Study of Stability Constant of Cu(II)-Simazine Complex Spectrophotometric ally

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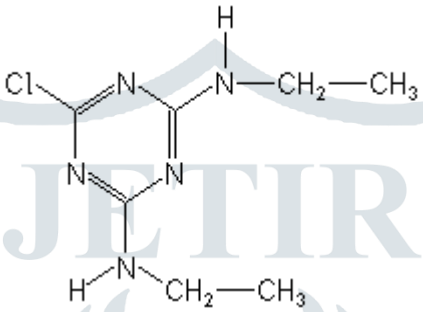
Abstract:- **Simazine is a herbicide. The formation of Cu(II) complex with simazine has been studied spectrophotometrically at an absorption maximum of 240 nm. The data shows that Cu(II) simazine form two types of complexes in the ratio1:3 and 3:1. The stability constant of complex was determined to be β3 (CuL3) = 2.74x 10^{10}.**

1. INTRODUCTION

The trade name of [2-chloro-4,6 -bis (ethylamino)-1,3,5- triazine] is simazine



It is widely used as herbicide. Simazine has been reported to be used as an outstanding pre- emergence and post-emergence herbicide for weed control in corn, tomatoes, potatoes, asparagus and grapes [1]. The metal ions are important catalysts for a variety of enzyme reaction for e.g.group transfer, proton transfer etc. It is very much necessary to assess quantitatively the interaction of metal ions with these ligands. The transition metal ions are micro-nutrients for plants and animals. The coordination compounds of transition metal ions play vital role in biology [2, 3] .Therefore, a study of transition metal ion complexes with simazine is of great importance for the biological point and it is likely to contribute to a better understanding of interaction of it with metal ions. Due to the presence of lone pair of electrons with nitrogen & chlorine atoms, Simazine can function as a Lewis base to transition metal ions which are Lewis acids.

2. EXPERIMENTAL

- **APPRATUS**

Spectrophotometric measurements were performed on UV spectrophotometer VSU2.A systronic model 331 pH meter with glass and calomel electrode assembly was calibrated with buffer solution of pH 4.0and 7.0.

- **REAGENTS**

Simazine [2-chloro-4,6 -bis (ethylamino)-1,3,5- triazine] was crystallized from methanol and crystals dried under vacuum over anhydrous calcium chloride (m.pt. 226ºC).Copper chloride of A.R grade was procured from BDH. Double distilled water was used throughout the study.

- **PREPERATION OF REAGENT SOLUTIONS**

0.01M simazine solution: 0.05038g (0.01M) of simazine was dissolved in minimum quantity of 5N HCl and diluted to 250ml in a measuring flask.

0.01M metal salt solution**:** Metal salt solution was prepared by dissolving the calculated quantity of salt in double distilled water. The solution was standardized by standard methods.

Buffer solution: Buffer solution of pH 4.0 and 7.0 were prepared by dissolving the standard pH buffer tablets. Other reagents:0.01M sodium hydroxide and 1.0M sodium perchlorate solution was prepared.

- **PROCEDUCERS**

Continuous variation method

0.5 mL of $1x10^{-2}$M Copper (II) chloride solution (0.1,0.2…….1.0ml) was pipetted out into 11 flasks of 10 ml capacity and (1.0,0.9…… 0 ml) of simazine solution was added. To each flask was added 0.5 ml of 1.0M sodium perchlorate solution then volume was made to the mark. The wave length of maximum absorbance was noted against reagent blank, which appeared at 240 nm. All the measurements were made at 240 nm and 3.4 pH.

3. RESULTS AND DISCUSSION

Simazinepossesses lonepair of electron with nitrogen and chlorine atom. Therefore, it is expected to form metalions whichare Lewis acids. As no visible colour of high intensity appeared,the study was completed in the UV region(200-400 nm). The composition and other characteristics of the complex such as selection of maximum wavelength, pH and nature of complex were studied. Experimental results obtained are given in the table and figures.

- **COMPLEXATION AND SELECTION OF WAVELENGTH**

In order to study complexation and select wavelength for maximum absorbance following three solutions were prepared in 10 mL measuring flask.

