



Synthesis, Characterization, Spectroscopic, Thermal and Biological Studies for New Complexes with N1, N2-bis(3-hydroxyphenyl) oxalamide

Abbas Ali Salih Al-Hamdani ^{a*}, Thamer A. M. Al-Alwany ^b, Marwa Abdulameer Mseer ^c, Areeg Malek Fadhel ^a, Yahya F Al-Khafaji ^c

^a Department of chemistry, Collage of Science for women, University of Baghdad, Baghdad, Iraq.

^b Al-Mustaqbal University College, Babylon 51001, Iraq

^c Department of chemistry, Collage of Science, University of Babylon, Babylon, Iraq.



CrossMark

Abstract

The synthesis, characterization and thermal analysis of mononuclear M(II) [M= Mn(II), Co(II), Ni(II), and Pd(II)] or M(IV) [M=VO(II) and Pt(IV)] complexes with the ligand namely [N¹,N²-bis(3-hydroxyphenyl)oxalamide](LH²) derived from oxalic acid and 3-aminophenol. Pure complexes of [VO(L₂)], [Co(L₂)(H₂O)₂], [Ni(L₂)(H₂O)₂], [Pd(L₂)], [Pt(L₂)(Cl)(H₂O)] have been isolated and characterized by FT-IR, UV-Vis, Mass spectra, ¹H-NMR spectra, TGA analysis, chloride containing, molar conductivity and atomic absorption. The spectroscopic data revealed mononuclear complexes and octahedral geometry for each Mn(II), Co(II), Ni(II) and platinum complexes otherwise Palladium complex gave a square planar geometry and Vanadium complex gave a square pyramidal geometry. The biological activities for the new compounds were evaluated against two types of bacteria and fungi and their results were good in inhibition.

Keywords: N1,N2-bis(3-hydroxyphenyl) oxalamide, Oxalic acid, Complexes, Biological activity, Thermogravimetric analysis.

Introduction

Amides is a compound with the general formula: RC (=O) NR'R'', where R, R', and R'' represent organic compounds or hydrogen atoms [1, 2]. Amides are a derivative of a carboxylic acids RC=OOH with the hydroxyl group -OH replaced by an amine group -NR'R''; or, equivalently, an acyl (alkonyl) group RC=O joined to an amine group. It is one of the essential and worthy organic functional groups in naturally occurring molecules, pharmaceutical, agrochemicals and polymers. They have the ability to form a number of complexes with metals ions so that it will have high importance from the biological and industrial application [3] due to the important feature than the amides compounds [4, 5]. Metal amides are a class of coordination compounds composed of a metal center with amide ligand of the form NR₂ [6, 7]. Exploring amide complexes still remain rare. Herein we synthesized and characterized

a new family of amide complexes and investigate their thermal properties these complexes derived from, N¹, N²-bis (3-hydroxyphenyl) oxalamide with di or tetra valance metals ions. Their biological activity also investigated.

Experimental

Materials:

The following chemicals were commercially available products of analytical reagent grade. 3aminophenol, Oxalic acid, DMSO, pure ethanol, Diethyl ether, NiCl₂.6H₂O, CuCl₂.2H₂O, PdCl₂, MnCl₂.4H₂O, CoCl₂.6H₂O, VOSO₄.H₂O were obtained from Fluka and Aldrich.

Instrumentation:

The (FT-IR) were recorded in the range (4000-400) cm⁻¹ on a Shimadzu3800 spectrometer. The electronic spectra registered by using (Shimadzu-

*Corresponding author e-mail: sci.yahya.alkhafaji@uobabylon.edu.iq.; (Yahya F Al-Khafajic).

Receive Date: 12 June 2022, Revise Date: 14 July 2022, Accept Date: 08 August 2022, First Publish Date: 08 August 2022

DOI: 10.21608/EJCHEM.2022.144403.6297

©2023 National Information and Documentation Center (NIDOC)

160) Spectrophotometer. Mass analysis of compounds has been done with LC-Mass 100P Shimadzu. TGA studies of all compounds were performed on perkin-Elmer pyris Diamond DTA/TG. $^1\text{H-NMR}$ spectra were recorded using Bruker 400-MHz spectrometer and elemental analysis (C,H,N and O) were carried out on a perkin-Elmer automatic equipment model 240B. Metals were determined using a Shimadzu (A-A) 680G atomic absorption spectrometer. Conductivity measurements using a jenway 4071. The chlorine content was determined gravimetrically. Magnetic properties were measured using balance magnetic susceptibility model MSR-MKi.

Synthesis of ligand N^1, N^2 -bis (3 hydroxyphenyl) oxalamide [8]

An ethanolic solution (10ml) of 3-aminophenol (0.132g, 0.002mol) was added to a mixture containing an ethanolic solution (10ml) of Oxalic acid (0.121g, 0.001mol), the mixture was heated on water bath at 50-60 °C for 4 hours. A white color was formed then the product was dried, collected and weighted. Yield: 86.9% (0.300g), m.p (90-92°C). $^1\text{H-NMR}$ (DMSO- d_6 , ppm): (2.48-2.50)(7.58-7.69) ((8H) m, aromatic), (8.58)((2H) s, NH), (10.58)(2H) s OH phenolic group). Figure 1 and table(1)

Synthesis of complexes[9]

A solution of the ligand (0.108g, 0.0004mol) in ethanol (10ml), an ethanol: water (1:1) solution (10ml) of the metal salt (0.0008mmol) (0.103g, 0.103g, 0.141g, 0.158g, 0.414g) ($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, PdCl_2 , $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$, $\text{H}_2\text{PtCl}_6 \cdot 6\text{H}_2\text{O}$) respectively, (0.072g, 0.0004mmol) $\text{VOSO}_4 \cdot \text{H}_2\text{O}$. The resulting mixture was refluxed in water bath for

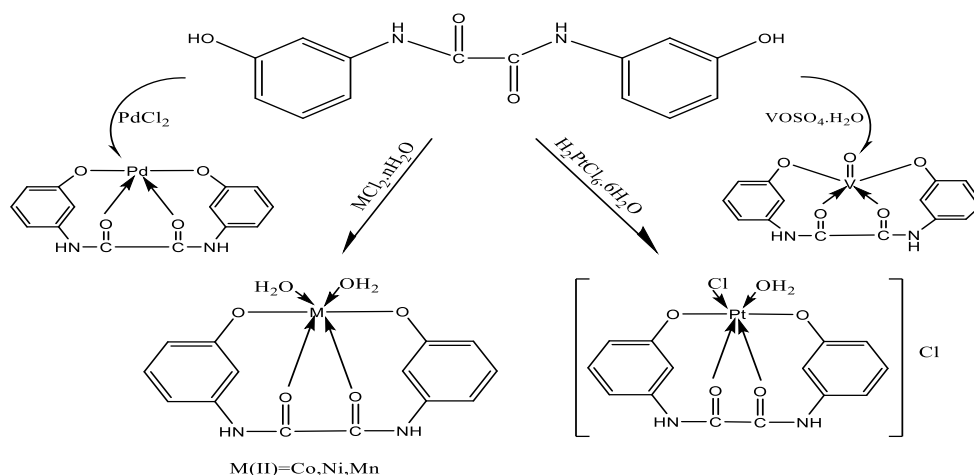
6 hours, a solid mass was formed, which was dried, collected and weighted. Physical properties for the complexes are given in table 1. The analytical results are in good agreement with the suggested stoichiometry of the organic complexes. The ligand to the metal ratio of organic complexes was found to be (1:1) [10]. The reaction illustrated in Scheme (1).

