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Synthesis and Study of Some Structural Properties for New Complexes derived from α-(phenyl)-N-phenyl nitrone with Cu(II), Co(II) and Ni (II) and Study of Their Anti-Bacterial Activity

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Abstract:

A new series of transition metal complexes of Cu (II), Co (II) and Ni (II) has been synthesized from the α-(phenyl)-N-phenyl nitrone derived from N-phenyl hydroxyl amine and benzaldehyde. Their structures were elucidated using spectroscopic techniques, elemental analyses and molar conductivity. The IR and UV-Vis spectral data of the complexes suggest, square planer geometry for all complexes. The theoretical calculations of nitrone complexes were studied by quantum chemical calculations. The optimized structures of the nitrone complexes were obtained by DFT/B3LYP level of theory using the basis set 6-311+G(d) for ligand and LANL2DZ for the complexes. The dipole moment of co-complex found to have high values compared with the complexes and ligand. Global descriptors such as the MO energies of HOMO, LUMO levels, ΔE and hardness (η) were determined and used to identify the differences in the stability and reactivity of compounds. In general the calculated the values lead to favorable state for stabilities (high chemical reactivity and low kinetic stability) (Li>Co >Ni>Cu). In addition the calculations show the effect of coordination and this leads to the change of the bond length and angles. The biological activity shows that the Cu (II) complex was sensitive to *S. aureus* and Co (II) complex was sensitive to *E. coli*.

Key Words*:* Nitrone complexes, Spectrophotometric, Conductivity, Antibacterial Activity, DFT/B3LYB.

1. Introduction:

The first report on the synthesis and characterization of nitrone-metal (II) complexes were explored in 1982 [1], even though the chemistry of nitrones is well recognized for a long time. Nitrones are significant synthetic intermediates that have been used widely in organic chemistry [2]. Nitrones can react as 1, 3-dipolar cycloadditions with a large variety of dipolarophiles has been extensively studied in 1960-70 [3]. The nitrones reactivity and diastereo-selectivity of the 1,3-dipolar cycloaddition reactions between electron-deficient olefins and nitrones catalyzed by several metal complexes or Lewis acids have been described [4]. Kanemasa and Tsuruoka [5] have reported the participation of nitrone-$MgBr_2$ complexes in some cycloaddition reactions with allylic alcohols. The asymmetric type of the cycloaddition reaction between C-(2-furyl)-N-benzyl nitrone and acrylates has been used in the preparation of numerous protected derivatives of 4-hydroxy-pyroglutamic acids of synthetic utility [6]. Nitrone complexes of iron have been wholly characterized and their acidic hydrolysis investigated by Pierre et.al. [7]. Some tin (IV) complexes with nitrones providing pentacoordinated metal compounds have been prepared [8]. Crist et.al. [9] have synthesised and characterized complexes of N-tert-butyl-C-(2-pyridyl) nitrone with Cu(II), Mn(II), Co(II), Ni(II), Fe(II) and Fe(III). Computational chemistry foundations of modern chemistry have been well developed through 70 years ago and in principle it became possible to be used for the predication of the interaction of atoms in molecule. Theoretical calculation methods are helpful tools for elucidating structure and behavior of molecules, atoms and electrons properties of chemical systems, molecular orbital density, charge on atoms and the bonding that is involved in the molecular systems [10-12]. Electronic structure methods provide useful information on the molecular structure and charge distribution, so they are useful to understand and describe systems where electronic effects and molecular orbital interactions are dominant. One of the most common methods of computational chemistry, density Functional Theory (DFT) has been accepted by the ab initio quantum chemistry community as a cost effective general procedure for studying physical properties of the molecules, because it is based on total electron density rather than wave functions [13-17].

The purpose of the present work is to synthesis and characterizes new complexes of Cu (II), Co (II) and Ni (II) with α-(phenyl)-N-phenyl nitrone and the predication of structure, electronic properties and relative stabilities and also study of anti-bacterial activity of these complexes.

2. Experimental:

FT-IR spectra were obtained on a Shimadzu FT-IR84005 spectrometer at College of Education Pure Science. The UV-Vis spectra were recorded in the range (200-700) nm on a PG Instruments Ltd spectrophotometer, in freshly prepared 10^{-3} M solutions in (DMF) at room temperature using quartz cell (1.000) cm. Molar conductivity measurements of the complexes at 25°C in freshly prepared 10^{-3} M solutions in DMF were determined using HI 2315 Digital Conductivity meter. Elemental analysis was carried out on CHNS, elementar, Vario microcube, (Germany). All chemicals were supplied by Merk, Ridel and Fluka Co.

2.1. Synthesis of N-phenyl hydroxylamine [18]:

Nitrobenzene (9.59 g, 8 ml, 77.94 mmol) and ammonium chloride (5 g, 93.47 mmol) were added to 160 ml water. This yellow mixture was stirred for 60 min, and then during a period of 30 min zinc powder (12 g, 183.51 mmol) was slowly added. The temperature of the reaction mixture kept at 55 C^o. The reaction mixture was stirred for 15 min after which time the reaction was complete added of zinc powder. The reaction was then stirred for 15 min, and the solution was filtered while still hot to remove zinc oxide. The solid was washed with 50 mL of hot water. The combined aqueous portions were saturated with sodium chloride and cooled to 0 C^o. The crystalline N-phenyl hydroxylamine which precipitated from the solution was removed by suction filtration, recrystallized from ether. These crystals after being dried in a vacuum desiccator overnight gave (6 g, 71% yield) with melting point (80-82) ^oC.

2.2. Synthesis of α-(phenyl)-N-phenyl nitrone (L) 1[19]:

In a 50 ml one-necked, round bottomed flask N-phenyl hydroxylamine (0.50 g, 4.58 mmol) was dissolved in absolute ethanol (10 ml) and warmed to 50 C^o. To this solution, benzaldehyde (0.54 g, 5.1 mmol) was then added. The reaction mixture was heated under reflux for 1 hrs., and the reaction was stirred at room temperature overnight in the dark. The crude nitrone product was filtered from the brown colored solution and recrystallized from hot absolute ethanol. The yellow crystals obtained after filtering and vacuum drying weighed (0.43 g, 2.37 mmol, 52% yield) with melting point (110-112) ^oC.

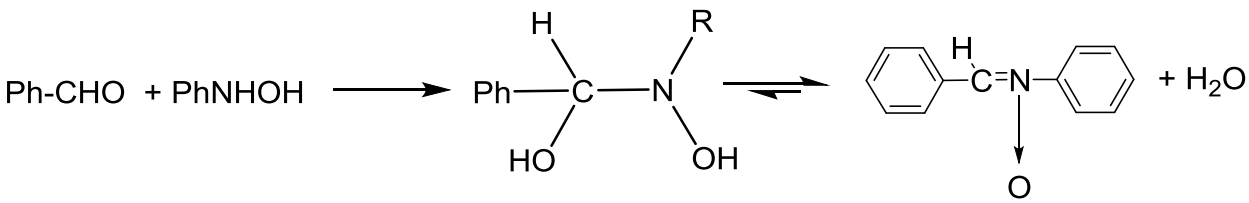

Fig. 1 Synthesis of the nitrone ligand.