(1) 0.5 mL of $1x10^{-2}$M metal ion solution.
(2) 0.5 mL of $1x10^{-2}$M metal ion solution +1.0 ml of $1x10^{-2}$Msimazine solution.
(3) 1.0 mL of $1x10^{-2}$M simazine solution

To each flask, 0.5 M $NaClO_4$ was added to make final volume was 10 mL in measuring flask while 1MNaOH was added to adjust the pH to 3.The metal ion solution containing $NaClO_4$ was used as reagent blank. Experimental data is given in Table 1 and Figure 1 which shows that the title complex has maximum absorbance at 240 nm.

Table 1: Data for absorbance of Simazine, Simazine+Cu(II)

Wave Length (nm)	Absorbance	
	Simazine	Simazine+Cu(II)
210	0.40	0.10
215	1.85	0.15
220	2.35	0.23
225	2.85	0.80
230	1.84	1.80
235	1.93	2.64
240	0.43	2.85
245	-	2.80
250	-	2.66
255	-	2.60
260	-	1.04

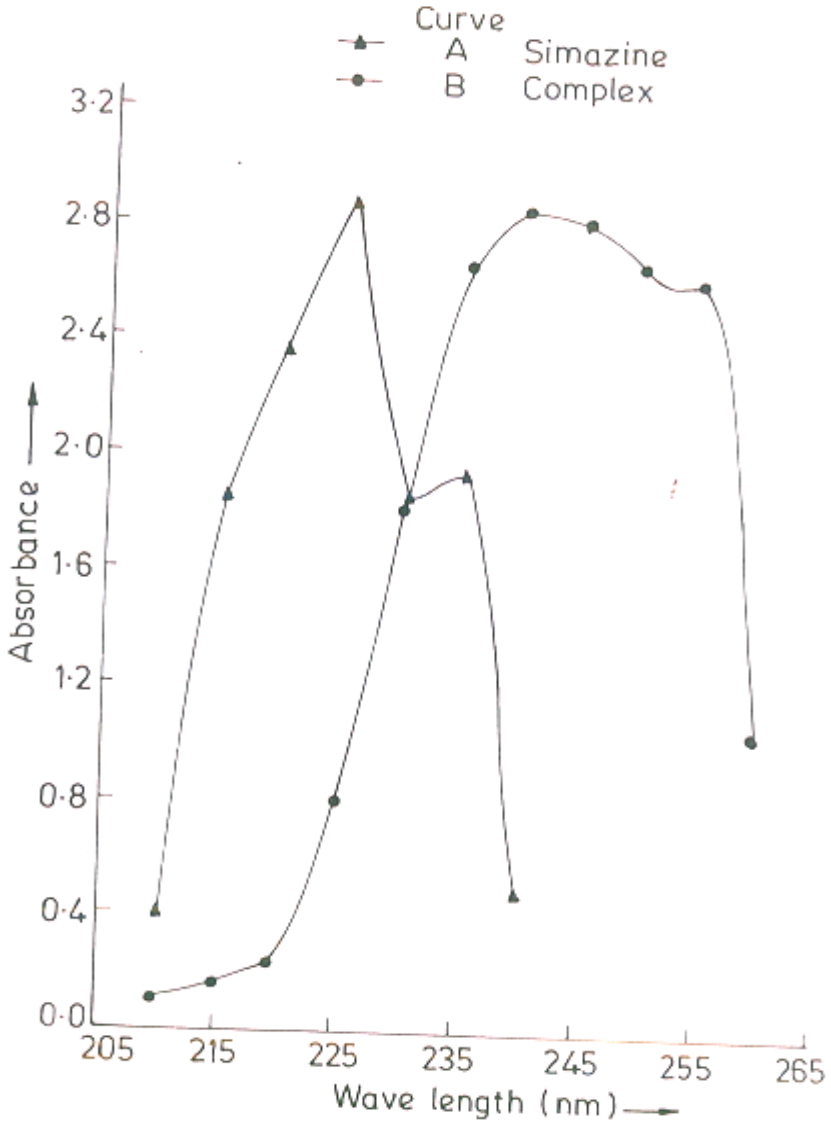


Figure 1: Curve for Selection of λmax of Copper Complex

- **SELECTION OF pH**

The pH curve indicates that precipitation occurs at pH 3.5. Hence the suitable pH value for complex formation is 3.4 (Table 2 and Figure 2)

