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Physico-chemical studies and antimicrobial evaluation of novel 1,2,3- triazole derivative and its complexes

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Abstract: *This study involves synthesis and characterization of some biologically important metal complexes of Cu(II), Ni(II), and Co(II) with novel ligand derived from 1,2,3- triazole. The synthesized ligand and complexes were examined for antibacterial activity. The antimicrobial analysis was carried out using disc diffusion method. The effected zone values of the compounds against the growth of microorganisms are observed for ligand and metal complexes. The results indicate that the metal complexes are more active than parent ligand.*

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I. Introduction

The chemistry of 1,2,3-triazole derivatives has received much attention due of their wide range of applications. They have been used as fungicides, anti bacterial agents, herbicides, light stabilizers, fluorescent whiteners, optical brightening agents, corrosion inhibitors and photo stabilizers for fibers, plastics or dyes[1,2]. Some 1,2,3-triazole derivatives have seldom been found in nature as constituents of natural products. For a number of these compounds there have been found diverse uses in medicinal and pharmaceutical chemistry as cytostatic, virostatic, ant proliferative agents, synthetic intermediates for antibiotics, antihistaminic agents and polyheterocyclic compounds with neuroleptic activity[3-9]. There are few numbers of complexes with benzotriazole[10,11] and 1,2,3- triazole derivatives[12].

Moreover, novel ligands derived from various heterocycles have been reported to possess cytotoxic[13], anticonvulsant[14], antiproliferative[15], antimicrobial[16], anticancer[17], and antifungal activities[18]. Antimicrobial resistance is fast becoming a global concern with rapid increase in multidrug resistant bacteria. To overcome the alarming problem of microbial resistance to antibiotics, the discovery novel active compounds against new targets is a matter of urgency. Many of the crude drugs, which are sources of medicinal preparations, still originate from wild growing material. This revival interest was generated by discovery of the antibacterial and antifungal activity of several metal complexes (saha *et al.,* 2009)[19].

II. Experimental Techniques

2.1 Materials and Methods

All the chemicals used were of AR grade supplied by MERK. All the solvents were purified by distillation as per procedure. Cu(II) acetate, $Co(II)Cl_2.2H_2O$ and $Ni(II)Cl_2$ were used as respective metal sources.

2.2 synthesis of the ligand 4-Chlorobenzyl phenyl triazole [4-CBPT]

The ligand were synthesized by coupling reaction between 4- chloro benzylchloride (20 mmol), phenylacetylene(10 mmol) and sodium azide (10 mmol) in t-butanol water mixture in the presence of catalytic amount of sodium ascorbic acid and copper acetate. The mixture was refluxed for 12 hrs, cooled and extracted with DCM and finally purified by coloum chromatography. (yield: 87%)

2.3 preparation of M- 4-CBPT complexes

The ligand 4-Chlorobenzyl phenyl triazole [4-CBPT](20mmol) and respective metal salts ie Cu(II), Co(II) and Ni(II) were dissolved in ethanol in a clean 100ml RB flask and refluxed for 4 hrs. The mixture was cooled, added water and filtered. The residue was washed with water and finally with hexane then dried.

III. Result and Discussion

3.1 IR spectrum

Characteristic frequencies of ligand and its complexes were shown in table-1. The ligand shows a C-H bending at 758cm^{-1}, a characteristic stretching peak at 810 cm^{-1}due to C-Cl bond, ν N=N at 1649, ν CH str at 2922 and a peak at 3076 due to aromatic CH str.the complexes show a small variations in these peaks which

evident the complex formation. In Co-4-CBPT there is a broad peak at 3381 which is due to the presence of water of hydration.

3.2 UV-VIS spectrum

Electronic spectra of the ligand and complexes reveal some idea about the structure. The characteristic absorption frequencies are tabulated in Table-2. The characteristic bands due to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions exhibited by the ligand in its electronic spectrum at 29351cm^{-1} and 28612cm^{-1} respectively. During complexation a red shift is detected for these absorption bands which indicate the involvement of triazole in coordination.

