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A quantitative analysis of N & O donor chelating ligand complexes

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Abstract

In the present manuscript di & tri positive transition metal complexes with mixed chelating ligands viz., 5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide and 5-iodo-7-chloro-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide were synthesized in 1:3 stoichiometric ratio, and characterized by elemental analysis, magnetic susceptibility measurement, IR spectra, UV-visible and mass spectra measurement. Studies suggested distorted octahedral coordination geometry in all cases of isolated complexes. Compounds assayed for their *in vitro* antimicrobial activities against four bacterial and two fungal strains, were found to be metal chelates are more noxious than the free ligands. Antimicrobial analysis of chelating ligands and their complexes type ML_3 & ML'_3 against bacterial-fungal strains had been done by disk diffusion method. CuL_3 & CuL'_3 chelates manifest overwhelming activity against microbes than the other metal chelates.

Keywords: IR, UV-visible spectra, ligands, complexes, diffusion method, antimicrobial activities

Introduction

The coordination, analytical as well as industrial chemistry are highly important to understand the formation and stability of quinoline and p-toluenesulphonamide with a number of metal complexes have attracted special attention because of their therapeutic properties and to know the exact experimental methods of their investigation have already been discussed¹. Some of the sulphonamides were used as drugs for diseases like diabetes, dengue, tuberculosis, leprosy, malaria, cancer and convulsion and they were found to be active against different types of bacteria. It has been observed recently that some drugs have increased activity when administered as metal complexes more so than their metal chelates. Similar indication was found in our previous work. In continuation of our previous work and to test the change in antibacterial activity of ligands on chelation, we report here the synthesis of metal chelates viz., 5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide and 5-iodo-7-chloro-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide with di and tri positive transition metals. Beside their synthesis and characterization of number of mixed chelating complexes of transition metals have been reported in our research lab^[2, 4]. Some of the research work has predicted that normal geometries of the compounds experience distorted as the 'bite' of the bidentate ligands change.

Material and Method: All chemicals and reagents for this research work used were of A.R. grade. The ligands 5-iodo-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide(L) and 5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide(L') were prepared by the action of chlorosulphonic acid on 5-iodo-8-hydroxyquinoline and 5-iodo-7-chloro-8-hydroxyquinoline, thus getting their sulphonylchlorides. These sulphonylchlorides were allowed to react with p-toluene in ethanolic medium. This resulted in the formation of precipitate of both ligands, precipitate was filtered, washed well with absolute ethanol and recrystallized. The metal- ligand ratio was determined by conductometric titration⁵ which showed 1:3 complexation. Metal salt in double distilled water and ligands in methanol and ethanol (absolute) solution were added (pH- 8-9) with constant magnetic stirrer at 60°C for 2 hrs. The pH was maintained by using a solution of 0.1M NaOH and 0.1M H₂BO₃. White-blue coloured solid adducts of type ML_3/ML'_3 were obtained.

The solid complexes that separated out were washed with distilled water and dried over P_4O_{10} in vacuum desiccator. Ligands and their complexes were subjected to analysis for C, N, S, Cl, I, whereas metal was estimated gravimetrically in the lab ⁶. IR spectra of the ligands and their complexes were recorded in FT/IR-4100 type in KBr / nujol mull phase $4000-200\text{ cm}^{-1}$, IITL Labs Pvt. Ltd. Delhi. Electronic spectra of the complexes were recorded with the help of UV-Beckman Du-2 spectrophotometer. Molar conductance of the complexes in different solvents viz., nitrobenzene, DMF & DMSO in 10^{-3} M dilution were observed at 27°C by Philips conductivity-bridge RP-9500 with a dip type conductivity cell. Magnetic susceptibility measurement were carried out by Gouy balance using $\text{HgCo}(\text{SCN})_4$ as standard. Mass spectra of the ligands and their complexes were recorded at the ToF magnetic sector and Quadrupole-SIMS instrument at New Delhi. The molecular weight determination ^[7] was carried out by Rast's method using camphor as a solvent. The biological activities were tested against antimicrobial and anti-fungal activities as compared to respective standard drugs using the disc diffusion methods ^[8].