Table 2: Absorbance of Copper complex at different pH

pH	Absorbance
	Copper complex at λmax=240nm
2.0	-
2.4	2.76
2.8	2.80
3.2	2.82
3.4	2.86
3.6	2.88
3.8	Precipitation _

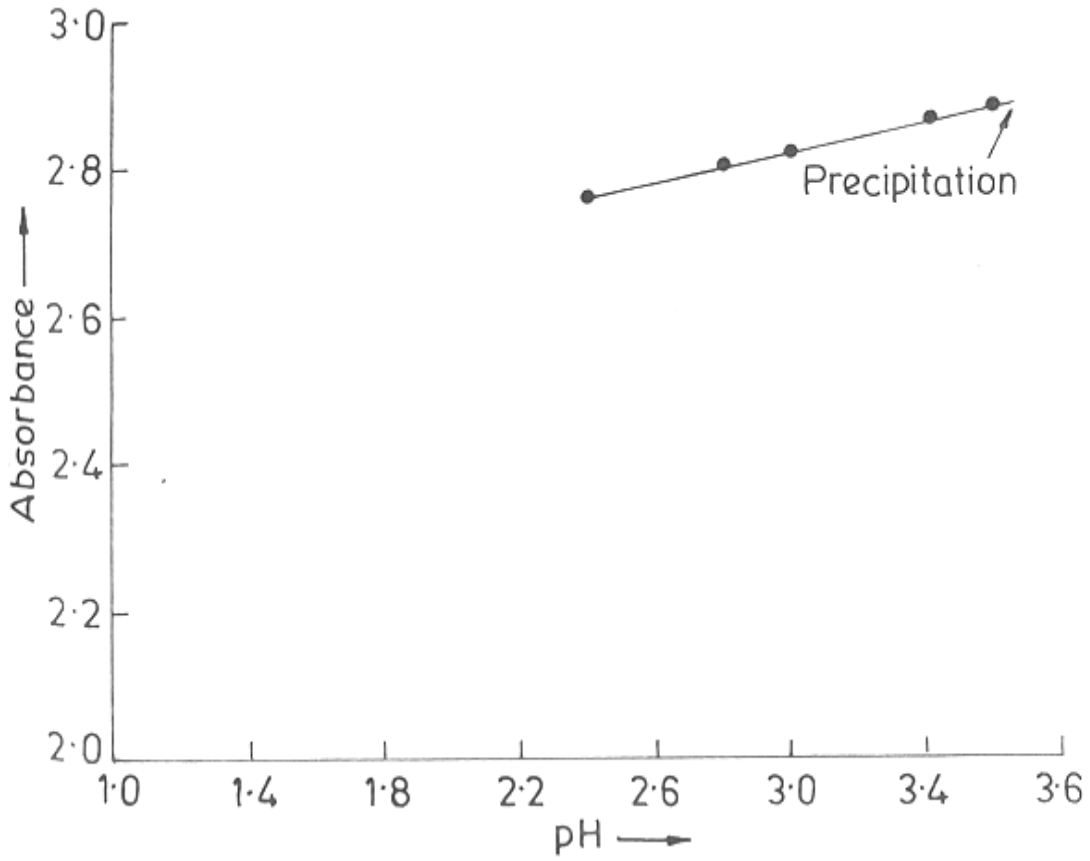


Figure 2: Curve for Selection of pH for Copper Complex

- **NATURE OF THE COMPLEX**

The nature of the complex was studied by using the method of Vosburg & Cooper [4]. Experimental data is given in Table 3 and Figure 3.

Table 3: Absorbance of Copper complex with different composition a various wave lengths in 0.05 M $NaClO_4$

Wave Length (nm)	Absorbance for the Metal:Ligand Ratio		
	(1:1)	(1:2)	(1:3)
210	0.06	0.10	0.20
215	0.09	0.15	0.22
220	0.20	0.23	0.25
225	0.75	0.80	0.80
230	1.75	1.80	1.85
235	2.60	2.64	2.70
240	2.80	2.85	2.90
245	2.75	2.80	2.85
250	2.60	2.66	2.70
255	1.42	2.60	-
260	-	1.04	1.53

