

Preparation, Spectroscopic, Bioactive and Theoretical Studies of Mixed Ligand Complexes

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Abstract

The mixed ligands complexes of 8-hydroxyquinoline and Schiff base 1, 5-dimethyl-4-(5-oxohexan-2-ylideneamino)-2-phenyl-1H-pyrazol-3 (2H)-one (L) with Cr^(III), Mn^(II), Fe^(II), Co^(II), Ni^(II), Cu^(II) and Zn^(II) ions were prepared. The compounds have been characterized by NMR, FT-IR, UV-Vis and mass spectra, elemental microanalysis (C.H.N.), magnetic moment, chloride contain, atomic absorption and molar conductance. All prepared complexes were octahedral geometry. Compound structures treated theoretically using the program hyper chem. 8 in gas phase at 298°K. The compounds were also screened for their bioactive property such as antifungal and antibacterial. [DOI: [10.22401/JNUS.20.3.09](https://doi.org/10.22401/JNUS.20.3.09)]

Keywords: Mixed ligand Complexes, 8-hydroxyquinoline, Bioactive, Theoretical Studies.

Introduction

Schiff bases are a class of important compounds in medical and pharmaceutical field. They show biological activities including antibacterial, antifungal^[1,2], anticancer and herbicidal activities^[3]. The concept of mixed ligand complexes is always fascinating to the chemist interested in synthesis because of their ease of synthesis and generally less time requirement for these reactions to occur than normal complex formation reaction using synthesized ligand and metal salt. These facts have prompted many researchers to publish their research work in this fascinating and interesting area of research^[4-6]. Mixed ligand complexes play an important role in numerous chemical and biological systems like water softening, ion exchange resin. Many of these metal complexes showed good biological activity against pathogenic micro organisms^[7-10]. The 8-hydroxyquinoline is used in many processes for the preparation of mixed ligand complexes form^[11]. Its ability to get bonded with metal ion with its phenolic oxygen and ring nitrogen results in forming stable chelates with metals in combination with some other ligands, thus producing stable mixed ligand complexes^[12-14]. In report here in the synthesis and spectroscopic studies as well as the thermal investigation of a new mixed ligands 8-hydroxyquinoline and Schiff base complexes

with some transition metals ions such as Cr^(III), Mn^(II), Fe^(II), Co^(II), Ni^(II), Cu^(II) and Zn^(II)

Materials and Methods

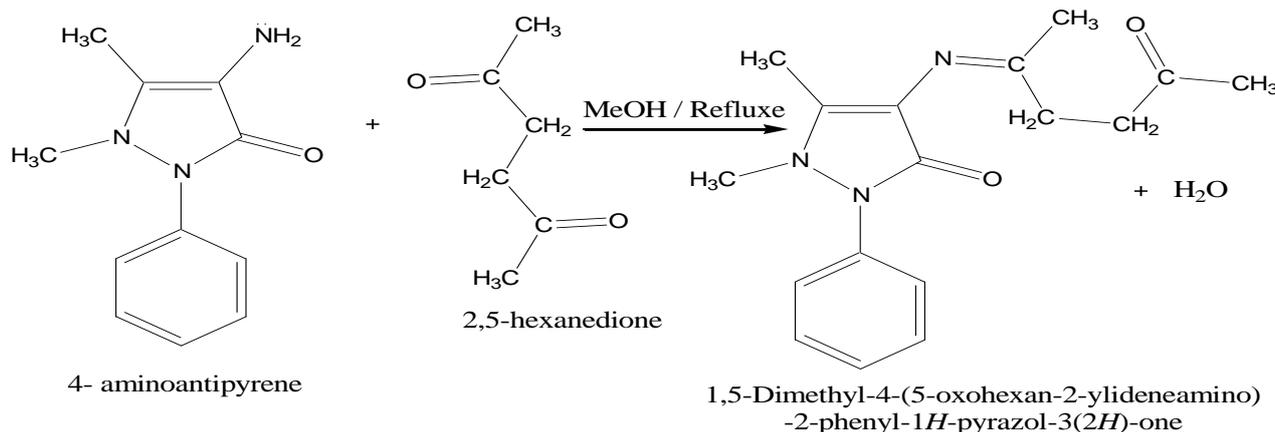
The following chemicals were commercially available and were used without further purification: (2,5-hexanedione, 4-aminoantpyrene, FeCl₂. H₂O, Aldrich) (diethyl ether, CaCl₂, CrCl₃.6H₂O, NiCl₂.6H₂O, CuCl₂.2H₂O, ZnCl₂.H₂O BDH) (DMSO, pure ethanol, methanol, Fluka) (MnCl₂.4H₂O, CoCl₂. 6H₂O, Reedel).

FT-IR spectra were recorded on a Shimadzu 3800, spectrometer. Electronic absorption spectra were recorded for solution in DMSO (1×10⁻³) on a Shimadzu 160 Spectrophotometer. ¹H- and ¹³C-NMR spectra were recorded using Bruker 400 MHz spectrometer Elemental (C.H.N.) analyses were carried out on a Perkin-Elmer automatic equipment model 240.B. Mass spectra were obtained by using LC-Mass 100P Shimadzu. Melting points were obtained on a Buchi SMP-20 capillary melting point apparatus and are uncorrected. Metal ratio was identified using a shimadzu 680 G. Conductivity measurements were measured for solution in DMSO(1×10⁻³) using a Jenway 4071 digital conductivity meter, Chloride ion content was determined by using potentiometric titration method on a 686-Titro processor–665 Dosimat

Metrohm Swiss. Magnetic properties were measured using (Magnetic susceptibility balance model MSR-MKi).