Result and Discussion: Ligands and their complexes were subjected to elemental analysis and results are reported in Table-1 the exact melting points could not be determined but were more than 300°C , data revealed that the ligands have reacted with metals in 1:3 ($M:L_n$) ratio where $n=3$. On

the basis of analysis the general formula of the complexes came out to be ML_n . There is a significant difference in the melting point of all complexes formed with ligands, which indicates that the complexes may have been formed. All the complexes were found to be insoluble in common organic solvents but soluble in nitrobenzene, DMF and DMSO. The molecular conductance at 27°C indicated the non-electrolytic nature of the complexes. The low values of molar conductance (~ 20) $\text{ohm}^{-1}\text{cm}^2\text{mol}^{-1}$ in nitrobenzene, DMF and DMSO medium (Table-1) indicate that the complexes are non-electrolytes.

The electronic spectra of all complexes were recorded in solid state. Since the colour of all complexes were different, the spectra of all were found to be almost the same in nature. The Ti^{+3} complexes shows magnetic moment (1.74-1.78 B.M.) for one unpaired e^- . The higher values may be due to orbital contribution ^[9, 10]. A single broad band has been observed at range $19221-19225\text{ cm}^{-1}$ for Ti^{+3} complexes derived from the transition ${}^2T_{2g} \rightarrow {}^2E_g$ for an octahedral geometry ^[9, 10]. These bands are unsymmetrical in shape are indeed made up of two closely shaped bands. The second band appears as a hump and may be due to the presence of John-Teller distortion in the complexes. But regular octahedral stereo chemistry would experience distortion due to the presence of chelating agents that too of a dissimilar nature. Hence, it is concluded that Ti^{+3} complexes reported in this manuscript are mixed chelating complexes and possessing distorted octahedral geometry.

Table 1: Physico-chemical analysis of the complexes

S.N.	Complexes	Mol. Formula	Colour	m.p. ($^\circ\text{C}$)	Elemental Analysis						$(\text{ohm}^{-1}\text{cm}^2\text{mol}^{-1})$			μ_{eff} (B.M.)
					%C	%N	%S	%Cl	%I	%M	NB	DMF	DMSO	
1.	TiL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{STi}$	grey	269	13.80 (13.60)	1.51 (2.11)	2.73 (2.41)		26.73 (28.6)	3.85 (3.757)	2.	11	13	1.74 (d1)
2.	VL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SV}$	yellow	258	13.10 (13.53)	1.87 (2.11)	2.67 (2.41)		24.23 (28.8)	3.40 (3.99)	2.2	12	18	2.63 (d2)
3.	VOL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SVO}$	cream	289	12.87 (12.89)	1.64 (2.08)	2.03 (2.38)		26.76 (28.27)	4.83 (5.24)	2.1	10	15	1.78 (d1)
4.	CrL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SCr}$	grey	314	13.10 (13.53)	1.73 (2.10)	2.02 (2.41)		27.44 (28.64)	3.64 (4.06)	2	19	13	3.5 (d3)
5.	MnL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SMn}$	brown	324	13.08 (13.35)	1.60 (2.08)	2.13 (2.85)		27.03 (28.50)	3.82 (4.30)	1.6	15	17	5.22 (d5)
6.	FeL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SFe}$	brown	308	12.79 (13.50)	2.06 (2.07)	1.91 (2.43)		27.32 (28.17)	3.67 (4.38)	1.7	13	19	3.24 (d4)
7	CoL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SCo}$	black	314	13.12 (13.46)	1.59 (2.02)	2.14 (2.38)		27.62 (28.50)	4.11 (4.62)	18	11	20	3.74 (d3)
8	NiL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SNi}$	green	287	13.28 (13.50)	1.85 (2.00)	2.15 (2.37)		26.84 (28.52)	4.08 (4.54)	14	16	21	3.10 (d2)
9	CuL_3	$\text{C}_{15}\text{H}_{11}\text{IN}_2\text{O}_3\text{SCu}$	Light blue	254	13.02 (13.42)	1.83 (2.08)	2.19 (2.38)		26.98 (28.41)	5.08 (4.93)	16	18	19	1.83 (d1)
10	TiL'_3	$\text{C}_{15}\text{H}_9\text{ClIN}_2\text{O}_3\text{STi}$	cream	249	12.05 (12.67)	1.09 (1.96)	1.98 (2.23)	2.15 (2.50)	24.98 (26.74)	3.03 (3.48)	17	11	14	1.78 (d1)
11	VL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SV}$	pink	284	12.00 (12.63)	1.58 (1.96)	2.12 (2.18)	1.98 (2.51)	25.14 (26.68)	3.01 (3.70)	19	17	18	2.78 (d2)
12	VOL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SVO}$	cream	267	11.58 (12.44)	1.64 (1.93)	1.89 (2.10)	2.04 (2.46)	24.89 (26.38)	3.98 (4.86)	14	16	20	1.82 (d1)
13	CrL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SCr}$	brown	302	11.85 (12.57)	1.58 (1.96)	1.95 (2.17)	2.06 (2.48)	25.11 (26.62)	3.09 (3.77)	18	10	18	3.5 (d3)
14	MnL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SMn}$	purple	290	11.45 (12.54)	1.65 (1.95)	2.18 (2.14)	2.01 (2.52)	25.48 (26.76)	3.11 (3.99)	19	14	19	5.61 (d5)
15	FeL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SFe}$	brown	285	11.36 (12.54)	1.64 (1.96)	1.97 (2.14)	2.11 (2.54)	24.79 (26.81)	3.54 (4.08)	17	16	18	3.43 (d4)
16	CoL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SCo}$	blue	302	11.25 (12.51)	1.59 (1.93)	1.69 (2.11)	2.08 (2.58)	25.18 (26.95)	3.58 (4.24)	12	11	21	3.98 (d3)
17	NiL_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SNi}$	brown	319	11.57 (12.51)	1.62 (1.95)	1.86 (2.12)	2.17 (2.61)	25.11 (26.92)	3.84 (4.31)	19	13	17	3.25 (d2)
18	CuL'_3	$\text{C}_{15}\text{H}_{11}\text{ClIN}_2\text{O}_3\text{SCu}$	blue	287	11.58 (12.47)	1.84 (1.94)	2.08 (2.26)	2.20 (2.65)	24.69 (26.45)	43.98 (4.42)	12	10	18	1.85 (d1)