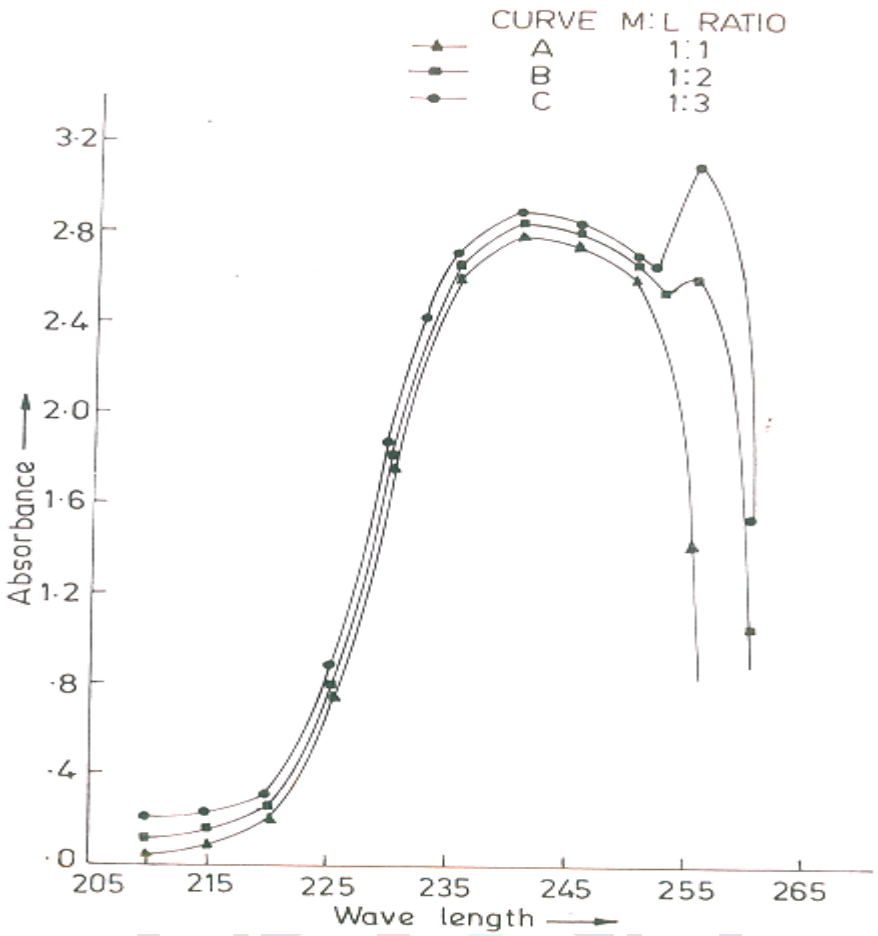


Figure 3: Absorbance Curve for Copper Complex

The plots of absorbance versus wavelength indicate that the curve for different simazine:metal ratios are similar in shape but the curves exhibits a trend which on the smaller wavelength side of 240nm is different from that on the longer wave length side. This may be due to the formation of more than one type of complex.The exact stoichiometry was determined by method of continuous variation.

- **COMPOSITION OF COMPLEX**

Job's method of continuous variation method was used to study the composition of the complex. Experimental data is given in Table 4 and Figure 4.

Table 4: Absorbance of Copper complex at different metal: ligand ratio to find the composition and stability by Job's method.

Metal ligands:Ratio	Absorbance	
	Molar concentration 0.01M	Molar concentration 0.02M
1:9	0.16	0.22
2:8	0.52	0.57
3:7	0.78	0.86
4:6	1.00	1.07
5:5	1.21	1.28
6:4	1.44	1.50
7:3	1.64	1.70
8:2	1.76	1.82
9:1	1.80	1.86

