

# Medicinal Aspects of Coordination Complexes in Human Health and other Living Beings

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**ABSTRACT:** Coordination chemistry has very impressive and valuable aspects in medicinal view. Today metal toxification is a worldwide problem where this branch of chemistry provides very effective study for the solution of this problem by interacting metal ions with suitable mono, di, tri, and tetra or polydentate ligands forming metal chelates under good experimental conditions as the present work which is an advanced computational study of divalent toxic metal ions  $Hg^{++}$  and  $Cd^{++}$  with 2- AHPPA and 5- MU as ligand having different chemical nature.

**KEYWORDS:** Metal Chelates, 2-AHPPA, 5- MU, Computational Study, Formation Constant.

## I. INTRODUCTION

Among the various subjects of chemical sciences coordination chemistry is much advanced branch of chemistry. It proves its value in the field of education, pharmaceutical industry, agriculture, medicinal and several other fields fruitful for human and other living beings. It also proves its importance in most advanced therapy chelation therapy which is very effective in treatment of various dangerous diseases today. This paper contains the study of various binary, ternary and quaternary complexes of bivalent toxic metal  $Hg^{++}$  and  $Cd^{++}$  with two ligand 2-Amino-3-(4-hydroxyphenyl) propanoic acid (2-AHPPA) as primary ligand and 5- methyluracil (5-MU) as secondary ligand through chelation. In the chelation, metal ion interacted with electron donating anions or neutral molecules called ligands binds single metal forming heterocyclic ring structure which is known as chelating ligand whereas complex is formed metal chelate [1].

## II. RELATED WORK

Researchers of this field show the value of coordination complexes with publication in various reputed national and international journals. B. K. Magare and M. B. Ubale [2] studied the mixed ligand stability constants of Co (II), Ni (II), Cu (II) and Zn (II) transition metal complexes with chlorpheniramine maleate drug and amino acids. P. R. Shirode [3] reported the synthesis and physicochemical studies of mixed ligand complexes of Mn(II), Fe(III), Co(II), Ni(II) and Cu(II) with acetophenone semicarbazone and acetone semicarbazone. Prachi Arya, Neha Singh, Ranu Gadi and Sulekh Chandra [4] studied the preparation, characterization and antiulcer activity of mixed ligand complex of Zn (II) with famotidine and glycine. A.B. Patil [5] described the stability constants of ternary complexes of transition metal (II) ions with aspartic acid and glutamic acid as primary ligands and ampicillin and cephalexin as secondary ligands. Chaudhary Rakhi and Shelly [6] described the synthesis, spectral and pharmacological study of Cu (II), Ni (II) and Co (II) coordination complexes. G.V. Mane, L.P. Shinde and D.G. Kolhatkar [7] described the pH metric study of proton-ligand and metal-ligand stability constant complexes of transition and inner transition metal ions with some organic acids.

## III. PROPOSED METHODOLOGY

Stock solutions (0.01M) of ligand were prepared by constant stirring in double distilled water and had been standardized against a standard oxalic acid solution. In the present study metal nitrate solutions were prepared in doubly distilled and standardized by EDTA titrations [8]. An electric digital pH meter (Eutech 501) having a reproducibility of  $\pm 0.01$  with a glass electrode used for potentiometric titration by Irving & Rossetti Technique [9-10]

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followed by advanced computational study through SCOGS [11-13] and ORIGIN computer programs. An ultra thermostat type U<sub>10</sub> (VEB MLW Sitz, Freital, Germany) was used to maintain a constant temperature in all the experiments.