Results and discussion

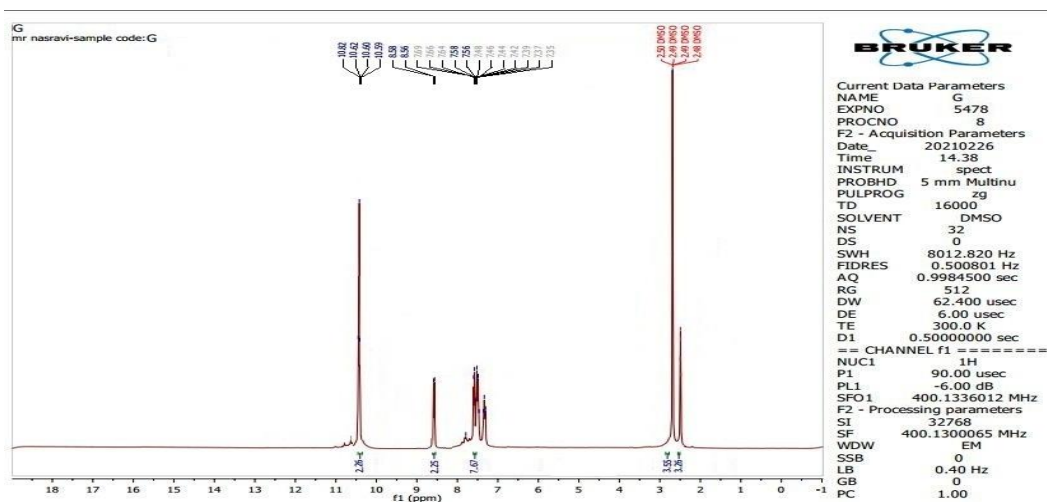
C.H.N Analysis were conducted and it was found that the practical results match the theory as shown in the table (2). The molar conductivity showed that all the complexes were non-electrolyte. But the Pt complex is electrolyte (1:1) which is proved by chlorine contain test was found(6.98). According to the results as mention in table (2) by using DMF as a solvent.

UV-Visible for the ligand and its complexes

The electronic spectrum of the ligand show intense absorption at 290, 332.5nm belongs to ($\pi \rightarrow \pi^*$), ($n \rightarrow \pi^*$) respectively. The electronic spectrum of Ni(II) complex showed four peaks at 270, 370, 695 and 860nm assigned to ($\pi \rightarrow \pi^*$), $\nu_3(n \rightarrow \pi^*)$, $\nu_2(^4\text{T}_1\text{gF} \rightarrow ^4\text{T}_1\text{g(P)})$ and $\nu_1(^4\text{T}_1\text{gF} \rightarrow ^4\text{A}_1\text{g(F)})$ respectively. The electronic spectrum of Pd(II) complex showed four peaks at 242, 381, 560 and 685nm assigned to ($\pi \rightarrow \pi^*$), ($n \rightarrow \pi^*$), ($^1\text{A}_1\text{g} \rightarrow ^1\text{B}_1$), ($^1\text{A}_1\text{g} \rightarrow ^1\text{A}_2$) respectively. The electronic spectrum of V(IV) complex showed four peaks at 263, 340, 380 and 597nm assigned to ($\pi \rightarrow \pi^*$), ($n \rightarrow \pi^*$), ($^2\text{B}_2\text{g} \rightarrow ^2\text{B}_1\text{g}$), ($^2\text{B}_2\text{g} \rightarrow ^2\text{Eg}$) respectively.



Scheme 1. Preparation of the ligand and their complexes

Fig. 1 $^1\text{H-NMR}$ spectrum of LH_2 ligandTable 1 $^1\text{H-NMR}$ spectra for the LH_2 ligand and the chemical shift in ppm

Ligand	Functional group	$\delta(\text{ppm})$
LH_2	Ar-H	(7.58-7.69) (8H-m)
	O-H Phenolic	(10.58) (2H-s)
	N-H amide	(8.58) (2H-s)
	DMSO (Solvent)	(2.48-2.50)

Table 2 Elemental analysis and physical properties for the ligand LH_2 and their metal complexes

Compounds	Formula M.wt	Color	m.p $^\circ\text{C}$	Yeild%	molar conductivity $\text{S.cm}^{-1}\text{mol}^{-1}$	Element analysis %Calcu (Found)			
						M	C	H	N
LH_2	$\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_4$ 272.26	White	90-92	86.9	--	-	61.7 61.16	4.34 4.40	10.28 10.27
$[\text{Mn}(\text{L})(\text{H}_2\text{O})_2]$	$\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_6\text{Mn}$ 361.21	reddish brown	235-236	68	9	15.20 (15.72)	46.55 (46.01)	3.87 (3.82)	7.75 (7.66)
$[\text{Co}(\text{L})(\text{H}_2\text{O})_2]$	$\text{C}_{14}\text{H}_{14}\text{CoN}_2\text{O}_6$ 365	dark blue	200-202	71	14	16.11 (16.35)	46.06 (46.22)	3.83 (3.82)	7.67 (7.66)
$[\text{Ni}(\text{L})(\text{H}_2\text{O})_2]$	$\text{C}_{14}\text{H}_{14}\text{N}_2\text{NiO}_6$ 364.96	White	160-162	79	3	16.13 (16.41)	46.07 (45.59)	3.83 (2.97)	7.67 (7.42)
$[\text{Pd}(\text{L}_2)]$	$\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_4\text{Pd}$ 376.66	Light green	198-202	58	8	28.25 (26.11)	44.64 (44.81)	2.65 (3.03)	7.34 (8.29)
$[\text{VO}(\text{L})]$	$\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_5\text{V}$ 337.18	dark brown	199-202	68	18	15.10 (17.18)	49.87 (48.31)	2.96 (2.15)	8.30 (8.04)
$[\text{Pt}(\text{L})(\text{Cl})(\text{H}_2\text{O})\text{Cl}]$	$\text{C}_{14}\text{H}_{12}\text{ClN}_2\text{O}_5\text{Pt}$ 520.76	reddish brown	>300	87	60	37.46 (30.21)	32.29 (30.50)	2.30 (3.86)	5.37 (6.74)

