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Metal-organic frame works of transition metal Co (II), Ni (II), Zn (II), Cd (II) and Cu (II) ions derived from streptomycin and chloramphenicol and their molecular modeling

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ABSTRACT

Metal organic frame works of transition metal ions complexes have been synthesized with streptomycin and oxime. Conformational changes and binding abilities of the organic frame works toward metal ions were identified by various physical -chemical and spectroscopic measurements including IR, ^{1}HNMR, UV-Vis, molecular modeling and X-ray powder diffractometery. The lattice parameters were calculated by CRYSFIRE software programme. Molecular model represent a better understanding of the arrangement of the atoms in the molecules in three dimensions. The synthesized complexes were highly antibacterial effective.

Keyword: Antibiotic, streptomycin, chloramphenicol, TGA, molecular modeling

INTRODUCTION

The interaction of ligand donor atoms with a metal is very important in coordination chemistry and it affects the physiochemical properties of the resulting metal-organic frame work. Metal-organic frame works (MOFs) are very useful in the field of antibiotic drugs and utilization in various physiochemical systems. This is due to the variability in the bond formation between donor atoms and metals. Spectroscopic characterization of synthetic MOFs helps to determine their coordination abilities [1]. Other spectroscopic parameters were calculated to understand this new bond formation. Simple ligands containing significantly different donor atoms, such as oxygen, sulphur and nitrogen, find increasing use in chemistry because of their selectivity. It introduces a new approach to understand

metal-ligand interactions and their possible dynamic behaviuor.These are important topics in drug science and theraptic research[2-4].Organic ligands, such as antibiotics contain a flexible backbone and due to this flexibility and conformational freedom, allow the formation of complexes having great structural diversity. Ligands bearing O and N coordinating sites can coordinate metals with different modes (forming a great variety of molecular structures. The elemental analysis, infrared, electronic, mass spectra and X-ray powder diffractometry spectra were investigated to elucidate the activity, stability, solubility and coordination parameters of metal ions [5].

Lattice parameters, crystal size, spectroscopic characterization, stability measurements and atomic coordinates were also calculated. These parameters provide significant information about the molecular structure of the organic framework and its MOFs [6]. Molecular modeling representation and their relative parameters were utilized to provide a better understanding of the correct sequences of the atomic arrangements in the molecules.

The present work details the fundamental coordination chemistry of the metal ions with streptomycin and oxime [7-9]. Particularly emphasis will be placed on the spectroscopic properties structures and molecular modeling. Not only the knowledge of the thermodynamic stability of such complexes but also the mechanisms, decomposition path ways, ligand-exchange dynamic of substitution and redox reactions further provide a better understanding of how MOFs can be utilized in medical applications[10]. The organic frame work to be used in this study is shown in figures.

MATERIAL AND METHODS

All the chemicals used in this study were of analytical grade which obtained from Merck. Streptomycin tetracycline and chloramphenicol were purchased from CDH (India). Solvents used were of analytical grade and were purified by standard procedures [11]. The stoichiometric analyses(C, H and N) of the complexes were performed using Elementar vario EL III (Germany) model. Metal contents were estimated on an AA-640-13 Shimadzu flame atomic absorption spectrophotometer in solution prepared by decomposing the respective complex in hot concentrated HNO_3. Their IR spectra were recorded on Perkins–Elmer FTIR spectrophotometer in KBr and polyethylene pellets. The electronic spectra were recorded in water on Beckman DU-64 spectrophotometer with quartz cells of 1 cm path length. ^1H NMR spectra were recorded in $CDCl_3$ solvent on a Bruker Advance 400 instrument The XRD powder pattern were recorded on a vertical type Philips 1130/00 X-

ray diffractometer, operated at 40kVand 50Ma generator using the Cukα line at 1.54056 A° as the radiation sources. Sample was scanned between 5° to 70°(2θ) at 25°C. The crystallographic data was analyzed by using the CRYSFIRE –2000 powder indexing software package and the space group was found by the CHECK CELL program. Debye – Scherer relation with the help of 100% peak width determined the particle size. The experimental density was determined by Archimedes method.

Synthesis of legands

Synthesis of novel ligand 12-((1R)-2,2-dichloro-1-(1,3-dihydroxy-1-(4-nitrophenyl)propan-2-ylamino)-1-hydroxyethoxy)-3,6,10,12a-tetrahydroxy-4-isopropyl 6 methyl-1,11-dioxo-1,2,5a,6,11,11a,12,12a-ctahydrotetracene-2-carboxamide.The mixed ligands were prepared by mixing of cholramphenicol(0.5mmol) and tetracycline(0.5 mmol) in a aqueous solution of methanol and again mix chloramphenicol(0.5 mmol) and streptomycin(0.5 mmol) in a aqueous solution methanol in separate round bottom flask. The reaction mixture was refluxed with stirring for 5 h under reduced pressure followed by cooling to room temperature. The product obtained was washed with a small amount of methanol and air dried .The above product was redissolved in excess warm methanol and clear solution was left undisturbed for weeks to give beautifull crystals of the ligands separately. The other ligand 1,-(4-((R)-2,2-dichloro-1 ((1R,2S)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-ylamino)-1-hydroxyethoxy)-6-(3-(3,4oxy-6-5-tetrahydro-2H-pyran-2-yloxy)-5-formyl-5-hydroxy-4-methyltetrahydrofuran-2-yloxy)-2,5-dihydroxycyclohexane-1,3- was synthesized by mixing of 0.05(mmol) of chlramphenicol and streptomycin 0.05(mmol) in a round bottom flask adopting a similar method. The legands characterized by different physical techniques. Pertinent analytical and physico-chemical data for these ligands and their complexes are table in 1