*Values in parenthesis are calculative value

The electronic spectrum of V^{+3} complexes were recorded which showed band at 15992 - 15996 cm^{-1} with shoulder at 21017-21023 cm^{-1} . The low energy band has been assigned to ${}^3T_{1g} \rightarrow {}^3T_{2g}$ whereas the high energy band ${}^3T_{1g} \rightarrow {}^3T_{1g}$ transition, respectively, characteristics of octahedral geometry [11]. Which is further confirmed by absorption spectrum and magnetic moment values 2.63-2.78 B.M. for V^{+3} complexes. The spectral result for the six coordinated VL_3 and VL'_3 complexes are characteristic of an octahedral geometry around the central V^{+4} ion of the three expected low energy ligand field bands, two are easily observed in the 12868-13330 and 16945-17854 cm^{-1} ranges and are assigned as ${}^2B_{2g} \rightarrow {}^2A_{1g}$ and ${}^2B_{2g} \rightarrow {}^2B_{1g}$ transitions, respectively. Since, the energy separation between the ${}^2B_{1g}$ and ${}^2B_{2g}$ levels occur at ca. 2000 cm^{-1} . The frequency of this electronic transition is taken to correspond to 10Dq. The strong high energy band in the 27395-27775 cm^{-1} range may be assigned to a spin forbidden charge transfer transitions.

The magnetic moment of the examined Cr^{+3} metal complexes as well as the electronic absorption spectra in DMF (10^{-3} cm^{-1}) were measured at room temperature. The Cr^{+3} complexes displayed two absorption band at 15037 and 16529 cm^{-1} correspond to be the transitions ${}^4A_{2g}(F) \rightarrow {}^4T_{2g}(F)$ and ${}^4A_{2g}(F) \rightarrow {}^4T_{1g}(P)$, respectively, in an octahedral configuration [12]. The octahedral geometry around the Cr^{+3} ion was confirmed by the Cr^{+3} complexes magnetic moment values 3.4-3.5 B.M.

The octahedral geometry of Mn^{+2} complexes were confirmed by the magnetic moment values 5.22-5.61 BM. One absorption band exhibited in the electronic spectrum of Mn^{+2} complexes at range 17064-17301 cm^{-1} as a result ${}^6A_{1g} \rightarrow {}^4T_{2g}(G)$ transition in the octahedral geometry [13].

