



“SCOGS METHOD TO DETERMINE THE METAL –LIGAND FORMATION CONSTANTS”

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ABSTRACT: *Inorganic compounds have a specific property that is formation constant which can be determine easily and exactly by very advance computer programme “SCOGS” taking titration values of various investigating species like binary, ternary, and quaternary compounds where their graphical representation can be completed by another advanced computer programme ORIGIN.*

Keywords: Formation constant, Inorganic Compound, ORIGIN, SCOGS.

Introduction: Formation constant is very important factor for any inorganic compound so its determination should be correct and exact. In this paper we studied the formation constant of some binary, ternary and quaternary compounds of Hg(II), Pb(II), 2- amino 3-(4-hydroxyphenyl) propanoic acid (2-AHPPA) and 2,4-dihydroxypyrimidine (2,4-DHP). The 2-AHPPA, acts as primary ligand while 2,4-DHP acts as secondary ligand and give out several complex species and this primary ligand is a precursor to neurotransmitters would be useful during conditions of stress, cold, fatigue¹ loss of a loved one such as in death or divorce, prolonged work and sleep deprivation² with reductions in stress hormone levels, reductions in stress-induced weight loss seen in animal trials, improvements in cognitive and physicals performance seen in human trials.

Materials and Procedures:

In our study EDTA titrations³ were used for standardization of metal solution while the formation constants were determined with the help of very advanced computer program SCOGS⁴⁻⁶ (Stability constant of generalized species) and the potentiometric titration were completed with the help of Bjerrum’s⁷ method modified by Irving & Rossoti Technique^{8,9} using an electric digital pH meter (Eutech 501) having a reproducibility of ± 0.01 .



Solutions for various investigations:

Acid Solution: 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + H₂O

Ligand (A) Solution: 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5mL 2-AHPPA (A) (0.01M)
+ H₂O

Ligand (B) solution: 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5mL 2,4-DHP (B) (0.01M)
+ H₂O

Binary Solution: I - 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5mL 2-AHPPA (A) (0.01M) + 5mL
Hg/ Pb (II) (0.01M) + H₂O

Binary Solution: II - 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5mL 2,4-DHP(B) (0.01M) + 5mL Hg
/Pb (II) (0.01M) + H₂O

Ternary Solution: (1:1:1): 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5mL 2-AHPPA (A)
(0.01M) + 5mL Hg/ Pb (II) (0.01M) + 5mL 2,4-DHP (B) (0.01M) + H₂O

Quaternary Solution: (1:1:1:1): 5mL NaNO₃ (1.0M) + 5mL HNO₃ (0.02M) + 5 mL 2-
AHPPA (A) (0.01M) + 5 mL Hg (II) (0.01M) + 5mL 2,4-DHP (B) (0.01M) + 5 mL Pb (II) (0.01M)
+ H₂O

RESULTS AND DISCUSSION

Titration Curve and Species Distribution Curve:

The titration and species distribution curves were sketched by using 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. Some research worker¹⁰⁻¹³ studied in this field as we were completed our investigations.



Table.1

Hg(II) - Pb (II) - 2-AHPPA (A) - 2,4-DHP (B) system

Volume of NaOH (mL)	pH				
	A	B	C	D	E
0.0	2.52	2.74	2.92	3.20	3.10
0.2	2.62	2.86	3.14	3.65	3.30
0.4	2.73	3.04	3.59	4.48	3.66
0.6	2.87	3.37	4.69	5.21	4.35
0.8	3.11	5.84	5.77	5.87	5.59
1.0	3.65	8.68	6.50	6.71	6.20
1.2	9.70	9.20	7.16	8.41	6.94
1.4	10.29	9.61	8.04	8.96	7.80
1.6	10.53	9.95	8.79	9.35	8.32
1.8	10.68	10.20	9.38	9.67	8.49
2.0	10.79	10.39	9.86	9.95	8.60
2.2	10.88	10.54	10.15	10.16	8.76
2.4	10.95	10.66	10.34	10.33	8.86
2.6	11.00	10.75	10.47	10.45	8.96
2.8	11.05	10.83	10.58	10.55	10.06
3.0	11.10	10.89	10.67	10.63	10.16
3.2	11.14	10.95	10.74	10.70	10.26
3.4		10.99	10.80	10.76	
3.6		11.04	10.85	10.82	
3.8		11.07	10.90	10.86	
4.0		11.10		10.91	
4.2				10.95	
4.4				10.99	