Study of Bioactivity

All the metal ion complexes, ligands and metal salts were screened against *staphylococcus aureus* (gram positive) and *Pseudomonas aeruginosa* (gram negative) bacteria as well fungi like *Penicillium expansum*, *Fusarium graminearum*, *Macrophomina phaseolina*, and *Candida albicans*, by using the wall agar diffusion method. The concentration of the compounds in this exposure was ($1 \times 10^{-3} \text{M}$) in DMSO solvent by using disc sensitivity test. This method involves the exposure of the zone inhibition toward the diffusion of microorganism on agar plate. The plates were incubated for 24 and 48 hours of bacteria and fungi respectively at 37°C .



Scheme (1): Preparation of the Ligand (L).

Synthesis of Mixed Ligand Complexes

A solution of the Schiff base ligand (0.25g, 0.836 mmole) in methanol was added gradually with stirring to the metal salts (0.105g Fe^(II), 0.222g Cr^(III), 0.165g Mn^(II), 0.198g Co^(II), 0.198g Ni^(II), 0.142g Cu^(II) or 0.128g Zn^(II) individually. 0.121g, 0.833mmol) of 8-hydroxyquinoline dissolved in (10) cm³ methanol was added to the mixture gradually while stirring. The reaction mixture was allowed to reflux and the solids were collected by filtration then recrystallized from ethanol. Physical properties for the compounds are given in Table (1).

Synthesis of Schiff base Ligand: [16]

A solution of 4-aminoantipyrene (1 g, 4.92 mmol) in methanol (25 ml) was mixed with a solution of 2,5-hexanedione (0.56g, 4.92mmol). The reaction was stirred and heated at 40°C for four hrs. A colorless precipitated was formed which was washed with diethyl ether and recrystallized from (1:1) ethanol: water mixture. The product was dried via anhydrous CaCl₂ in vacuum. The preparation of L is shown in Scheme (1). The yield was (1.38g), 93.66%, mp. 179°C .

Theoretical calculations

Program hyper chem.-8 is a sophisticated molecular modeler, editor and powerful computational package that are known for its quality, flexibility and ease of use. It's also uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics and dynamics. In the present work, parameterization method (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 method due to the availability of algorithms and it is more accurate than other method. PM3/ TM is an extension of the PM3 method to include orbital's with transition metals^[17].

Results and Discussion

The LC-Mass for ligand (Schiff base) (299.3m/ z) with (C₁₇H₂₁N₃O₂), (244.2 m/ z) with (C₁₄H₁₈N₃O), (243.3m/ z) with (C₁₄H₁₇N₃O) and (144.2m/ z) with (C₆H₁₄N₃O). ¹H-NMR (DMSO-*d*₆, ppm): δ 2.044 (s,3H, N=C-CH₃), 2.147 (s,3H, O=C-CH₃), 3.11 (s, 3H, C=C-CH₃), 3.31 (s,3H, N-CH₃), 5.88 (tri, 4H, CH₂-CH₂), 7.282-7.513 (m, 5H, Ar-H), figure (1). ¹³C-NMR (100.622 MHz, DMSO-*d*₆): δ 162.22 (C₁₆), 153.25 (C₁₂), 134.67 (C₄), 129 (C₂, 6), 127 (C₈, 10), 124.31 (C₉), 109.83 (C₁₁), 105.95(C₇), 77.25(C₅, 15), 76.93(C₃), 50.41(C₁₇), 36.09 (C₄), 12.5 (C₁₃), 10.62 (C₁), Fig.(2) shown Schiff base structure

Molar conductance values in (DMSO) solution (10⁻³M) were found in the range (24-46) S. cm² mol⁻¹ for, all complexes of Cr^(III), Mn^(II), Fe^(II), Co^(II), Ni^(II), Cu^(II) and Zn^(II) which

indicates that they are non electrolytes in nature [18,19]. Physical properties and elemental microanalysis are listed in Table (1).

Mass spectra for complexes

High resolution mass spectra of the [Cr(L) (8-HQ)Cl₂], [Mn(L) (8-HQ)Cl(H₂O)] and [Co(L)(8-HQ)Cl(H₂O)] mixed ligands complexes, Shows parent ion peak m/z=566.2(M), 552(M), 556(M) respectively [19]. Further details for the fragmentation and their relative abundances for each compound are listed in Table (2), see Fig.(3).

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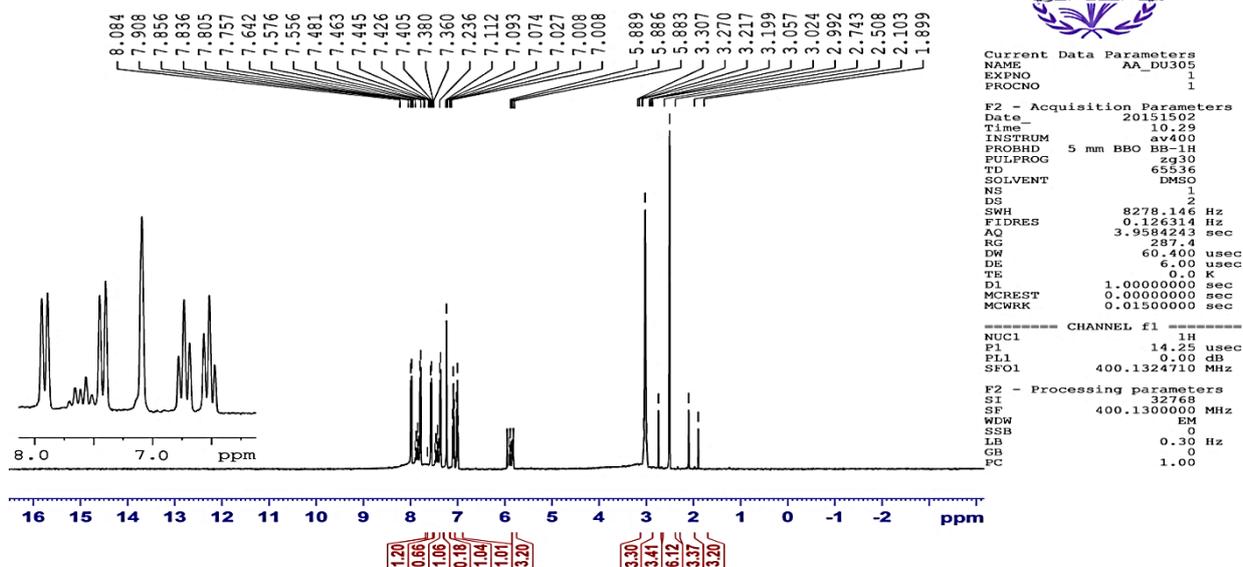


Fig.(1): ¹H-NMR Spectrum of Ligand.