In the Fe^{+2} complexes a shoulder band at range 27027-27030 cm^{-1} in the spectrum is attributed to $n \rightarrow \pi^*$ transition. The band at range 18018-18020 cm^{-1} with a shoulder around 20202 cm^{-1} is assigned to $T_{2g} \rightarrow \pi^*$ transition which is responsible for intense colour of Fe complexes. Dq value of about 924 cm^{-1} calculated from the maximum of the major ($d \rightarrow d'$) band suggested octahedral structure for these complexes [12, 13].

In the Co^{+2} complexes bands at range 9523-9528 and 20747-20749 cm^{-1} are assigned to the transitions ${}^4T_{2g}(F) \rightarrow {}^4T_{2g}(F)$ and ${}^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$, respectively. The energy of ${}^4T_{1g}(F) \rightarrow {}^4A_{2g}(F)$ transition has been calculated to be 22886 cm^{-1} . The spectrochemical parameters of these complexes, $Dq = 838.23 \text{ cm}^{-1}$, $\beta = 0.78$, $B' = 8.73.2 \text{ cm}^{-1}$ and magnetic moment of 3.74-3.98 B.M. confirm their octahedral structure [14, 15].

In the Ni^{+2} complexes the electronic spectral bands at ranges 30310-30312 cm^{-1} , 17852-17854 cm^{-1} and 10750-10752 cm^{-1} are due to ${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(P)$, ${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(P)$, ${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(F)$ and ${}^3A_{2g}(F) \rightarrow {}^3T_{2g}(F)$ transitions. All these transitions are spin allowed transition and are designated as V_3 , V_2 and V_1 , respectively. The ratio of V_2/V_1 (17850/10750) comes out to be 1.66 which suggested octahedral geometry to these complexes. Values of various ligand field parameters viz., Dq (1075 cm^{-1}), B' (1060 cm^{-1}) and β (0.98) further substantiate the above conclusion. The magnetic moment of 3.10-3.25 B.M. for both the complexes of nickel also confirm the assigned geometry [15].

The magnetic moment of the Cu^{+2} complexes at room temperature lie in the range (1.83-1.85 B.M.). These spin allowed transition may be expected in the visible region and the E_g and T_{2g} levels of ${}^2D$ free ion will split in to B_{1g} , A_{1g} ,

B_{2g} and E_g levels, respectively. The electronic spectrum of six coordinated copper complexes display band at 13698, 15151, and 23202 cm^{-1} corresponding to the transitions ${}^2B_{1g} \rightarrow {}^2B_{2g}$, ${}^2B_{1g} \rightarrow {}^2E_g$ and ${}^2B_{1g} \rightarrow {}^2A_{1g}$ indicate that the both complexes of copper also confirm the octahedral geometry [15].

The ir spectrum data of the ligands and their complexes were recorded. A broad distinct band at 2960 cm^{-1} in the spectrum of 5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide and another at 3110 cm^{-1} in 5-iodo-7-chloro-8-hydroxyN(4-methylphenyl) quinolyl-4-sulphonamide ligands were found [4, 13, 16]. These values are less than the prescribed limit (3700-3300 cm^{-1}) for -OH group. It is due to hydrogen bonding. On the basis of intramolecular hydrogen bonding chelate structure (-O-H...N-) have been proposed for the ligands. A critical examination of the spectra of metal chelates indicate that the bonds at 2960 cm^{-1} and 3110 cm^{-1} present in the ligands shift to higher values (3600-3300 cm^{-1}) in the chelates. Thus on the metal chelate formation the band between 3600-3300 cm^{-1} which appears in all chelates are not present in the original ligands. The disappearance of H-bonded -OH in the ligand and its reappearance in the metal chelates are suggestive of O-M-N bond formation, where M is a metal atom. The bands of medium intensity around 1610 cm^{-1} in the spectra of ligands due to $\gamma(>C=N-)$ shift to lower values with weak intensity in the spectra of chelates. It is due to $M \leftarrow N$ bond formation. The bands between 1610-1495 cm^{-1} are due to 520 cm^{-1} and 810 cm^{-1} are due to $>CH-I$ and $>CH-Cl$, respectively [13, 16]. The presence of sulphonamide group has been established by a characteristics band in the vicinity of the region 1375 cm^{-1} .

