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The role and significance of metal - ligand complexes in our society

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ABSTRACT

Complexes formed through mutual interaction between metal ions and electron donating groups by bind single metal ion and form a heterocyclic ring structure named as metal chelates which play an important role in biological, analytical, industrial and medicinal field to serving the society. Like this present study have been completed by evaluating the metal ligand stability constant of hazardous bivalent Pb(II) metal ion with 2- amino-succinic acid (2-ASA) and 5-methyl uracil (5-MU) in 1:1:1 and 1:2:1 ratio to investigate the metal ligand complexes.

1. Introduction

As we know that science is a very valuable subject to read, teach and various other fields serving to our society such as agriculture, medical, pharmaceutical and industries etc. Among various subjects of science, chemistry is totally involved in about all essential needs in human life and other living beings. Here a good piece of study in co-ordination chemistry with bivalent toxic metal ion Pb(II) and 2- amino-succinic acid (2-ASA) as primary ligand (A) and 5- methyl uracil (5-MU) as secondary ligand (B) forming metal –ligand complexes in 1:1:1 and 1:2:1 ratio which plays important role in our society providing a very effective method to remove the toxic effect of metal using potentiometry technique followed by very advanced computer study. Some valuable studies were also completed in this field by researchers[1-5] time to time which shows their importance in the service of our society.

2. Materials and procedures

For the study of metal ligand complexes metal nitrate solutions have been taken which is standardized by EDTA titrations[6] while binary complexes of Pb^{++} with primary ligand 2-ASA, Pb^{++} with secondary ligand 5-MU and ternary complexes of Pb^{++} with primary ligand 2-ASA and secondary ligand 5-MU in two different ratios 1:1:1 and 1:2:1 were studied by preparing solution in the way given as under. An electric digital pH meter (Eutech 501) having a reproducibility of ±0.01 with a glass electrode used for potentimetric titration of binary and ternary complexes with the help of Bjerrum's[7] method modified by Irving & Rossoti Technique[8-9]. The pH meter was calibrated with buffer solutions of pH (4.0) and pH (9.2). All the experiments were completed at a constant temperature of 37 $\pm 1^0$C using an ultra thermostat type U_{10} (VEB MLW Sitz, Freital, Germany).

Solutions for various investigations

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

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

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

Binary Solution: I - 5ml $NaNO_3$ (1.0M) + 5ml HNO_3 (0.02M) + 5ml 2-ASA (A) (0.01M) + 5ml Pb (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 Pb (II) (0.01M) + H_2O

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

Ternary Solution: (1:2:1): 5ml $NaNO_3$ (1.0M) + 5ml HNO_3 (0.02M) + 10 ml 2-ASA (A) (0.01M) + 5 ml Pb (II) (0.01M) + 5ml 5-MU (B) (0.01M) + H_2O

3. Results and discussion

In the present paper a study of metal –ligand interaction were discussed with the help of advanced computer program SCOGS[10-12] (Stability constant of generalized species) as applied in our research papers[13-21] calculating the metal ligand constant while the titration and species distribution curves were sketched by using another advanced computer program named as ORIGIN 6.0. Titration curves were plotted by taking pH value of acid, ligand, binary and ternary complexes vs. volume of NaOH and species distribution curves were plotted by taking percent (%) concentration of the species against pH.

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pH metric study of above solutions

TABLE. 1 Pb(II)- 2-ASA (A) - 5-MU (B) (1:1:1) system

Volume of NaOH (mL)	pH A	B	C	D
0.0	2.52	2.61	2.41	2.90
0.2	2.62	2.72	2.65	3.07
0.4	2.73	2.85	2.70	3.31
0.6	2.87	3.02	3.75	3.66
0.8	3.11	3.26	3.86	3.81
1.0	3.65	3.60	4.93	4.15
1.2	9.70	4.20	5.12	5.12
1.4	10.29	8.54	6.31	6.33
1.6	10.53	9.40	7.56	7.29
1.8	10.68	9.89	8.74	7.82
2.0	10.79	10.24	9.08	8.62
2.2	10.88	10.47	9.38	9.12
2.4	10.95	10.63	10.21	9.48
2.6	11.00	10.74	10.32	9.75
2.8	11.05	10.83	10.63	10.02
3.0	11.10	10.91	10.74	10.26
3.2	11.14	10.97	10.86	10.48