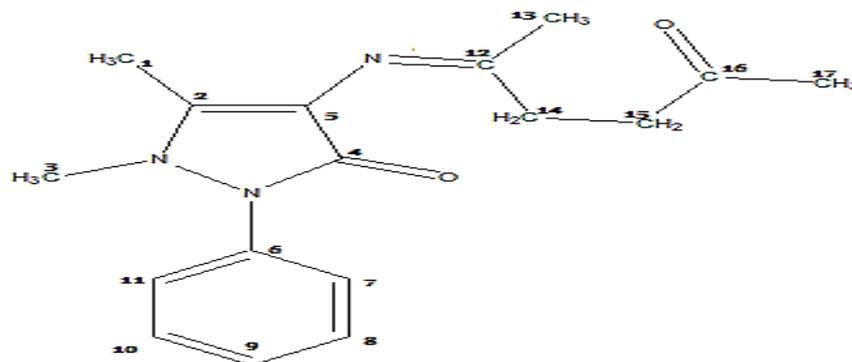


Fig.(2): Structure of Schiff base Ligand.

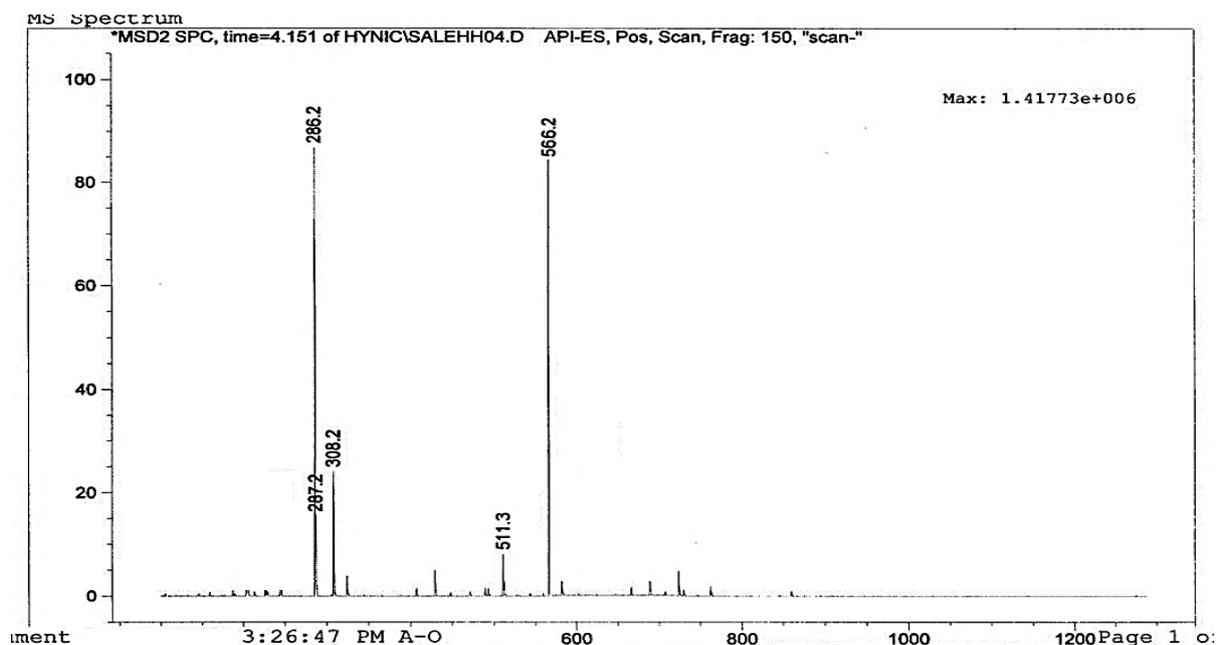


Fig.(3): Mass spectrum for $[Cr(L)(8-HQ)Cl_2]$ complex.

Table (1)

Metal and element analysis and some physical properties of the ligands and its complexes.

Sample Formula	M. wt. Yield%	Color m. p °C	Molar conductance S. cm ² . mol ⁻¹	Elemental micronalysis % Calc				
				Experimental				
				C	H	N	M	Cl
L C ₁₇ H ₂₁ N ₃ O ₂	299.37 89	Colorless 179	-	68.20	7.07	14.04	-	-
				68.95	6.68	14.44	-	-
8-HQ C ₉ H ₇ NO	145.16	White 74	-	-	-	-	-	-
				-	-	-	-	-
CrL+8-HQ C ₂₆ H ₂₇ N ₄ O ₃ CrCl ₂	566.42 67	dark brown 207	46	55.56	5.14	9.09	9.91	13.01
				55.13	4.80	9.89	9.18	12.52
MnL+8-HQ C ₂₆ H ₂₉ N ₄ O ₄ MnCl	551.92 90	Yellow 125	24	56.98	5.93	11.01	9.05	6.04
				56.58	5.30	10.15	9.95	6.42
FeL+8-HQ C ₂₆ H ₂₉ N ₄ O ₄ FeCl	552.83 89	Brown 289	37	56.65	5.92	10.31	11.01	6.14
				56.49	5.29	10.13	10.10	6.41
CoL+8-HQ C ₂₇ H ₂₉ N ₄ O ₄ CoCl	555.92 87	Green 270	37	56.57	5.66	10.76	6.08	11.15
				57.10	5.15	9.87	6.24	10.38
NiL+8-HQ C ₂₆ H ₂₉ N ₄ O ₄ ClNi	555.68 77	Light greenist 230d	31	56.20	5.26	10.08	10.56	6.38
				55.43	4.40	11.13	9.18	6.01
CuL+8-HQ C ₂₆ H ₂₉ N ₄ O ₄ ClCu	560.53 83	Brown 210d	35	55.71	5.21	10.00	11.34	6.32
				54.31	4.98	11.03	12.01	5.70
ZnL+8-HQ C ₂₆ H ₂₉ N ₄ O ₄ ZnCl	562.38 78	Light brown	27	55.53	5.20	9.96	11.63	6.30
				55.97	5.39	10.83	10.98	6.93