2.3. Synthesis of complexes [20]:

2.3.1. Synthesis of complex 2:

A solution of α-(phenyl)-N-phenyl nitrone (0.20 g, 1.014 mmol) in ethanol (5 ml) was added with stirring to a hot solution of copper chloride $CuCl_2.2H_2O$ (0.17 g, 1.014 mmol) in ethanol (5 ml). After cooling, a dark yellow precipitate was filtered off and washed with cold ethanol to give the required complex **2** (43% yield) with melting point (160-162) ^oC.

2.3.2. Synthesis of complex 3:

A solution of α-(phenyl)-N-phenyl nitrone (0.20 g, 1.014 mmol) in ethanol (5 ml) was added with stirring to a hot solution of cobalt chloride $CoCl_2.6H_2O$ (0.24 g, 1.014 mmol) in ethanol (5 ml). After cooling, a bluish green precipitate was filtered off and washed with cold ethanol to give the required complex **3** (44% yield) with melting point (118-120) ^oC.

2.3.3. Synthesis of complex 4:

A solution of α-(phenyl)-N-phenyl nitrone (0.20 g, 1.014 mmol) in ethanol (5 ml) was added with stirring to a hot solution of nickel chloride $NiCl_2.6H_2O$ (0.24 g, 1.014 mmol) in ethanol (5 ml). After cooling, a light yellow precipitate was filtered off and washed with cold ethanol to give the required complex **4** (46% yield) with melting point (230-232) ^oC.

Table 1: Physical Properties for Ligand and its metal complexes

Number of compound	Compound formula	Color	M.P ^oC	Yield %
1	α-Ph.NPh	yellow	110-112	52
2	$[Cu(\alpha\text{-Ph.NPh})(H_2O)_2Cl]Cl$	Dark yellow	160-162	43
3	$[Co(\alpha\text{-Ph.NPh})(H_2O)_2Cl]Cl$	Bluish green	118-120	44
4	$[Ni(\alpha\text{-Ph.NPh})(H_2O)_2Cl]Cl$	Light yellow	230-232	46

3. Computational Methods

Theoretical calculation was performed using Gaussian 03 program, running on a Pentium V PC-CPU 3400GHz. A full quantum mechanical geometry optimization were done at the DFT/B3LYP (Becke3-Lee–Yang–Parr) level of theory using the basis set 6-311+G(d) for ligand and LANL2DZ for the complexes(Cu, Co and Ni). This basis set has proved its stability for treating transition metal complexes [21-23].

4. Antibacterial Activity:

The antibacterial activity has been evaluated by agar plate diffusion technique [24] against of medicinally important gram negative bacteria (*Escherichia coli*) and gram positive bacteria (*Staphylococcus aureus*). Here in the nutrient agar plates have been seeded with 0.1ml of the broth culture of the tested microorganism containing (10^6) cells/ml by well-variant method at100 μg/ml concentration, the solvent used was dimethylsulfoxide (DMSO). The plates were incubated at 37 ^oC for 24 hrs. The zones of inhibition have been measured using a special calibrated lences.

5. Results and Discussion:

The synthesized ligand and its complexes were characterized by elemental analysis, IR and UV-Vis spectra and conductivity measurements. Apart from this, biological activity of the ligand and its complexes were studied.

5.1. Elemental Analysis:

The stoichiometry of the ligand and its complexes were confirmed by their elemental analysis. The metal / ligand ratio was found to be 1:1 by estimating the carbon, hydrogen and nitrogen contents of the complexes. Elemental analysis of ligand and its Cu(II), Co(II) and Ni(II) complexes show good agreement with the proposed structures of the ligand and its complexes (Table 2).

Table 2: Elemental Analysis data for Ligand and its metal complexes

Number of compound	Compound formula	C% Calc / C% Expr	H% Calc / H% Expr	N% Calc / N% Expr
1	α-Ph.NPh	79.16	5.62	7.10
		79.01	5.12	7.03
2	[Cu(α-Ph.NPh)$(H_2O)_2$Cl	47.07	3.34	4.22
		47.11	3.25	4.15
3	[Co(α-Ph.NPh)$(H_2O)_2$Cl]Cl	47.74	3.39	4.28
		47.60	3.20	4.20
4	[Ni(α-Ph.NPh)$(H_2O)_2$Cl]Cl	47.77	3.39	4.29
		47.70	3.30	4.23

5.2. Infrared spectra:

The IR spectra provide valuable information regarding the nature of functional group attached to the metal atom (Table 3). The IR spectra of the ligand showed strong absorption band in the 1192 cm^{-1} attributed to the (N→O) stretching vibration , which is shifted to lower frequencies in the spectra of all the complexes (1180–1070) cm^{-1} indicating the involvement of (N→O) oxygen in coordination to the metal ion. Consequently, the spectrum of the ligand shows the medium band in the 1548 cm^{-1} attributed to the (C=N) stretching vibration, which is shifted to higher frequencies in the spectra of all the complexes (1685-1600) cm^{-1}. Accordingly, the ligand acts as a monodentate chelating agent, bonded to the metal ion via the oxygen (N→O) atom of the nitrone ligand for the Co(II), Ni(II) and Cu(II) complexes. Assignment of the proposed coordination sites is further supported by the appearance of medium bands at (937–684) cm^{-1} which could be attributed to νM–O for complexes with ligand. All the complexes exhibit a broad band (3200-3600) cm^{-1} indicating the presence of water molecules in the complexes [25-26].

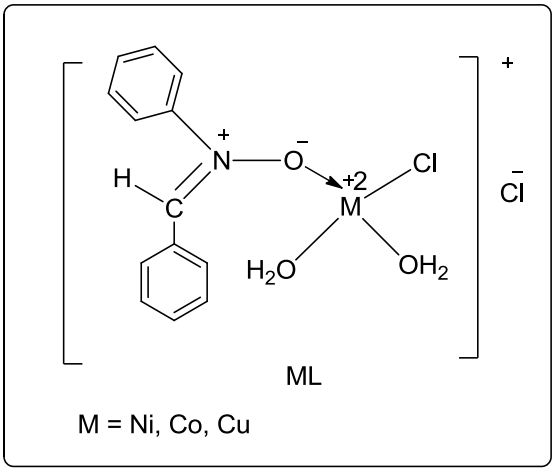

Fig. 2 Suggested structure of the complexes.

Table 3: Characteristic IR bands (cm^{-1}) of the compounds studied

Number of compound	Compound formula	M–O $str.cm^{-1}$	C-O $str.cm^{-1}$	N-O $str.cm^{-1}$	C=C $str.cm^{-1}$	C=N $str.cm^{-1}$
1	α-Ph.NPh	-	1298(m)	1192(s)	1483-1438(m)	1548(m)
2	[Cu(α-Ph.NPh)$(H_2O)_2$Cl]Cl	900-804	1261(m)	1101(s)	1480-1409(m)	1600(w)
3	[Co(α-Ph.NPh)$(H_2O)_2$Cl]Cl	937-833	1294(m)	1180(s)	1454-1421(m)	1685(w)
4	[Ni(α-Ph.NPh)$(H_2O)_2$Cl]Cl	763-684	1300(m)	1070(s)	1483-1436(m)	1635(w)