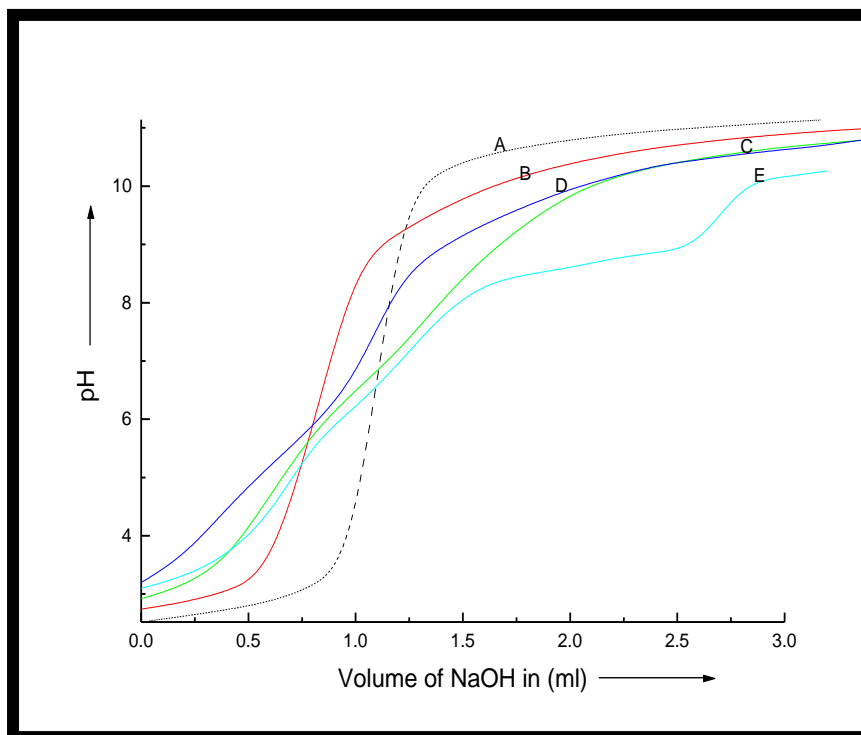


Fig. 1. Titration Curves of 1:1:1:1 Hg(II)-Pb(II)- 2-AHPPA (A) - 2,4-DHP(B) system
(A) Acid (B) Ligand (C) Hg(II)- 2-AHPPA (D)Hg(II)- 2-AHPPA - 2,4-DHP (E)Hg (II)-Pb(II) 2-AHPPA
- 2,4-DHP

Hg(II)-Pb (II)- 2-AHPPA (A) - 2,4-DHP (B) system

The distribution diagram of present system is represented in given fig. Distribution diagram provide evidence for existence of following species Hg^{2+} , Pb^{2+} , H_3A , H_2A , HA , $\text{Hg}(\text{OH})_2$, $\text{Hg}(\text{OH})^+$, PbB , HgAB , PbAB and Hg Pb AB .

It is clearly evident from species distribution diagram that the protonated ligand species viz H_3A , H_2A , HA are found to be in decreasing manner. Binary complex of Hg A and Hg B shows their no existence and binary complex of another metal with ligand PB- A is not found also. Pb B complex attain the maximum concentration $\sim 23\%$ at the start of titration. Ternary complexes of Hg AB existed with maximum concentration $\sim 22\%$ at the ~ 7.2 pH while the PbAB existed with maximum concentration $\sim 75\%$ at the ~ 9.0 pH. The major species which is quaternary complex of Hg Pb AB attain the maximum concentration $\sim 78\%$ at the ~ 7.3 pH. Hydroxo species $\text{Hg}(\text{OH})_2$ shows very well existence in this system.