Table 2: Mass spectra data of ligands and their metal complexes

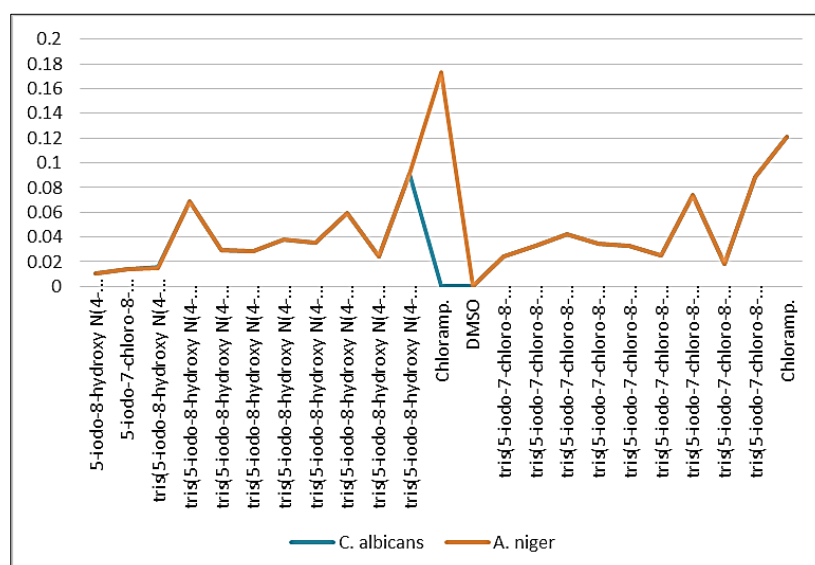
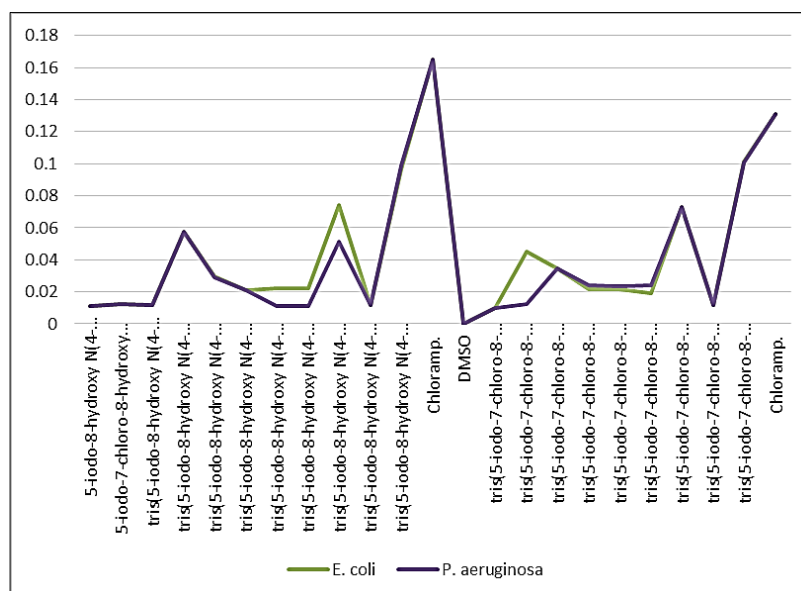
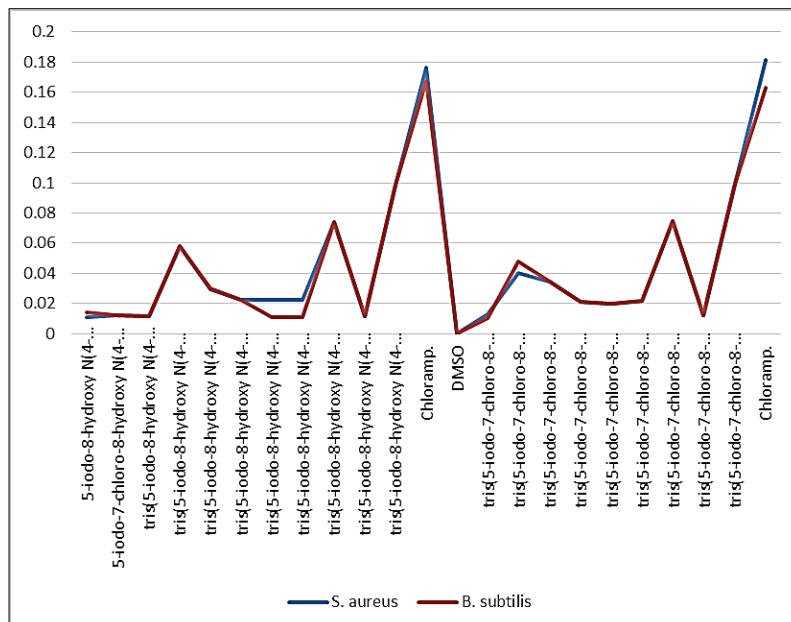
Ligands/Complexes	Calculated Mass	Observed Mass	Peak
5-iodo-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide (L)	426	426.19	M
5-iodo-7chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide(L')	459	458.06	M
TiL_3	1326	1325.83	M
VL_3	1329	1328.67	M
VOL_3	1345	1345.26	M
CrL_3	1330	1329.51	M
MnL_3	1333	1333.85	M
FeL_3	1334	1336.76	M+2
CoL_3	1337	1336.05	M
NiL_3	1336	1338.45	M+2
CuL_3	1341	1340.65	M
TiL'_3	1425	1425.41	M
VL'_3	1428	1427.81	M
VOL'_3	1444	1443.87	M
CrL'_3	1429	1429.26	M
MnL'_3	1432	1432.09	M
FeL'_3	1433	1435.43	M+2
CoL'_3	1436	1435.89	M
NiL'_3	1435	1437.61	M+2
CuL'_3	1440	1439.88	M