S: strong ; w: weak str.: stretching ; m: medium

5.3. Electronic Spectra:

The electronic spectral data for the ligand and its metal complexes were recorded in DMF solution in the range of 200 to 700 nm regions and the data are presented in Table 4. The ligand shows two bands, the week band at 200 nm which related to the electronic transitions in the individual benzene nuclei, and the strong band at 300 nm (ε= 765 $mol^{-1}cm^{-1}$) attributed to the electronic transition n $\rightarrow\pi^*$ of the conjugated electronic system of nitrone group in conjugation with phenyl group. These transitions are found also in the spectra of the complexes, but they effect red shifting of the bands confirming the coordination of the ligand to the metallic ions. Copper (II) complex **1** shows bands at 210 nm attributed to the electronic transition $\pi \rightarrow\pi^*$ of the conjugated electronic system of phenyl group, and the other band at 310 nm (ε= 1646 $mol^{-1}cm^{-1}$) attributed to the electronic transition n $\rightarrow\pi^*$ of the electronic system of nitrone group with a shoulder at 690 nm (ε= 12 $mol^{-1}cm^{-1}$) may be assigned to the d-d transition. Coordination of ligand to copper (II) ion affects a red shifting of the bands, suggesting a square planar geometry arrangement around the Cu (II) ions. Co (II) complex **2** shows bands at 210 nm attributed to the electronic transition $\pi \rightarrow\pi^*$ of the conjugated electronic system of phenyl group, and the other band at 305 nm (ε= 892 $mol^{-1}cm^{-1}$) attributed to the electronic transition n $\rightarrow\pi^*$ of the electronic system of nitrone group with a shoulder at 550 nm (ε= 111 $mol^{-1}cm^{-1}$) may be assigned to d-d transition. Coordination of ligand to cobalt (II) ion affects a red shifting of the bands, suggesting a square planar geometry arrangement around the Co (II) ions. Ni (II) complex **3** shows bands at 210 nm attributed to the electronic transition $\pi \rightarrow\pi^*$ of the conjugated electronic system of phenyl group, and the other band at 335 (ε= 2384 $mol^{-1}cm^{-1}$) nm attributed to the electronic transition n $\rightarrow\pi^*$ of the electronic system of nitrone group with a shoulder at 625 (ε= 117 $mol^{-1}cm^{-1}$) nm may be assigned to d-d transition. Coordination of ligand to nickel (II) ion affects a red shifting of the bands, suggesting a square planar geometry arrangement around the Ni(II) ions. [27, 28]

Table 4: U.V-Visible spectra data of free ligand and its complexes in 10^{-3} M in DMF

λMax nm					
Number of compound	**Compound formula**	**Band I**	**Band II**	**Band III**	**Solvent**
1	α-Ph.NPh	200	300	-	Dimethyl formamide
2	[Cu(α-Ph.NPh)$(H_2O)_2$Cl]Cl	210	310	690	Dimethyl formamide
3	[Co(α-Ph.NPh)$(H_2O)_2$Cl]Cl	210	305	550	Dimethyl formamide
4	[Ni(α-Ph.NPh)$(H_2O)_2$Cl]Cl	210	335	625	Dimethyl formamide

5.4. Molar conductance measurements:

The molar conductance (Λm) values of the ligand and its metal complexes in DMF at (10^{-3} M) lie in the (13, 102, 156 and 210 Ohm^{-1} cm^2 mol^{-1}) respectively (Table 5), indicating their electrolytic nature. [29, 30]

Table 5: Molar Conductance ($Cm^2.\Omega^{-1}.Mol^{-1}$) of the ligand and its complexes in DMF (10^{-3})

Number of compound	Compound formula	Λ_m($Cm^2.\Omega^{-1}.Mol^{-1}$) DMF
1	α-Ph.NPh	13
2	[Cu(α-Ph.NPh)$(H_2O)_2$Cl]Cl	102
3	[Co(α-Ph.NPh)$(H_2O)_2$Cl]Cl	156
4	[Ni(α-Ph.NPh)$(H_2O)_2$Cl]Cl	210

5.5. DFT Calculation:

The lowest energy conformations are obtained by the final optimized geometries of the ligand and their complexes were obtained by performing the DFT/B3LYP level of theory. The optimized geometries are shown in figure .4.this figure illustrates the geometry of the molecules in the sticks model. For all molecules, optimized geometric structures, total energies, dipole moments, the HOMO, LUMO and energy band gap (Δ*E*) calculation have been investigated after total optimization, the structural data are summarized in Table 6. It can be seen from Table 6 that, the total energy determines the occurrence or non-occurrence of chemical reactions and stereospecific paths in intra- and intermolecular processes. The total energy of the system composed of the internal, potential, and kinetic energy [25]. The total energy (absolute values) for compounds are L>Co>Cu>Ni.

While in the other hand the dipole moment (μ in Debye) is another important electronic parameter used to describe the polarity of the molecule. This parameter that helps in the understanding of interaction between atoms in the same or different molecules dipole moment increases with the increase in electronegativity of atoms. Chemical reactivity usually increases with the increase in dipole moment as well as attractive for the interaction with other systems and to form complexes, from Table 6 that, the dipole moment has maximum values for co-complex compared with compounds. The high dipole moment may make the compound co-complex attract other systems to interact, and to indicate highly polar molecules. Also the dipole moment values are also considered for locating the coordination site [31, 32].

The highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and energy gaps (ΔE) for compounds are shown in figure3. The eigenvalues of LUMO and HOMO and their energy gap reflect the chemical activity of the molecule. LUMO as an electron acceptor represents the ability to obtain an electron, while HOMO as an electron donor represents the ability to donate an electron. The smaller the LUMO, HOMO and energy gaps are the easier is it for the HOMO electrons to be excited; the higher the HOMO energies, the easier it is for HOMO to donate electrons; the lower the LUMO energies are the easier is it for LUMO to accept electrons. The energy gap of the ligand is larger than complexes.

A compound with a small HOMO-LUMO gap can be associated with a high chemical reactivity and low kinetic stability as well as more polarizable (it is evident from the magnitudes of their high dipole moments)

this termed as soft molecule, so we expect the co-complex have high biological activity compare with other compounds, while the compound with a large energy gap implies higher stability and lower chemical reactivity [33-34]. There is relationship between hardness and stability, the principle of maximum hardness (PMH) represents that the system would be more stable if the global hardness related to HOMO-LUMO gap, is a maximum. As well as based on the principle it has been suggested after extensive study that a system of maximum chemical hardness value would have minimum energy, so from the table 6 the ligand more stable than complexes because of have high energy gap ΔE and hardness η, PMH is a qualitative tool to study the stability of the system. So that from table 6, it is obvious that the ligand have maximum hardness and high stability according to the values of hardness, energy gap [35- 37].

Table 6: Calculated The Molecular descriptors of observed compounds.

