International Journal of Applied Chemistry.
ISSN 0973-1792 Volume 20, Number 1 (2024) pp. 1-15

http://www.ripublication.com

"Computational Calculation of Hydrolytic and Association Constants of Inorganic Complex Compounds Through Various Concentration Profile"

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Abstract

The reactivity and stability of any inorganic complex compound is depends upon its association constants which is an important and specific property of any complex species for providing most of the information about them while hydrolytic constant says about equilibria between water molecule and bivalent metal ions forming mono and dihydroxo species during complexation and their study can be done by using an advanced computer software programme (SCOGS) and their concentration profile provide information about extent of particular species which can be seen and understand by graphical representation by using another advanced computer software programme (ORIGIN 6.0).

Keywords: Association Constant, Hydrolytic Constant, Computational Calculation, Software Programme (SCOGS, ORIGIN), Concentration profile.

INTRODUCTION

As we know that human life is pushes towards danger by all world exposing different type of hazardous elements and chemical in most essential need of human such as water and air from industries and these elements enters in our body by inhalation, ingestion, direct contact with skin and harms various organs that causes even death. Chelation is one of the best method for solution of these exposed materials problem. In this paper me and my coworkers studied various inorganic complex compound through chelation which provide an easy and valuable method to penetrate to hazardous chemicals using potentiometric analytical technique by taking three different biologically significant ligands 2-ASA,2-AHPPA,5-MU and two very hazardous heavy metal ions Hg and Cd where toxic metal problem in tissues of various organs can be checked out through chelation process using various concentration profile as well as pH profile for various inorganic complex compounds and their binding constant were find out through computational calculation method. Some research workers[1-2] also completed their work in this field in the above way.

MATERIALS AND METHODS

In this work we studied about computational calculation to find out exact binding constants of some binary ternary and quaternary complex compounds of 2-ASA ,2-AHPPA, and 5-MU binding ligands with bivalent Hg and Cd heavy metal ions using the following sets of solutions:

Acid Solution: 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + H_2O

Ligand (A) Solution: I- 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 2-ASA (A) (0.01M) + H_2O

Ligand (A) Solution: II-5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 2-AHPPA (A) (0.01M) + H_2O

Ligand (B) solution: 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL5-MU (B) (0.01M) + H_2O

Binary Solution: I - 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL2-ASA (A) (0.01M) + 5mL Cd (II) (0.01M) + H_2O

Binary Solution: II - 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 5-MU (B) (0.01M) + 5mL Cd (II) (0.01M) + H_2O

Binary Solution: III - 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL2-AHPPA (A) (0.01M) + 5mL Hg (II) (0.01M) + H_2O

Binary Solution: IV- 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 2-AHPPA (A) (0.01M) + 5mL Cd (II) (0.01M) + H_2O

Binary Solution: V- 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 5-MU (B) (0.01M) + 5mL Hg(II) (0.01M) + H_2O

Ternary Solution: I- (1:1:1): 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 2-ASA (A) (0.01M) + 5mL Cd (II) (0.01M) + 5mL 5-MU (B) (0.01M) + H_2O

Ternary Solution: II- (1:1:1): 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL2-AHPPA (A) (0.01M) + 5mL Hg (II) (0.01M) + 5mL 5-MU (B) (0.01M) + H_2O

Ternary Solution: III- (1:1:1): 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5mL 2-AHPPA (A) (0.01M) + 5mL Cd (II) (0.01M) + 5mL 5-MU (B) (0.01M) + H_2O

Quaternary Solution: (1:1:1:1): 5mL $NaNO_3$ (1.0M) + 5mL HNO_3 (0.02M) + 5 mL 2-AHPPA (A) (0.01M) + 5 mL Hg (II) (0.01M) + 5mL 5-MU (B) (0.01M) + 5 mL Cd (II) (0.01M) + H_2O

Here the standardization of the metal nitrate solutions of Hg and Cd through the EDTA titrations[3] method and pH titration profile of different binary, ternary and quaternary sets of above solution were find out with the using Eutech 501 digital pH meter having a reproducibility of ±0.01 with the help of Bjerrum's[4] and Irving &Rossoti[5,6] methods which is very good method to provide most of the information about electrochemical behavior of equilibria of complex compounds formed in complexation or chelation process.