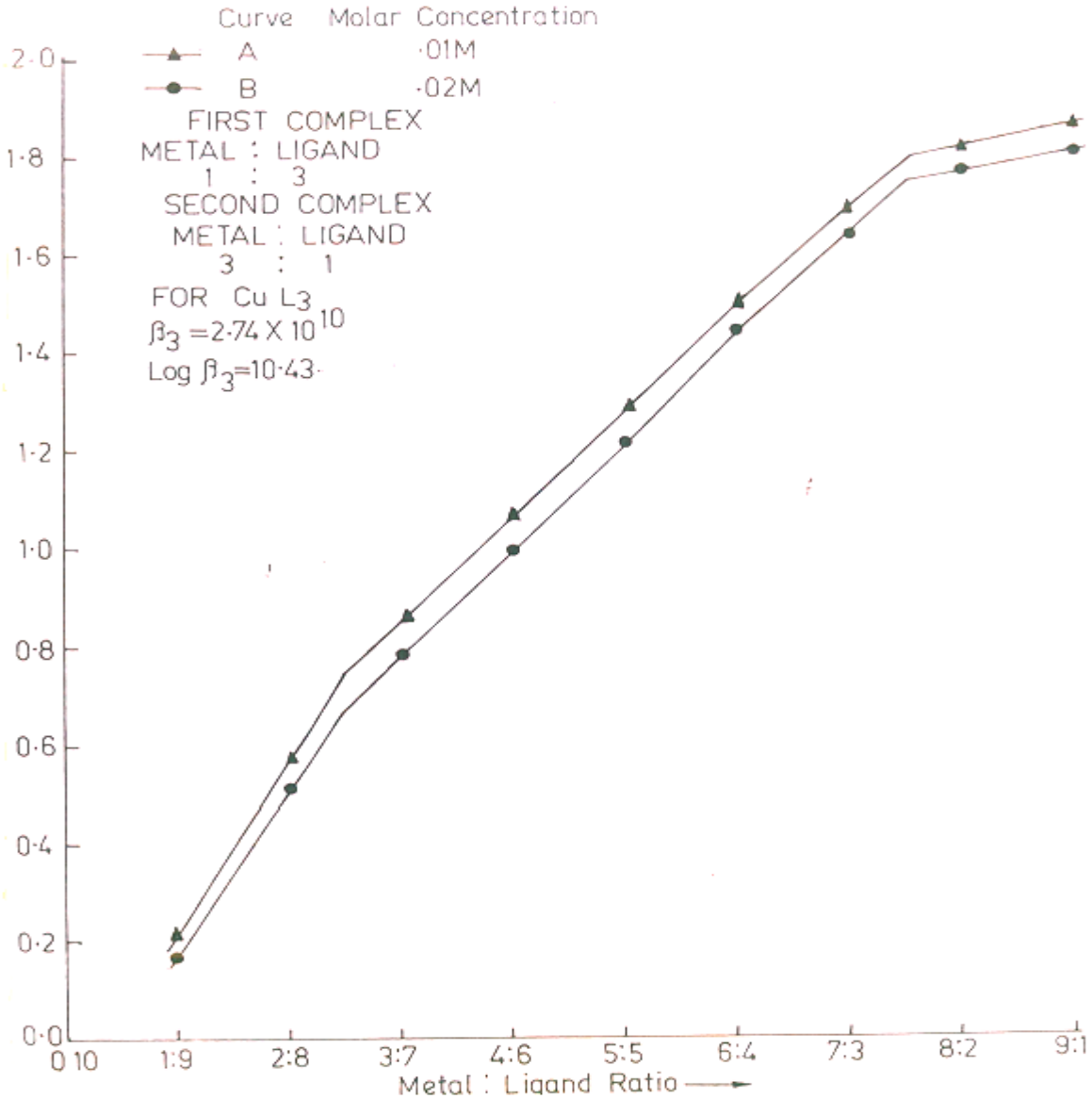


Figure 4: JOB'S Method for Composition & Stability of Copper Complex

The curves show the formation of two types of complexes. One type of complex show metal:ligand ratio 1:3 and other 2:1. First type of complex is formed when ligand is excess and second when metal ion is in excess.

- **STABILITY CONSTANT**

The overall stability constantß3 for CuL3 was determined to be 5.87x109. This indicates that the complexe is very stable. This may affect the uptake of Cu from the soil.

4. CONCLISION

The overall stability constant was determined to be β3(CuL3) = 5.87 x 109. The value indicates that the complex is highly stable. The optimum pH for complex formation was found to be 3.4 and maximum wavelength of absorption (λmax) of the complex was determined to be 240nm.

REFERENCES

[1] Bartley, E..Nyton 1957. "Simazine and related triazine compound as pre-emergence and post-emergence herbicides" Proc. N. Central Weed Control Conf., 13th Meeting.

[2] R.R. Holmes, J.C. Brown 1955. "Soil Sci",: 80-169.

[3] Tassanert 1798. "cf. an introduction to coordination chemistry by Gradoon, 1961."

[4] W.C. VosburG, G.R. Cooper, J.Am.Chem. Soc. 1941 : 63-427.