### Solutions for various investigations:

*Acid Solution:* 5ml NaNO<sub>3</sub> (1.0M) + 5ml HNO<sub>3</sub> (0.02M) + H<sub>2</sub>O

*Ligand (A) Solution:* 5ml NaNO<sub>3</sub> (1.0M) + 5ml HNO<sub>3</sub> (0.02M) + 5ml 2-AHPPA (A) (0.01M) + H<sub>2</sub>O

*Ligand (B) solution:* 5ml NaNO<sub>3</sub> (1.0M) + 5ml HNO<sub>3</sub> (0.02M) + 5ml 5-MU (B) (0.01M) + H<sub>2</sub>O

*Binary Solution:* 5ml NaNO<sub>3</sub> (1.0M) + 5ml HNO<sub>3</sub> (0.02M) + 5ml 2-AHPPA (A)/5-MU (B) (0.01M) + 5ml Hg (II)/Cd (II) (0.01M) + H<sub>2</sub>O

*Ternary Solution:* 5ml NaNO<sub>3</sub> (1.0M) + 5ml HNO<sub>3</sub> (0.02M) + 5ml 2-AHPPA (0.01M) + 5ml Hg (II) / Cd (II) (0.01M) + 5ml 5-MU (B) (0.01M) + H<sub>2</sub>O

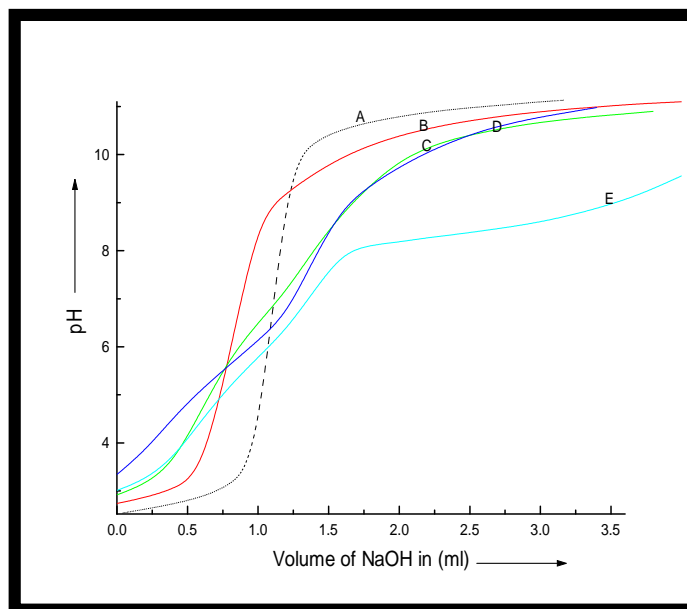
*Quaternary Solution:* 5 ml NaNO<sub>3</sub> (1.0 M) + 5ml HNO<sub>3</sub> (0.02M) + 5ml 2-AHPPA(A) (0.01M) + 5 ml Hg(II)(0.01M) + 5ml 5-MU(B) (0.01M) + 5ml Cd(II) (0.01M) + H<sub>2</sub>O

## IV. EXPERIMENTAL RESULTS

From the study of above solutions we get some findings on the basis of which we draw titration curves and species distribution curves showing exact percentage of complex formation. Sketching of titration curves and speciation or species distribution curves for study of various complexes have been done by plotting pH vs. volume of alkali and by plotting percent (%) concentration of the species against pH respectively. Both the curves are finally sketched by running through much advanced computer program also named as ORIGIN 6.0. Percentage concentration of different species and stability constant were studied through very advance computer program SCOGS (Stability constant of generalized species) as applied in our earlier research articles [14-21] published in reputed journals.

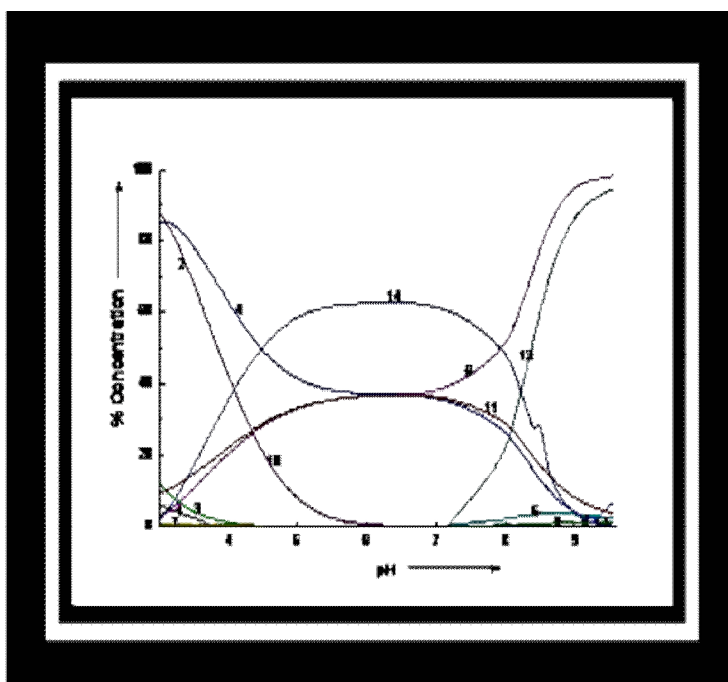
**Table.1**  
**Hg (II) - Cd (II) -2-AHPPA (A) - 5-MU (B) pH Metric Titration**