Table (2)
The Fragmentation pattern data for complexes.

complexes	Assignment	Peak m/z	Relative abundance%
[Cr (L)(8-HQ)Cl ₂]	M= (C ₂₆ H ₂₇ N ₄ O ₃ CrCl ₂)	566.2	86%
	M- C ₃ H ₅ N= M ₁	511.3	9%
	M ₁ -C ₈ H ₇ O ₃ Cr = M ₂	308.2	24%
	M ₂ -CH ₉ = M ₃	287.2	17%
	M ₃ -H	286.2	87%
[Mn(L)(8-HQ)Cl(H ₂ O)]	M= (C ₂₆ H ₂₉ N ₄ O ₄ MnCl)	552	97%
	M- C ₂ HO= M ₁	511.3	9%
	M ₁ -C ₉ H ₈ O ₂ Mn = M ₂	308.2	26%
	M ₂ -CH ₉ = M ₃	287.2	17%
	M ₃ - H = M ₄	286.2	87%
	M ₄ -C ₂ H ₄ N = M ₅	244.2	16%
	M ₅ -C ₃ H ₃ = M ₆	205.2	14%
	M ₆ - H	204.2	63%
[Co(L)(8-HQ)Cl(H ₂ O)]	M= (C ₂₆ H ₂₉ N ₄ O ₄ CoCl)	556	91%
	M- C ₂ H ₅ O= M ₁	511.3	9%
	M ₁ -C ₁₀ H ₈ OC _o = M ₂	308.2	24%
	M ₂ -CH ₉ = M ₃	287.2	17%
	M ₃ -H = M ₄	286.2	87%
	M ₄ - C ₂ H ₄ N	244.2	16%

FT-IR spectra

1. Infrared Spectra of Free Ligands

The spectrum of ligands (L) and 8-HQ exhibited weak bands at 3035 and 3047 cm⁻¹, this could be attributed to $\nu(\text{C-H})$ aromatic respectively. The spectrum of ligand (L) bands belong to the $\nu(\text{C=N})$ were found at 1640 cm⁻¹, was noticed band at exhibited two bands 1740 and 1696 cm⁻¹ which were attributed to $\nu(\text{C=O})$ ring of pyrazol and $\nu(\text{C=O})$ respectively. The IR spectrum bands of 8-HQ showed abroad vibration band at 3128 cm⁻¹ which was assigned to phenolic OH group and vibration band at 1504cm⁻¹ which was assigned to $\nu(\text{C=N})$ ring functional groups^[20,21].

2. Infrared Spectra of Complexes

The infrared spectra of the mixed ligands complexes of Schiff base (L) and 8-HQ exhibited bands at rang (1620 -1627) cm⁻¹ due to the $\nu(\text{C=N})$ azomethine group to the lower frequencies in comparison with ligand Schiff base. This indicated the coordination of ligands with metal ions through the nitrogen atoms in their structures. The spectra of

complexes showed bands in the range of 1669-1678cm⁻¹ were characterized for the carbonyl group which suffers a shift. Thus, it is suggested that the oxygen atom of the carbonyl group is coordinated with the metal ion^[7,11,12]. The spectra of complexes showed bands at (552-493) cm⁻¹ referred to the $\nu(\text{M-N})$ and in the range of (486-424) cm⁻¹ which was attributed to the $\nu(\text{M-O})$ ^[20]. This indicates that the ligand was coordinated with the metal ions through O of carbonyl groups and N of azomethine group. The IR-spectral data for the ligands and prepared complexes were listed in Table (3).

UV-Vis Spectra and Magnetic Moments

The electronic spectrum of the ligands of Schiff base and 8-HQ exhibit intense absorption bands at (282 and 280) nm attributed to $n \rightarrow \pi^*$ respectively. The electronic spectra of complexes [Cr (L)(8-HQ)Cl₂], [Mn(L)(8-HQ)Cl(H₂O)], [Fe (L)(8-HQ)Cl(H₂O)] and [Co(L)(8-HQ)Cl (H₂O)] gave absorptions at (291, 299, 277, 280 and 339nm) assigned to ligand field respectively. The electronic spectrum of [Cr (L)(8-HQ)Cl₂]