Table 3 Electronic spectra data for the ligand and its complexes

Compound	ABS	λ_{nm}	(L.mol ⁻¹ .cm ⁻¹ ε	Assignment	$M_{eff}(BM)$	Suggested formula
LH ₂	1.1099	290	1109.9	$\pi \rightarrow \pi^*$		
	0.8	332.56	800	$n \rightarrow \pi^*$	--	Octahedral
[Co(L)(H ₂ O) ₂]	0.07	617	70	${}^4T_{1g}F \rightarrow {}^4T_{1g}(P)$	3.884	Octahedral
	0.1	679	100	${}^4T_{1g}F \rightarrow {}^4A_{1g}(F)$		
[Ni(L)(H ₂ O) ₂]	1.24	370	1240	$n \rightarrow \pi^* + C.T$		
	0.09	695	90	${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(p)$	2.217	Octahedral
[Pd(L)]	0.1	860	100	${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(F)$		
	0.54	381	540	$n - \pi^* + C.T$		
[VO(L)]	0.052	560	52	${}^1A_{1g} \rightarrow {}^1B_1$	--	Square planar
	0.051	685	51	${}^1A_{1g} \rightarrow {}^1A_2$		
[Mn(L)(H ₂ O) ₂]	0.045	380	45	${}^2B_{2g} \rightarrow {}^2B_{1g}$	1.519	Square pyramidal
	0.052	597	52	${}^2B_{2g} \rightarrow {}^2E_g$		
[Pt(L)(Cl)(H ₂ O)]Cl	0.87	290	870	$n \rightarrow \pi^* + C.T$		
	0.051	440	51	${}^6A_{1g} \rightarrow {}^4T_2(G)$	3.714	Octahedral
[Pt(L)(Cl)(H ₂ O)]Cl	0.054	600	54	${}^6A_{1g} \rightarrow {}^4T_1(G)$		
	0.06	540	60	${}^1A_{1g} \rightarrow {}^1T_{2g}$	--	Octahedral
	0.06	670	60	${}^1A_{1g} \rightarrow {}^1T_{1g}$		

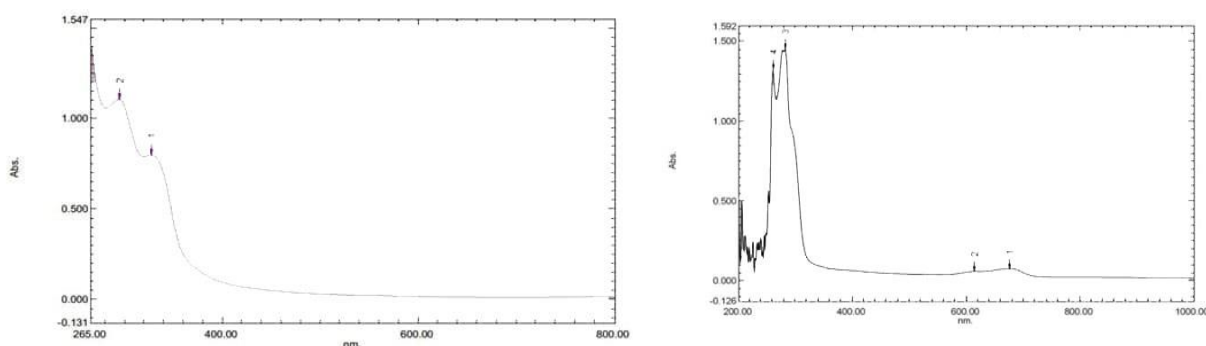


Fig. 2 the electronic spectra of the ligand and the selected complex (cobalt complex)

Infrared Spectral studies of the ligand and the complexes

The FTIR spectrum of ligand figure 3 shows bands at (3447, 3264, 1742) cm^{-1} , that belongs to $\nu(\text{O-H})$, $\nu(\text{N-H})$, $\nu(\text{C=O})$ respectively, which confirms ligand structure [11, 12]. Also the complexes are characterized and their spectra are compared with free ligand spectrum. It is noticed the disappearance of phenolic (O-H) band in all complexes spectra compared with ligand

spectrum[13]. This indicates that the coordination with metals and new bands are appeared that belongs to (M-O) at (453, 521, 481, 500, 505, 400) cm^{-1} for the complexes (Mn, Co, Ni, Pd, VO, Pt) respectively which confirms coordination occurrence. Besides (C=O) group bands are shifted in complexes compared to ligand which supports coordination occurrence through the oxygen [14-17]. Characteristic vibrations and assignments of the ligand and its complexes are reported in table (4).

Table 4 The Infrared Spectra Data of the ligand and its complexes

compounds	$\nu(\text{O-H})$	$\nu(\text{N-H})$	$\nu(\text{C=C})$	$\nu(\text{C-H})$ aromatic	$\nu(\text{C=O})$	$\nu(\text{M-O})$	Other band
LH ₂	3447	3264	1595	3084	1742	-	-
[Co(L)(H ₂ O) ₂]	-	3250	1558	3090	1620	451,521	3590,779,677,aqua
[Ni(L)(H ₂ O) ₂]	-	3275	1558	3071	1620	453,481	3398,779,677,aqua
[Pd(L)]	-	3286	1570	3057	1604	447,500	
[VO(L)]	3500	3289	1566	3011	1601	469,505	910(V=O)
[Mn(L)(H ₂ O) ₂]	-	3275	1550	3095	1618	453	3575,734,678
[Pt(L)(Cl)(H ₂ O)]Cl	-	3270	1557	3098	1618	440,410	3577,750,H ₂ O aqua

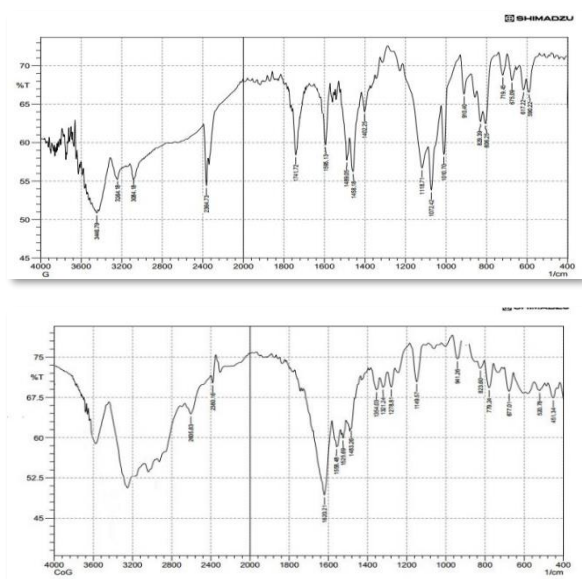


Fig. 3 The IR spectrum of the ligand and cobalt complex

Mass spectra Analysis

The mass spectra of the ligand and Ni,VO complexes are shown in figure (4-5), the peak at $m/z = 272.26$, 364.96 and 337.18 due to the molecular ion peak, which coincides with its formula weight, and table (5) shows mass spectra data for ligand and its complexes [18, 19].