Number of compound	Compound formula	Total energy in kcal/mol	HOMO in eV	LUMO in eV	Δ*E* in eV	Dopole (debye) (μ)	η
1	α-Ph.NPh	-631.93946	-2.173390	-5.848044	3.674654	3.1902	1.8373
2	[Cu(α-Ph.NPh)(H_2O)$_2$Cl]Cl	-944.76406	-2.533944	-3.78867	1.25472	7.9045	0.6273
3	[Co(α-Ph.NPh)(H_2O)$_2$Cl]Cl	-969.034603	-5.938115	-2.53149	3.40662	7.7283	1.7033
4	[Ni(α-Ph.NPh)(H_2O)$_2$Cl]Cl	-995.83174	-2.23924	-5.11305	2.87381	5.7290	1.4369

The bond lengths and angles for compounds are listed in Table 7; as shown from this table, there are slight changes in the bond lengths and angles of compounds, like the changes of the bond length and angles between ligand and metals indicate the presence of -conjugation which causes of the electrostatic attraction between atoms. And this leads to redistribution of electron cloud in the compounds. In all complexes the ligands can coordinate to the metals (Co, Ni, Cu), through the nitrones oxygen. The bond lengths N9-O2 in ligand are shorter than all complexes. In all complexes Co(L1) the distance between [d(O-Co) =1.914 A^{o}] and the distance between [d(O-Ni) =1.996 A^{o}] while [d(O-Cu) =1.911 A^{o}]. In cu-complex the distance between [d(O-Cu) =1.911 A^{o}] is shorter than in complexes Co, Ni, due to the presence of π-conjugation in the coordinated nitrones oxygen with metal which causes electrostatic attraction between both oxygen and copper cation. [38-44].

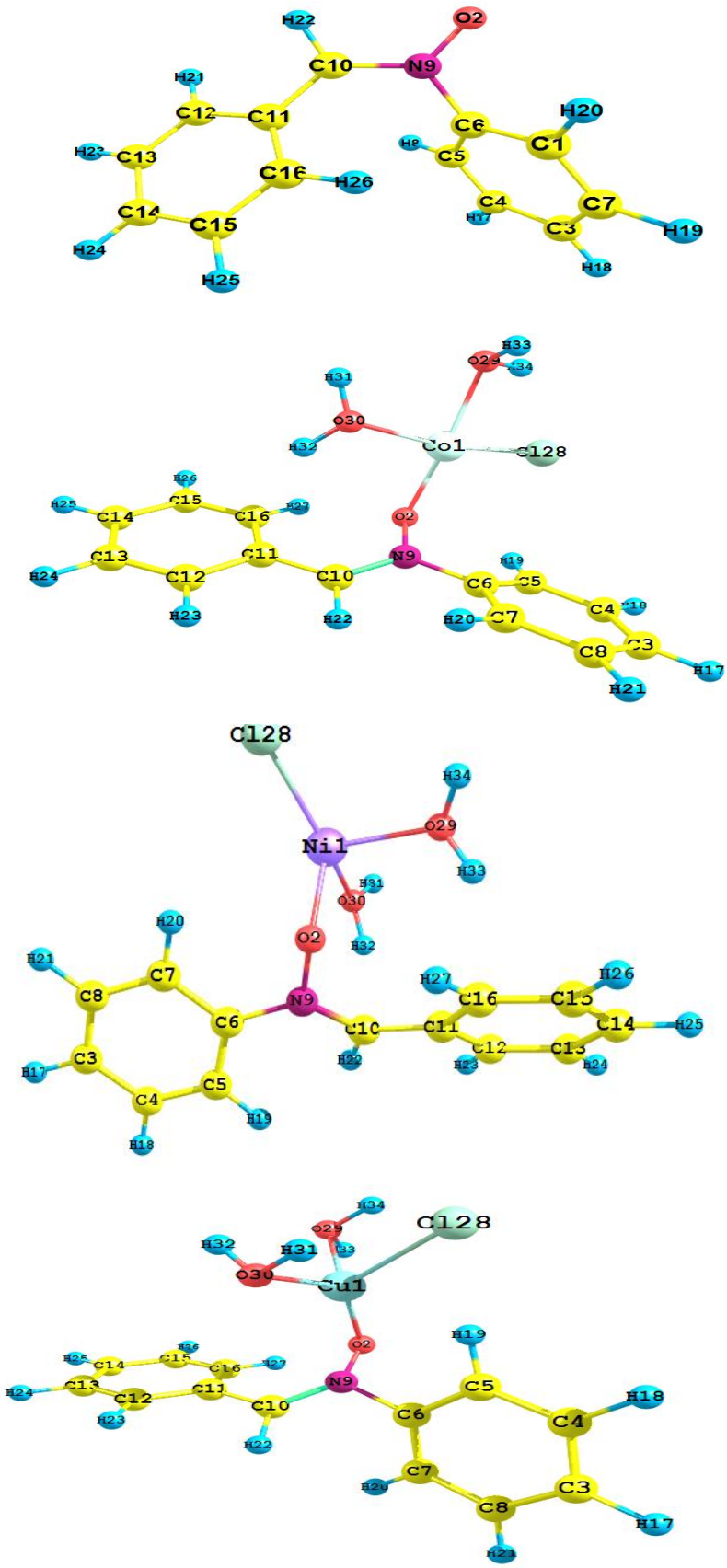

Fig. 3 Calculated Optimized Structures of the Possible Predication for the Compounds in Gas Phase.

