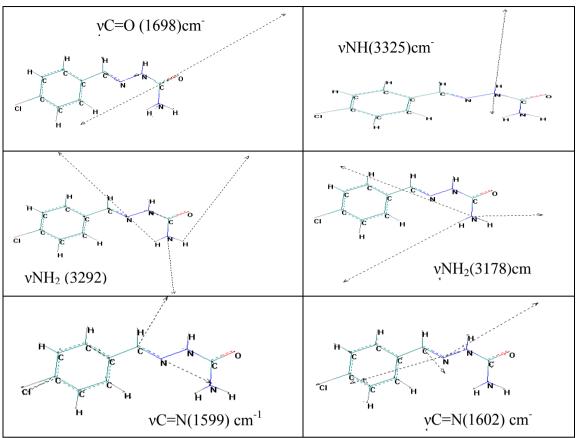**Fig. (1): Conformational Structure L1 and their Complexes**

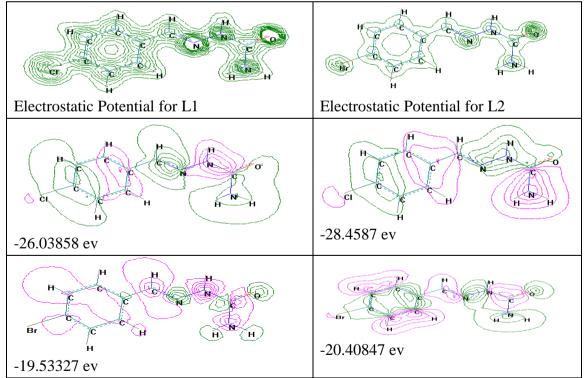**Fig. (2): The calculated vibration frequencies of L1**

Electrostatic Potential for L1

Electrostatic Potential for L2

-26.03858 ev

-28.4587 ev

-19.53327 ev

-20.40847 ev

Fig. (3): HOMO and Electrostatic Potential for L1 and L2

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تحضير،تشخيص طيفي،دراسة تراكيب وفعالية بكتيرية لمعقدات قواعد شف ثنائية السن

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الخلاصة :

تحضير سلسلة من معقدات المعادن الايونية الجديدة للـفناديوم بتكافؤه الرباعي، الكروم والسيريوم بتكافؤهم الثلاثي والمنغنيز، الخارصين، الكادميوم بتكافؤهم الثنائي مع قواعد شف المحضرة (4- كلوروبنزلدين)- يوريا امين و(4-بروموبنزلدين)-يوريا امين. المركبات المحضرة تم تشخيصها بوساطة تحليل الدقيق للعناصر، الحساسية المغناطيسية والتوصيلية المولارية، ودرست طيفياً بالاشعة تحت الحمراء، الفوق بنفسجية ـ المرئية، الكتلة والرنين النووي المغناطيسي. على ضوء نتائج أطياف الاشعة فوق البنفسجية ـ المرئية، الحساسية المغناطيسية والتوصيلية المولارية أظهرت النتائج ان المعقدات ذات شكل رباعي السطوح بينما اعطى الفناديوم شكل هرم مربع القاعدة ومعقدي الكروم والسيريوم شكل ثماني السطوح .

أجريت معالجة تكوين المعقدات نظريا في الطور الغازي بأستخدام برنامج (Hyper Chem-6) بتطبيق الميكانيك الجزيئي والشبه تجريبي في الحساب وذلك بأستخدام الدوال ZINDO/IوPM3 لحساب حرارة التكوين (ΔH_f °) وطاقة الترابط (ΔE_b) وبدرجة حرارة 298 كلفن كما أجري حساب الجهد الالكتروستاتيكي لبيان المواقع الفعالة في قاعدتي شف وجرى حساب التردد الاهتزازي نظريا وبأستخدام الدالة PM3 لقاعدتي شف ومقارنتها مع القيم المقاسة عمليا ووجد ان هناك توافق كبير بين القيم العملية والمحسوبة نظريا . كما تم حساب الجهد الألكتروستاتيكي وتحديد المواقع الفعالة (HOMO) و (LUMO) لليكاندين المحضرين. درست الفعالية البكتيرية لكل من الليكاند (4-كلوروبنزلدين)-يوريا امين ومعقداته ضد انواع منتخبة من البكتريا *Escherichia coli and Staphylococcus aureus*.وباستخدام تركيزين حيث اظهر التاثير زيادة الفعالية للمعقدات ويعزى ذلك الى تآزر كل من المعدن والليكاند ضمن المعقد.

الكلمات المفتاحية:4-كلوروبنزلدين، يوريا امين ، معقدات شف، فعالية حيوية.