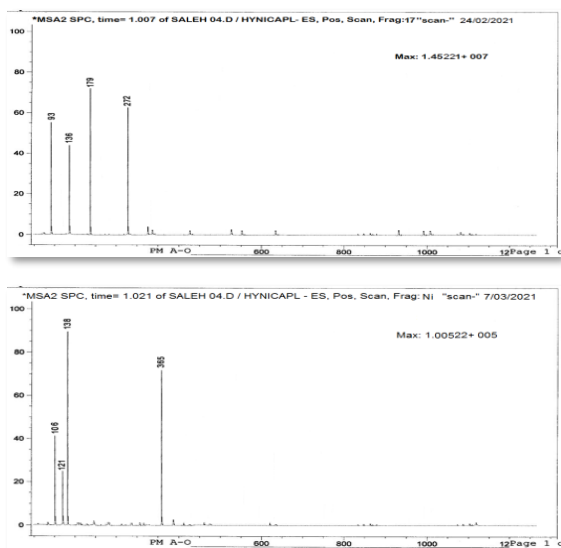


Fig 4. Mass spectrum of (LH_2) ligand and $[Ni(L)(H_2O)_2]$

Thermal gravimetric analysis

The results of thermogravimetric analysis of LH_2 and their complexes are given in Table (6) and figure (6). The thermograms have been carried out in the range of $25 - 600\text{ }^\circ\text{C}$ at a heating rate of $10\text{ }^\circ\text{C}/\text{min}$ in nitrogen atmosphere, they showed an agreement in weight loss between their results obtained from the thermal decomposition and the calculated values, which supports the results of elemental micro analysis and confirms the suggested formulae [20-22].

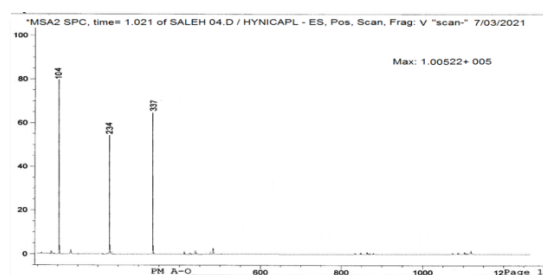


Fig. 5 Mass Spectrum of $[VOL_2]$

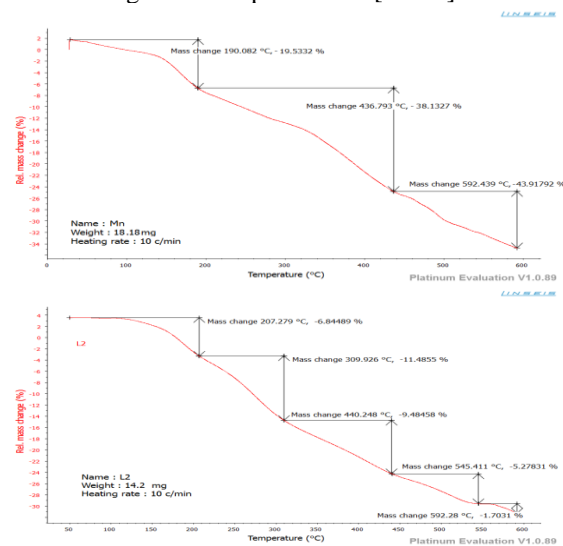


Fig. 6 TGA and Curve for ligand and Mn complex

Microbiological investigations

The biological activity of ligand and all complexes were tested against two types of bacteria figure 7. We used the organisms in investigation included gram positive bacteria (*S.aureus*) and gram negative bacteria (*E.coli*). The bactericidal screening results of the prepared compounds are recorded in table (7). The influence of the central ion of the complexes in the antibacterial activity against the tested gram positive and negative bacteria shows the complexes have an activity in inhibition [23-26].

Table 5 Mass spectra Data for ligand and its complexes

Compounds	Assignment	Peak m/z	Abundance
LH ₂	M=C ₁₄ H ₁₂ N ₂ O ₄	272.26	62%
	C ₈ H ₇ N ₂ O ₃ ⁺	179.15	72%
	C ₇ H ₆ NO ₂ ⁺	136.13	44%
	M=C ₆ H ₅ O ⁺	93.10	55%
[Co(L)(H ₂ O) ₂]	M=C ₁₄ H ₁₄ CoN ₂ O ₆	365	71.5%
	M=C ₇ H ₈ CoNO ₅ ⁺	245.08	72%
	M=C ₇ H ₆ NO ⁺	120	35%
[Ni(L)(H ₂ O) ₂]	M=C ₁₄ H ₁₄ N ₂ NiO ₆	364.96	72%
	M=C ₇ H ₈ NO ₂ ⁺	138.14	90%
	M=CH ₂ NiO ₃ ⁺	121	25%
	M=C ₆ H ₄ NO ⁺	106	41%
[Pd(L)]	M=C ₁₄ H ₁₀ N ₂ O ₄ Pd	376.66	73%
	M=C ₇ H ₆ NO ⁺	120.13	35%
	M=CH ₂ O ₂ Pd ⁺	152.45	80%
	M=C ₆ H ₃ NO ⁺	105	46%
[VO(L)]	M=C ₁₄ H ₁₀ N ₂ O ₅ V	337.18	65%
	M=C ₇ H ₄ NO ₅ V ⁺	234	55%
	M=C ₇ H ₆ N ⁺	104	80%
[Mn(L ₂)(H ₂ O) ₂]	M=C ₁₄ H ₁₄ MnN ₂ O ₆	361.21	60%
	M=C ₇ H ₈ NO ₂ ⁺	138.14	89%
	M=CH ₂ MnO ₃ ⁺	117	80%
	M=C ₆ H ₄ NO ⁺	106	41%

