Section A -Research paper

SYNTHESIS AND EVALUATION OF TRIAZINE BASED SCHIFF BASE METAL COMPLEXES AND THEIR STABILITY CONSTANTS AND BIOLOGICAL ACTIVITY

S. T. Sankpal[1] and R. R. Surve[2]

[1]Assistant Professor, Department of Chemistry A.S.P. College, Devrukh, Ratnagiri, India
[2]Assistant Professor, Department of Chemistry, A.C.S. College, Lanja, Ratnagiri India

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Abstract

The Hugo Schiff base comprises the Azomethine moiety formed by the reaction between The Carbonyl moiety and Amine groups. Schiff bases of aminotriazine treated with isatin have been synthesized in this project. Complexes of Nickel, Cobalt, Iron, and Chromium's transition metals have also been produced. They were identified using IR, NMR, Mass spectra and UV-Vis spectra. Utilizing spectrophotometric methodology, their stability constants were determined. It has been determined that the stability constants of Cobalt and Nickel are greater than those of Chromium and Iron owing to their higher binding capacities. They were discovered to have good antibacterial activity after screening with a few bacteria.

Keywords: Triazine, Schiff Base, Isatin, Stability constant, Transition metal

1. INTRODUCTION

Schiff base is simply considered by the presence of an Azomethine group which is produced through the condensation reaction of the carbonyl moiety with the primary amine group (1, 2). This Hugo Schiff base is distinguished by its capacity to form bonds with a variety of metal ions, which significantly expands its usefulness across a variety of domains. Schiff bases find widespread use in a variety of fields, including the analytical chemistry, catalysts, food industry, the dye industry, agrochemical, fungicidal and biological activity. This Schiff bases have vast applicability in maximum of the fields, particularly in the pharmaceutical area; as a result, the attention of many researchers is increasing on the growth of more unique Schiff base and their transition metal complexes. Primary emphasis of the current research is a unique synthesis of Schiff base achieved by mixing a Triazine derivative with isatin, as well as an investigation into the antibacterial properties of this compound. Triazine and isatin are heterocyclic compounds consists of an amino group and keto group as their main moiety respectively. Modern potent

antibiotics have replaced Triazine. Because of the prevalence of antibiotic resistance in the pharmaceutical area, triazine and isatin combination Schiff base and their metal complexes are of considerable research attentiveness.

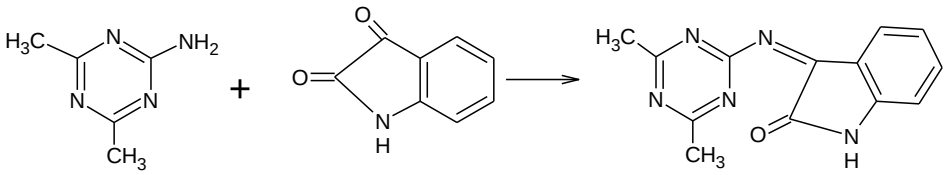
2. METHODS AND MATERIAL

- **Experimental methods**

The preparation of Schiff base with metal complexes was accomplished by adhering to the standard operating procedures. The substances were all purchased from Merck.

- **Synthesis of depicted Schiff Base:**

The following Schiff bases is synthesized by refluxing mixture of isatin and triazine based amine in ethanol. 1 milimole of each isatin and triazine based amino compound in 10 cm^3 ethanol was taken in the RBF. This refluxed for a total of three hours.. After the process of refluxing had been completed, the substance was allowed to cool in air. After being collected in its solid condition, the Schiff base was then cleaned, recrystallized through the use of ethanol and dried and desiccated for a few minutes. The ligand is steady at room hotness. It is solvable in chloroform and alcohol at elevated temperature even in DMSO and DMF (3, 4).



- **Synthesis of Metal Complexes:**

The complexes of metal are prepared by the reflux in the ethanol solution of the ligand that was prepared earlier in a 2:1 mole ratio with metal chloride. To produce the metal complex, 2 mill moles of the ligand that was prepared earlier in a small excess were taken in an RBF with 25 ethanol. It is capable of dissolving Schiff bases. One millimole of metal chloride was added to 5 cm^3 of alcohol and stirred. The metal chloride solution was then slowly drizzled into the heated ligand. The pH is kept between 7.5 and 8.0 with the help of a few drops of diluted ammonia. The contents went through a three-hour process of refluxing. After being filtered, the precipitate of compound that had formed was washed with diluted ammonia, and then it was dried out in a desiccator. (4, 5, 6)

3. RESULTS AND DISCUSSION

In accordance with the instructions in the experiments section, Schiff base was synthesized, crystallized, dried, and submitted to an elemental analysis.

- **Physical Properties of Schiff Bases**

Molecular formula of the ligand formed is found to be C13H11N5O and color id dark red with melting point above 300 ^{o}C. The molecular weight of the compound is 253.26 with practical yield 92.25 percent. Elemental analysis found to be C (61.65%) H (4.38%) N (27.65%) O (6.32%) (7, 8)

IR Spectral Analysis

Compound	Wavelength (cm^{-1})			
	v (C-0)	**v (C=N)**	**V (M-N)**	**v (M-O)**
Ligand L	1072.93	1714.32	-	-
Co-L	1054.49	1713.70	662.21	732.04
Ni-L	1100.10	1697.50	640.30	672.46
Cr-L	1074.07	1712.06	656.42	668.39
Fe-L	1077.35	1716.74	636.13	674.05