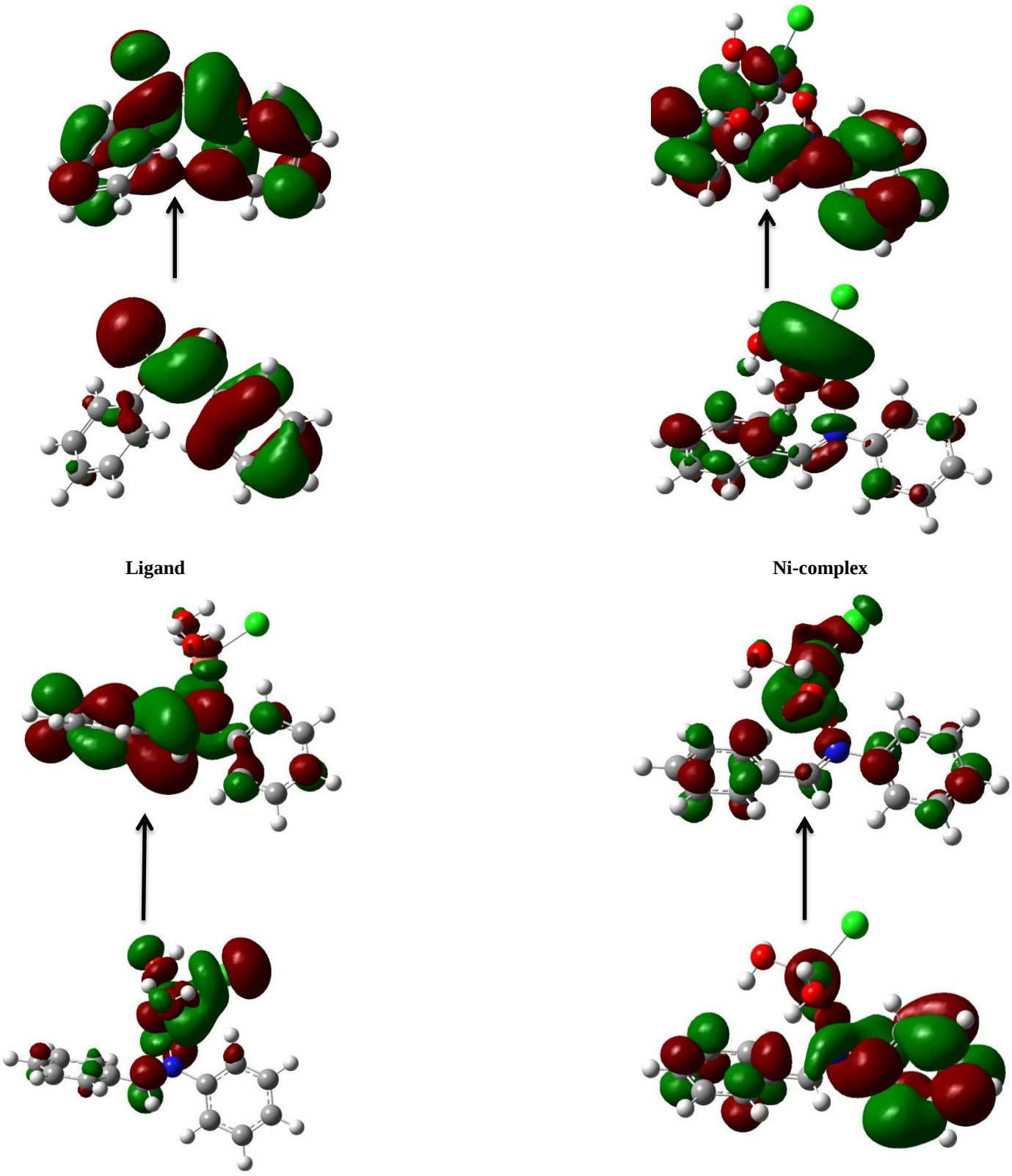

Fig. 4. Electronic Distribution in HOMO and LUMO Orbitals.

Table 7: Selected Structural Parameters of the Optimized Compounds, By DFT/B3LYP/6-311G+(d) for ligand and LANL2DZ for the complexes (Cu, Co, Ni).

BondS/Angles (A°)	Compounds			
	L	Cu	Ni	Co
N9-O2	1.286	1.330	1.390	1.387
N9-C6	1.470	1.496	1.429	1.453
N9-C10	1.321	1.337	1.380	1.341
C10-H22	1.080	1.103	1.085	1.084
O2-Co1	----	----	----	1.914
O2-Cu	----	1.911	----	----
O2-Ni	----	----	1.996	----
O2-N9-C10	123.15	125.65	119.51	120.38
O2-N9-C6	115.65	116.96	116.32	116.97
C6-N9-C10	121.21	114.39	123.91	122.07
N9-O2-Co1	----	----	----	112.70
N9-O2-Ni	----	----	119.15	----
N9-O2-Cu	----	92.13	----	----
C11-C10-H22	116.28	115.12	118.58	117.25

Antibacterial activity:

Table (8) shows inhibition zones diameter of *E. coli* growth yielded by ligand and its complexes (Cu, Co and Ni) tested by well variant diffusion method at 100 µg/ml concentration. According to evaluation of the data obtained only the complex 3 was sensitive to *E. coli* with the inhibition diameter of 10 mm. Only the complex 2 was sensitive to *S. aureus* with the inhibition diameter of 15 mm (figures 5 and 6).

Table 8: Calculated inhibition zones diameter of the ligand and its complexes.

Zones of growth inhibition			
Compound (1mg)	**Compound formula**	***E. coli* (100µg/ml)**	***S. aureus* (100 µg/ml)**
1	α-Ph.NPh	-	-
2	$[Cu(\alpha\text{-Ph.NPh})(H_2O)_2Cl]Cl$	-	15
3	$[Co(\alpha\text{-Ph.NPh})(H_2O)_2Cl]Cl$	10	-
4	$[Ni(\alpha\ Ph.NPh)(H_2O)_2Cl]Cl$	-	-

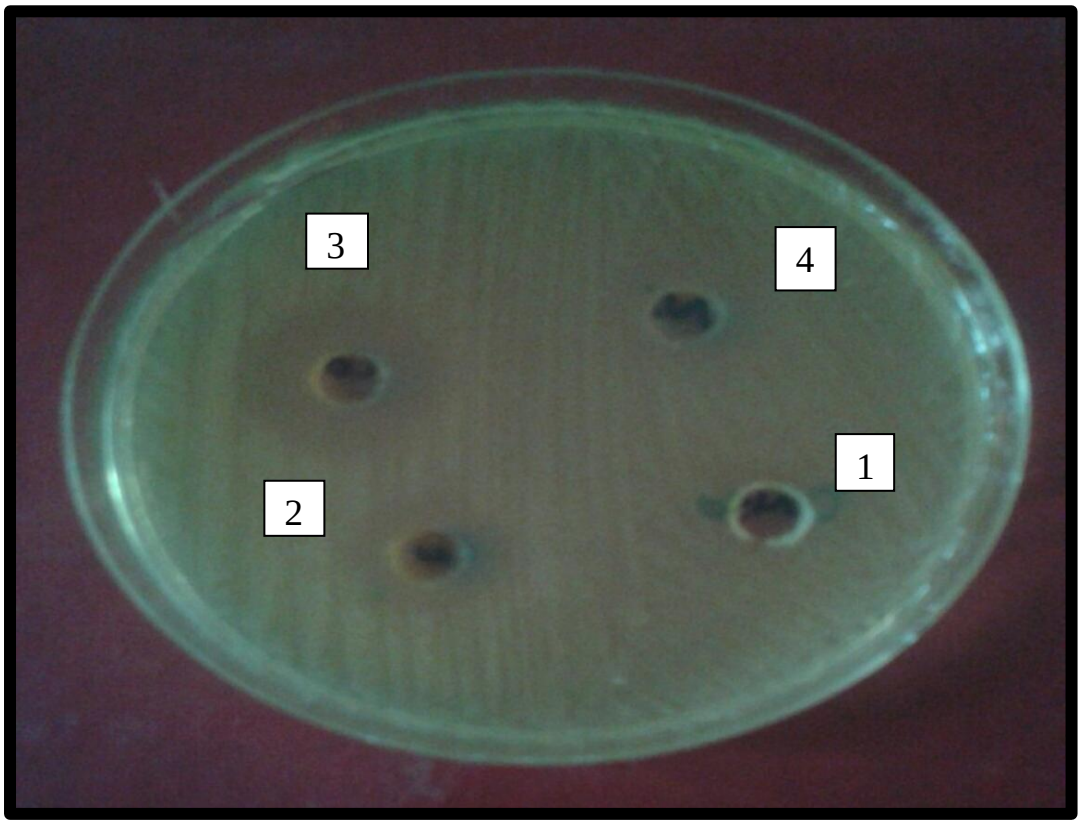

Fig. 5 Antibacterial activity of 100 µg/ml concentration of complexes on *Escherichia coli*.