Cobalt complex of the ligand 4-CBPT, give its on characteristic peaks at 29044, 40816 and 44964cm^{-1} due to $^4T_1g(F) \rightarrow {}^4T_2g(F)$, $^4T_1g(F) \rightarrow {}^4A_2g(F)$ and $^4T_1g(F) \rightarrow {}^4T_1g(P)$ transitions[20]. Octahedral geometry for Co(II) complex can be ascertained based on these data.

The absorption bands at 49751cm^{-1} given by Cu(II) complex in its electronic spectrum can be assigned to charge transfer transition. Also Ni(II)complex shows peaks at 41203cm^{-1} and 49727cm^{-1} as expected.

3.3 mass spectral studies

In mass spectrum of ligand 4-CBPT the molecular ion peak is observed at 269.04 which confirm the structure.

3.4 nmr analysis

^{1}HNMR spectrum of ligand gives peaks corresponding to 12 H atoms which correlate the molecular formulae. Peak at 5.54δ s(2H) is due to CH_2 group, the peak at 7.66δ s(1H) is due to triazole H. and all the other peaks are due to the presence of 9 aromatic H atoms. ^{13}CNMR studies shows 11 signals as we expected, since the ligand contains 15 carbon atoms about which 11 are un identical carbons.

3.5 Magnetic moment measurements

The values of the magnetic moment of the complexes are represented in Table-1. The Co(II) complex exhibited a magnetic moment value of 4.78 BM. It is reported that an octahedral high spin geometry can be assigned to Co(II) complex, if the measured μ_{eff} value is in the range 4.5-5.1 B.M.

The Cu(II) complex exhibited slightly higher magnetic moment value of 2.22BM than expected for one unpaired electron of the d^9 electronic configuration (1.8 BM) . This accounts for a slight orbital contribution to the spin only value and absence of spin- spin interactions in the complex. Therefore a monomeric square planar geometry is assigned to Cu(II) complex. Complex of Ni(II) is diamagnetic as expected due to the formation of low spin complex.

3.6 Molar conductance measurements

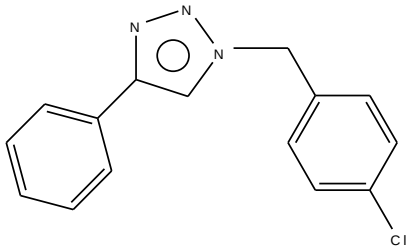
The molar conductance data of Co(II), Cu(II) and Ni(II) complexes in DMSO at a concentration of 10^{-4} mol^{-1} at 28± 2^{o}c are presented in Table-3. All these complexes exhibited very low value of molar conductance, below 13 ohm^{-1} cm ^{2}mol^{-1} indicating their non-electrolytic behaviour in DMSO.

3.7 Metal percentage data

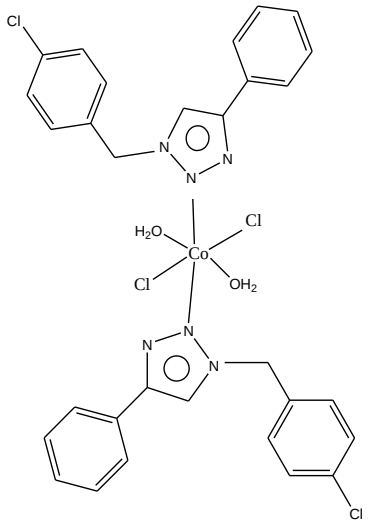
The empirical formulae, physical appearance, melting point and metal percentage data of the complexes of Co(II), Cu(II) and Ni(II) are presented in Table-3. The analytical data of the complexes shows that there is 1:2 stoichiometry exists between metal ion and ligand in all complexes

3.8 structure of ligand and complexes

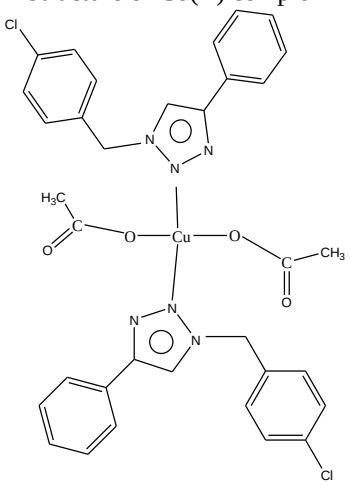
Based upon the above physico-chemical studies, octahedral geometry is suggested for Co(II) complexe and a square planar geometry for both Cu(II) and Ni(II) complexes. The structures of the complexes are as follows.