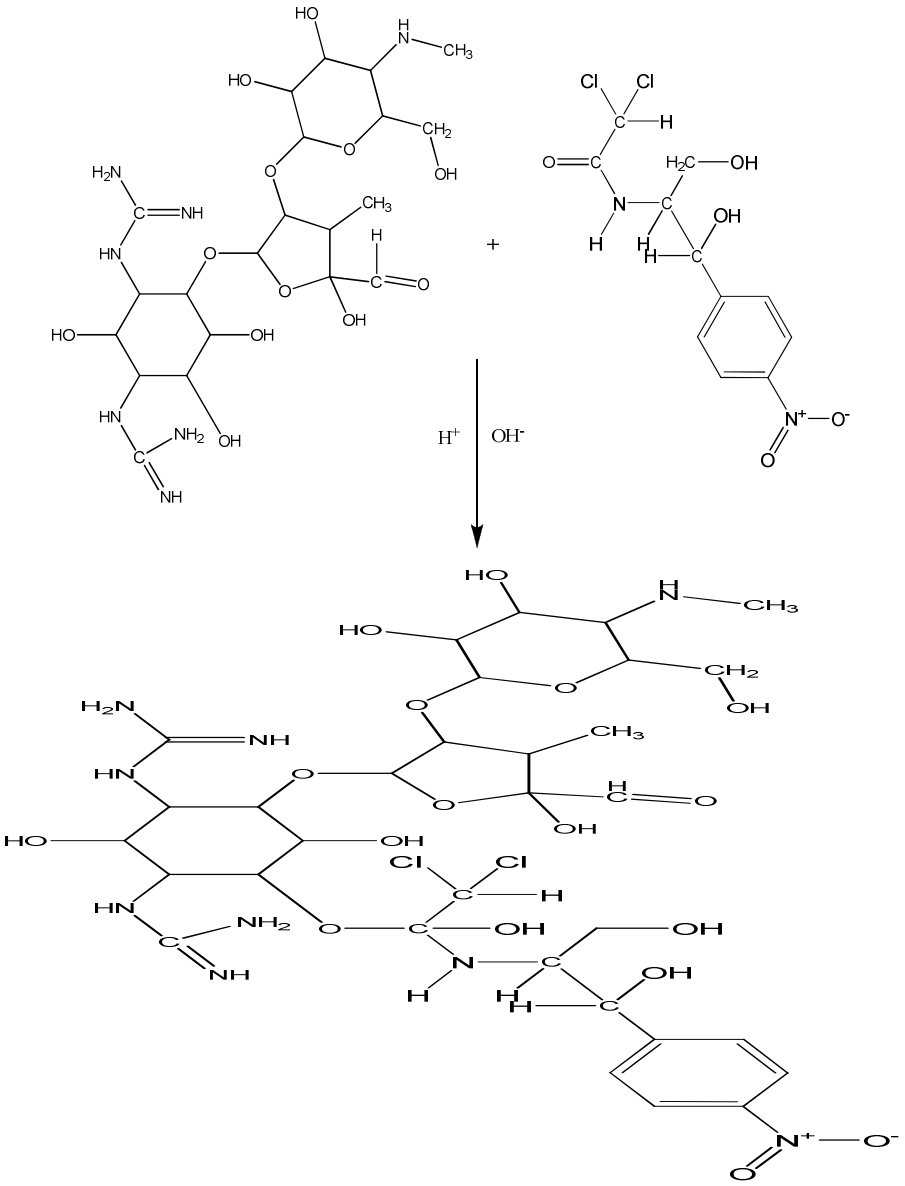

Fig. 1: 1,-(4-((R)-2,2-dichloro-1-((1R,2*S*)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-ylamino)-1-hydroxyethoxy)-6-(3-(3,4-dihydroxy-6-(hydroxymethyl)-5-(methylamino)tetrahydro-2Hpyran-2-yloxy)-5-formyl-5-hydroxy-4-methyltetrahydrofuran-2-yloxy)-2,5 dihydroxycyclohexane-1,3-diyl) diguanidine(Novel Ligand)

Synthesis of complexes

A hot solution of metal chloride (1mmol, 20ml) in 80% methanol (20ml) was added to another solution of ligand and was mixed in 100ml round bottom flask. The mixture was refluxed for several hours at a temperature of 75°C .The mixture was cooled at room

temperature and the precipitate was filtered and washed with 50% methanol and dried at room temperature too[13]

RESULTS AND DISCUSSION

Satisfactory results of elemental analysis (Table 1) and spectral studies revealed that the complexes were of good purity. Various attempts to obtain the single crystals have so far been unsuccessful. X-ray diffraction studies indicate crystalline nature of the metal complexes. The complexes were soluble in polar solvents [14].