RESULTS AND DISCUSSION

Potentiometric titration studies of above solutions were done by pH meter and the end point noted and tabulated according to result on display of the experimental instrument as in the various table given bellow.

pH Titration Table:1

Cd (II)- 2-ASA(A) - 5-MU (B) Ternary System

Volume of NaOH (mL)	pH			
	A	**B**	**C**	**D**
0.0	2.52	2.61	2.67	2.98
0.2	2.62	2.72	2.75	3.15
0.4	2.73	2.85	2.87	3.38
0.6	2.87	3.02	3.02	3.72
0.8	3.11	3.26	3.24	4.34
1.0	3.65	3.60	3.55	6.93
1.2	9.70	4.20	4.07	7.89
1.4	10.29	8.54	5.66	8.53
1.6	10.53	9.40	6.77	8.98
1.8	10.68	9.89	7.59	9.23
2.0	10.79	10.24	8.00	9.45
2.2	10.88	10.47	8.14	9.69
2.4	10.95	10.63	8.46	9.93
2.6	11.00	10.74	8.60	10.14
2.8	11.05	10.83	8.72	10.32
3.0	11.10	10.91	8.82	10.46
3.2	11.14	10.97	8.86	10.58

pH Titration Table: 2

Hg (II)- 2-AHPPA (A) - 5-MU (B) System

Volume of NaOH (mL)	pH			
	A	**B**	**C**	**D**
0.0	2.52	2.74	2.92	3.34
0.2	2.62	2.86	3.14	3.84
0.4	2.73	3.04	3.59	4.53
0.6	2.87	3.37	4.69	5.12
0.8	3.11	5.84	5.77	5.63
1.0	3.65	8.68	6.50	6.13
1.2	9.70	9.20	7.16	6.67
1.4	10.29	9.61	8.04	7.87
1.6	10.53	9.95	8.79	8.90
1.8	10.68	10.20	9.38	9.37
2.0	10.79	10.39	9.86	9.74
2.2	10.88	10.54	10.15	10.05
2.4	10.95	10.66	10.34	10.30
2.6	11.00	10.75	10.47	10.51
2.8	11.05	10.83	10.58	10.66
3.0	11.10	10.89	10.67	10.78
3.2	11.14	10.95	10.74	10.88
3.4		10.99	10.80	10.98

pH titration Table- 3

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

0	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

Titration Curves and Species Distribution Curves

From the above titration table, we plotted titration curves with the help of pH value of acid, ligand, binary and ternary complexes species against the volume of the NaOH which is found at the end point of the titration procedure using computer software ORIGIN 6.0 for sketching the curves. The binding constants of all the investigated complex compounds were calculated by the SCOGS[7-9] (Stability constant of generalized species) which is a specific and one of the best computer software programme for the study of information about the complex formation and determination of their binding constants and the species distribution curves were sketched by taking percent (%) concentration of the species against pH with the help of ORIGIN 6.0 which is also used in plotting the titration curves as earlier in our research aurticles.[10-15]

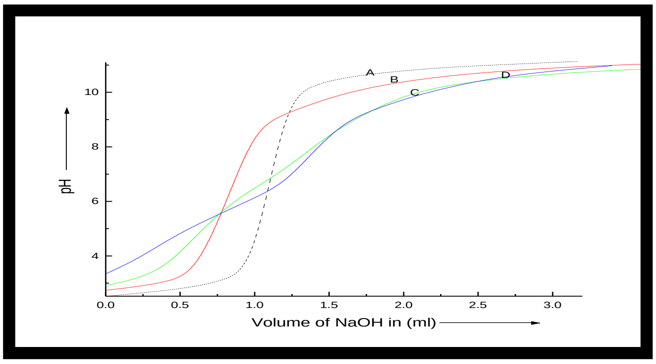


Figure.1- Potentiometric Titration Curves of 1:1:1 Cd (II)- 2-ASA (A) - 5-MU (B)System