Table 6 thermal analysis data of the ligand and its complexes

Compounds	Step	TGA				Reaction	Total mass loss%
		T _i /°C	T _f /°C	T _{DTG} _{max}	Weight mass loss% found(cal)		
LH ₂	1	113.5	209.8	169.8	17.013(16.528)	-OH,CO	99.78 (106)
	2	209.8	318.7	251.3	17.775(18.051)	-CO ₂ ,CH ₄	
	3	118.7	442.5	377.8	28.951(29.991)	C ₅ H ₃ N	
	4	442.5	541.1	489.4	21.631(20.311)	C ₄ H ₄ N	
	5	541.1	596.5	569.3	14.41(15.119)	C ₂	
Total wt. loos= 99.78%Found (100 % Cal) and final residue:0.22 % Found(0% Cal)							
MnL	1	40.115	188.632	151.01	17.162(18.313)	-2H ₂ O,2CO	85.956 (87.231)
	2	188.632	436.212	309.67	39.661(39.956)	C ₆ H ₈ N ₂	
	3	436.212	596.445	489.95	29.133(28.962)	C ₆ H ₂ O	
MnO							
Total wt. loos= 85.956%Found (87.231 % Cal) and final residue: 14.044 % Found(12.769% Cal)							
NiL	1	40.115	205.5	108.71	23.321(22.661)	2H ₂ O,2CO	87.884 (87.781)
	2	205.51	440.14	316.84	22.612(23.059)	C ₆ H ₇ N	
	3	440.14	596.695	498.7	41.951(42.061)	C ₆ H ₃ O	
NiO							
Total wt. loos=87.884 %Found (87.781% Cal) and final residue:12.116 % Found(12.219% Cal)							
PtL	1	103.32	218.821	151.136	14.410(15.551)	-H ₂ O,2CO	89.458 (88.596)
	2	218.821	321.123	277.71	18.681(17.771)	2Cl	
	3	321.123	447.188	378.87	23.321(22.321)	C ₃ H ₄ N	
	4	447.188	541.110	497.794	14.441(15.05)	C ₅ H ₆	
	5	541.110	596.51	569.962	18.605(17.911)	C ₂ H ₂ N	
PtO ₂							
Total wt. loos= 89.458%Found (89.458 % Cal) and final residue:10.542 % Found(11.406% Cal)							

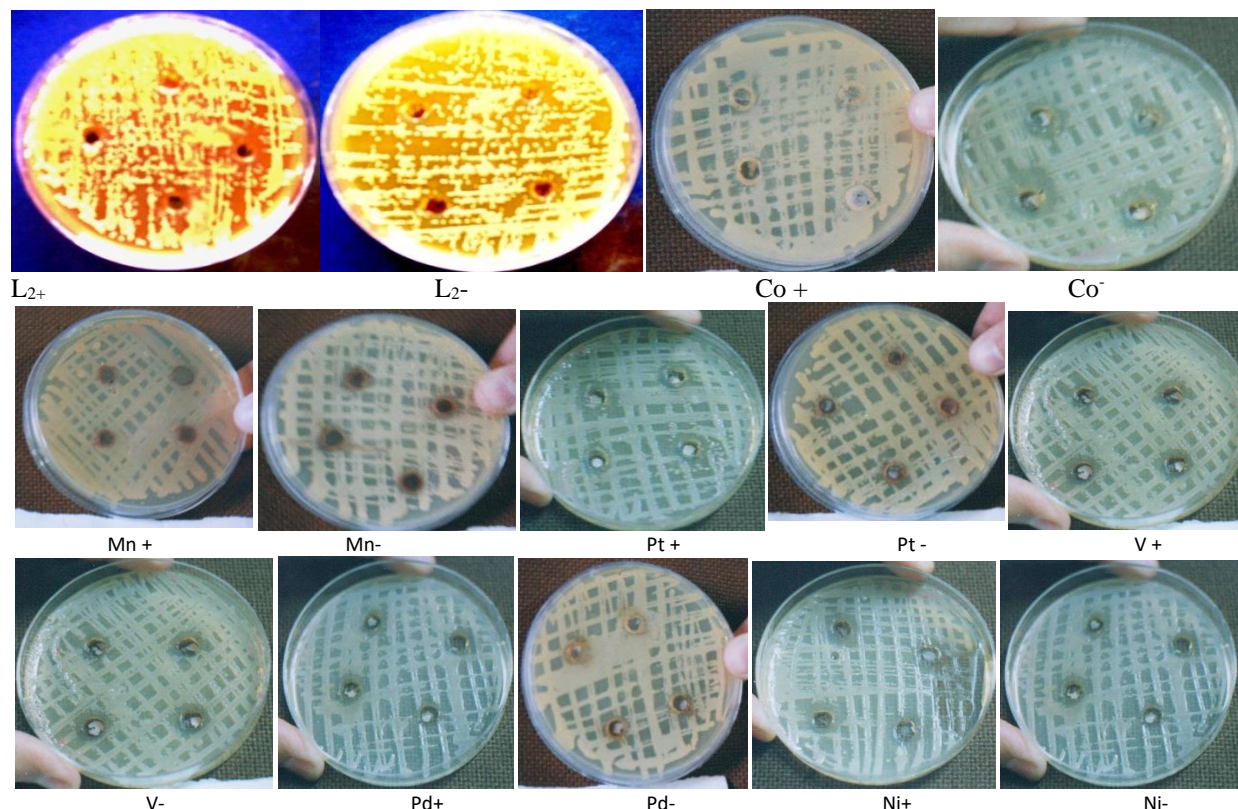


Fig. 7 Effect of the ligand and its complexes towards gram positive bacteria and gram negative bacteria

Table 7 MIC of different chemical compounds with different microorganisms

No.	Compounds	G+(<i>Staph</i>)	G-(<i>E-Coli</i>)
1	LH ₂	1.2	1.2
2	[VO(L ₂)]	1.1	1.2
3	[Mn(L)(H ₂ O) ₂]	0.6	0.8
4	[Co(L)(H ₂ O) ₂]	0.7	1.5
5	[Pt(L)(H ₂ O)Cl]Cl	1.5	1.6
6	[Pd(L)]	0.7	1.2
7	[Ni(L)(H ₂ O) ₂]	1.1	1.9

