IJESRR International Journal of Education and Science Research Review
ISSN 2348-6457
www.ijesrr.org February-2015, Volume-2, Issue-1 Email- editor@ijesrr.org

THEORY OF BIOLOGICAL STUDIES ON TRANSITION METAL COMPLEXES OF SUBSTITUTED OXAZOLE

Ms. Anju
M.Sc. Chemistry
Department of Chemistry
Kurukshetra University
Kurukshetra, Haryana

ABSTRACT:

The chemistry of transition metal complexes of biologically active ligands has attracted attention of several workers for the last few years. There are various heterocyclic compounds known which form complexes with various metal ions. These metal complexes are of great importance in the field of medicines and analytical chemistry. Various complexes of platinum and palladium with sulphur and nitrogen donar ligands are used in cancer chemotheraphy[1], metal complex of amino acids have been found to possess antitumour activity.

KEY WORDS: Biologically active ligands

INTRODUCTION

The chemistry and wide range of application of oxazole compounds have been reported in literature. These compounds have shown wide range of applications, they can be used as hypertensive, analgesic, anti-inflammatory, antibacterial, antiviral, anti-tubercular, anticonvulsant urinary tract infection sedative, cardiac stimulant[8], antihistaminic muscle relaxant and hypotensive.

Recently Pattanayak has reported, that addition of chlorine increases the fungicidal activity, he also reported that with increase of chlorine atom in the molecule the activity increases regularly. Survey of the literature shows that few references[11-15] are available but no systematic study has been done so far so is worthwhile to study the preparation and characterization of substituted oxazole. The present paper with the preparation of 2-Amino-4-(p-hydroxy phenyl)-5-chloro oxazole and its metal complexes. The stoichiometry of the newly synthesized complexes was established by their elemental analysis. They U.V., I.R., far I.R., magnetic measurements were carried out to establish their structure. The ligand as well as the metal complexes was screened for their fungicidal activity against various fungi at different concentration.

EXPERIMENTAL:

(a) SYNTHESIS OF THE LIGAND:

The ligand 2-Amino-4-(p-hydroxy phenyl)-5-chloro oxazole was prepared by the method reported in literature.

(b) PREPARATION AND ISOLATIONOF METAL COMPLEXES:

All the complexes were prepared by mixing ethanolic solution of ligand with appropriate metal salts in the same solvent and in proper ratio. The mixed solutions were refluxed on water bath. The contents were concentrated and cooled, crystals were separated out. These crystals were filtered washed thoroughly with ethanol and dried.

I.R. SPECTRAL STUDIES:

On comparison of the spectra of ligand with that of metal complexes it is observed that the υ (C– N) stretching frequency observed at 3450 cm^{-1} in the free ligand remains practically unchanged after complexation, they show that ring nitrogen is not taking part in complexation. The antisymmetric and symmetric υ (NH) stretching frequencies appeared in the region 3440-3400, 3340-3300 cm^{-1} in the free ligand get shifted to lower frequency after complexation. This shows that nitrogen of the amino group is taking part in complex formation. In all the complexes a band appeared in the region 375-280 cm^{-1} assigned to υ (M– O) bond. This shows that the oxygen of the oxazole ring is taking part in coordination. The characteristic band of oxazole system were observed in the region 1640-1600, 1595-1580 and 1560-1530 cm^{-1} . In the ligand as well as in all the complexes a band appeared in the region 600-500 cm^{-1}. This is due to υ (C– Cl) band.

MAGNETIC AND ELECTRONIC SPECTRAL STUDIES:

Fe (III) COMPLEXES:

The magnetic moment values of Fe (III) complexes were found in the region 4.9-5.3 B.M. The electronic spectra shows bands in the region 14000-15000, 16000-17000, 24500-25500 cm^{-1} assigned to $^6A_{1g} \rightarrow {}^4T_1\,({}^4D)$ (υ_1) $^6A_{1g} \rightarrow {}^4T_{1g}\,(\upsilon_2)$ and $^6A_{1g} \rightarrow {}^4A_{2g}$ (υ_3) transitions respectively the spectral and magnetic suggest octahedral structure of Fe (III) complexes.

Co (II) COMPLEXES:

In the case of Co(II) nitrate, chloro and sulphato complexes bands are observed in the range 8000-8500,15000-18000, 20000-23000 cm^{-1} . These bands are assigned to $^4A_2$ (F) $\rightarrow {}^4T_2$, (υ_1), $^4A_2$ (F) $\rightarrow {}^4T_1$ (υ_2) and $^4A_2$ (F) $\rightarrow {}^4T_1$ (P) (υ_3) respectively[16]. The magnetic moment value 4.0-4.42 B.M. and spectral data suggest tetrahedral structure[17]. In the acetato complexes bands are observed at 8600, 17000, 21000 cm^{-1} assigned to $^4T_{1g}$ (F) $\rightarrow {}^4T_{2g}$ (F) (υ_1), $^4A_{2g}$ (F) (υ_2) and $^4T_{1g}$ (P) (υ_3) respectively. The magnetic moment value observed 5.0 B.M. This and the spectral studies shows into octahedral geometry.

