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# Synthesis, Spectral and Microbiological Activity of Cr(II) Mn(II) and Cu(II) Complexes of Quinazoline Based Schiff Bases (QSB)

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## ABSTRACT

The paper emphasizes strictly on the characterization of Complexes of 3-„amino-2-phenyl-4(3H)-quinazoline-3,4 dimethoxy benzaldehyde with Cr(II), Mn(II) and Cu(II) using several techniques such as elemental analysis, FTIR spectroscopy, UV–Vis spectroscopy, Mass spectroscopy,‟ $^{1}$H NMR, magnetic susceptibility and conductivity measurements. The bidentate co-ordination by the ligand through azomethine nitrogen and amido oxygen can be done by Infrared spectra. The Cr(II) and Mn(II) is known to possess octahedral complexes in which the study of toxic effect has been elaborated. The presence of the substituted groups in the quinazoline ring indicates its toxicity deficiency.

**Keywords:** Magnetic Moment, IR, Proton NMR& Electronic Spectra

## INTRODUCTION

Quinazoline based Schiff bases ligands synthesis and characterization with Fe(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) along with the isolation number of Cr (II), Mn (II) and Cu(II) complexes with 3-amino-2-phenyl-4(3H)- quinazoline3, 4-dimethoxybenzaldehyde have been dealt. The ligand containing quinazoline-4(3H)-one moiety may have biological potency[2-3] and has the ability to coordinate with metal ions. High stability, greater solubility and chelating ability[5] enables Schiff‟s base to be widely used as ligands of coordination compounds in common solvents [4].

**Results and Discussion**

The formulation of analytical data of complexes has been featured in Table 1 on the basis of elemental analysis and conductance, magnetic, IR and electronic spectral data. These complexes are soluble in DMF and has low molar conductivity values of 10-18$\Omega^{-1}$ $cm^{-1}mol^{-1}$ for Cu and Mn complex that indicates their non-electrolytic nature[6]. Molar conductivity of 85$mhocm^{-1}mol^{-1}$ for the Cr (II) complex along with 1:1. Ionic nature [7].The IR spectra of the ligands N-C=O stretch at 1670 $cm^{-1}$ indicates co-ordination through amido oxygen[10] along with C=N, C=C and C-H bending vibrations[8] within expected values. The ligand band at 1615 $cm^{-1}$ in all complexes shows co-ordination through azomethine nitrogen[9] and amido oxygen[5] were further confirmed by ν M-N and νM=N bands of 545-610 and 480-530$cm^{-1}$ respectively[11-12]. Weak intensity bands at 270-280 $cm^{-1}$ in the spectra may be assigned to ν M-X bands whereas strong intensity bands at 1265 $cm^{-1}$ in the ligand spectrum may be assigned to ν CO[13]. All other characteristics of this band are retained which indicates non participation of O-atoms of the methoxy groups in co-ordination.

**$^1$H-NMR Spectra**

Sharp singlet at$\delta$3.80 is recorded for –$OCH_3$ protons in the free ligand whereas in other spectral complexes it remained at the same position thereby confirming non participation of O-atom of the –$OCH_3$ groups in co-ordination. All the ligand and complexes signals at $\delta$2.4(S, $CH_3$) and(m, ArH)[14] indicates co-ordination through the nitrogen of azomethine group to the metal ion[15] as azomethine proton deshielding appeared at $\delta$8.4-7.8 in all the complexes.

**Electronic Spectra of $[Cr(SQDB)_2X_2]$**

Three bands observed at 16400-16600 $cm^{-1}$ , 23900-24100 $cm^{-1}$ and 39500-39800 $cm^{-1}$ can be assigned to $^4A_{2g}(P) \rightarrow {}^4T_{2g}(F)$ and $^4A_{2g}(P) \rightarrow {}^4T_{1g}(F)$ and $^4A_{2g}(P) \rightarrow {}^4T_{1g}(P)$ transitions in the electronic spectra of Cr(II) complexes. Several ligand field parameters have been calculated for Cr(II) complexes[16] that agreed with the reported values of octahedral Cr(II) complexes. 1$^{st}$ spin allowed transition is taken as Dq along the parameters B, $\nu_2/\nu_1$ and β values that have been found to be 8.40 $cm^{-1}$, 1.46 and 0.91 $cm^{-1}$ respectively. The range of magnetic moment values were found between 3.82-3.88 B.M. at room temperature which are slightly less than spin only values[17].

**Electronic Spectra of $[Mn(SQDB)_2X_2]$**

Bands at 17000-17150 $cm^{-1}$, 26600 $cm^{-1}$ and 28500-28650$cm^{-1}$ are attributed to $^6A_{1g}(S) \rightarrow {}^4T_{1g}(G)$ and $^6A_{1g}(S) \rightarrow {}^4T_{2g}(S)$ and $^6A_{1g}(S) \rightarrow {}^4E_g(G)$ transition for the electronic spectra. The spectral parameters, Dq/B, $\nu_2/\nu_1$ and β values have been found to be 7.60 $cm^{-1}$, 1.55 and 0.88

$cm^{-1}$ respectively that agrees with the recorded values for octahedral Mn(III) complexes[17]. Magnetic moment values ranged between 5.90-5.93 B.M. at room temperature which corresponds to five unpaired electrons.