The mass spectra data of ligands and their metal complexes given in table-2, which exhibit some peaks illustrate the power fragmentation. In most cases instance molecular ion peaks were recorded, which were in good agreement for expected values ^[17]. The mass spectra of the ligands give some peaks at 425 m/z and 458 m/z, respectively, due to the loss of e⁻ C₁₃H₁₀IN₂O₃S¹⁺ and C₁₅H₈ClIN₂O₃S¹⁺ which are assigned for molecular ion peaks at H/L⁺ 425 m/z and 458 m/z are attributed to the presence of base peaks C₁₀H₅INO₂S¹⁺ and C₁₀H₃ClINO₂S¹⁺ at 100%≤ relative abundance¹⁷. All complexes give some peaks at 1325.8, 1425.41 m/z, 1328.6, 1427.81 m/z, 1345.2, 1443.87 m/z, 1329.51, 1429.26 m/z, 1333.85, 1432.09 m/z, 1336.05, 1435.89 m/z, and

1340.65, 1439.88 m/z, respectively which assigned as M⁺ peak in all cases but in the spectra of Ni(II) & Fe(II) complexes, these peak were at 1338.45, 1437.72 m/z and 1336.76, 1435.43 m/z which assign to M+2 peak. These M+2 peaks were recorded along with the molecular ion peaks due to the presence of isotopes of Ni & Fe atoms in the complexes. The mass spectra proved that the isotopic pattern of detected complexes corresponds to the characteristic isotopic pattern ⁶⁰Ni(17.8%) & ⁵⁶Fe (15.6%) table-2 present the assumed composition and m/z values of prominent coordination complexes of the ⁶⁰Ni & ⁵⁶Fe isotopes ^[18, 19].

Table 3: Antimicrobial activity of the ligands and their metal complexes MIC in µmol/ml, Gram (+) bacteria Gram (-) bacteria-fungi (Microorganism Inhibition Zone)