Ni (II) COMPLEXES:

The electronic spectra of Ni(II) complexes show bands in the region 8500-9000 cm^{-1} , 14000-15750 cm^{-1} and 24050-24200 cm^{-1} characterstic of octahedral Ni(II) ion. These observed energies of three spin allowed transitions $^3A_{2g} \rightarrow {}^3T_{2g}$, $^3A_{2g} \rightarrow {}^{33}T_{1g}$ (F) and $^3A_{2g} \rightarrow {}^3T_{1g}$ (P) agree well with those predicted from Liehr and Ballhausen[18] energy level diagram for Ni(II) in a ligand field of octahedral symmetry. The magnetic moment value is in between 2.90-3.20 B.M. which is in support of high spin octahedral structure.

Cu(II) COMPLEXES :

The electronic spectra of Cu (II) complexes show absorption bands in the region 15500-16000, 18500-20000 cm^{-1} assignable to $^2B_{1g} \rightarrow {}^2A_{1g}$ and $^2B_{1g} \rightarrow {}^2E_g$ transitions respectively. A unique peaks also obtained in all the cases around 14000 cm^{-1} this is characteristic of planar geometry. The Cu(II) complexes are paramagnetic in nature and are having magnetic moment value suggest squareplanar configuration of Cu(II) complexes.

FUNGICIDAL ACTIVITY:

The fungicidal activity of ligand and metal complexes were determined using growth method. The fungi toxicity data (table-I) revealed that the ligand is more toxic than its metal complexes. The Fungi toxicity also varies from fungus to fungus as well as on the change of concentration. At higher concentration the ligands as well as the metal complexes are more toxic. The toxicity decreases with decrease of concentration.

Table -1

Growth responses of Phoma-exigua, Macrophomina- phaseoli and Collectotrichun-capsici at three concentrations in relation to the ligand and its metal complexes

Test Samples	AVERAGE PERCENTAGE INHIBITION AFTER 168 HOURS								
	Phoma-exigua			Macrophomina-phaseoli			Colletotrichum-capsici		
	Concentetrations used in ppm.								
	100	50	20	100	50	20	100	20	50
ABPO	74.4	56.4	40.8	65.7	50.8	43.6	75.6	44.3	54.0
[Mn (L)$_2$ Cl$_2$]	52.3	36.6	208	45.7	30.6	23.4	55.4	24.2	24.4
[Mn (L)$_2$ (NO$_3$)$_2$]	52.2	36.4	20.7	45.5	30.4	22.9	54.8	23.9	24.2
[Mn (L)$_2$ (CH$_3$ COO)$_2$]	52.0	36.3	20.6	45.0	30.3	22.8	54.7	23.8	24.2
[Mn (L)$_2$ SO$_4$)]	52.0	36.2	20.6	45.0	30.2	22.8	54.6	23.7	24.2
[Fe (L)$_3$] Cl$_3$	32.2	16.0	1.0	25.1	10.8	2.2	34.7	4.1	4.2
[Fe (L)$_3$] (NO$_3$)$_3$	32.8	16.6	1.2	25.7	11.0	2.7	35.3	4.7	4.8
[Fe (L)$_3$] (CH$_3$ COO)$_3$	33.0	17.2	1.4	26.7	11.2	3.0	35.5	4.9	5.0
[Fe$_2$ (L)$_6$] (SO$_4$)$_3$	32.6	16.0	1.0	25.7	10.8	2.5	35.1	4.4	5.5
[Co (L)$_2$] Cl$_2$ .2H$_2$O	47.8	31.2	15.8	40.7	25.0	17.6	50.6	19.8	19.7
[Co (L)$_2$] (NO$_3$)$_2$ .2H$_2$O	47.0	30.7	15.2	40.4	25.2	17.8	50.0	19.2	19.12
[Co (L)$_2$ (CH$_3$ COO)$_2$]. 2H$_2$O	47.2	29.6	15.0	40.1	25.0	17.9	49.8	19.0	19.1
[Co (L)$_2$] (CH$_3$ CO$_4$) . 2H$_2$O	47.3	30.5	15.4	40.4	25.4	18.3	50.0	19.3	19.4
[Ni (L)$_2$ Cl$_2$] .H$_2$O	46.6	31.2	14.7	39.8	24.5	17.6	49.2	19.6	19.5
[Ni (L)$_2$ (NO$_3$)$_2$].H$_2$O	46.2	30.6	14.2	39.6	24.3	17.2	49.2	19.4	19.2
[Ni (L)$_2$ (CH$_3$ COO) $_2$]. H$_2$O	46.8	31.5	14.8	39.9	24.7	17.8	49.6	19.8	19.7
[Ni (L)$_2$ (SO$_4$)]. H$_2$O	46.4	31.1	14.5	39.4	24.4	17.3	49.4	19.4	19.3
[Cu (L)$_2$] CL$_2$	42.2	26.5	13.2	35.1	20.4	13.2	45.3	14.2	15.2
[Cu (L)$_2$] (NO$_3$)$_2$	42.3	26.4	13.4	35.0	20.6	13.3	45.5	14.3	15.4
[Cu (L)$_2$] (CL$_3$COO)$_2$	42.4	26.4	13.2	35.1	20.8	13.4	45.8	14.6	15.5
[Cu (L)$_2$] ((SO$_4$)	42.2	26.6	13.0	34.9	20.6	13.2	45.6	14.4	15.3