TABLE. 2 Pb(II)- 2-ASA(A) - 5-MU (B) (1:2:1) system

Volume of NaOH (mL)	pH A	B	C	D
0.0	2.52	2.61	2.41	2.90
0.2	2.62	2.72	2.65	2.93
0.4	2.73	2.85	2.70	2.98
0.6	2.87	3.02	3.75	3.10
0.8	3.11	3.26	3.86	3.21
1.0	3.65	3.60	4.93	3.35
1.2	9.70	4.20	5.12	3.51
1.4	10.29	8.54	6.31	3.71
1.6	10.53	9.40	7.56	3.93
1.8	10.68	9.89	8.74	4.23
2.0	10.79	10.24	9.08	4.65
2.2	10.88	10.47	9.38	5.59
2.4	10.95	10.63	10.21	6.37
2.6	11.00	10.74	10.32	6.96
2.8	11.05	10.83	10.63	7.52
3.0	11.10	10.91	10.74	8.87

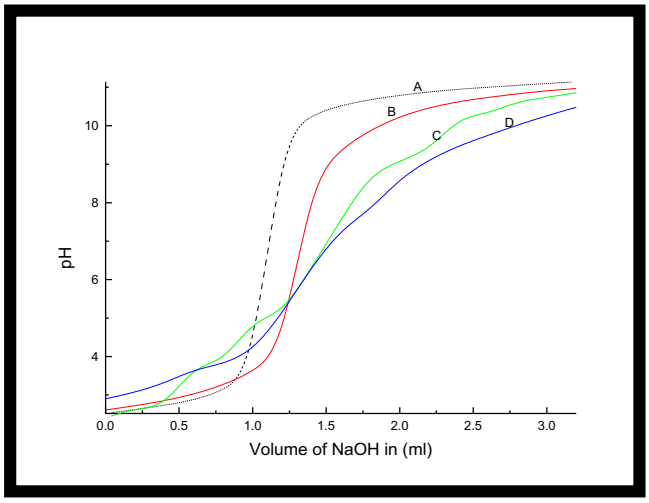


Figure 1. Potentiometric titration curves of (*1:1:1*) Pb (II)- 2-ASA (A)-5-MU(B) system

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

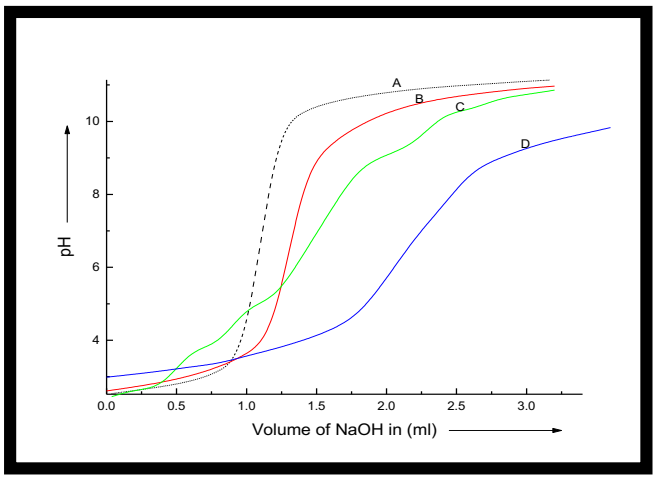


Figure 2. Potentiometric titration curves of (*1:2:1*) Pb (II)-2-ASA(A)-5-MU (B) system