**Electronic Spectra of $[Cu(SQDB)_2X_2]$**

One asymmetrical peak at 12850$cm^{-1}$ attributable to $^2E_g(S) \rightarrow {}^2T_{2g}$ transition with John Teller effect, 10Dq values and 12850 along wth $\mu_{eff}$ values is 1.92 B.M. and 1.90 B.M. at room temperature has been shown in accordance with the distorted octahedral geometry of the Cu(II) complexes[18].

**Micro Biological Activity**

The toxicity of the complexes, ligands and metal chlorides were studied on growth of a green algae chlorello and it was concluded that the metal chlorides are more toxic than their respective complexes and ligands whereas the lesser toxicity nature of the ligands may be due to the presence of the substituted groups in the Quinazoline ring. The order of toxicity of complexes ligands and metal chlorides were observed as :

**Metal Chloride > Ligands > Complexes**

**Experimental**

The chemicals used were of A-R grade and utilised the same way as received. The solvent (BDH) were purified by standard methods and Ethanol was distilled before use.

3- amino-2pyr-phenyl quinazoline-4(3H)-one was prepared by the reported methods[19] whereas the ligand was prepared by refluxing a mixture of ethanolic solutions of 3, 4-dimethoxy-benzaldehyde and 3-amino-2-phenylquinazoline-4(3H)-one (1:1 molar ratio) on a water bath for about 6 hrs followed by cooling and the the resulting solid was washed, crystallized from DMF and dried over anhydrous $CaCl_2$.By refluxing ethanolic solutions of the metal salts (0.25 mol) with the ligand (0.01 mol) for 7-8 hrs on a water bath, the metal complexes were prepared and a pH 7-8 was maintained at all times. The resulting complexes were washed with ethanol and dried under reduced pressure over anhydrous $CaCl_2$. C and N were determined with micro analytical at CDRI, Lucknow. The estimation of Metals were done by standard methods[20] and its Magnetic susceptibility at room temperature was determined by Gouy method using $Hg[Co(SCN)_4]$ as the calibrant. Molar conductance was measured using a systonics -303 conductivity bridge. IR spectra(KBr) were recorded on a Beckmans FR20A. Spectrophotometer. Electronic spectra (DMF) on a Perkin-Elmer 400A. Spectrophotometer at CDRI, Lucknow and 1H-NMR spectra (DMSO-db) on an EM-930 Spectrophotometer at RSIC, Madras.

**Table – 1**

**Analysis and Physical Data of Complexes**

| Name of Compound | Analysis % : Found(cal.) M | N | Molar Conductance $\Omega^{-1}$ $Cm^2$ $mol^{-1}$ | $\mu_{eff}$ B.M |
|---|---|---|---|---|
| $[Cr(C_{19}H_{19}N_3O_3)_2Cl_2]Cl$ | 6.456(6.518) | 10.492(10.535) | 90 | 3.88 |
| $[Cr(C_{19}H_{19}N_3O_3)_2Br_2]Br$ | 5.803(5.865) | 9.401(9.479) | 85 | 3.85 |
| $[Cr(C_{19}H_{19}N_3O_3)_2I_2]I$ | 5.295(5.302) | 8.501(8.570) | 88 | 3.82 |
| $[Mn(C_{19}H_{19}N_3O_3)_2Cl_2]$ | 6.812(6.862) | 10.413(10.417) | 19 | 5.91 |
| $[Mn(C_{19}H_{19}N_3O_3)_2Br_2]$ | 6.101(6.175) | 9.398(9.447) | 17 | 5.90 |
| $[Mn(C_{19}H_{19}N_3O_3)_2I_2]$ | 5.502(5.586) | 8.945(8.544) | 16 | 5.93 |
| $[Cu(C_{19}H_{19}N_3O_3)_2Cl_2]$ | 7.804(7.855) | 10.301(10.388) | 12 | 1.92 |
| $[Cu(C_{19}H_{19}N_3O_3)_2Br_2]$ | 7.04(7.09) | 9.30(9.37) | 10 | 1.90 |
| $[Cu(C_{19}H_{19}N_3O_3)_2I_2]$ | 6.38(6.40) | 8.49(8.47) | 14 | 1.91 |

## Conclusion

On the basis of elemental analysis, magnetic moment data, conductivity measurements and spectral studies, octahedral structure for Cr, Mn, and Cu may be proposed. The toxic effect of complexes, ligands , metal chlorides were studied on the growth of green algae chlorella.

## Scope of Future Work:

The complexes can be useful in minimising the toxicity effects from the useful compounds.


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