Table 1: Color, reaction yield and elemental analysis of complexes

Complex	Empirical formula	Color	Yield (%)	Analysis: found (calculated)(%) C	H	N	M	M.P.^{0}C
Ligand	$C_{34}H_{37}Cl_2N_3O_{13}$	Pale	80	53.27 (53.32	4.86 (4.87)	9.25 (4.62)	- -	35
Complex 1	$C_{34}H_{35}CoCl_5N_3O_{25}$	white	70	39.64	5. 51	7.31	6.08	65
Complex 2	$C_{34}H_{35}NiCl_5N_3O_{25}$	white	80	39.65 (39.61)	5.51 (5.54)	7.31 (7.32)	10.11 (10.12)	6.05 (6.04) 67
Complex 3	$C_{34}H_{35}ZnCl_5N_3O_{25}$	white	75	39.37 (39.76)	5.47 (5.43)	10.04 (10.41)	6.70 (6.71)	71.23
Complex 4	$C_{34}H_{35}CdCl_5N_3O_{25}$	white	65	37.57 (37.52)	5.22 (5.21)	10.99 (10.91)	9.58 9.52	75.43
Complex 5	$C_{34}H_{35}CuCl_5N_3O_{25}$	bluish	60	39.45 (39.41)	5.48 (5.43)	10.06 (10.61)	6.52; (6.51)	75.34

VIBRATIONAL SPECTRA

Novel ligand exhibits absorptions 1056, 1765, 29488cm^{-1}. These bands are very metal complexes indicating non – involvement of the oxygen atoms of hydroxyl group in coordination with the metal ions [15]. The stretching frequencies of streptomycin hydroxyl and give bands at 3368 and 3434 cm^{-1} with a shoulder at about 3560 cm^{-1}. These bands appear in the complexes as strong band absorption in the region 3425- 3448 cm^{-1}. These bands appear for the new complex at the same wave number, ruling out the participation of hydroxyl oxygen in the coordination. These results confirm that complexation occurred and suggest that the oxygen of the hydroxyl group is involved in the coordination sphere. The vibrational bands due to rocking & wagging modes of water and metal – oxygen stretching modes are observed in the 800 – 350 cm^{-1} region for all the complexes may be attributed to coordinated of hydroxyl . This can be confirmed with the help of thermo grams. A new band in the 615 – 300 cm^{-1} regions in the spectra of the complexes is assignable to ν (M - O).

Table 2: IR spectral data (cm^{-1}) of the metal complexes

Frequency	ν_{N-H}	OH	OH	NH_2	NH_2	M - O
$C_{34}H_{37}C_{l2}N_3O_{13}$	3328(s,b)	1640(m)	1515(s)	1224m)	689(s)	
$C_{34}H_{35}CoCl_5N_3O_{25}$	3339(s,b)	1645(m)	1523 (s)	1344(s)	695(m)	419(s),1340
$C_{34}H_{35}NiCl_5N_3O_{25}$	3327(s,b)	1685(s)	1529(m)	1317(w)	613(m)	472(m)
$C_{34}H_{35}ZnCl_5N_3O_{25}$	3395(s,b)	1624(m)	1475(s)	1216(w)	627(s)	419(s)
$C_{34}H_{35}CdCl_5N_3O_2$	3371	1637	1532	1318	637	464
$C_{34}H_{35}CuCl_5N_3O_2$	3385	1625	1543	1385	635	450

^{1}H N M R

The ^{1}HNMR spectra of the complexes of Co(II),Ni(II)Zn(II)Cd(II) and Cu(II)in a DMSO-d_6 solvent of the ligand and complexes show well-resolved signals.^{1}HNMR spectrum of complex (I). The N-H protons of amine, which would have undergone very rapid exchange with the solvent, appear as quite broad ragged doublet around 4.58(ppm) and 3.65 (ppm) coordinated with metals(II) which disappeared in the metal complex spectra. In complex 3,

peaks range 1.21-1.71 ppms are from coordinated water. The various assignments of ^{1}HNMR of the complexes are summarized in table3.Chemical shift are in ppm from TMS & multiplicity in parentheses (bd, broad; d, doublet; m, multiplet).

Table 3: ^{1} H N M R data of free novel ligands and their complexes

Compounds	δ (ppm)
$C_{30}H_{46}N_8O_{13}$	[3.35(s)1H,OH],16.77(s)1H,OH,16.77(s),1H,OH,3.65(m),5H,OH,2.0(s)1H,NH,7.16(s)!H,N $H_2$3.83(m)1H,CH,8.19(d)1H,CH(Ar),9..00(s)1H,CH(Ar),8.62(m) 1H,CH(Ar),7.78(s)1H,CH(Ar),2.52---3.98(m)4H,(m)CH,3.98—4.73(d),2H,CH,1.35(s) 3H,$CH_3$1.06(s)6H,CH_3].
Complex1	8.17(bd)1H 3.26(m)2H, 1.95(bd),2.05,1.94(d)6.54(d).104,4.45(m),3.76(m0,6.12(d),
Complex2	8.12(bd)8.17(bd)1H3.26(m)2H, 1.95(bd),2.05,1.94(d)6.54(d).104,4.555(m),3.76(m0,6.13(d),
complex 3	8.16(bd)1H3.16(m)2H,.8.5(bd),2.05,1.71(d)6.54(d).1.14(m),4.45(m),3.16(m)6.12(d),
complex 4	8.28(bd)1H3.25(m)2H,.8.7(bd),2.05,1.75(d)6.54(d).1.01(m),4.15(m),3.66(m0,6.22(d),
complex 5	8.17(bd)1H3.16(m)2H,.25(bd),2.05,1.64(d)6.55(d).1.14(m),4.55(m),3.77(m0,6.22(d),