(A) Acid (B) Ligand (C) Cd(II)- 2-ASA (D) Cd(II)-2-ASA - 5-MU

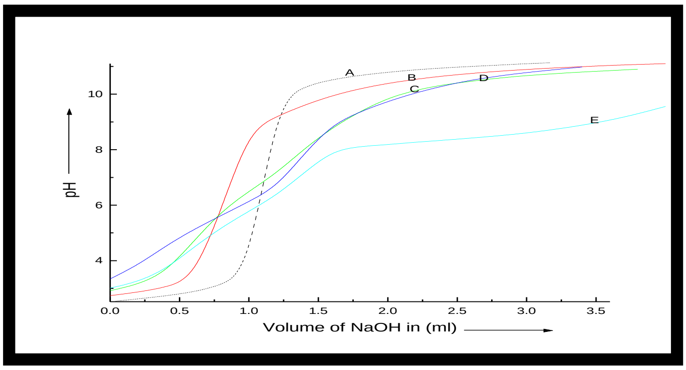


Figure.2. Potentiometric titration Curves of 1:1:1 Hg (II) - 2-AHPPA (A)- 5-MU (B)System

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

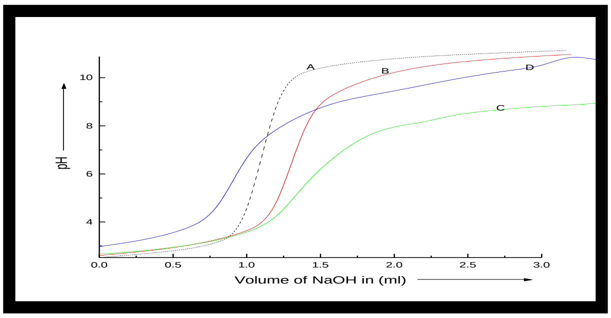


Figure. 3-Titration Curves of 1:1:1:1 Hg(II)–Cd(II)-2-AHPPA (A) - 5-MU (B) system

(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

STUDY OF SPECIES DISTRIBUTION CURVES

Cd(II)- 2-ASA(A)- 5-MU (B) System

The species distribution curves for Cd-2-ASA-5MU (1:1:1) ternary complex compound can be seen and understood by the related graph Fig-4 given as under where total nine species were identified. These are protonated ligand species (H_3A, H_2A, HA, BH), hydroxo species $Cd(OH)_{2,}$.free metal ion Cd^{2+} (aq.), binary species (Cd-(2ASA, Cd-5-MU) and ternary species Cd-2ASA-5-MU. Cd^{2+} (aq.) species shows higher value at initial stage of titration which shows decline trend with increasing pH. H_2A species shows maximum concentration ~ 78% at the very initial stage also which decreases with the increase in pH range. HA has maximum concentration ~ 64% at the pH~ 4.4, binary complex of metal and ligand A (Cd-2-ASA) is existed with maximum concentration ~ 5.0% at the pH range ~4.8. while another binary complex metal ion with secondary ligand B (Cd-5-MU) is found to be maximum concentration ~ 86% at the pH ~4.0. The major complex species in this investigation is ternary complex is Cd-2-ASA_5_MU which attains maximum concentration ~ 98% at the very high pH ~ 9.8.

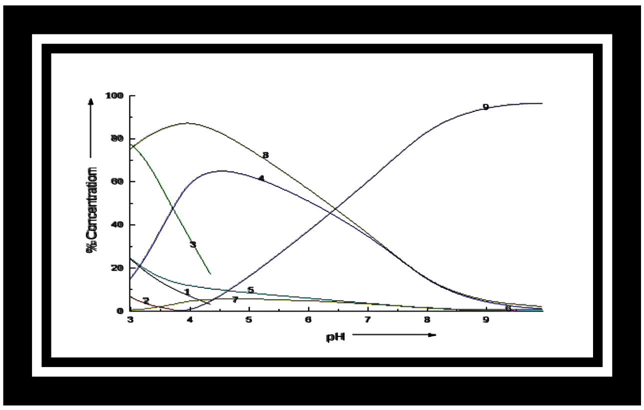


Figure 4- Distribution Curves of 1:1:1 Cd (II)-2-ASA (A) - 5-MU (B) System

(1) Cd^{2+} (2) H_3A (3) H_2A (4) HA (5) BH (6)$Cd(OH)_2$ (7)Cd A (8)CdB (9)CdA

Hg (II)- 2-AHPPA (A) - 5-MU (B) System

There were various species like H_3A, H_2A, HA and BH as protonated ligand species, Hg^{2+} (aq.) as free metal ion species, Hg $(OH)_2$ as hydroxo species, Hg-5-MU as binary species and Hg-2-AHPPA-5-MU as ternary species were identified in the graph while other species were in negligible amount as given in fig 5. In this system protonated ligand species shows their remarkable presence. The binary complex of Hg-5-MU exist in good concentration ~ 98% at start of the titration and gradually decreases with increase in pH range. Ternary complex of Hg-2-AHPPA-5-MU exist with higher value having maximum concentration ~ 98 %at higher pH ~ 9.5 hydroxo species $Hg(OH)_2$ also seen in this system in good concentration.