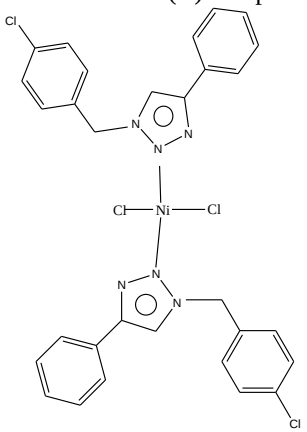
structure of ligand



Structure of Co(II) complex



Structure of Cu(II) complex



Structure of Ni(II) complex

3.9 Antimicrobial activity

The ligand and its complexes were checked against the bacterial species: *Proteus*, *Escherichia coli*, *Staphylococcus and Pseudomonas.*The studies were carried out by KB Disc method. *Gentamicin was* used as the standard for anti bacterial activities. The test organisms were grown on Nutrient Agar medium in petri dishes for bacterial species. The compound was dissolved in Rectified Spirit and soaked in filter paper disc of 5mm diameter and 1mm thickness. The discs were placed on the previously seeded plates and incubated at 37^0C and the diameter of effected zone around each disc was measured after 24 hrs for bacterial and 48 hrs for fungal species. The in vitro antibacterial investigation results are given in table- 4 . It has been observed that most of the compounds shows significant antibacterial activity. The free ligand has very low antibacterial activity about

which it shows higher activity against staphylococcus bacteria. Among all compounds Co(II) complex exhibited much more antibacterial activity towards bacteria Proteus with zone inhibition value of 18 mm. The results are tabulated.

IV. Tables and Figures

4-CBPT	Ni-4-CBPT	Co-4-CBPT	Cu-4-CBPT	Assignments
758	754	758	759	C-H bending
810	823	810	812	C-Cl str
1209	1392	1207	1207	C-N str
1649	1629	1633	1529	N=N
2922	2791	3103	2881	CH str
3076	3211	3381 (due to water of hydration)	3070	Aromatic CH str

Table-1 Characteristic IR frequencies of ligand and its complexes

Substance	$\bar{\upsilon}$ in cm^{-1}
4-CBPT	29351, 28612
Ni-4-CBPT	41203and 49727
Co-4-CBPT	29044, 40816 and 44964
Cu-4-CBPT	40850,44883 and 49751

TABLE – 2 Electronic spectral data of the ligand and its complexes

Complex	Molecular weight	M.P. ^0C	Metal percentage		Molar conductance ($ohm^{-1} cm^2 mol^{-1}$)	Magnetic moment (μ_{eff})	Geometry
			Found	Calculated			
$[NiL_2Cl_2]$	668.59	201	9.60	8.78	12.3	D	Square planar
$[CoL_2Cl_2(H_2O)_2]$	704.83	189	8.80	8.36	4.2	4.78	Octahedral
$[CuL_2Ac_2]$	720.55	218	8.21	8.82	5.1	2.22	Square planar

Table 3: Magnetic moment, molar conductance and metal percentage data of transition metal complexes of 4-CBPT

	Escherichia coli Zone of inhibition (in mm)	Staphylococcus Zone of inhibition (in mm)	Proteus Zone of inhibition (in mm)	Pseudomonas Zone of inhibition (in mm)
Gentamicin (+ve control)	19	28	20	27
A1[Ligand]	7	9	6	6
A2 $[NiL_2Cl_2]$	7	12	7	7
A3$[CoL_2Cl_2(H_2O)_2]$	14	10	18	7
A4$[CuL_2Ac_2]$	6	7	8	7

Table -4: Anti bacterial study conducted

V. Conclusion

Triazole based ligand 1-[4-chlorobenzyl]4-phenyl-1,2,3-triazole and its Ni(II), Co(II) and Cu(II) complexes were synthesized and characterized. Antibacterial analysis of all compounds have been evaluated with bacterial species *Proteus*, *Escherichia coli*, *Staphylococcus and Pseudomonas*. Among which Co(II) complex is found to have better antibacterial activity.

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