Kinetics of thermal decomposition

Recently, there has been increasing interest in determining the rate- dependent parameters of solid-state non- isothermal decomposition reactions by analysis of TG curves. Thermogravimetric (TG) and differential thermo gravimetric (DTA) analyses were carried out for different metal–streptomycin complexes in ambient conditions. The thermogravimetric analysis revealed that the complexes of Zn & Cd loses mass between 65°C and 140°C, corresponding to nearly 15 % of the total mass, followed by considerable decomposition up to 600°C, which corresponds to the decomposition of the ligand molecule leaving metal oxide (NiO & CuO, respectively) as residue. The complexes of Zn & Cd decomposes nearly 9% of the total mass up to temperature 170°C, followed by considerable decomposition of the ligand molecule up to 650°C, leaving metal oxide (CoO and ZnO respectively) as residue. On the basis of thermal decomposition, the kinetic analysis parameters such as activation energy (E*), enthalpy of activation (ΔH*), entropy of activation (ΔS*), free energy change of decomposition (ΔG*) were evaluated graphically by employing the Coats – Redfern relation.

$\text{Log } [-\text{Log } (1- \alpha) /T^2] = \log [AR/ \theta E^*(1-2RT/E^*)]-E^*/2.303RT$

Where α is the mass loss up to the temperature T, R is the gas constant, E*is the activation energy in J mole^{-1}, θ is the linear heating rate and the term (1-2RT/E*) ≅ 1.A straight line plot of left hand side of the equation (1) against 1/T gives the value of E* while its intercept corresponds to A (Arrhenius constant). The Coats and Redfern linearization plots, confirms the first order kinetics for the decomposition process . The calculated values of thermodynamic activation parameters for the decomposition steps of the metal complexes are reported in Table 4. According to the kinetic data obtained from the TG curves, the activation energy relates the thermal stability of the metal complexes. Among metal complexes, activation energy increases as complex 3 ~ complex 2 < complex 4 < complex 1, same trends happens with thermal stability of metal complexes. All the complexes have negative entropy, which indicates that the complexes are formed spontaneously. The negative value of entropy also indicates a more ordered activated state that may be possible through the chemisorptions of oxygen and other decomposition products. The negative values of the entropies of activation are compensated by the values of the enthalpies of activation, leading to almost the same values for the free energy of activation.

Table 4: Thermodynamic activation parameters of the metal complexes

Complex	Order/n	Steps	E*/Jmol^{-1}	A/sec^{-1}	ΔS*/JK^{-1}mol^{-1}	ΔH*/Jmol^{-1}	ΔG*/ kJmol^{-1}	k×10^{2}s^{-1}
$C_{34}H_{35}CoCl_5N_3O_{25}$	1	I	56.66	1.125×10^{5}	-91.49	112.745	61.228	1.62
		II	68.804	1.256×10^{5}	-109.175	96.114	89.18	1.01
$C_{34}H_{35}NiCl_5N_3O_{25}$	1	I	58.066	6.27×10^{5}	-80.136	74.10	55.29	3.25
		II	7.178	1.16×10^{5}	-109.603	125.89	93.104	1.718
$C_{34}H_{35}ZnCl_5N_3O_{25}$	1	I	56.35	1.4501×10^{5}	-66.345	118.76	44.135	1.41
		II	61.08	1.171×10^{4}	-74.96	54.691	74.96	1.142
$C_{34}H_{35}CdCl_5N_3O_{25}$	1	I	54.59	2.28×10^{6}	-56.01	70.98	36.566	1.01
		II	67.88	1.53×10^{6}	-80.731	28.16	80.547	0.611
$C_{34}H_{35}CuCl_5N_3O_{25}$	1	I	55.67	2.38×10^{6}	-55.32	69.91	37.87	1.o32
		II	69.54	1.54×10^{6}	-79.732	36.32	81.23	0.321