Volume of NaOH (mL)	pH				
	A	B	C	D	E
0.0	2.52	2.74	2.92	3.34	3.01
0.2	2.62	2.86	3.14	3.84	3.24
0.4	2.73	3.04	3.59	4.53	3.69
0.6	2.87	3.37	4.69	5.12	4.48
0.8	3.11	5.84	5.77	5.63	5.19
1.0	3.65	8.68	6.50	6.13	5.78
1.2	9.70	9.20	7.16	6.67	6.36
1.4	10.29	9.61	8.04	7.87	7.18
1.6	10.53	9.95	8.79	8.90	7.96
1.8	10.68	10.20	9.38	9.37	8.12
2.0	10.79	10.39	9.86	9.74	8.18
2.2	10.88	10.54	10.15	10.05	8.27
2.4	10.95	10.66	10.34	10.30	8.34
2.6	11.00	10.75	10.47	10.51	8.42
2.8	11.05	10.83	10.58	10.66	8.50
3.0	11.10	10.89	10.67	10.78	8.60
3.2	11.14	10.95	10.74	10.88	8.73
3.4		10.99	10.80	10.98	8.88
3.6		11.04	10.85		9.06
3.8		11.07	10.90		9.29
4.0		11.10			9.56



**Fig. 1. Titration Curves for (1:1:1) Hg (II) - Cd (II) -2-AHPPA (A) - 5-MU (B)**

(A) Acid (B) Ligand (C) Hg(II)- 2-AHPPA (D)Hg(II)-2-AHPPA - 5-MU (E)Hg(II) Cd (II)- 2-AHPPA -5-MU



**Fig.2 -Distribution Curves of (1:1:1) Hg (II) - Cd (II)- 2-AHPPA (A)- 5-MU(B) System**

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- (1)  $Hg^{2+}$ (II) (2)  $Cd^{2+}$ (II) (3)  $H_3A$  (4)  $H_2A$  (5)  $HA$  (6)  $Hg(OH)_2$  (7)  $Hg(OH)^+$  (8)  $Cd(OH)_2$  (9)  $Cd(OH)^+$  (10)  $CdA$  (11)  $CdB$  (12)  $HgAB$  (13)  $CdA$  (14)  $HgCdAB$

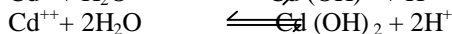
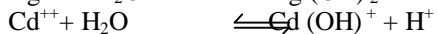
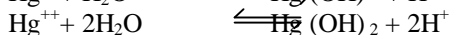
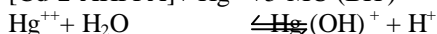
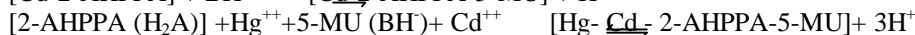
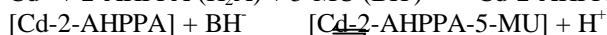
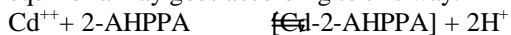
### STUDY OF SPECIES DISTRIBUTION DIAGRAM:

#### (Hg (II)-Cd (II)-2-AHPPA (A)- 5- MU (B) system.)

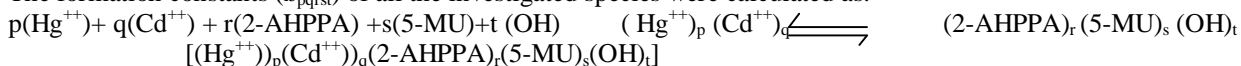
Species distribution diagram reveals the following species in this system:

$Hg^{2+}$ (aq.),  $Cd^{2+}$ (aq.),  $H_3A$ ,  $H_2A$ ,  $HA$ ,  $Hg(OH)_2$ ,  $Hg(OH)^+$ ,  $Cd(OH)_2$ ,  $Cd(OH)^+$ ,  $CdA$ ,  $CdB$ ,  $HgAB$ ,  $CdAB$  and  $HgCdAB$ . The graphical representation reveals that quaternary species is the dominant species, attaining maximum concentration ~63% at the ~6.5pH value. Free metal ion  $Cd^{2+}$ (aq.) attain maximum concentration ~88% at the start of titration which shows decline trend with increase in pH while  $Hg^{2+}$ (aq.) have low existence ~6.0% at the start of titration.  $H_2A$  have the maximum existence ~84% at the start of titration which shows decline trend with increase in pH. Binary complex of Hg A and Hg B were not present. Cd- A complex have maximum concentration ~89% at the start of titration shows decline trend with increase in pH while the Cd B complex attain the maximum concentration ~40% at the ~6.5 pH. Ternary species Hg AB existed with very low amount attaining maximum concentration ~5.0% at the ~ 9.2 pH value and ternary complex of Cd AB existed with very good concentration ~ 9.4 pH. Hydroxo species  $Hg(OH)_2$ , shows very good existence in the present system.

In the present investigation formation of different binary, ternary, quaternary complexes and general hydrolytic equilibria may goes according to this way:



The formation constants ( $\beta_{pqrst}$ ) of all the investigated species were calculated as:



$$\beta_{pqrst} = \frac{[Hg^{++}]^p [Cd^{++}]^q [2-AHPPA]^r [5-MU]^s [OH]^t}{[Complex]}$$

Table. 2

- Proton-ligand formation constant ( $\log \beta_{00r0t} / \log \beta_{000st}$ ) of 2-AHPPA - 5-MU at  $37 \pm 1^\circ C$   $I = 0.1 NaNO_3$

Complex	$\log \beta_{00r0t} / \log \beta_{000st}$
$H_3A$	21.35
$H_2A$	19.18
$HA$	10.14
$BH$	9.94

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**Table. 3**

- Hydrolytic constants ( $\log \beta_{p000t} / \log \beta_{0q00t}$ )  $M^{2+}$  (aq.) ions.

Complex	log $\beta$ Value
Hg(OH) <sup>+</sup>	-3.84
Hg(OH) <sub>2</sub>	-6.38
Cd(OH) <sup>+</sup>	-6.89
Cd(OH) <sub>2</sub>	-14.35

**Table.4**

- Metal-Ligand constants ( $\log \beta_{p0r00} / \log \beta_{0qr00} / \log \beta_{p0o0s0} / \log \beta_{0qo0s0}$ ) Binary System

Binary Complexes	log $\beta$ Value
Cd-2-AHPPA	3.57
Cd - 5-MU	11.33

**Table. 5**

- Metal-Ligand constants ( $\log \beta_{p0rs0} / \log \beta_{0qrs0}$ ): Ternary System(1:1:1)