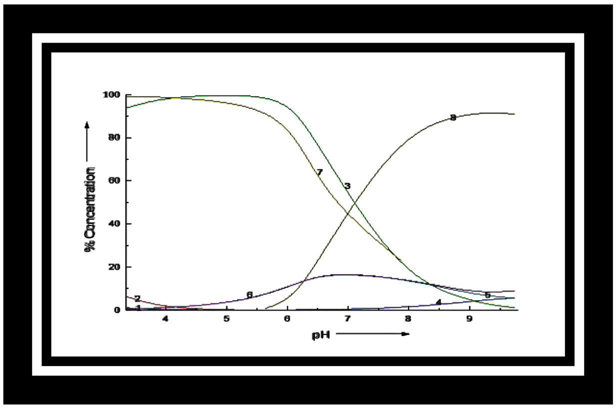


Figure-5-Distribution Curves of 1:1:1 Hg (II)-2-AHPPA (A) - 5-MU (B)System

(1) Hg^{2+} (2) H_3A (3) H_2A (4) H A(5) BH (6) Hg $(OH)_2$(7)Hg B (8) Hg A

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

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-2-AHPPA and Hg-5-MU were found in low extent. Cd-2- AHPPA complex have maximum concentration ~89% at the start of titration shows decline trend with increase in pH while the Cd -5MU complex attain the maximum concentration ~40% at the ~6.5 pH. Ternary species Hg- 2-AHPPA-5-MU existed with very low amount attaining maximum concentration ~5.0% at the ~ 9.2 pH value and ternary complex of Cd-2-AHPPA-5-MU existed with very good concentration ~ 9.4 pH. Hydroxo species Hg $(OH)_2$, shows very good existence in the present system.

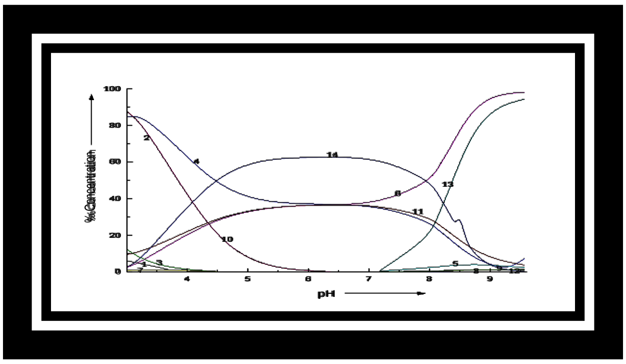


Figure. 6-Distribution Curves of 1:1:1:1Hg (II) - Cd (II)- 2-AHPPA (A)- 5-MU(B) System

(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)Cd A (11)Cd B (12)Hg AB (13)Cd A B(14)Hg Cd AB

Formation of Binary and Ternary Species with Cd(II)- 2-ASA(A)- 5-MU (B) (1:1:1)

Binary species

Cd^{++}+ 2-ASA (H_2A) ⇋ [Cd-2-ASA] + $2H^+$

Cd^{++}+ 5MU(BH^-) ⇋ [Cd-5-MU] + H^+

Ternary Species

[Cd^{++}-2-ASA] + BH^- ⇋ [Cd-2-ASA-2,4-DHP] + H^+

Cd^{++}+ 2-ASA (H_2A) + 5-MU (BH^-) ⇋ [Cd-2-ASA – 5-MU] + $3H^+$

Formation of binary and ternary species with Hg(II)- 2-AHPPA (A)- 5-MU (B) (1:1:1)

Binary species

Hg^{++}+ 2-AHPPA (H_2A) ⇋ [Hg-2-AHPPA] + $2H^+$

Hg^{++}+ 5-MU (BH^-)⇋ [Hg-5-MU] + H^+

Ternary Species

[Hg^{++}-2-AHPPA] + 5-MU (BH^-) ⇋ [Hg-2-AHPPA -5-MU] + H^+

Hg^{++}+ 2-AHPPA (H_2A) + 2,4-DHP (BH^-) ⇋ [Hg-2-AHPPA – 5-MU] + $3H^+$

Formation of binary ternary and quaternary species with Hg(II)- Cd(II)- 2-AHPPA (A)- 5-MU (B) (1:1:1:1) molar ratio