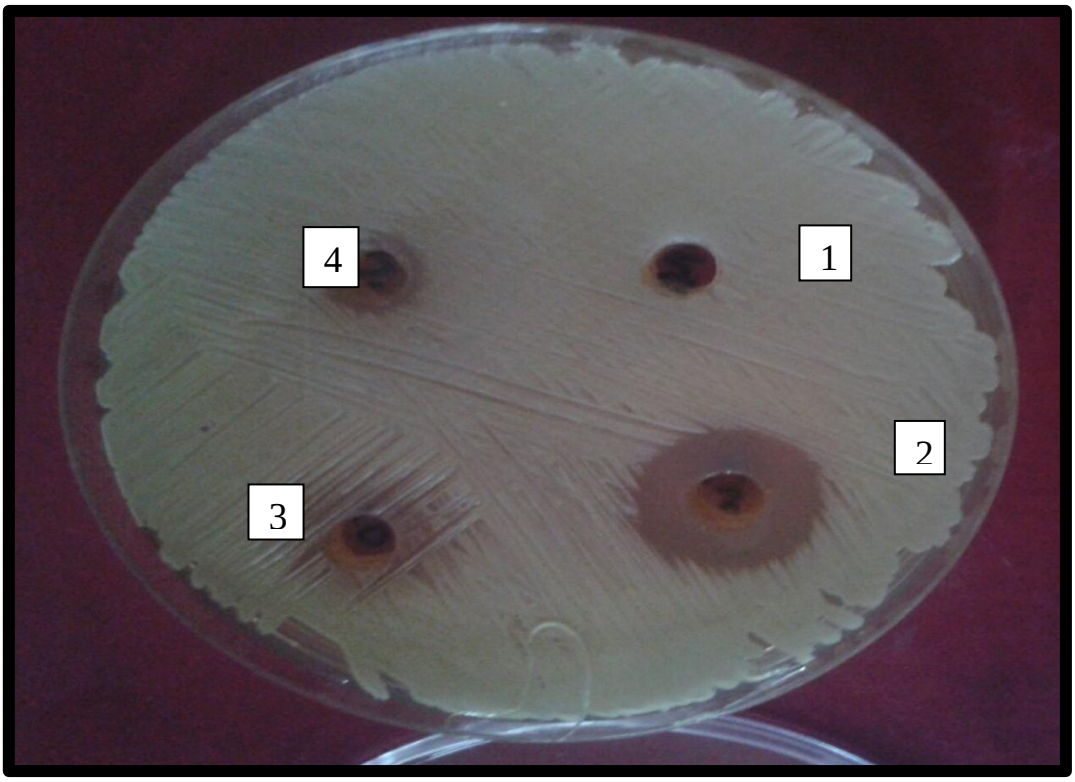

Fig. 6 Antibacterial activity of 100 µg/ml concentration of complexes on *Staphylococcus aureus*.

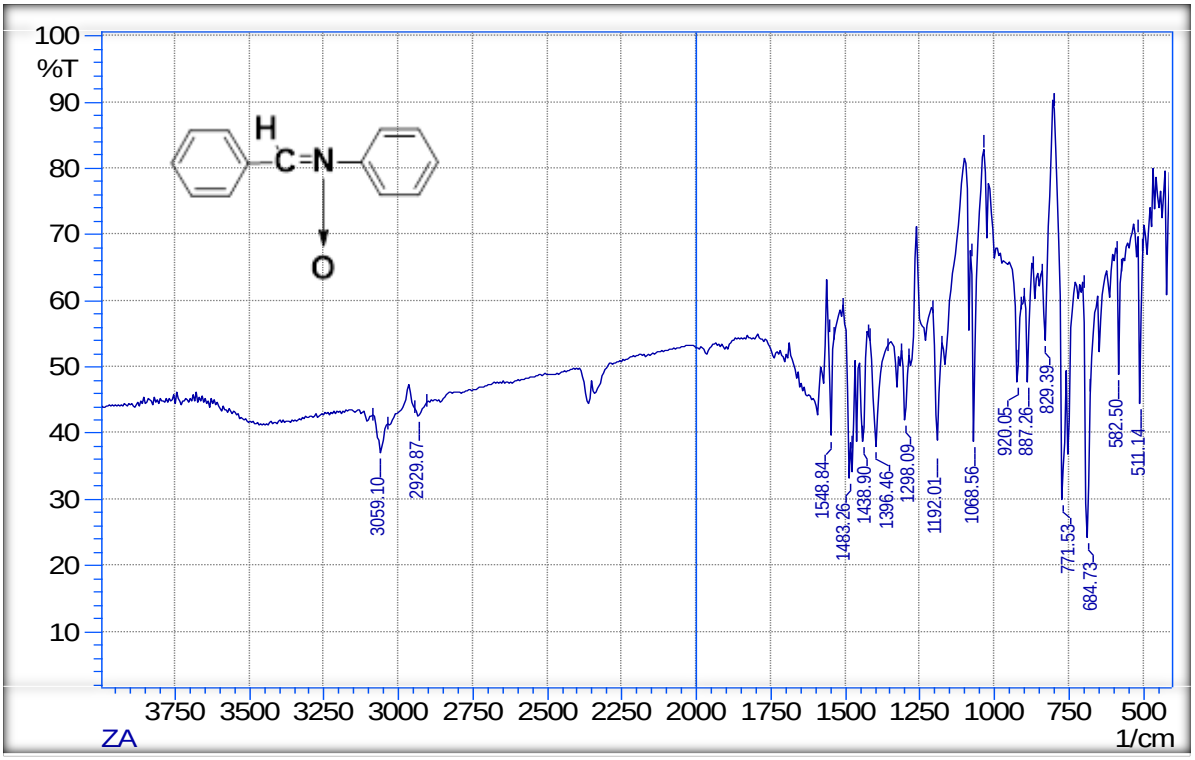

Fig. 7 The IR spectrum of L (α-Ph.NPh) 1.

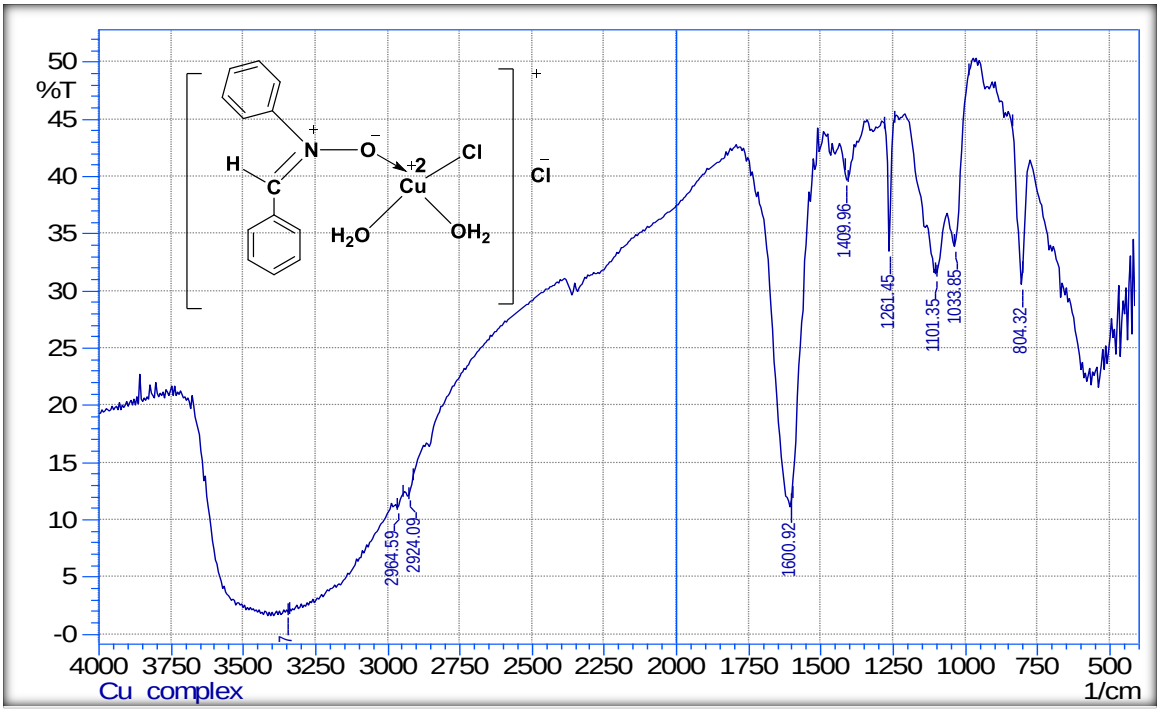

Fig. 8 The IR spectrum of [Cu(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 2.