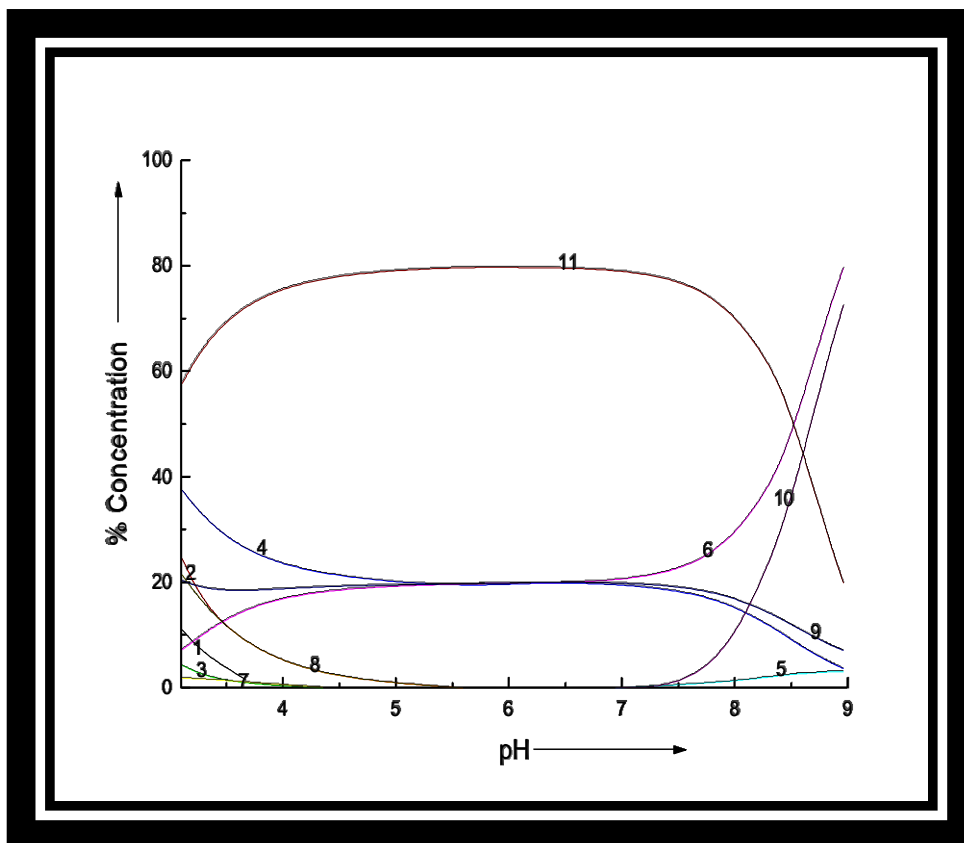
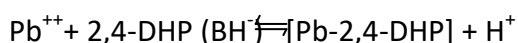
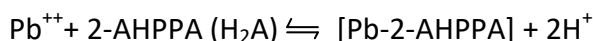
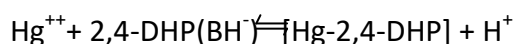
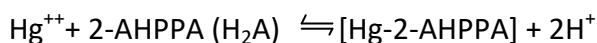


Fig 2- Distribution Curves of 1:1:1:1Hg (II) - Pb (II)-2-AHPPA (A)- 2,4-DHP (B)System

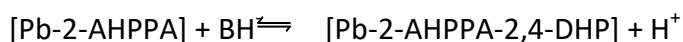
(1) $\text{Hg}^{2+}(\text{II})$ (2) $\text{Pb}^{2+}(\text{II})$ (3) H_3A (4) H_2A (5) HA (6) $\text{Hg}(\text{OH})_2$ (7) $\text{Hg}(\text{OH})^+$ (8) Pb B (9) HgAB (10) Pb A B (11) Hg Pb AB

Equilibria of complex formation:

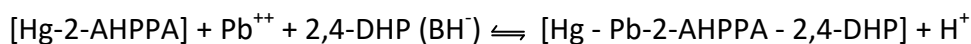
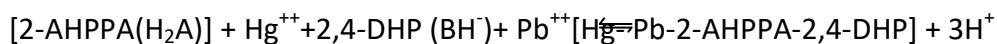
Formation of binary complexes:



Ternary complex formed through two ways:

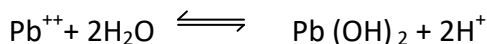
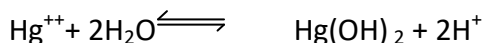
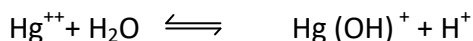


Quaternary complex formed through two ways:



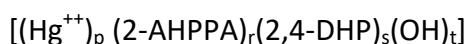
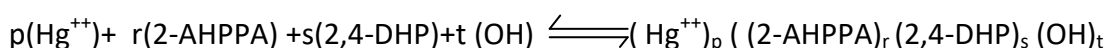


General hydrolytic equilibria are as follow:

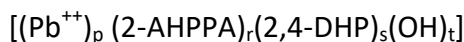
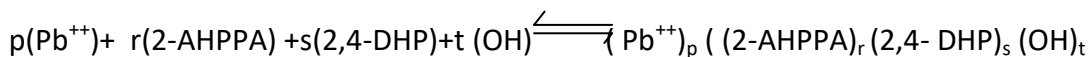