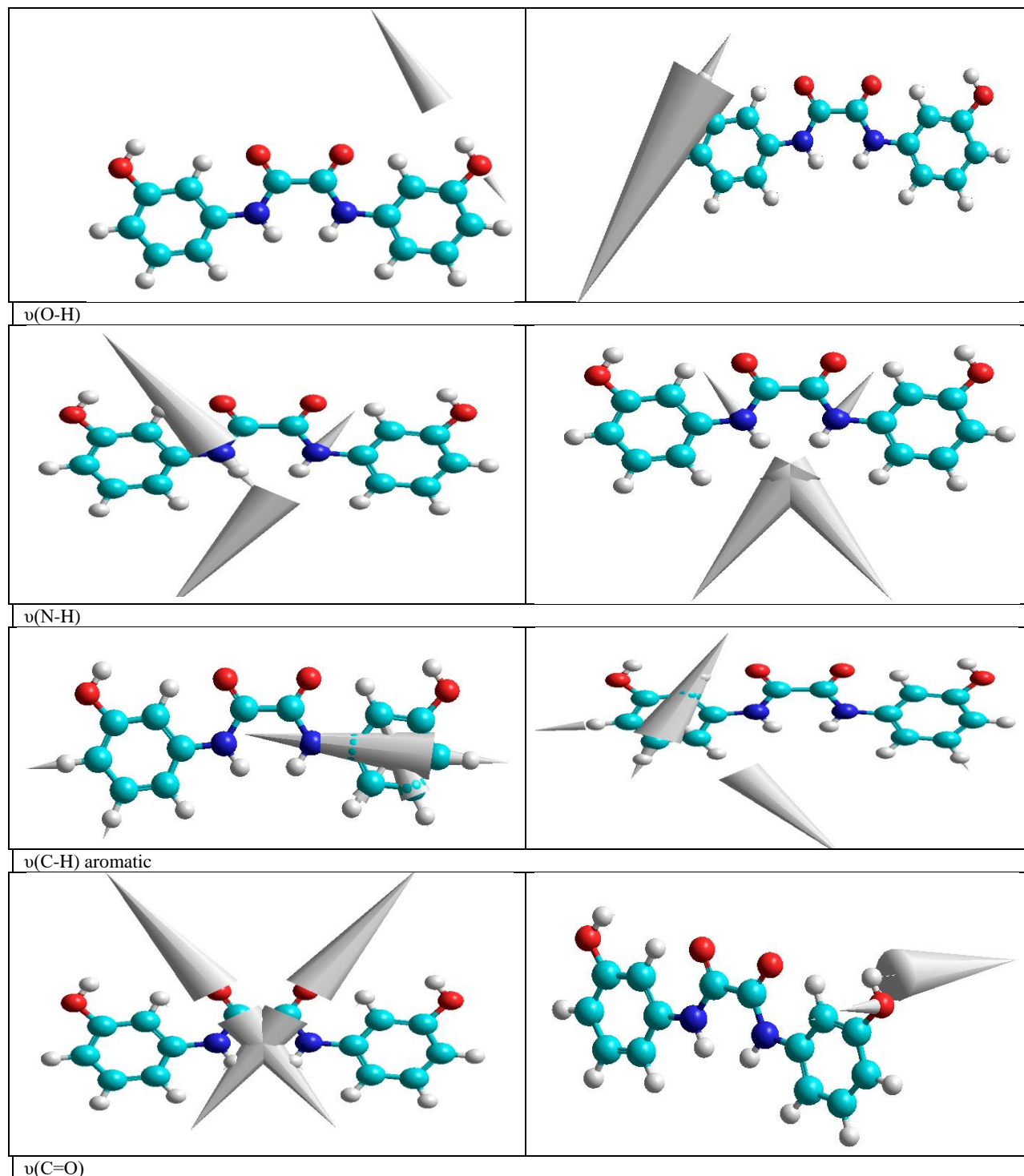
Theoretical Study

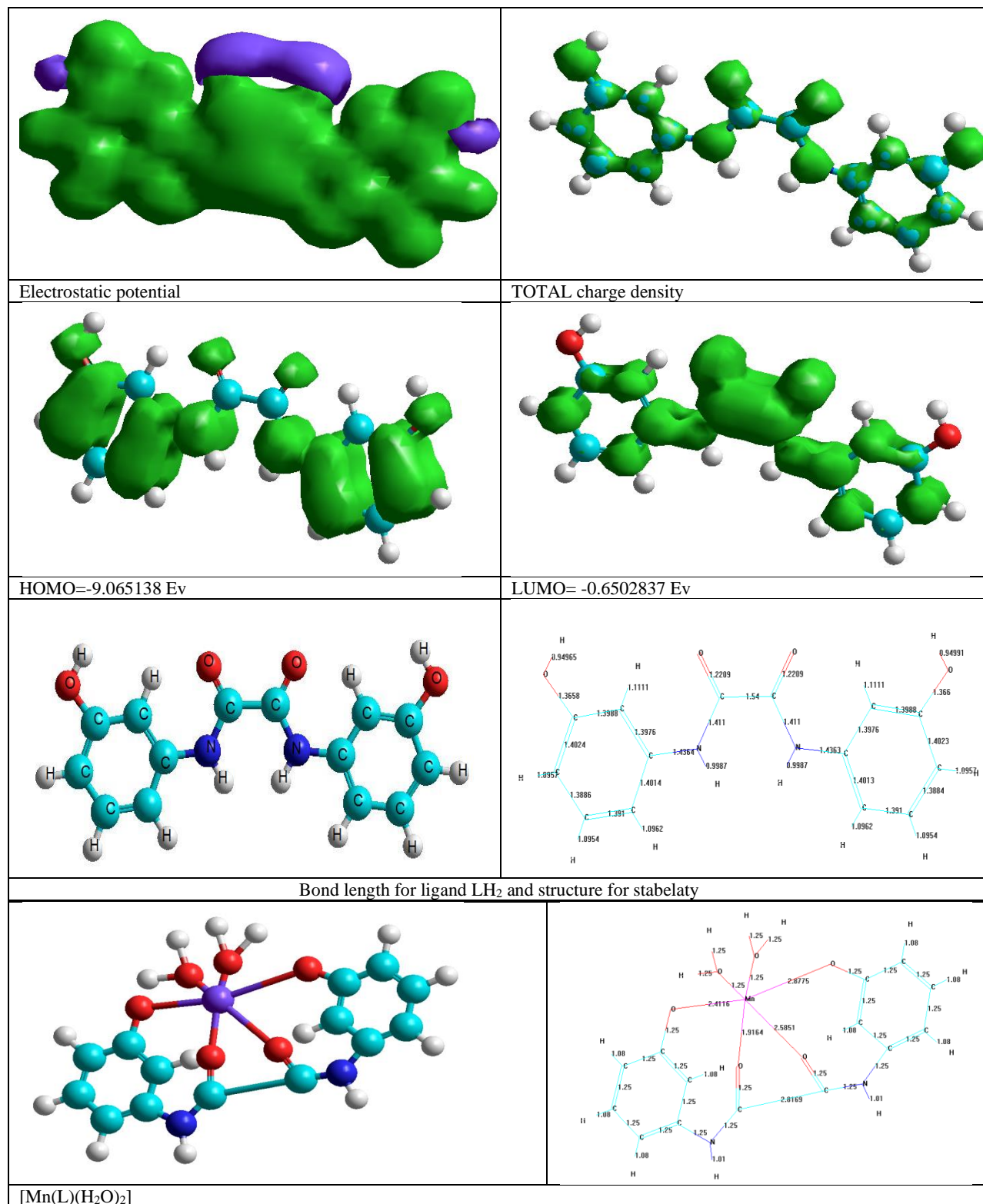
The vibration spectra of amide ligand were calculated by using a Hyber chem.8 method. The results obtained for wave numbers are presented in