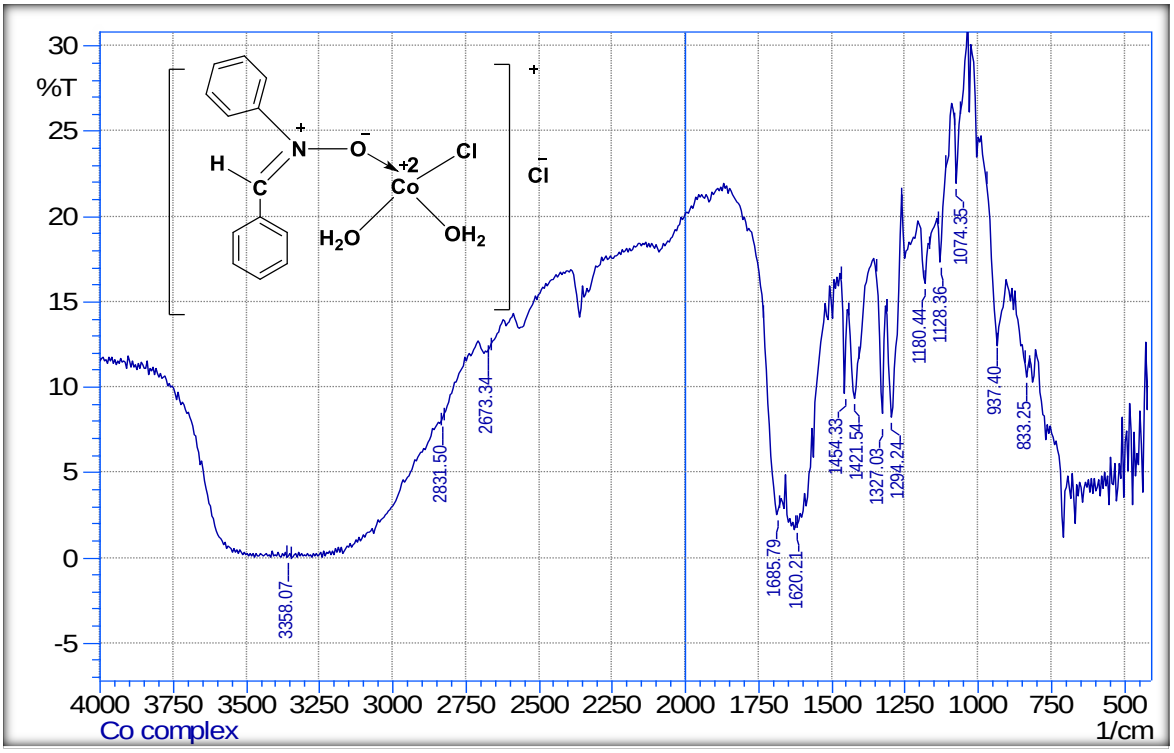

Fig. 9 The IR spectrum of [Co(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 3.

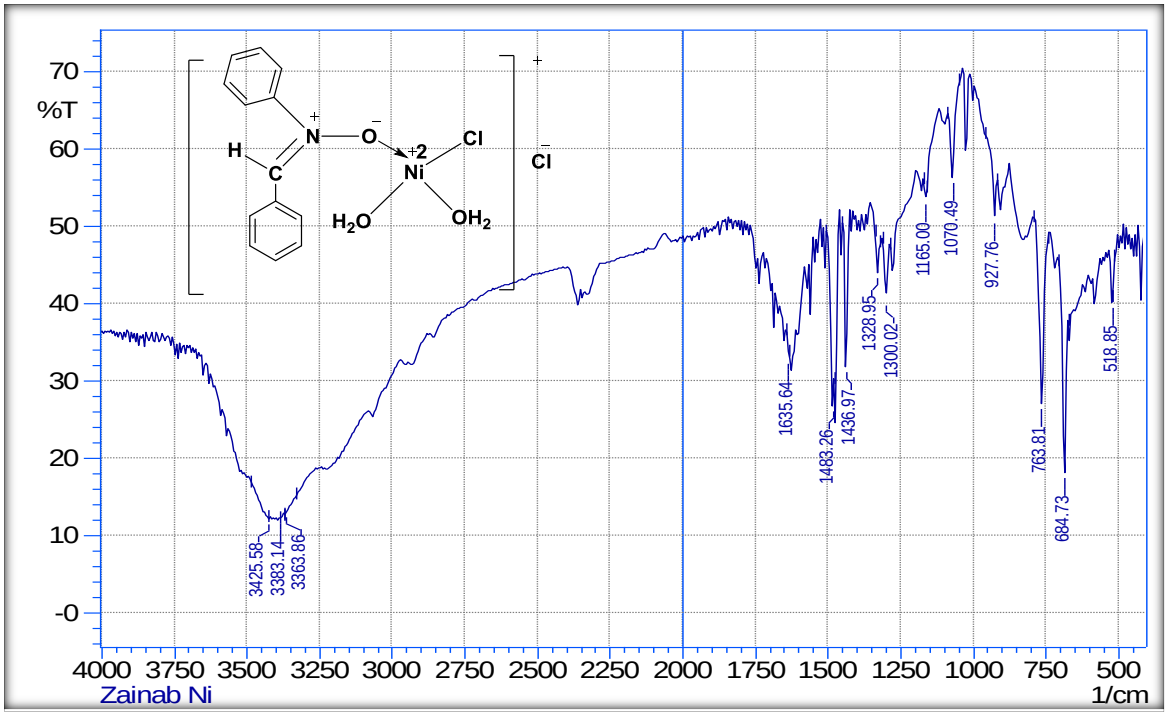

Fig. 10 The IR spectrum of [Ni(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 4.

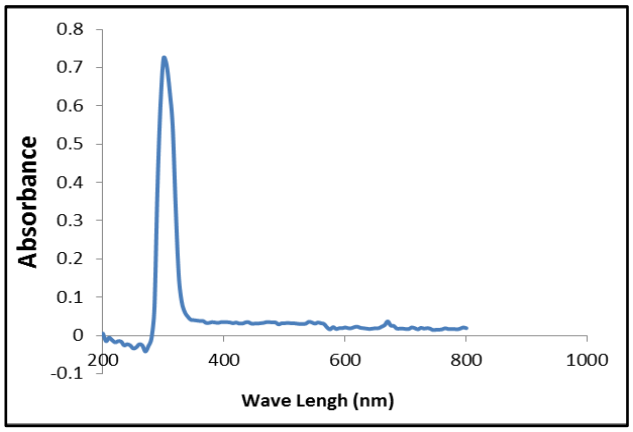

Fig. 11 UV-Visible spectrum of L (α-Ph.NPh) 1.