complex showed three broad peaks at 601, 689 and 802 nm assigned to (d-d) electronic transition type ${}^4A_{2g} \rightarrow {}^4T_{1g(p)}$, ${}^4A_{2g} \rightarrow {}^4T_{1g(f)}$ and ${}^4A_{2g} \rightarrow {}^4T_{2g(f)}$ respectively and the given two peaks at 345, 404 nm due to charge transfer (C.T). The electronic spectrum of [Mn(L)(8-HQ)Cl(H₂O)] complex showed three broad peaks at 396, 599 and 676 nm assigned to (d-d) electronic transition type ${}^6A_{1g} \rightarrow {}^4T_{2g(f)}$, ${}^6A_{1g} \rightarrow {}^4A_{1g}$ and ${}^4E_{g(4G)}$, ${}^6A_{1g} \rightarrow {}^4T_{2g(4G)}$ respectively and the given peak at 351 nm due to (C.T). The electronic spectrum of [Fe(L)(8-HQ)Cl(H₂O)] complex showed one broad peak at 676 nm assigned to (d-d) electronic transition type ${}^5T_{2g(D)} \rightarrow {}^5E_{1g(D)}$ and peak at 391 nm due to charge transfer (C.T). The spectrum of [Co(L)(8-HQ)Cl(H₂O)] complex showed three broad peaks at 576, 672 and 752 nm assigned to (d-d) transition type ${}^4T_{1g(F)} \rightarrow {}^4T_{1g(p)}$, ${}^4T_{1g(F)} \rightarrow {}^4A_{2g(F)}$ to ${}^4T_{1g(F)} \rightarrow {}^4T_{2g(f)}$ respectively and two peaks at 353 and 407 nm due to charge transfer (C.T). The (d-d) electronic transition for all prepared complexes were in a good agreement for octahedral geometry around Cr^(III), Mn^(II), Fe^(II) and Co^(II) central ion. The magnetic moment value (3.80), (5.88), (5.01) and (3.88) B.M. of Cr^(III) (d³), Mn^(II) (d⁵), Fe^(II) (d⁶) and Co^(II) (d⁷) complexes respectively are typical for octahedral geometry [12, 14]. All these electronic spectra data can be shown in Table (4).

Electrostatic Potentials

The electrostatic potential (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 electrostatic potential is strongly negative (electrophilic attack)^[17]. The (E.P) of the free ligand was calculated and plotted as 2D contour to investigate the reactive sites of the molecules shown in Fig.(5). Also one can interpret 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 two-donor atoms of oxygen carbonyl and nitrogen of azomethen group for free

ligand^[11,16], Fig.(4). All theoretically probable structures of compounds have been calculated in gas phase to search for the most probable model building stable structure. 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 Table (5)

Antimicrobial activity of ligands and all complexes

Schiff base, 8-hydroxyquinoline, metal salts and their complexes were screened for antifungal and antibacterial activity. The entire tested compounds exhibited variable.

Schiff base activity exhibited antibacterial against *Staphylococcus aureus* and *Pseudomonas aeruginosa* but activity was found to be lower than the metal ion complexes and salts metals. 8-HQ also exhibited activity antibacterial against *Staphylococcus aureus* and *Pseudomonas aeruginosa* but activity high in complexes and metal salts, Schiff base which did not exhibit have antifungal activity but exhibited activity was in some metal complexes and salts metals. While the 8-HQ and some salts metals exhibiting antifungal strong activity against *Penicillium expansum* and *Candida albicans*, not exhibited antifungal activity against *Fusarium graminearum* and *Macrophomina phaseolina* as compared with the antimicrobial activity with some mixed ligand metal ion complexes which exhibited antifungal activity top than ligands, exhibited some complexes. Prepared antifungal activity strong against *Fusarium graminearum* and *Macrophomina phaseolina* as compared with the ligands which did not exhibit antimicrobial activity. From the data shown in Table (6) a lot of compounds exhibited bio activity against two kinds of bacteria and four kinds of fungus.

Table (3)
The Infrared spectra data of the free ligand and its metal complexes in(cm^{-1}).

Comp.	$\nu\text{C-H}$ aliph.	$\nu\text{C-H}$ arom.	$\nu\text{C=O}$ ring	$\nu\text{C=O}$	$\nu\text{C=N}$	$\nu\text{C=N}$ ring	$\nu\text{H}_2\text{O}$	$\nu\text{M-N}$	$\nu\text{M-O}$	$\nu\text{O-H}$
L	-	3035	1740	1696	1640	-	-	-	-	-
8-HQ	-	3047	-	-	-	1504	-	-	-	3128
CrL+8-HQ	2927	3037	1741	1677	1627	1467	-	552 499	456 429	-
MnL+8-HQ	2920	3040	1744	1678	1624	1466	3446-883	551 497	459 424	-
FeL+8-HQ	2922	3033	1741	1672	1622	1462	3451-882	552 493	454 422	-
CoL+8-HQ	2920	3039	1745	1678	1624	1466	3437-883	552 497	459 424	-
NiL+8-HQ	2890	3080	1743	1677	1620	1449	3398-880	540 501	488 460	-
CuL+8-HQ	2980	3030	1739	1671	1629	1460	3440-870	509	480-434	-
ZnL+8-HQ	2959	3039	1737	1669	1630	1463	3457-890	530 500	486-463	-

Table (4)
Electronic spectral data and magnetic moments of the prepared compounds.

Compound Geometry	μ_{eff} B.M	ν (cm^{-1})	ABS	λ_{max} (nm)	ϵ_{max} L $\text{mol}^{-1}\text{cm}^{-1}$	Assignments
L	-	35460.99	2.48	282	24800	$n \rightarrow \pi^*$
8-HQ	-	33222.5	2.251	301	2251	$n \rightarrow \pi^*$
[Cr (L)(8-HQ)Cl ₂] Octahedral	3.80	34364.2 28985.5 24752.4 16638.9 14513.7 12468.8	2.209 1.430 1.206 0.886 0.220 0.029	291 345 404 601 689 802	2209 1430 1206 886 220 29	L.F C.T C.T ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{1g}(\text{p})$ ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{2g}(\text{F})$ ${}^4\text{A}_{2g} \rightarrow {}^4\text{T}_{1g}(\text{F})$
[Mn(L)(8-HQ)Cl(H ₂ O)] Octahedral	5.88	33444.8 28490.0 25252.5 16694.4 14792.8	2.383 1.391 2.112 0.099 0.087	299 351 396 599 676	2383 1391 2112 99 87	L.F C.T ${}^6\text{A}_{1g} \rightarrow {}^4\text{T}_{2g}(\text{f})$ ${}^6\text{A}_{1g} \rightarrow {}^4\text{A}_{1g}, {}^4\text{E}_{g(4G)}$ ${}^6\text{A}_{1g} \rightarrow {}^4\text{T}_{1g}(\text{G})$
[Fe (L)(8-HQ)Cl(H ₂ O)] Octahedral	5.01	36101.0 24154.5 17574.6	1.836 0.391 1.302	277 414 676	1836 391 1302	L.F C.T ${}^5\text{T}_{2g(\text{D})} \rightarrow {}^5\text{E}_{1g(\text{D})}$
[Co(L)(8-HQ)Cl(H ₂ O)] Octahedral	3.88	35714.2 29498.5 28328.6 24570.0 17636.6 14869.8 13297.8	2.03 1.086 0.722 1.283 0.062 1.153 0.071	280 339 353 407 576 672 752	2031 1086 722 1283 62 1153 71	L.F L.F C.T C.T ${}^4\text{T}_{1g(\text{F})} \rightarrow {}^4\text{T}_{1g(\text{p})}$ ${}^4\text{T}_{1g(\text{F})} \rightarrow {}^4\text{A}_{2g(\text{F})}$ ${}^4\text{T}_{1g(\text{F})} \rightarrow {}^4\text{T}_{2g(\text{F})}$