S. No.	Ligands/Complexes	S. aureus	B. subtilis	E. coli	P. aeruginosa	C. albicans	A. niger
1	5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide	0.0112	0.0142	0.0112	0.0112	0.0103	0.0103
2	5-iodo-7-chloro-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide	0.0123	0.0123	0.0123	0.0123	0.0141	0.0141
3	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Ti	0.0117	0.0117	0.0117	0.0117	0.0153	0.0152
4	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)V	0.0578	0.0578	0.0578	0.0578	0.0686	0.0686
5	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)VO	0.0293	0.0299	0.0299	0.0293	0.0293	0.0293
6	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Cr	0.0225	0.0225	0.0212	0.0212	0.0282	0.0282
7	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Mn	0.0225	0.0112	0.0225	0.0112	0.0384	0.0382
8	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Fe	0.0224	0.0111	0.0224	0.0111	0.0351	0.0351
9	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Co	0.0742	0.0742	0.0742	0.0511	0.0598	0.0598
10	tris(5-iodo-8-hydroxy N(4-methylphenyl)quinolyl-4-sulphonamide)Ni	0.0119	0.0119	0.0119	0.0119	0.0246	0.0246
11	tris(5-iodo-8-hydroxy N(4-methylphenyl) quinolyl-4-sulphonamide)Cu	0.0985	0.0985	0.0965	0.0992	0.0910	0.0910
12	Chloramp.	0.1763	0.1678	0.1651	0.1651	0.1702	0.1730
13	DMSO	-	-	-	-	-	-
14	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Ti	0.0131	0.0101	0.0101	0.0101	0.0242	0.0242
15	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)V	0.0401	0.0476	0.0450	0.0124	0.0332	0.0332
16	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)VO	0.0346	0.0346	0.0346	0.0345	0.0425	0.0425
17	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Cr	0.0212	0.0212	0.0216	0.0241	0.0345	0.0344
18	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Mn	0.0201	0.0201	0.0216	0.0233	0.0326	0.0326
19	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Fe	0.0221	0.0221	0.019	0.0241	0.0251	0.0251
20	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Co	0.0746	0.0746	0.0731	0.0731	0.0741	0.0740
21	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Ni	0.0120	0.0120	0.0120	0.0120	0.0184	0.0184
22	tris(5-iodo-7-chloro-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide)Cu	0.0993	0.0993	0.1012	0.1009	0.0889	0.0888
23	Chloramp.	0.1812	0.1631	0.1311	0.1314	0.1210	0.1210
24	DMSO	-	-	-	-	-	-