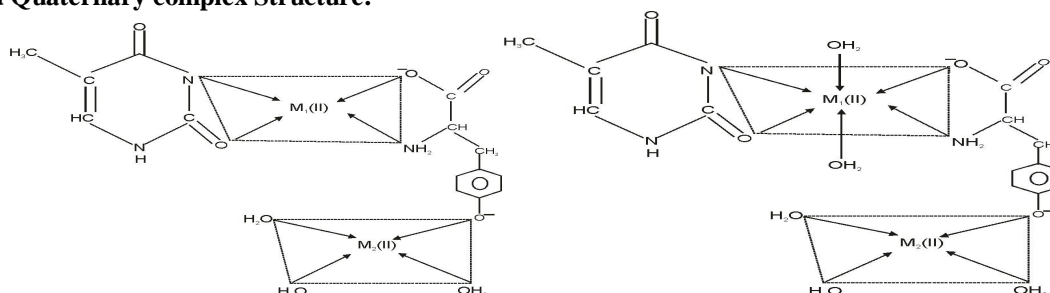
Ternary Complexes	log $\beta$ Value
Hg-2-AHPPA-5-MU	21.25
Cd-2-AHPPA-5-MU	16.95

**Table. 6**

- Metal-Ligand constants ( $\log \beta_{pqrst}$ ): Quaternary System (1:1:1:1)

Quaternary Complexes	log $\beta$ Value
Hg- Cd - 2-AHPPA-5-MU	28.25

## Proposed Quaternary complex Structure:



## V. CONCLUSION

Complexes formed by above method acts as scavenger due to their interaction with metal ions and suitable ligand to dislodging the toxic metals and remove them as soluble chelates. It is well known fact that a lot of drugs actions are based on chelation which is possible only by coordination chemistry so this branch of chemistry plays very fruitful role in human life as well as other living beings through medicinal way. Study of coordination chemistry and coordination complexes in special reference of chelation help to understood drug actions for students and researchers working in the chemical, medical and pharmaceutical fields.

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## REFERENCES

- [1] F.L.; Grvan 'Chelating Agents and Metal Chelates' (Ed. F.P. Dwyer and D.P. Mellor) *Academic Press, New York*, Ch. 7, 283, 1964.
- [2] B. K Magare. and M. B Ubale, *Der Pharma Chemica*, 3 (4):323-329, 2011.
- [3] P. R. Shiode *Chem Sci Trans.*, 396-400, 2012.
- [4] Prachi Arya, Neha Singh, Gadi Ranu and Chandra Sulekh *J. Chem. Pharm. Res.*, 2(6):253-257, 2010.
- [5] A.B. Patil *OJCHEG*, Vol. 28, No. (3): 1509-1512, 2012.
- [6] Chaudhary Rakhi and Shelly *Research Journal of Chemical Sciences*, Vol. 1(5), 1-5, 2011.
- [7] G.V. Mane, L.P. Shinde. and D.G. Kolhatkar, *Alfa Universal An International Journal of Chemistry* Vol 2 (3), 181-187, 2011.
- [8] F.J. Welcher, "The analytical uses of ethylene diamante tetraacetic acid" *D. Van Nostarand Company, New York* P. 169 , 1957.
- [9] H. M. Irving and., H.S. Rossotti *J. Chem. Soc.* 3397, 1953.
- [10] H. M. Irving and H.S. Rossotti, *J. Chem. Soc.* 2904, 1954.
- [11] I.G Sayce, *Talanta*, 15, 1397-1411, 1968.
- [12] I.G. Sayce, *Talanta*, 18, 653, 1970.
- [13] I.G Sayce and V. Sharma, *Talanta*, 19, 831, 1972.
- [14] K. Kumar and D.K Dwivedi, *RJPBCS*, 8(2), 1427-1433, 2017.
- [15] K. Kumar and D.K Dwivedi, *JUC*, 13(2), 44- 49, 2017.
- [16] K. Kumar and D.K Dwivedi, *J. Chem. Pharm. Res.*, 6(9):81-88, 2014.
- [17] K. Kumar and D.K Dwivedi, *IJSR*, 3(7), 2336-2340, 2014.
- [18] K. Kumar and D.K Dwivedi, *IMPACT: IJRANSS*, 2(8):79-88, 2014.
- [19] K. Kumar and D.K Dwivedi, *IJIRSET*, 3(7):14711-14718, 2014.
- [20] K. Kumar and D.K Dwivedi, *Res. J. Chem. Sci.*, 4(10):37- 42, 2014.
- [21] K. Kumar and D.K Dwivedi, *Trends in Biosciences*, 7(15):1994-1999, 2014.