Table (5)
Conformation energetic in ($K J.Mol^{-1}$) for the ligands and complexes.

Comp.	Total energy	Binding energy	Heat of formation	Electronic energy	Dipole (Debyes)
L	-78659.2647	-4472.7426	-15.35266	-600793.517	3.160
8-HQ	-37080.4358086	-1577.1730516	498.1099484	-188148.4562257	3.444
CrL+8-HQ	-135971.5636626	-6410.0689746	223.4820254	-1434661.6938480	10.174
MnL+8-HQ	-139411.4000761	-6590.0024281	151.0215719	-1455264.5261658	7.932
FeL+8-HQ	-142464.6998421	-6532.0043181	240.6196819	-1485785.5198371	4.943
CoL+8-HQ	-148689.5868695	-6824.9564375	-49.2324375	-1516503.5091923	6.143

Table (6)
Antibacterial and antifungal activities for ligands, metal Salts and complexes.

No	Compound	Staphylococcus aureus G(+)		Pseudomonas aeruginosa G(-)		Penicillium expansum		Fusarium graminearum		Macrophomina phaseolina		Candida albicans	
		A	B	A	B	A	B	A	B	A	B	A	B
2	8-HQ	60	55	60	50	***	56	—	—	—	—	***	***
3	CrCl ₃ .6H ₂ O	15	12	16	15	38	28	38	33	—	—	—	—
4	CoCl ₂ .6H ₂ O	40	25	23	18	30	18	26	15	—	—	20	10
5	MnCl ₂ .4H ₂ O	40	18	20	14	—	—	—	—	—	—	—	—
6	FeCl ₂ .H ₂ O	30	12	15	—	—	—	—	—	—	—	—	—
7	L	12	—	12	—	—	—	—	—	—	—	—	—
16	FeL+8-HQ	30	25	24	18	23	19	24	14	25	20	23	15
17	CrL+8-HQ	28	22	22	15	23	19	25	20	—	—	8	—
18	CoL+8-HQ	24	20	18	14	30	28	30	22	30	20	25	17
19	MnL+8-HQ	38	30	28	18	23	17	19	12	—	—	29	18
20	Con.	0	0	0	0	0	0	0	0	0	0	0	0