CONCLUSION

This paper deals with the preparation and characteristic of few transition metal complexes. In general metal complexes were prepared by refluxing the respective metal salts with ligand in 1:2 molar ratios in case of divalent metal ions and 1:3 in case of trivalent metal salts in appropriate solvent on water bath. The resulting solution were refluxed and then concentrated and kept for overnight. The respective complexes separate out which were filtered washed and dried. On analysis it is found that the stoichiometry of the complexes is 1:2 in the case of Mn (II), Ni (II), Co(II), Cu (II) and 1:3 in Fe (III). The electronic and magnetic studies shows that the Mn (II), Fe (III), Ni (II), Fe (II) and acetato complexes of Co (II) are octahedral while chloro and nitrato complexes of Co (II) are tetrahedral. The magnetic moment values of Cu (III) complexs are in the range of 1.90-2.20 B.M. These values suggest square planar configurations. The fungicidal activities of the ligand as well as of metal complexes were screened against *Phoma-exigua*, *Macrophomina- Phaseoli* and *Colletotrichum-capsici* at 100, 50 and 20 ppm. in Czepecks dox agar medium. It is cleared that the fungitoxicity of the ligand decreases on complex formation. The ligands as well as the metal complexes are more toxic at higher concentration than the lower one i.e. the fungicidal activity decreases with decrease of concentration.

REFERENCES

1. Blain S, Appriou P, Chaumeil H and Handel H 1990, "Application of a tetraaza macrocycle immobilized on an organic polymer to the determination of trace amounts of manganese in sea water", *Anal. Chim. Acta*, 1990, **232,** 331.
2. Cunha S, Oliveira S M , Rodrigues Jr M T , Bastos R M , Ferrari J, de Oliveira C M A , Kato L, Napolitano H B, Vencato I , Lariucci C , Structural Studies of 4-Aminoantipyrine Derivatives *J. Mol. Struct.*, 2005, ***752,*** 32-39.
3. Eilmes J, "Jager benzoylation of macrocyclic Ni(II) complex efficiently and year demetalation of γ γ '-dibenzoylated products", *Polyhedron*, 1985, **6**, 943.
4. Kubaszewski Eugeniusz and Malinski Tadeusz, "5,7,12,14-Tetramethyldimethoxybenzo [b,l][1,4,8,11] tetraazacyclodecane, a new tumoricidal pseudo-porphyrin" *J. Heterocyclic Chem.*, 1992, **29**, 1417.
5. Maurya, M. R. & Bharatia, N. 1993. Transition Metals Chemistry, 23, 5-15.

6. Filho V C, Corréa R , Vez Z , Calixto J B , Nunes R J , Pinheiro T R, "Andricopulo A D, Yunes R A, "Further Studies on Analgesic Activity of Cyclic Imides," *Farmaco*, 1998, **53,** 55-57.
7. Guillemot D, "Antibiotic use in humans and bacterial resistance," *Current Opinion in Microbiology*. 1999, **2,** 494-498.
8. Vaum R, Heindel N D, Burns H D, Emrich J, "Synthesis and evaluation of an III In –labeled porphyrin for lymph no deimaging", *J. Pharm. Sci.*, 1982, **7l**, 1223.
9. Xie, L. Q. Yang, Z. Q. Zhang, Z. X. & Zhang, D. K. 1992. Applied Organometallic Chemistry, 6: 193-199.
10. Hassan, M. Scozzafava, A. Chohan, Z. H. & Supuran, C. T. 2003. Journal of Enzyme Inhibition and Medicinal Chemistry, 18: 495-503