TOF–MS SPECTRA

Mass spectrometry has been successfully used to investigate molecular species $[MH]^+$ in solution . The molecular ion peaks of the ligands and complexes have been used to confirm the proposed formula .The pattern of the mass spectrum gives an impression of the successive degradation of the target compound with the series of peaks corresponding to the various fragments. Their intensity gives an idea of stability of fragments. The ligand starts degradation and finally forms [C7H15NO5]=193, (100 % m/z values. In the TOF–mass spectra of metal complexes initial fragmentation pattern is again similar (loss of two water molecules), a mononuclear nature for these complexes $[M(L)]^+$ can be deduced. The last two fragments appears in nearly all the complexes at positions (m/z values) 163(100% complex 1, 100 % complex 2, 100 % complex 3 and 57 % complex (4) and 263/264/267 (10 % complex I, 50% complex 2 and 100 % complex 4) corresponds to $[C_8H_{18}N_6O_4]^+$ and $[C_{21}H_{41}N_7O_{12}]^+$ respectively, which could be the result of degradation & demetallation of the complexes (Figure 5a-b. Scanned TOF-MS spectrum of complexes 3 and 4 with specific fragments). m/z: 968.21 (100.0%), 970.21 (68.8%), 969.21 (37.9%), 971.21 (23.2%), 972.20 (10.2%), 972.21 (6.8%), 970.22 (6.3%), 973.21 (3.8%), 971.22 (2.1%), 971.20 (1.7%), 973.22 (1.4%), 974.21 (1.2%),for comple1, m/z: 975.20 (100.0%), 973.21 (82.4%), 977.20 (71.5%), 976.21 (37.3%), 979.20 (30.0%), 974.21 (29.6%), 978.20 (20.1%), 978.21 (14.6%), 977.21 (12.8%), 980.20 (10.4%), 976.20 (9.5%), 975.21 (9.0%), 979.21 (6.2%), 981.20 (5.7%), 980.21 (2.5%), 974.20 (2.1%), 981.21 (1.8%), 982.20 (1.5%)for complex2, m/z: 975.20 (100.0%), 973.21 (82.4%), 977.20 (71.5%), 976.21 (37.3%), 979.20 (30.0%), 974.21 (29.6%), 978.20 (20.1%), 978.21 (14.6%), 977.21 (12.8%), 980.20 (10.4%), 976.20 (9.5%), 975.21 (9.0%), 979.21 (6.2%), 981.20 (5.7%), 980.21 (2.5%), 974.20 (2.1%), 981.21 (1.8%), 982.20 (1.5%)for complex3 m/z: 972.21 (100.0%), 974.20 (64.0%), 974.21 (55.5%), 975.21 (40.6%), 976.20 (39.3%), 973.21 (35.9%), 977.21 (12.6%), 976.21 (11.5%), 978.20 (4.9%), 977.20 (4.5%), 978.21 (4.2%), 975.20 (2.8%), 973.20 (2.6%), 979.20 (1.8%) for complex 5.

X-ray powder diffraction studies

In absence of single crystal, x-ray powder data is especially useful to deduce accurate cell parameters. The diffraction pattern reveals the crystalline nature of the complex. The

indexing procedure were performed using (CCP4,UK) Crysfire programme giving different crystal system with varying space group. The merit of fitness and particle size of the metal(II) complexes has been calculated. The crystallographic data of the complexes are shown in table 5.

Molecular structures & analysis of bonding modes

In order to ascertain the structural preferences and coordination behavior of streptomycin to metal ions, molecular mechanics calculations on the $[ML]^{n+}$ species were undertaken. The optimized molecular structure of complex 1,2,3 ,4 and 5 are given in figures (2-7).

Energy minimization was repeated several times to find the global minimum. The energy minimization values for the optimized structure for the complex 1,2,3 ,4 and complex 5 are 35.12 , 25.31,38.24 and 41.34 kcal/mol respectively. The selected bond length and bond angles of all the complexes are represented in Table5. The optimized structure of complex 1 is octahedral, complex 2 is square planar, complex 3 & 4 are trigonal planar and complex 5 is tetrahedral geometrical structure respectively.

Table 5: Crystallographic data of complexes

Compound	**Complex1**	**Complex2**	**Complex3**	**Complex4**	**Complex5**
Formula	$C_{34}H_{35}CoCl_5N_3O_{25}$	$C_{34}H_{35}NiCl_5N_3O_{25}$	$C_{34}H_{35}ZnCl_5N_3O_{25}$	$C_{34}H_{35}CdCl_5N_3O_{25}$	$C_{34}H_{35}CuCl_5N_3O_{25}$
FW	969.64	970.40	973.28	1023 .243	966.23
Temp (K)	293	293	293	293	293
Wavelength	1.54056	1.54056	1.54056	1.54056	1.54056
Crystal System	Monoclinic	Orthorhombic	Monoclinic	Tetragonal	Triclinic
Space group	P2/m	Pmmm	P2/m	Pmm	P1

Unit cell dimension					
a(Å)	20.083	23.242	18.1357	12.717	3.380
b(Å)	5.4594	9.6204	8.842287	12.717	9.252
c(Å)	10.2398	8.0821	8.708652	16.652	22.039
α^o	90.00	90	90.00	90.00	51.31
β^o	122.322	90	96.346856390	90.00	87.39
γ^o	90.00	90	90.00	90.00	96.07
Volume (A^3)	3429.47	1805.60	1387.97	2693.37	529.3
θ range (0)	21.696-75.106	13.811-61.987	10-65	12-67	12-67
Limiting indices	$0 \le h \le 4$ $0 \le k \le 6$ $0 \le l \le 3$	$-6 \le h \le 4$ $0 \le k \le 7$ $0 \le l \le 4$	$-3 \le h \le 1$ $-4 \le k \le 4$ $0 \le l \le 4$	$-7 \le h \le 5$ $0 \le k \le 8$ $0 \le l \le 5$	$-7 \le h \le 5$ $0 \le k \le 8$ $0 \le l \le 5$
Particle size(nm)	11.922	80.82	55.99	10.92	11.92
Intensity (%)	7.2–100	5.9–100	4.5-100	3.4-100	3.4-100
R indices	0.0000156	0.0000615	0.0000754	0.0000362	0.0000362
Density	1.07405	1.7437	1.034	1.151	1.151
Z	2	2	1	1	1