***= highly active, A=conc., B=dilu.

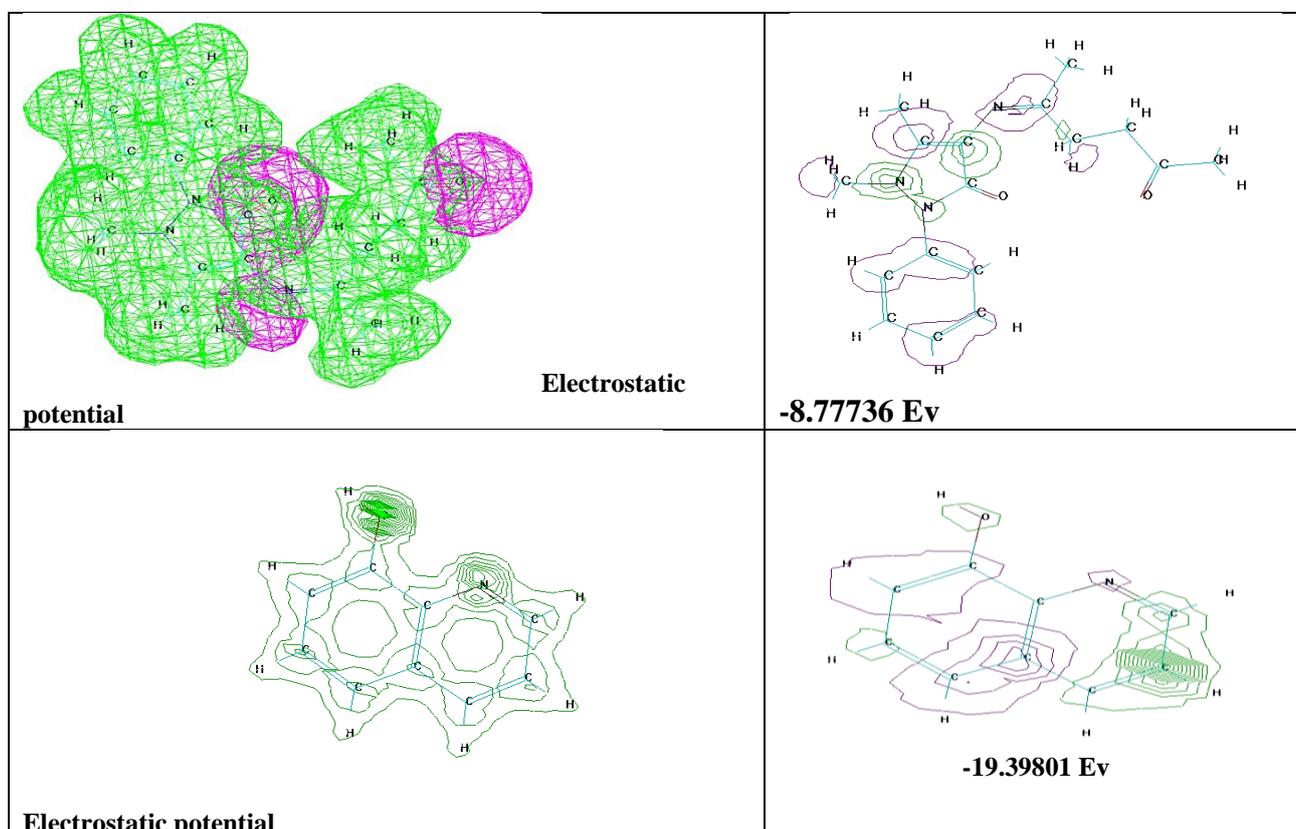


Fig.(4): Electrostatic potential (HOMO and LUMO) contours for ligands.

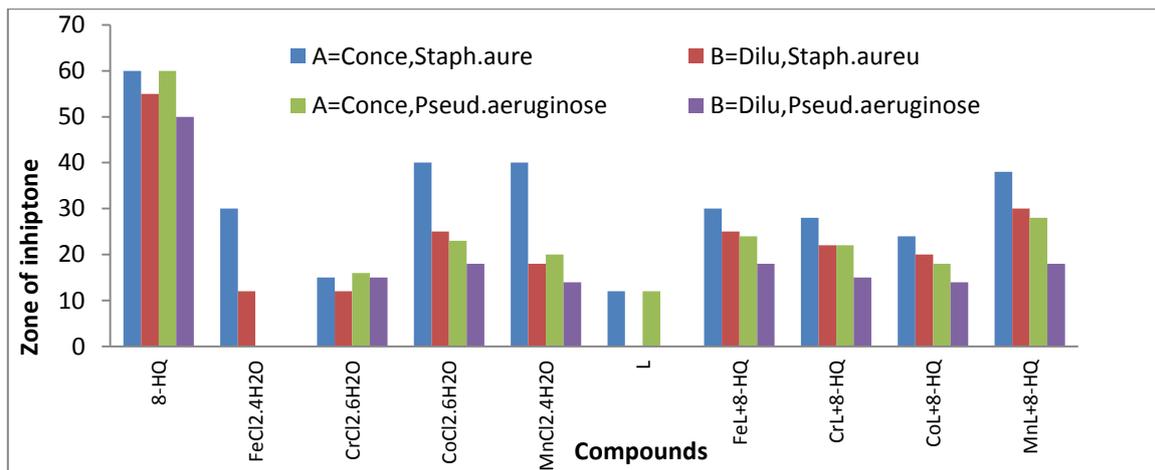
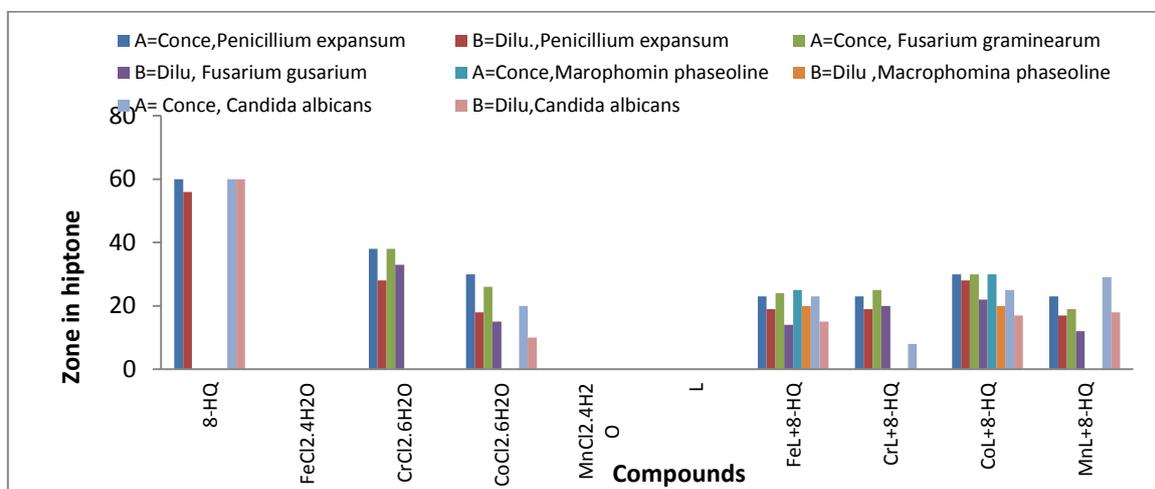


Fig.(6): The antibacterial activity of compounds against *S. aureus* and *P. aeruginosa*.