Hg^{++}+ 2-AHPPA (H_2A)⇋[Hg-2-AHPPA] + $2H^+$

Hg^{++}+ 5-MU (BH^-)⇋ [Hg-5-MU] + H^+

Cd^{++}+ 2-AHPPA (H_2A) ⇋ [Cd-2-AHPPA] + $2H^+$

Cd^{++}+ 5MU(BH^-) ⇋ [Cd-5-MU] + H^+

[Hg^{++}-2-AHPPA] + 5-MU (BH^-) ⇋ [Hg-2-AHPPA -5-MU] + H^+

Hg^{++}+ 2-AHPPA (H_2A) + 2,4-DHP (BH^-) ⇋ [Hg-2-AHPPA – 5-MU] + $3H^+$

[Cd^{++}-2-AHPPA] + BH^- ⇋ [Cd-2-AHPPA-5-MU] + H^+

Cd^{++}+ 2-AHPPA(H_2A) + 5-MU (BH^-) ⇋ [Cd-2-AHPPA – 5-MU] + $3H^+$

[2-AHPPA(H_2A)] + Hg^{++}+5-MU (BH^-) + Cd^{++} ⇋ [Hg- Cd-2-AHPPA-5-MU] + $3H^+$

[Hg-2-AHPPA] + Cd^{++} + 5-MU (BH^-) ⇋ [Hg - Cd-2-AHPPA – 5-MU] + H^+

Hydrolytic Species

Hg^{++}+ H_2O ⇋ Hg $(OH)^+$ + H^+

Hg^{++}+ $2H_2O$ ⇋ $Hg(OH)_2$ + $2H^+$

Cd^{++}+ H_2O ⇋ Cd $(OH)^+$ + H^+

Cd^{++}+ $2H_2O$ ⇋ Cd $(OH)_2$ + $2H^+$

Calculation of association constants of investigated complex species

The equation for binding or stability constants or log ß value ($ß_{p/qrst}$) of the Cd – 2-ASA -5MU ternary species given as:

p(Cd^{++})+ r(2-ASA) +s(5-MU)+t (OH) ⇋ $(Cd^{++})_p$ ($(2\text{-ASA})_r$ $(5\text{-MU})_s$ $(OH)_t$

$$\beta_{p/qrst} = \frac{[(Cd^{++})_p (2\text{-ASA})_r (5\text{-MU})_s (OH)_t]}{[Cd^{++})]^p [2\text{-ASA}]^r [5\text{-MU}]^s [OH]^t}$$

The equation for binding or stability constants or log ß value ($ß_{p/qrst}$) of the Hg – 2-AHPPA-5-MU ternary species given as:

p(Hg^{++})+ r(2-AHPPA) +s(5-MU)+t (OH) ⇋ $(Hg^{++})_p$ ($(2\text{-AHPPA})_r$ $(5\text{-MU})_s$ $(OH)_t$

$$\beta_{p/qrst} = \frac{[(Hg^{++})_p (2\text{-AHPPA})_r (5\text{-MU})_s (OH)_t]}{[Hg^{++})]^p [2\text{-AHPPA}]^r [5\text{-MU}]^s [OH]^t}$$

The equation for association constants or log ß value ($ß_{pqrst}$) for Hg-Cd- 2-AHPPA -5-MU quaternary species were calculated as:

p(Hg^{++})+ q(Cd^{++}) + r(2-AHPPA) +s(5-MU)+t (OH) ⇋ $(Hg^{++})_p$ (Cd^{++})q $(2\text{-AHPPA})_r$ $(5\text{-MU})_s$ $(OH)_t$

$$\beta_{p/qrst} = \frac{[(Hg^{++})_p (Cd^{++})q (2\text{-AHPPA})_r (5\text{-MU})_s (OH)_t]}{[Hg^{++})]^p [Cd^{++})]^q [2\text{-AHPPA}]^r [5\text{-MU}]^s [OH]^t}$$

Table 4

Association Constants for Cd(II)- 2-ASA(A)- 5-MU (B) (1:1:1) ternary System

Protonated Ligand Species	**Association Constant (log □)Value**
H_3-2-ASA	15.26
H_2-2-ASA	13.33
H-2-ASA	9.63
H-5-MU	9.94