The Infrared spectra of aforementioned synthesised Schiff Base show a -C=N- (azomethine) stretch band at 1714.32 cm^{-1}, allotted to the azomethine -C=N- moiety, confirming the reaction condensation in between the primary amino (-NH_2) group of aminotriazine and the Schiff base's ketone of isatin. The presence of an infrared band with a wavelength of around 1713.70 cm-1 in the IR spectra of the Schiff base Co complex is evidence that azomethine contributes electrons to Co^{2+} producing metal complex. The IR spectra of Schiff Base shows that the azomethine group's IR band around 1714.32 cm^{-1} shifts to 1697.50 cm^{-1}, confirming that azomethine transfers electrons to the Ni^{2+} producing metal complex. This verifies that azomethine contributes its electrons to the Cr^{2+} producing metal complex, as seen by the shift in the position of the IR band around 1712.06 cm^{-1} in the IR spectra of the Schiff Base Cr complex, which was originally at 1714.32 cm^{-1}. The Schiff base Fe complex's IR spectra reveal an IR band at about 1716.74 cm^{-1}, indicating that azomethine provides their electrons to the Schiff base metal complex's Fe^{2+} formation. (9, 10).

- **NMR Spectral Analysis**

Benzene is indicated by a peak at the 7.4 to 7.9 ppm with multiplet. The -NH_2 peak group is typically produced at 8.9 ppm, but the absence of the peak for the -NH2 group indicates that

condensation activity is taking place. The peak for –CONH- remains same around 9.1 singlet. Other H, of triazine ring remains same at 6.1 Singlet (11).

- **Mass Spectral Analysis**

According to the mass spectral study, the Schiff base complex ligand's synthesis is indicated by the molecular ion with the peak at 256.23 m/e, which is subsequently fragmented to produce other smaller peaks.

Conductance and Electronic absorption Spectra

Sr. no.	**Compound**	**Molar Conductance Ω -1cm2mol-1**	**Magnetic Properties**	**Absorption Maxima cm-1 (nm)**	
				3A2g →3T2g(F) Weak	Charge transfer Strong
1	Co-L	34.3	Paramagnetic	7200, 10,000	19000
2	Ni-L	29.2	Diamagnetic	450nm(27000)	270nm(35714), 350nm (27700)
3	Cr-L	33.2	Paramagnetic	8300, 11,000	20000
4	Fe-L	35.1	Paramagnetic	8500, 12,000	21000

Octahedral Complexes typically have three bands, with the first one ranging from 7000 to 13000 cm^{-1}, the second from 10,000 to 20,000 cm^{-1}, and the lastly from 19,000 to 27,000 cm^{-1}. Contrarily, square planar geometry complexes exhibit substantial absorption bands from 15,000 to 25,000 cm^{-1} and also with 25,000-35,000 cm^{-1}, as well as a actual little absorption group near 13,000 to 11,000 cm^{-1}. These bands can be found in the spectral region. As a result, it is clear from the information presented above that the Nickel complexes that are formed have a square planar structure, while all the other structures have an octahedral geometry. (4, 12, 13)

- **Stability constant of complexes**

The equilibrium constant of the compounds was determined by measuring the absorbance of five solutions of complex compounds with known concentrations. The respective concentrations measured were 0.001, 0.002, 0.003, 0.004, and 0.005moldm-3. Using Beer's Lambert law, the stability constants were derived. From the Beer's law plot, the complex's molar absorption

coefficient was calculated. Using Beer's law and the dilution formula, the molar absorptivity was used to figure out the equilibrium concentration of each complex compound. (14, 15, 16).

Following is an expression that was used to define the equilibrium concentration of both the metal ion and the ligand.

$[M^{2+}]_{eqm} = [M^{2+}]_0 - [Complex]$

$[L]_{eqm} = [L]_0 - x\ [Complex]$

Because of this, the equilibrium constant, Kf, was determined using the relation;

$[complex] /[M^{2+}]_{eqm}\ [L]^x{}_{eqm}$

Gibbs free energy can be calculated by using relation: $\Delta G=RT\ lnK$

Complexes	**Stability Constant**	**ΔG joule/mol**
Co-L	3.208×10^2	-14297.62
Ni-L	3.807×10^2	-14721.76
Cr-L	2.349×10^2	-13525.46
Fe-L	3.00×10^2	-14131.53

- **Antimicrobial activity**

By using the agar cup plate diffusion method and computing the inhibition zones in millimetres, the antimicrobial effect was analysed and evaluated. The in-vitro antibacterial action of the produced metal complexes and as well as that of the standard was evaluated using four different strains of bacteria. These bacteria included gram-positive bacteria like *S. Aurious* and *S. Pyogen* as well as gram-negative bacteria such as *P. Aeraginosa and E. Coli*. According to the findings of the antimicrobial activity of complexes, the synthesized complexes have effective antibacterial activity not only in contradiction of the gram-positive bacteria but also against gram-negative bacteria. Therefore, the molecule that was just described exhibits very strong antibacterial activity. (17, 18).

Bacterium	Zone Inhibition (mm) with 1000 ppm concentration of each solution			
	Co-L	Ni-L	Cr-L	Fe-L
E.Coli	15	07	24	17
P.Aeraginosa	15	09	13	12
S.Aurious	14	08	15	15
S.Pyogen	12	05	16	13

3. Conclusion

On treatment with isatin, Schiff bases of aminotriazine have been synthesised. Complexes of their transition metals, such as Nickel, Cobalt, Iron, and Chromium, have also been synthesised. They were identified using IR, Mass, NMR and UV-Vis spectra. From the data, it is clear that Nickel complex is having square planar geometry whereas all other have octahedral geometry. +- Utilizing spectrophotometric methodology, their stability constants were determined. It has been determined that the stability constants of Cobalt and Nickel are greater than those of Chromium and Iron owing to their higher binding capacities and also above mentioned compound have excellent antimicrobial properties.

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