References

- [1] Gazala M. H. and Ben Hander., “Ternary complexes of cobalt (II) involving nitrilotriacetic acid and some biological active ligands”, Res. J. Chem. Sci., 2(3), 12-20, 2012.
- [2] Al-Hamdani A.A. S., Balkhi A. M., Falah A. and Shaker Sh. A., “New Azo-Schiff base derived with Ni(II), Co(II), Cu(II), Pd(II) and Pt(IV) Complexes: Preparation, Spectroscopic Investigation, Structural Studies and Biological Activity”, J. Chil. Chem. Soc, 60 (1), 2774-2785, 2015.
- [3] Patel K. B., Patel R. B., Kartikvyas B. and Nimavat K. S., “Transition metal complexes of 5-(iso-propoxymethyl-8-quinolinol), synthesis, characterization and comparative antimicrobial screening with PMQ metal complexes”, Der Pharmacia Sinica, 3(4), 501-506, 2012.
- [4] Shivshankar V. S. and Takkar N. V., “Synthesis, characterization and antimicrobial activity of some mixed ligand Co(II) and Ni(II) complexes”, Acta Poloniae Pharmaceutica-Drug Research, 60(1), 45-50, 2003.
- [5] Sharma S., Ramani J., Bhalodia J., Patel N., Thakkar K. and Patel R., “Synthesis, Characterization and Antimicrobial Activity of Some Transition Metal Complexes (Mn, Co, Zn, Ni) With L-Proline and Kojic”, Acid. Advances in Applied Research., 2(4), 374-382, 2011.
- [6] Gaikwad S. T., Rajbhoj A. S. and Arbad B. R., “Study of mixed ligand complexes of copper (II) with enalapril maleate as primary ligand and some peptides as secondary ligand”, Der Chemica Sinica, 3(6), 1348-1351, 2012.

- [7] Al-Hamdani A. A. S. and Al-Zoubi W., "New metal complexes N3 tridentate ligand: Synthesis, spectral studies and biological activity", *Spectrochimica Acta Part A: Mole. and Biomol.*, 137, 75-89, 2015.
- [8] Girgaonkar M.V. and Shirodkar S.G., "Synthesis, characterization and biological studies of Cu(II) and Ni(II) complexes with new bidentate Schiff's base ligands as 4-hydroxy-3-(1-(arylimino) ethyl) chromen-2-one", *Res. J. Recent Sci.*, 1(ISC-2011), 110-116, 2012.
- [9] Al-Hamdani A.A. S., Jarad A. J. and Al-Atrakchi S. A., "Synthesis and Spectral Analysis of VO(II), Cr (III), Zn(II), Cd(II), Hg(II) and UO₂ (II) Complexes with Mixed Ligands of Bipyridyl and Novel Schiff Base", *Diala J.*, 36, 1-14, 2009.
- [10] Shaker Sh. A., Farina Y. and Al-Hamdani A. A. S., "Synthesis and Characterization of Mixed Ligand Complexes of 8-Hydroxyquinoline and hydroxybenzyl idene-1-phenyl-2,3-dimethyl-4-amino-3-pyrazolin-5-on with Fe(II), Co(II), Ni(II) and Cu(II) ions", *Euro. J. of Scie. Res.*, 33(4), 702-709, 2009.
- [11] Zhang H., Huang K., Chen Z., Liu Y., Ting Y., Meng T., Qin Q., Zou B. and Liang H., "Cobalt(II) 8-hydrxyquinoline complexes: Structure, Cytotoxicity and action mechanism", *Med. Chem. Commun.*, 7, 806-812, 2016.
- [12] Prachayasittikul V., Prachayasittikul S., Rirawatuc S. and Prachayasittikul V., "8-hydrxyquinoline: a review of their metal chelating properties and medicinal applications", *Drug Design, Dev. and Therapy*, 7, 1157-1178, 2013.
- [13] Shar G. A. and Soomro G. A., "8-hydrxyquinoline as a Complexing Reagent for the Determintion of Cd(II) in Micellar Medium", *J. Chem. Soc. Pak.*, 27(5), 471-475, 2005.
- [14] Hitendra D. R. and Yogesh S. P., "Synthesis, characterization and antifungal activityof metal complexes of 8-hydrxyquinoline based azo dye", *Adv.in Appl. Sci. Res.*, 6(2),119-123, 2015.
- [15] Mashaly M. M., Abd-Elwahab Z. H. and Faheim A. A., "Preparation, Spectral Characterization and Antimicrobial Activities of Schiff Base Complexes Derived from 4-Aminopyridine, 8-hydroxyquinoline and Oxalic Acid and their Pyrolytical Products", *J. Chin. Chem. Soc.*, 51, 901-915, 2004.
- [16] [16]- Al-Hamdani A. A. S. and Hamoodah R. G., "Transition Metal Complexes with Tridentate Ligand: Preparation, Spectroscopic Characterization, Thermal Analysis and Structural Studies", *J. Baghdad for science*, 13(4), 770-781, 2016.
- [17] Norman A., "Hyper Chem Computational Chemistry (Practical Guide and Theory and Methods)", New York, John Wiely and Sons, Inc, 1996.
- [18] Suresh M. S. and Prakash V., "Preparation, characterization and microbiological studies of Cr(III), Mn(II), Ni(II), Co(II), Cu(II), Zn(II) and Cd(II) chelates of Schiff base derived from vanillin and anthranilic acid", *Inter. J. phys. Sci.*, 5 (9), 1443-1449, 2010.
- [19] Shaker Sh. A., Mohammed H. A. and Al-Hamdani A. A. S., "Preparation, Physico-Chemical and Spectroscopic Investigation of Thiacetazone and Quinalizarin Complexes with Mn (II), Fe (II), Co (II), Ni (II), Cu (II), Zn (II), Cd (II) and Pb (II) " *Aus. J. Basic. And Ap. Sci.*, 4(10), 5178-5183, 2010.
- [20] Nakamoto N., "Infrared and Raman Spectra of Inorganic and Coordination Compounds", John Wiley & Sons, Inc., 6th Ed., New Jersey, 2009.
- [21] Sliverstien R. M. and Webser X. F., "Sptrometric Identification of Organic Compounds". 7th Ed., Jon Wiley and Son, Inc. USA, 2005.
- [22] Sarika R. Y., Amit R. Y., Gaurav B. P. and Anand S. A., "Synthesis and characterization of transition metal complexes with N, O-chelating Hydrazone Schiff base ligand, American-Eurasian Complexes Containing Heterocyclic Nitrogen Donor Ligands", *Chem. Pap .*, 57 (2), 91-96, 2003.
- [23] Lever A. B., "Inorganic electronic spectroscopy", Elsevier Amsterdam, 1984.