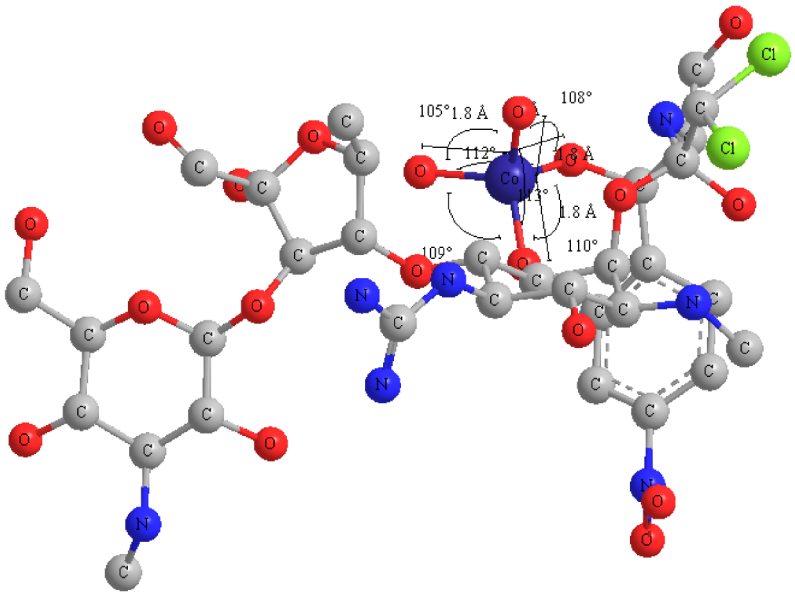

Fig. 2: Molecular structure of complex1

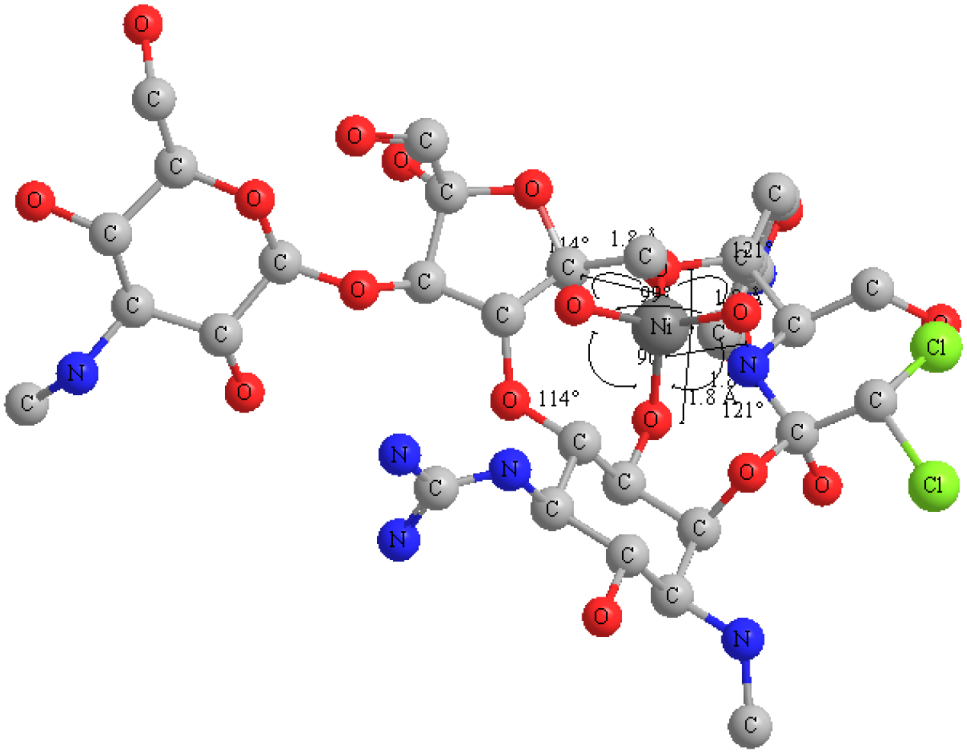

Fig. 3: Molecular structure of complex2

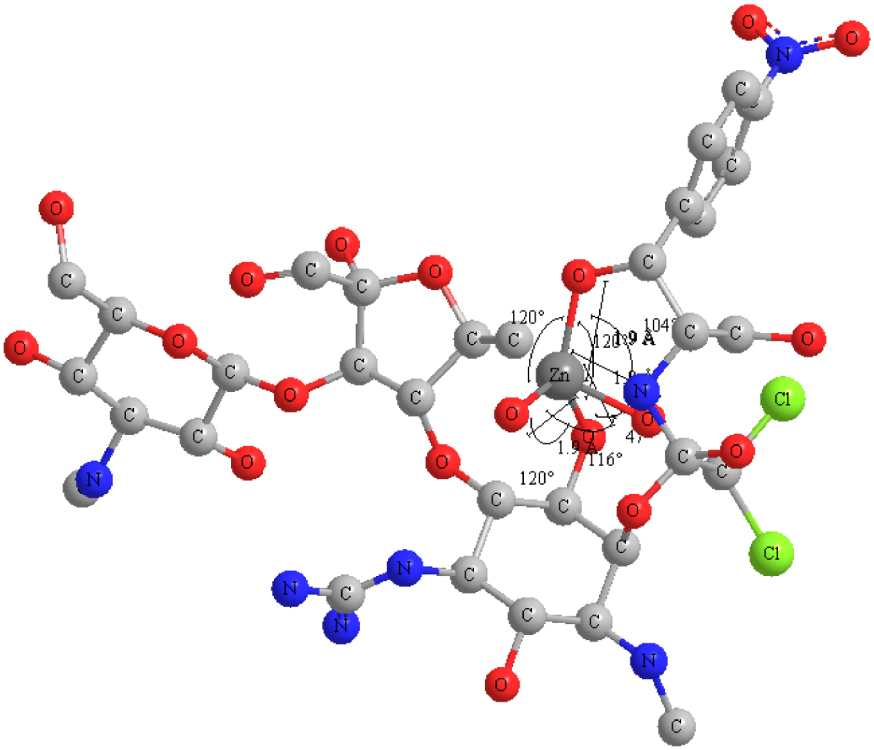

Fig. 4: Molecular structure of complex3

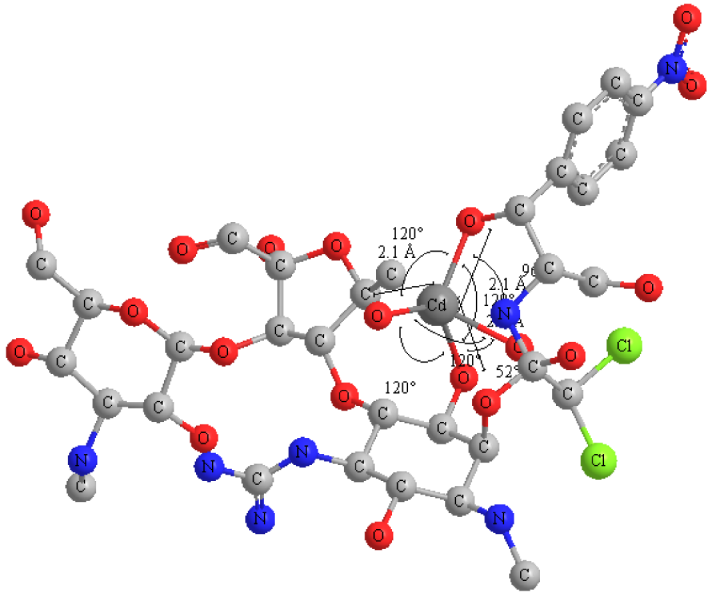

Fig. 5: Molecular structure of complex4

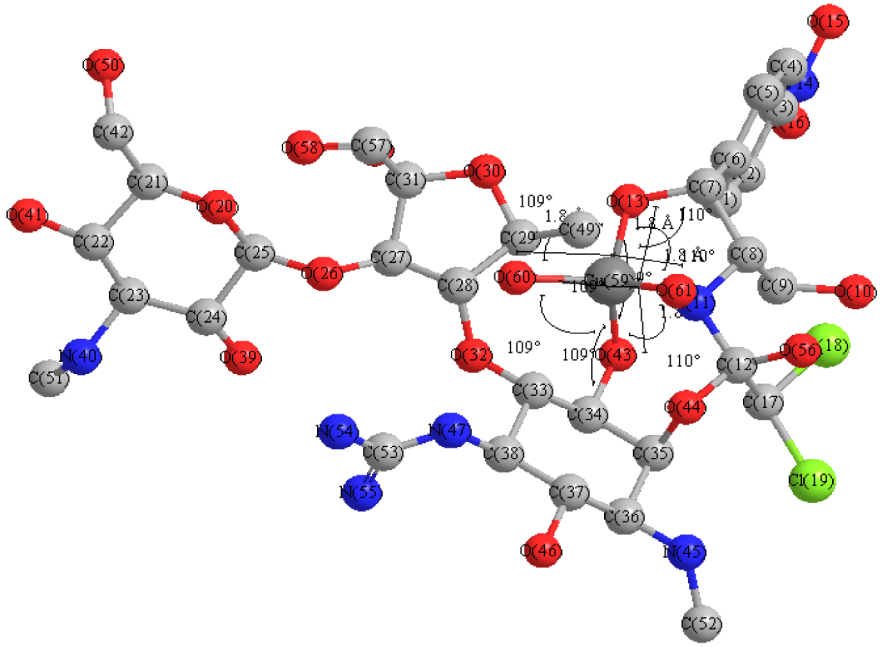

Fig. 6: Molecular structure of complex5

Table 6: Selected bond lengths and bond angles

Complex 1		**Complex 2**	**Complex3**	**Complex4**	**Complex5**
Bond lengths		Bond lengths	Bond lengths	Bond	Bond lengths
Co(59)-O(61)	1.8253	Ni(59)-O(61)	Zn(59)-O(61)	lengths	Cu(59)-
		1.790	1.8900	Cd(59)-	O(61)1.8100
Co(59)-O(60)	1.8174		Zn(59)-O(60)	O(61)	
		Ni(59)-O(60)	1.8900	2.1200	Cu(59)-
O(43)-Co(59)	1.7831	1.790	O(43)-Zn(59)	Cd(59)-	O(60)1.8100
			1.8900	O(60)	
O(13)-Co(59)	1.7851	O(43)-Ni(59)	O(13)-Zn(59)	2.1200	O(43)-
		1.790	1.8882	O(43)-	Cu(59)1.8100
Bond angles		O(13)-Ni(59)		Cd(59)	
O(61)Co(59)O(60)	104.9730	1.789	Bond angles	2.1200	O(13)-
			O(61)-Zn(59)-	O(13)-	Cu(59)1.8076
O(61)Co(59)O(43)	108.7214		O(60)115.8469	Cd(59)	
		Bond angles	O(61)-Zn(59)-	2.1	Bond angles
O(61)-Co(59)-		O(61)Ni(59)-	O(43)46.6956	19	O(61)-