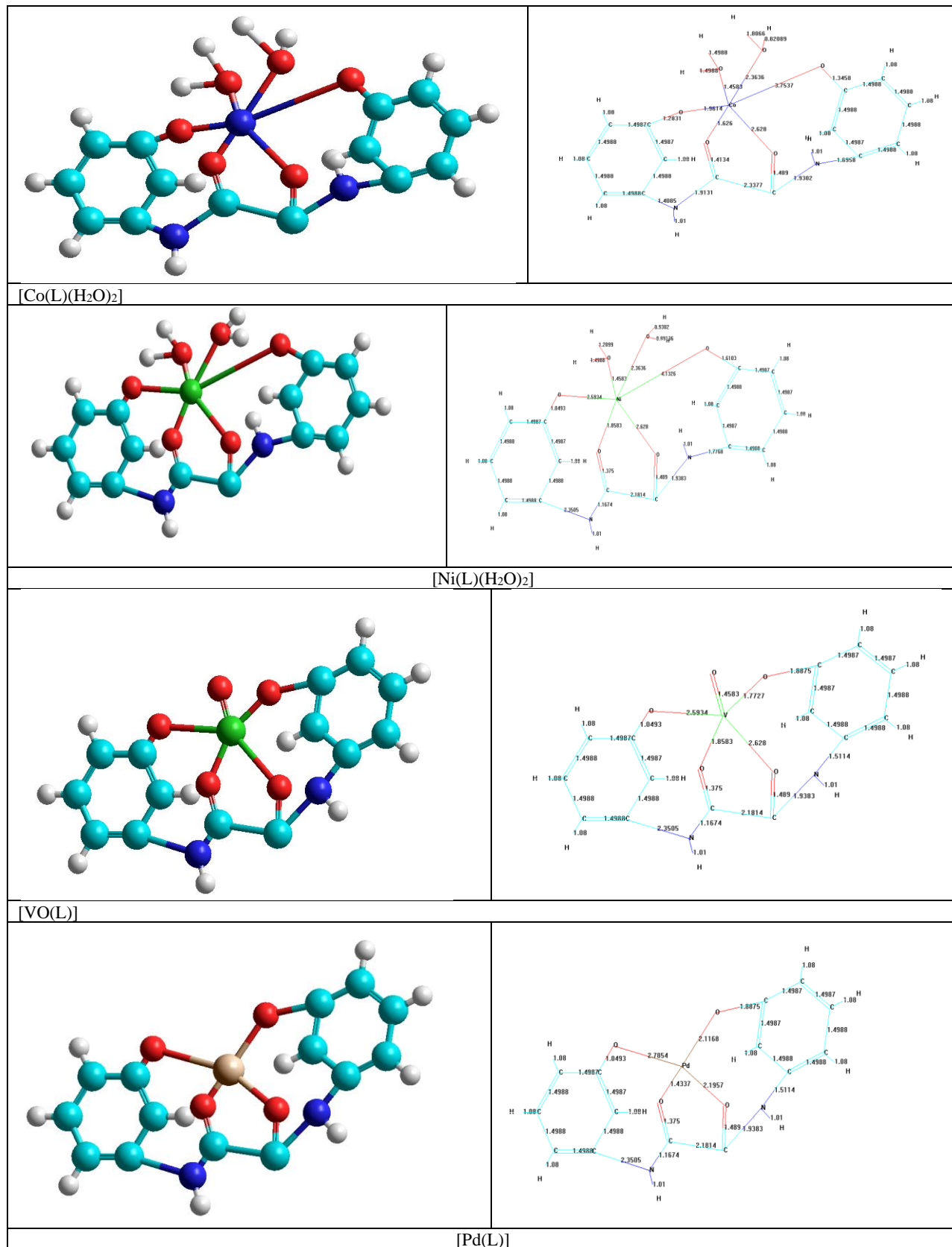
table (8) refers to all compounds are stable through results of formation heat, bonds energy and total energy and the comparison with the experimental values indicates some deviations. These deviations may be related to the approximation of the harmonic oscillator and the lack of electronic correlation [27]. It is reported that frequencies coupled with (HFT) approximation and quantum harmonic oscillator approximations tend to be 10% too high. The structures of ligand are calculated to search for the most probable model building stable structure [28-31]. These shapes show the calculated optima geometries for compounds prepared as shown in figure 10.

Table 8 Conformation Energetic in (K.J.Mol⁻¹) for the ligand and complexes

compounds	Total energy	Binding energy	Heat of formation	Electronic energy	Dipole (Debyes)
LH ₂	-77072.4233208	-3584.119108	-102.1991088	-480253.3122365	3.738
V-Complex	-100008.291114	-3325.348407	155.1675927	-590381.6460722	4.457
Mn-Complex	-66299.159734	-5522.48624	-56.552418	-951746.8521	4.016
Co-Complex	-362047.043750	-4479.970320	405.7256796	-1130444.552171	3.852
Ni-Complex	-134239.645784	-3331.820384	-17.3243845	-1876532.414264	7.084
Pt-Complex	-16299.159734	-5442.48624	-48.552418	-852746.8521	4.0124
Pd-Complex	-3235576.95172	-7444.137942	-13.84315922	-652111.85271	5.105