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

Study of species distribution curves

Pb (II)- 2-ASA(A)- 5-MU (B) *(1:1:1)* System

H_2A species attain the maximum concentration ~ 73% at the start of titration which is gradually decrease at increase the pH this the decline trend goes to ~ 5.1 pH while the HA species exist at ~ 4.5 pH having the maximum concentration of ~ 64%. Binary complex Pb A exist at ~ 4.1 pH with maximum concentration ~ 14%. Another binary complex Pb B exist a maximum concentration of ~ 91% at very initial stage of titration which shows gradual decline trend with raising pH range. The ternary complex Pb A B shows remarkable presence with maximum concentration of ~ 98% at higher pH range ~ 9.8. In this system free metal ion Pb^{2+} (aq.), and BH species shows their remarkable presence.

Pb(II)- 2-ASA(A) – 5-MU(B) (*1:2:1*) system

In this system binary species Pb A shows its maximum concentration ~13% at pH ~ 3.8. Another binary complex Pb B shows its maximum concentration ~ 90% at very start of the titration which gradually decrease with increase in pH. In this system ternary complex of Pb AB is major species having concentration ~ 89% at higher pH ~ 9.2. In present system protonated ligand species and free metal ion species its remarkable presence. H_2A shows the maximum concentration~ 49% at start of the titration while HA exist with maximum concentration ~ 70% at ~ 4.0 pH.

Formation of binary complexes goes on this way

Pb^{++}+ 2-ASA (H_2A) $\rightleftharpoons$ [Pb-2-ASA] + $2H^+$

Pb^{++}+ 5-MU (BH^-) $\rightleftharpoons$ [Pb-5- MU] + H^+

Ternary complex formed through two ways

[Pb-2-ASA] + BH^- $\rightleftharpoons$ [Pb-2-ASA-5-MU] + H^+

Pb^{++} + 2-ASA (H_2A) + 5-MU (BH^-) $\rightleftharpoons$ [Hg-2-ASA-5-MU]+ $3H^+$

General hydrolytic equilibria are as follow:

Pb^{++}+ H_2O $\rightleftharpoons$ Pb $(OH)^+$ + H^+

Pb^{++}+ $2H_2O$ $\rightleftharpoons$ Pb $(OH)_2$ + $2H^+$

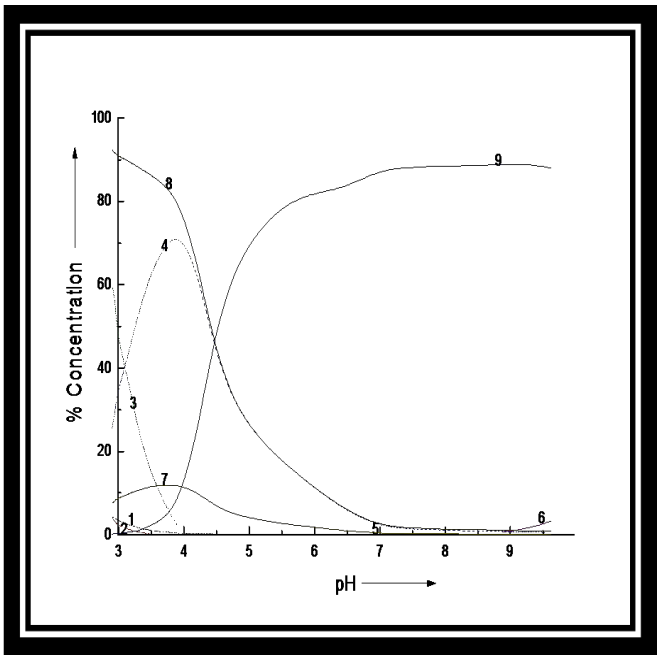


Figure 3. Distribution Curves of *(1:1:1)* Pb (II)-2-ASA (A) - 5-MU (B) System (1) Pb^{2+}(2) H_3A (3) H_2A (4) HA (5) BH (6) Pb A (7) PbB (8) Pb AB

The stability constants or log ß value ($ß_{p/qrst}$) of all the investigated species were calculated through the equation given as:

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

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

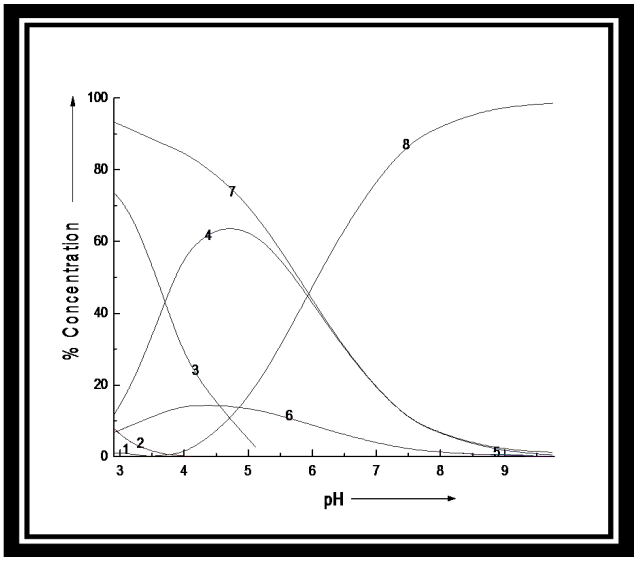


Figure 4. Distribution Curves of (*1:2:1*) Pb (II)-2-ASA (A) -5-MU (B) System
(1) Pb^{2+} (2) H_3A (3) H_2A (4) HA (5) BH (6) $Pb(OH)_2$ (7) Pb A (8) PbB (9) PbAB

Proton-ligand formation constant (log β_{00r0t}/ log β_{000st}) of 2-ASA - 5-MU at 37 ± 1^0C I = 0.1 $NaNO_3$

Complex	log β_{00r0t}/ log β_{000st}
H_3A	15.26
H_2A	13.33
HA	9.63
BH	9.94

Hydrolytic constants

Complex	(log β_{p000t}/ log β_{0q00t}) M^{2+} (aq.) ions
Pb $(OH)^+$	-9.84
Pb $(OH)_2$	-15.54

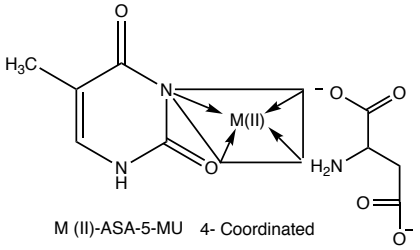
Metal-Ligand constants for Binary Systems

Complex	(log β_{p0r00}/ log β_{po0s0})
Pb -2-ASA	11.61
Pb- 5- MU	13.33

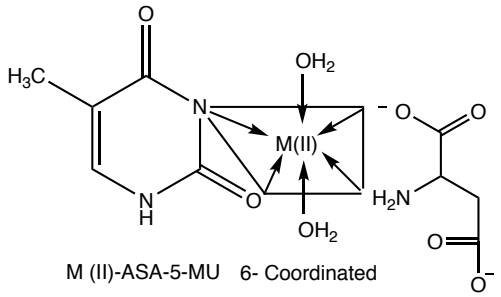
Metal-Ligand constants for Ternary Systems

Complex	(log β_{p0rs0}) value *(1:1:1)*	(log β_{p0rs0}) value *(1:2:1)*
Pb -2-ASA-5-MU	19.25	19.84

Structure of Complexes



M (II)-ASA-5-MU 4- Coordinated



M (II)-ASA-5-MU 6- Coordinated

4. Conclusion

The above study proves that the interaction between ligand and central metal Pb^{++} ion forming binary and ternary complexes through strong coordination bonds and remove them from the system in the form of soluble chelates and safe us from the bad effects of hazardous metal. These metals chelate have very impressive role in various fields such as agriculture, medical, biological, pharmaceutical and industrial fields etc. on which human as well as other living beings are totally dependent. So the metal ligand complexes have a great significance to serving our society.

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