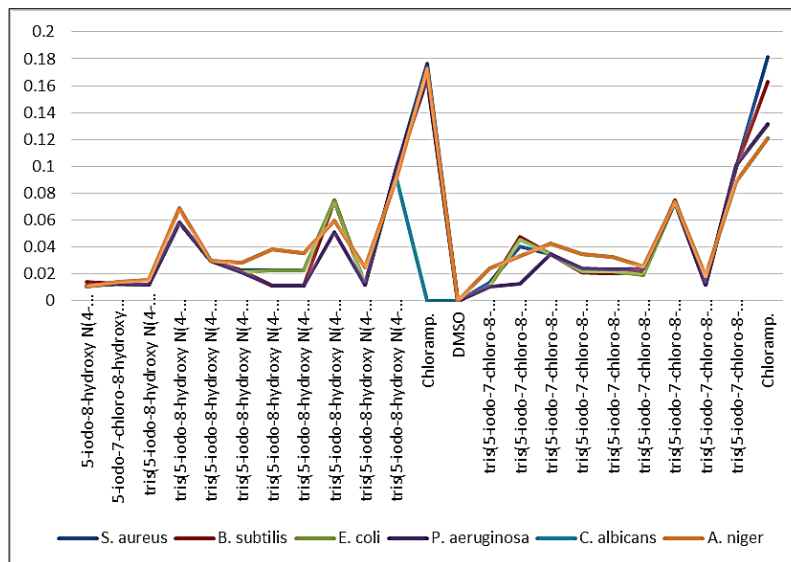


Fig d: Overall growth comparison bacterial-fungal strains

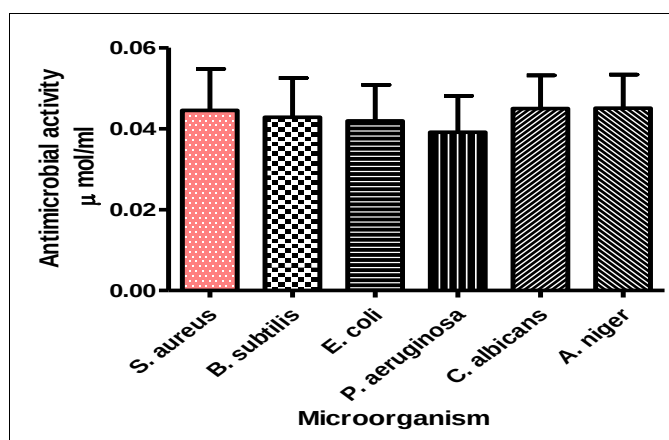


Fig e: Showing anti-microbial activities

All di & tri positive metal complexes (ML_3, ML'_3) reveal antimicrobial activity and they were found to be active inhibitors against bacteria-fungi strains (table-3). Responsiveness of both the testing coordinated complexes ML_3 & ML'_3 ($M=Ti^{+3}, V^{+3}, VO^{+2}, Cr^{+3}, Mn^{+2}, Fe^{+2}, Co^{+2}, Ni^{+2}, Cu^{+2}, L=$ 5-iodo-8-hydroxyN(4-methylphenyl)quinolyl-4-sulphonamide, $L' =$ 5-iodo-7-chloro-8-hydroxy(4-methylphenyl)quinolyl-4-sulphonamide) was evaluated based on the diameter of the inhibition zone against gram+ve (*S. aureus*, *B. subtilis*) and gram -ve (*E. coli*, *P. aeruginosa*) bacteria and two fungal (*C. albicans*, *A. niger*) strains. The analysis of results presented in table-3 shows the antibacterial activities of nine different metal-ligand complexes against gram+ve bacterial strain. Using this data an attempt has been made to explain the comparative studies through Fig. a, b, c, d, e. *In vitro* screening for all coordinated complex was performed at different concentration mentioned above and the result were compared with chloramphenicol antibiotic. The values of the diameter of inhibition zone of CuL_3 & CuL'_3 complexes show that these antimicrobial agent are effective in controlling the growth of all the bacteria strains studied when compared with the positive (chloramphenicol) and Cu complexes were also effective against *S. aureus*, *E. coli* and *P. aeruginosa*, respectively. The result also point out that the TiL_3 & TiL'_3 complexes are less active than other complexes but like other metal chelates these chelates also showing

significant inhibition activity against fungi *C. albicans* & *A. niger* [20]. In comparison of the standard drugs fluconazole all metal chelates exhibited anti-fungal activity. Among all testing complexes CuL_3 & CuL'_3 complexes were most active against all fungal strains. DMSO (-ve control) has shown negligible activity as compared to these complexes.

The metal complexes exhibited different levels of activities against various strains because of variation in cells wall permeability. Inhibition depends on metal complex concentration, culture medium and incubation conditions [20, 21]. The antimicrobial activity of the synthesized compounds might be explained on the basis of the overtone concept and chelation theory. Accordingly, polarity of metal-atom gets reduced due to sharing of the partial (+) charge of metal ion to the different donor atoms of the compounds and some p-electrons delocalization inside the entire chelates. Some metal complexes do not show good activity because of their limited lipid solubility, therefore, metal ions present on center may not be able to attack the required site of cell wall to interfere with the normal cell activity. Although chelation enhances the biological activity of the complexes along with other factors like dipole moment, geometry of the complexes, concentration, size of the molecules, bond length, coordination site and hydrophobicity effect activity. Hence it may be concluded that not only chelation but may other contributions also enhance the antimicrobial activity [22]

Conclusion

Di & tri valent transition metal complexes with biologically active mixed ligands were synthesized in stoichiometric ratio, the ligands function as anionic chelating ligands through deprotonated N, O atoms. The ligand field parameters of the synthesized complexes have been evaluated which suggested to be distorted octahedral geometry. Antimicrobial activities of free ligands and their metal complexes were measured, data prove that the complexes CuL_3 & CuL'_3 were found most active complexes followed by cobalt & vanadium, whereas TiL_3 & TiL'_3 complexes were found less active as compared to standard drugs fluconazole, all metal chelates exhibited significant anti-fungal activity. The significance of this investigation is to uncover shielding and constructive therapeutic agents that wield against bacterial and fungal infection, all chelates exhibited anti-fungal activity. The molecular docking of the both ligands and its complex with enzyme sterol 1, 4- α Demethylase suggested the hydrophobic binding. Furthermore, in the silico stressed that the compounds may be used as orally active drugs.

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