Fig. 8 The calculated vibrational frequencies of ligand L₁H₂ theoretically





- complexes of a hybrid ligand 4'-(4'''-benzo-15-crown-5)-methyloxy-2,2':6',2''-terpyridine," *Dalton Transactions*, pp. 2482-2489, 2009.
- [10] W. Al Zoubi, M. J. Kim, A. A. Salih Al-Hamdani, Y. G. Kim, and Y. G. Ko, "Phosphorus-based Schiff bases and their complexes as nontoxic antioxidants: Structure-activity relationship and mechanism of action," *Applied Organometallic Chemistry*, vol. 33, p. e5210, 2019.
- [11] S. V. Jirjees VY, Al-Hamdani AAS, Ahmed SD, "Preparation, Spectroscopic Characterization and Theoretical Studies of Transition Metal Complexes with 1-[(2-(1H-indol-3-yl) ethylimino) methyl] naphthalene-2-ol Ligand," *Asian J. Chem*, vol. 31, p. 8, 2019.
- [12] Y. F. Al-Khafaji, M. R. J. Elsegood, J. W. A. Frese, and C. Redshaw, "Ring opening polymerization of lactides and lactones by multimetallic alkyl zinc complexes derived from the acids Ph₂C(X)CO₂H (X = OH, NH₂)," *RSC Advances*, vol. 7, pp. 4510-4517, 2017.
- [13] F. Ge, Y. Dan, Y. Al-Khafaji, T. J. Prior, L. Jiang, M. R. J. Elsegood, *et al.*, "Vanadium(v) phenolate complexes for ring opening homo- and co-polymerisation of ε-caprolactone, l-lactide and rac-lactide," *RSC Advances*, vol. 6, pp. 4792-4802, 2016.
- [14] V. T. Suleman, A. A. S. Al-Hamdani, S. D. Ahmed, V. Y. Jirjees, M. E. Khan, A. Dib, *et al.*, "Phosphorus Schiff base ligand and its complexes: Experimental and theoretical investigations," *Applied Organometallic Chemistry*, vol. 34, p. e5546, 2020.
- [15] M. J. Kareem, A. A. S. Al-Hamdani, Y. G. Ko, W. Al Zoubi, and S. G. Mohammed, "Synthesis, characterization, and determination antioxidant activities for new Schiff base complexes derived from 2-(1H-indol-3-yl)-ethylamine and metal ion complexes," *Journal of Molecular Structure*, vol. 1231, p. 129669, May 01, 2021.
- [16] S. C. Moldoveanu, "Chapter 12 - Pyrolysis of Carboxylic Acids," in *Pyrolysis of Organic Molecules (Second Edition)*, S. C. Moldoveanu, Ed., ed: Elsevier, 2019, pp. 483-553.
- [17] Z. Chen, Y. Jiang, L. Zhang, Y. Guo, and D. Ma, "Oxalic Diamides and tert-Butoxide: Two Types of Ligands Enabling Practical Access to Alkyl Aryl Ethers via Cu-Catalyzed Coupling Reaction," *Journal of the American Chemical Society*, vol. 141, pp. 3541-3549, 2019/02/27 2019.
- [18] E. H. Copland and N. S. Jacobson, "Measuring Thermodynamic Properties of Metals and Alloys," in *Mass Spectrometry Handbook*, ed, pp. 1143-1180.
- [19] M. N. Matada and K. Jathi, "Pyrazole-based azo-metal (II) complexes as potential bioactive agents: synthesis, characterization, antimicrobial, anti-tuberculosis, and DNA interaction studies," *Journal of Coordination Chemistry*, vol. 72, pp. 1994-2014, 2019.
- [20] R. A. Saber, A. K. Attia, and W. M. Salem, "Thermal analysis study of antihypertensive drugs telmisartan and cilazapril," *Advanced pharmaceutical bulletin*, vol. 4, pp. 283-287, 2014.
- [21] A. K. Attia, M. M. Ibrahim, and M. A.-N. El-Ries, "Thermal analysis of some antidiabetic pharmaceutical compounds," *Advanced pharmaceutical bulletin*, vol. 3, pp. 419-424, 2013.
- [22] W. Al Zoubi, A. A. S. Al-Hamdani, S. D. Ahmed, and Y. G. Ko, "Synthesis, characterization, and biological activity of Schiff bases metal complexes," *Journal of Physical Organic Chemistry*, vol. 31, p. e3752, 2018.
- [23] T. Glomb and P. Świątek, "Antimicrobial Activity of 1,3,4-Oxadiazole Derivatives," *International journal of molecular sciences*, vol. 22, p. 6979, 2021.
- [24] M. A. El-Nakeeb, H. M. Abou-Shleib, A. M. Khalil, H. G. Omar, and O. M. El-Halfawy, "In vitro antibacterial activity of some antihistaminics belonging to different groups against multi-drug resistant clinical isolates," *Brazilian journal of microbiology : [publication of the Brazilian Society for Microbiology]*, vol. 42, pp. 980-991, 2011.
- [25] J. Sun, M. Li, M. Lin, B. Zhang, and X. Chen, "High Antibacterial Activity and Selectivity of the Versatile Polysulfoniums that Combat Drug Resistance," *Advanced Materials*, vol. n/a, p. 2104402.
- [26] J. Sabotič, J. Brzin, J. Erjavec, T. Dreo, M. Tušek Žnidarič, M. Ravnikar, *et al.*, "L-Amino Acid Oxidases From Mushrooms Show Antibacterial Activity Against the Phytopathogen *Ralstonia solanacearum*," *Frontiers in Microbiology*, vol. 11, 2020-May-19 2020.
- [27] M. Merdan, D. Jalal Al-den Fakar Al-den, Y. Al-khafaji, and A. S. Abbas, "Theoretical study for chromen azodyes derivative compounds as

- anti-corrosive," *Journal of Physics: Conference Series*, vol. 1234, p. 012054, 2019/07 2019.
- [28] M. Oftadeh, N. M. Mahani, and M. Hamadani, "Density functional theory study of the local molecular properties of acetamide derivatives as anti-HIV drugs," *Research in pharmaceutical sciences*, vol. 8, pp. 285-297, 2013.
- [29] N. Flores-Holguín, J. Frau, and D. Glossman-Mitnik, "Conceptual DFT as a chemoinformatics tool for the study of the Taltobulin anticancer peptide," *BMC Research Notes*, vol. 12, p. 442, 2019/07/19 2019.
- [30] A. S. Rad, M. Ardjmand, M. R. Esfahani, and B. Khodashenas, "DFT calculations towards the geometry optimization, electronic structure, infrared spectroscopy and UV-vis analyses of Favipiravir adsorption on the first-row transition metals doped fullerenes; a new strategy for COVID-19 therapy," *Spectrochimica acta. Part A, Molecular and biomolecular spectroscopy*, vol. 247, pp. 119082-119082, 2021.
- [31] A. Tariq, S. Nazir, A. W. Arshad, F. Nawaz, K. Ayub, and J. Iqbal, "DFT study of the therapeutic potential of phosphorene as a new drug-delivery system to treat cancer," *RSC Advances*, vol. 9, pp. 24325-24332, 2019.