Hydrolytic Species	**Hydrolytic Constant (log □) Value**
$Cd(OH)^+$	-6.89
$Cd(OH)_2$	-14.35

Binary Complex Species (1:1)	**Association Constant (log □$_{pr,}$ log □$_{ps}$)Value**
Cd-2-ASA	4.39
Cd-5-MU	11.33

Ternary Complex Species (1:1:1)	**Association Constant (log □$_{p\,r\,s}$) Value**
Cd-2-ASA-5-MU	15.35

Table- 5

Associaton constant for Hg (II) 2-AHPPA(A) - 5-MU(B) (1:1:1) ternary system.

Protonated Ligand Species	**Association Constant (log □)Value**
H_3-2-AHPPA	21.35
H_2-2-AHPPA	19.18
H-2-AHPPA	10.14
H-5-MU	9.94

Hydrolytic Species	**Hydrolytic Constant (log □$_{p000t}$) Value**
$Hg(OH)^+$	-3.84
$Hg(OH)_2$	-6.38

Binary Complex Species (1:1)	**Association Constant ($\log\beta_{pr}$ & $\log\beta_{ps}$) Value**
Hg-2-AHPPA	12.25
Hg-5-MU	13.45

Ternary Complex Species(1:1:1)	**Association Constant ($\log\beta_{p0rs0}$) Value**
Hg-2-AHPPA-5-MU	21.25

Table- 6

Association constant for Hg (II)- Cd (II) - 2-AHPPA(A) - 5-MU(B) (1:1:1:1) quaternary system.

Protonated Ligand Species	**Association Constant** ($\log\beta_{rt}$ & $\log\beta_{st}$) **Value**
H_3 -2-AHPPA	21.35
H_2 -2-AHPPA	19.18
H- 2-AHPPA	10.14
H- 5-MU	9.94

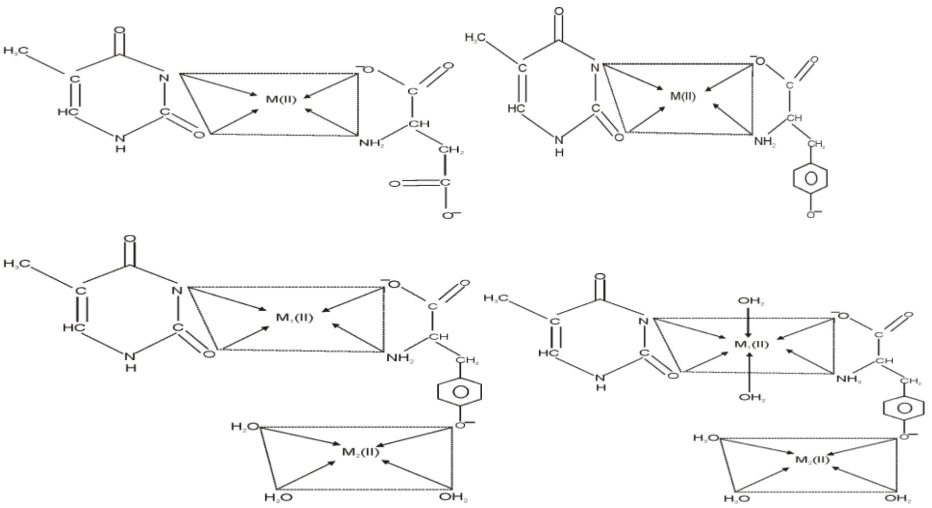
Hydrolytic Species	**Hydrolytic Constant ($\log\beta_{pt}$ & $\log\beta_{qt}$) Value**
$Hg(OH)^+$	-3.84
$Hg(OH)_2$	-6.38
$Cd(OH)^+$	-6.89
$Cd(OH)_2$	-14.35

Binary Complex Species (1:1)	**Association Constant ($\log\beta_{pr}$/ $\log\beta_{ps}$/$\log\beta_{qr}$/ $\log\beta_{qs}$) Value**
Hg-2-AHPPA	12.25
Hg-5-MU	13.45
Cd-2-AHPPA	3.57
Cd-5-MU	11.33