Determination of formation constant:

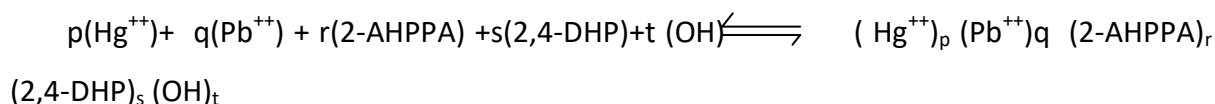
Formation constant of all the investigated complexes can be determined by the equation:



$$\beta_{p/qrst} = \frac{[(\text{Hg}^{++})_p (2\text{-AHPPA})_r (2,4\text{-DHP})_s (\text{OH})_t]}{[\text{Hg}^{++}]^p [2\text{-AHPPA}]^r [2,4\text{-DHP}]^s [\text{OH}]^t}$$



$$\beta_{p/qrst} = \frac{[(\text{Pb}^{++})_p (2\text{-AHPPA})_r (2,4\text{-DHP})_s (\text{OH})_t]}{[\text{Pb}^{++}]^p [2\text{-AHPPA}]^r [2,4\text{-DHP}]^s [\text{OH}]^t}$$



$$\beta_{p/qrst} = \frac{[(\text{Hg}^{++})_p (\text{Pb}^{++})_q (2\text{-AHPPA})_r (2,4\text{-DHP})_s (\text{OH})_t]}{[\text{Hg}^{++}]^p [\text{Pb}^{++}]^q [2\text{-AHPPA}]^r [2,4\text{-DHP}]^s [\text{OH}]^t}$$

β = Formation constant, $p = M_1, q = M_2$,

r = primary ligand, s = secondary ligand and t = hydroxo species.

Formation Constants of Investigated Complexes:

- Proton-ligand formation constant ($\log \beta_{00r0t} / \log \beta_{000st}$) of 2-AHPPA - 2,4-DHP at $37 \pm 1^\circ\text{C}$ $I = 0.1 \text{ NaNO}_3$

Complex	$\log \beta_{00r0t} / \log \beta_{000st}$
H ₃ A	21.35
H ₂ A	19.18



HA	10.14
BH	9.49

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

Complex	Hg	Pb
$M(OH)^+$	-3.84	-9.84
$M(OH)_2$	-6.38	-15.54

- Metal-Ligand constants ($\log \beta_{p0r00} / \log \beta_{0qr00} / \log \beta_{p00s0} / \log \beta_{0q0s0}$) Binary System

Complex	Hg	Pb
MA	12.25	4.14
MB	13.08	12.77

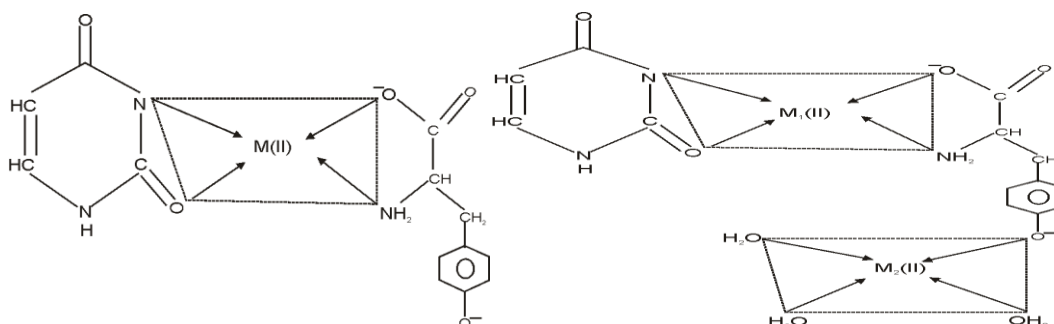
- Metal-Ligand constants ($\log \beta_{p0rs0} / \log \beta_{0qrs0}$) : Ternary System(1:1:1)

Complex	Hg	Pb
MAB	21.82	18.48

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

Complex	Hg-Pb
$M_1 - M_2 - A - B$	29.58

Proposed structures:



Conclusion:

It is well known fact that metal- ligand interaction depend on the formation constant, pH of the solutions and relevant pK. In our experiment we study the some binary, ternary and quaternary inorganic compound and formation constant of each species have a specific and definite value having a specific stability order. So our study provides an easy and qualitative method to determine the formation constant of different species.



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