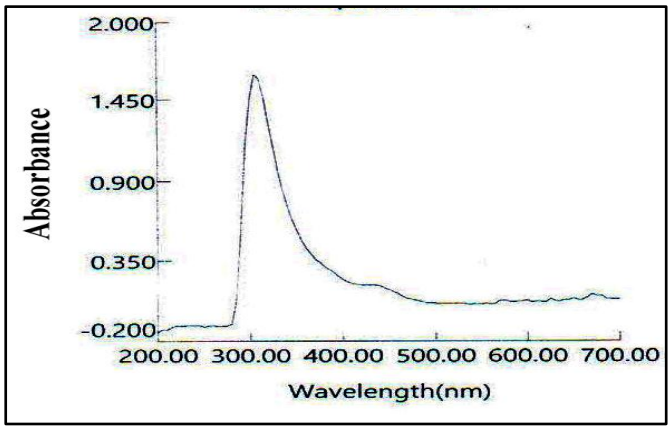

Fig. 12 UV-Visible spectrum of [Cu(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 2.

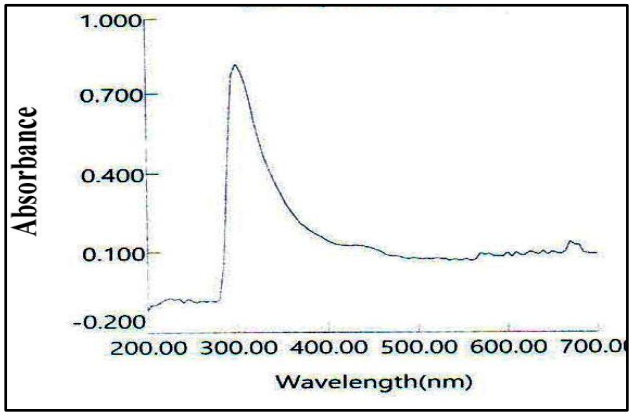

Fig. 13 UV-Visible spectrum of [Co(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 3.

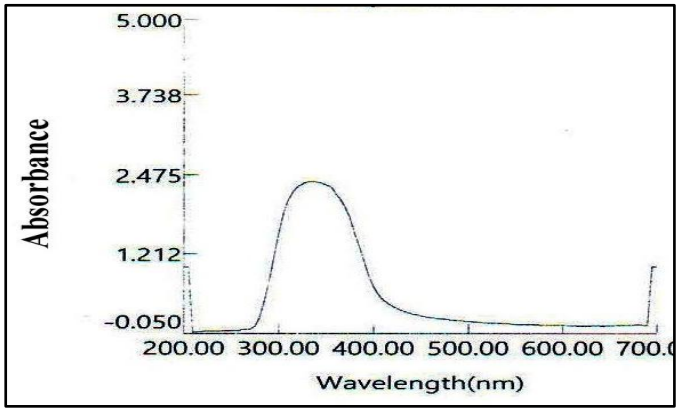

Fig. 14 UV-Visible spectrum of [Ni(α-Ph.NPh)(H_2O)$_2$Cl]Cl complex 4.

6. Conclusion:

In this paper reported the synthesis, isolation, and characterization of Cu(II), Co(II) and Ni(II) mono-chelates from the α-(phenyl)-N-phenyl nitrone derived from N-phenyl hydroxyl amine and benzaldehyde. Based on the above observations of FTIR, electronic spectral data, CHNS elemental analysis and conductance measurements, proposed the square planar geometry of Cu(II), Co(II) and Ni(II) complexes.Theoretically probable structures of metal complexes with nitrone have been calculated. In this study, the quantum chemical investigation of the geometries and electronic properties of nitrone ligand complexes, optimized geometric structures, dipole moments, total energies, the HOMO, LUMO and also the energy band gap (ΔE), Global hardness(η)calculation have been investigated after total optimization by B3LYP/6-31G for ligand and LANL2DZ for the complexes. From the results of the total optimized structures, it is noted that the total energy (absolute values) calculated using DFT for compounds are L>Co>Cu>Ni. The dipole moment has maximum values for co-complex as compared with compounds (Li, Cu and Ni). This high dipole moment may make the co-complex attract for the interaction with other systems and to form complexes and indicating that is highly polar molecules. The energy gap of the ligand is larger than complexes. The stabilities according to the values of the principle of maximum hardness (PMH), energy gap for compounds understudy are L>Ni>Cu>Co. because of the ligand have maximum hardness and high stability according to the values of hardness, energy gap while the co-complex with a small hardness and energy gap this can be associated with a high chemical reactivity and low kinetic stability. In ligand and all complexes there are slight changes in the bond lengths and angles of compounds, like the changes of the bond length and angles between ligand and metals indicate the presence of –conjugation which causes of the electrostatic attraction between atoms. And this leads to redistribution of electron cloud in the compounds.

This implies that different structures play key roles on electronic properties and the effect of slight structural variations. This calculation can be used as a model system for understanding the relationships between electronic properties and molecular structure and also can be employed to explore their suitability. As well as the antibacterial activity of the prepared ligand and its complexes was calculated against *E. coli* and *S. aureus* bacteria.

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تحضير ودراسة الخواص التركيبية لبعض المعقدات جديدة المشتقة من الفا- فنيل –N–فنيل نايترون مع نحاس(II) والكوبلت(II) والنيكل (II)ودراسة الفعالية البايولوجية

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الخلاصة

يتضمن البحث تحضير معقدات النحاس (II) والكوبلت (II) والنيكل (II) الجديدة للمركب [(α –فنيل)–N–فنيل نايترون] المشتق من تفاعل ن–فنيل هيدروكسيل امين مع البنزلديهايد. وقد تم تشخيص المعقدات باستخدام مطيافية الاشعة تحت الحمراء والاشعة فوق البنفسجية والمرئية ودرست قياسات التوصيلية لهذه المعقدات. أظهرت الدراسات الطيفية أن المعقدات تمتلك الشكل الهندسي المربع المستوي. كذلك درست الفعالية البايولوجية للمعقدات المحضرة وتبين بان معقد النحاس (II) له فعالية ضد البكتريا الموجبة لصبغة كرام ومعقد الكوبلت (II) له فعالية ضد البكتريا السالبة لصبغة كرام. كما تضمن هدا البحث دراسة نظرية للخصائص والصفات التركيبية والالكترونية لمعقدات النايترون بواسطة كيمياء الكم حيث انجزت الموائمة الهندسية للتراكيب باستخدام نظرية دالة الكثافة الالكترونية DFT بطريقة B3LYP وعند مستوى المجموعة الاساسية 6–311+G(d لليكاندLANL2DZ للمعقدات. الدراسة اظهرت أن القيمة العالية لعزم ثنائي القطب للمعقد الكوبلت مقارنة مع الجزيئات الاخرى. وتم حساب الخواص الالكترونية والتركيبية للدوال التالية طاقة االمدار الجزيئية LUMO., HOMO وقيمةΔE , η, للتحديد الاستقراريه للمركبات. قيم الحسابات تؤدي للحالة الاستقرارية المفضلة وكالاتي (Li>Co >Ni>Cu) اعتمادا على مبدأ فعالية كيميائية عالية وأقل استقرارية حركية . بالاضافة لذلك بينت الحسابات تأثير التناسق والذي يؤدي الى تغيرات في أطوال الاواصر والزوايا .

الكلمات المفتاحية: معقدات النايترون , المطيافية , التوصيلية , الفعالية البايلوجية, دالة الكثافة الالكترونية