O(13)112.3004
O(60)-Co(59)-
O(43)112.9117
O(60)-Co(59)-
O(13)107.9144
O(43)-Co(59)-
O(13)109.9817

O(60) 98.968
O(61)Ni(59)-
O(43)
120.5358

O(61)-Ni(59)-
O(13)
120.5
358
O(60)-Ni(59)-
O(43)
114.1
196
O(60)-Ni(59)-
O(13)
114.1
196
O(43)-Ni(59)-
O(13)
89.76
32

O(61)-Zn(59)-
O(13)
104.4420
O(60)-Zn(59)-
O(43)120.0384

O(60)-Zn(59)-
O(13)120.0384

O(43)-Zn(59)-
O(13)119.9231

Bond
angles
O(61)-
Zn(59)-
O(60)
115.8469

O(61)-
Zn(59)-
O(43)
46.6956

O(61)-
Zn(59)-
O(13)
04.4420

O(60)-
Zn(59)-
O(43)
20.0384

O(60)-
Zn(59)-
O(13)
20.0384

O(43)-
Zn(59)-
O(13)
19.9231

Cu(59)-O(60)
109.4
094
O(61)-
Cu(59)-O(43)
109.5
587
O(61)-
Cu(59)-O(13)
109.5
587
O(60)-
Cu(59)-O(43)
109.4
833
O(60)-
Cu(59)-O(13)
109.4
833
O(43)-
Cu(59)-O(13)
109.3
338
Cu(59)-
O(13)-C(7)
109.8
365

Antibacterial activities

The antibacterial sensitivity assay shows that there is reduction of inhibitory potentials of antibiotic Novel ligand by the formation of complex with metal. The bacterial strain sensitive to ligand easily grow in the presence of 200 µg/mL of complex1,2,3,4 and 5 N where as the complex 3 was not effective up to 100 µg/mL and less effective on the concentration of 150 µg/mL and more. It can be seen in the table and that only 25 µg/mL of ligand showed inhibitory effect on Agrobacterium sp BN-2A but the same strain is resistant to all concentrations of Co- Land Ni-L. The Bacterial Inhibition Index (BII) of novel ligand (L) was highest (4.2 ± 0.245) at the concentration of 200 µg/mL and minimum inhibitory concentration (MIC) was 25 µg/mL where BII was 0.8 ± 0.047.

Table7: Antibacterial sensitivity assay of novel ligand and its metal complexes with Agrobacterium sp BN-2A

Concentration (µg/mL)	BII of antibacterial Streptomycin-metal complexes[#]				
	Ligand	**Complex1**	**Complex2**	**Complex3**	**Complex4**
Control (-)	0 ± 0 (0)	0 ±0.024	0 ± 0 (0)	0 ± 0.01 (0)	0±0.321(0)
25	0.8±0.047 (0.2)	0 ± 0.4	0 ± 0.247	0 ± 0.02 (0)	0±0.245(0)
50	1.2±0.082 (0.002)	2 ± 0.17	0 ± 0.321	0±0.0214(0)	0±0.324(0)
100	1.6±0.163 (0.003)	1.5 ± 0.321	0±0.23145 (0.021)	0±0.0214(0)	0±0.245 (0)
150	2.2±0.245 (0.004)	2.32±0.654	0.6±0.082 (0.332)	0±0.214 (0)	0±00.214(0)
200	4.2±0.245 (0.001)	3.2 ± 1.254	1.0±0.082 (0.169)	0±0 .214(0)	0±0.3547(0)

Values shown is the average ± standard deviation of three readings performed three times

[#]value in the parenthesis indicates p-value of the data based on t-test (p≤ 0.005)

A number of studies have indicated the antimicrobial activities of many heavy metals due to their effects on iron uptake by bacteria Iron is a co-factor for many essential enzymes . Potant antimicrobial activity of complexes would result out of a combination of higher transport of the complex (1) through the cell membrane and iron limitation into the cells of the bacteria and less effective of complex 5.

CONCLUSION

Transport of organic ligands into bacterial cells can be facilitated by the formation of metal complexes. Hence, metal complexes of streptomycin were synthesized. They were characterized by UV, IR, TGA/DTA, XRPD and structure was optimized Chem Office Ultra-11 programme and elemental analysis. The complex was found to possess metal to ligand ratio of 1:4. It has been observed that complexation between metal ions and streptomycin takes place above pH 7. The Solubility of the complexes was found to be more than that of streptomycin. Agar diffusion method was used for antibacterial activity. The complexes were found to possess better activity (lesser MIC value) than that of streptomycin as well as metal chloride and streptomycin physical admixture. It was concluded that metal complexes can be a better alternative to streptomycin as an antibacterial agent as well as ailment of antituberclusis.

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