Ternary Complex Species (1:1:1)	**Association Constant ($\log\beta_{prs}$/ $\log\beta_{qrs}$) Value**
Hg-2-AHPPA-5-MU	21.25
Cd-2-AHPPA-5-MU	16.95

Quaternary Complex Species (1:1:1:1)	Association Constant (Log β_{pqrst}) Value
Hg-Cd- 2-AHPPA-5-MU	28.25

Proposed Binary, Ternary and Quaternary Structures of Investigated Inorganic Complex Compounds



CONCLUSION

In the above investigated inorganic complex compounds, all species has specific value for their association constants while hydrolytic constant for mono and dihydroxo species of metal and water molecule has also specific value as given in above table. The association constant is directly related to reactivity of any complex species it affects the reactivity in the inverse way. The complex having greater association constant value shows lower substitution or elimination reaction with attaching species and said to inert complex compound while the complex having lower binding constant value possess the liableness property of complexes and shows greater substitution reaction with attaching species. The association constant value also provides information about medicinal aspect of that particular complex species such as chelation processes applied in treatment of various indigenous problems.

REFERENCES

[1] Magare B. K and. Ubale M. B Der Pharma Chemica**, "**Mixed ligand stability constants of Co (II), Ni (II), Cu (II) and Zn (II) transition metal complexes with chloropheniramine maleate drug and amino acids. 3 (4):323-329 (2011).

[2] Shirode P. R Chem Sci Trans., "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".**1(2),** 396-400 (2012).

[3] Welcher F.J. (1957) “The analytical uses of ethylenediaminetetraacetic acid” *D. Van Nostarand Company, New York* P. 169

[4] Bjerrum, (1941)."Metal Amine Formation in Aqueous Solution". P. Masse &. Sons Copenhagen.

[5] lrving H. M.and. Rossetti, H.S. (1953) Methods for computing successive stability constants from experimental formation curves, J. *Chem. Soc*.. 3397-3405

[6] lrving, H. M and Rossetti H.S, (1954) Calculation of formation curves of metal complexes from pH titration curves in mixed solvents, *J. Chem. Soc*.. 2904-2910.

[7] Sayce I.G., (1968) “Computer Calculation of Equilibrium Constants of Species Present in Mixture of Metal Ions and Complexing Agents” *Talanta*, 15(12), 1397-1411.

[8] Sayce I.G., (1971) “Computer Calculation of Equilibrium Constants by use of the program SCOGS: A Correction,” *Talanta,* 18(6),653-654.

[9] Sayce I.G., and Sharma, (1972) “Computer Calculation of Equilibrium Constants using programme SCOGS: A further modification, *Talanta*, 19(6), 831.

[10] Kumar K and. Dwivedi D.K (2011) “Study on Formation of Some Mixed Ligand Ternary Metal Chevlates in Solution” **IJMIE**, **1(1)**:77-89

[11] Kumar K and Dwivedi D.K (2012) “Analysis of Electrochemical Behavior of Some Significant Inorganic Complexes” **IJAREAS**, **1(2)**:60-70

[12] Kumar K and Dwivedi D.K (2013). “Mode of Interaction and Behavior of Amino acid, Pyrimidine Base with Metal Ion in 4-Co-ordinated and 6-Coordinated Complexes” **Vidyawarta,1(4)**:0151-0155,

[13] Kumar K and Dwivedi D.K (2014). “An analytical study on complexation equilibria of non-essential amino acid and pyrimidine with heavy elements followed by specific computer programme” **J.Chem.Pharm. Res, 6(9)**:81-88,

[14] Kumar K and Dwivedi D.K (2017) “Multimetal - Multiligand complexes of Hg (II), Cd (II) and Pb (II) ions involving 2-aminosuccinic acid and 5-methyluracil”. **JUC, 13 (2),** 44- 49

[15] Kumar K, (2018). “Medicinal Aspects of Coordination Complexes in Human Health and Other Living Beings”. **IJIRSET, 6(8)**:17061-17066,

ABBREVIATIONS

β = Association or stability constant

p = M_1(first metal Hg), q = M_2(second metal Cd) for quaternary complex compound.

r = primary ligand, s = secondary ligand

t = hydroxo species

2-ASA =2-Aminosuccinic acid (primary ligand)

2-AHPPA = 2-Amino-3-(4-hydroxyphenyl) propanoic acid (primary ligand)

5-MU = 5-Methyl uracil (secondary ligand)