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1,2,4-TRIAZOLE DERIVED SCHIFF BASES AND THEIR BIOLOGICAL IMPORTANCE

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Abstract

The Zn(II) and Ni(II) complexes of Schiff base derived from 4-Amino -1,2,4-triazole with Salicylaldehyde has been synthesized keeping in view that metal complexes are found to be more powerful than their parent drugs. The synthesized complex has been characterized by, elemental analysis, IR, ESR studies. The spectroscopic studies showed that the presence of azomethine nitrogen in coordination to the metal ion and octahydral geometry of the metal complexes has been projected.

Keywords: *4-Amino -1,2,4-triazole, conductivity, metal complex, Schiff base,Spectral studies.*

2. Introduction

Schiff bases are aldehyde or ketone like compounds in which the carbonyl group is replaced by an imine or azomethine group.[1-2] These are used as chelating ligands in the field of coordination chemistry and their metal complexes are of great interest for many years.[3] Many Schiff bases and their complexes have been widely studied because of their industrial and biological applications. [4-5]Schiff bases, as an important class of ligands plays an important role in the development of coordination chemistry as they can easily form stable complexes with most of the transition metals.[6] The coordination compounds of transition metals are found to have added a great deal of interesting flexibility in the areas such as biological, industrial, pharmaceutical, catalysis and material chemistry.[7-10] Schiff base–transition metal complexes are one of the most adaptable and thoroughly studied systems.[11-12] These complexes have also applications in clinical[13] and analytical fields.[14]

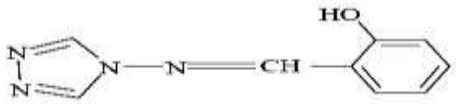
3. Materials and methods

3.1 Chemicals

All the chemicals used were of GR/AR grade. A pure sample of 4-Amino-1,2,4-Triazole, molecular formula $C_2H_4N_4$ was obtained from Loba Chem. Ltd. The metal salt of $ZnCl_2$ and $NiCl_2$ were from Hi-media Pharmaceuticals Ltd. Solvents used were ethanol, acetone, and DMF.

3.2 Synthesis of Ligand:

Equimolar mixture of 4-amino-1,2,4-triazole(0.1 mol) and 2-hydroxybenzaldehyde (0.1 mol) in 30 ml of ethanol was refluxed for about 2 hours followed by the addition of few drops of Sulphuric acid. The product, which was separated out as a crystalline solid on cooling, was collected and recrystallized from the ethanol.



4-(2-hydroxy arylidene-amino)-4*H*-[1,2,4]-triazole

3.3 Synthesis of Metal Complexes:

0.02 M concentration of Schiff base in 30 ml of ethanol and 0.01 M concentration of metal salt of $ZnCl_2$ and $NiCl_2$ in 30 ml of ethanol. The resulting solutions were mixed and refluxed for about 3 hours with occasional shaking until precipitation occurs. After precipitation, the resulting complex were collected by filtration, washed with the same solvent and recrystallized with acetone.

3.4. Physical Measurements:

Elemental analysis was performed on Perkin Elmer 24 ^{O}C Model Elemental Analyzer at Powai, IIT, Bombay. The infra-red spectra of Schiff base and derived complexes were recorded with FT-IR spectrophotometer Model RZX (Perkin Elmer) using KBr pellets in the range of 400 cm^{-1}-4000cm^{-1} at SAIF, Panjab University Chandigarh. Electronic spectra were also recorded on a UV-VIS-Spectrophotometer Model Synthesis Lambda 750 Perkin Elmer at SAIF, Panjab University, Chandigarh.

3.5.Biological Activity:

Schiff bases and its derived metal complexes were tested against one Gram-positive and one Gram-negative bacterial strains. *The in-vitro* antibacterial activity of the Schiff base and its derived metal complexes was determined by Disc diffusion method[15] against bacterial strains. The test organisms were grown on Nutrient Agar medium in Petri plates and then agar plates were left to solidify at room temperature. After solidification, the disc of Whatman filter paper with 20µL of prepared Schiff base and metal complex solutions was carefully placed with the help of forceps at the center of the Petri dish and then kept at 37±0.1^{o}C for 24 hours in an incubator. The zone of inhibition was measured.

4. Results and Discussion

The Schiff bases are subjected to elemental analyses. The results of elemental analyses (C, H, N, S) with molecular formula are presented in Table 1. The analytical data for the complexes suggested 1:2 stoichiometry for the entire synthesized complex.

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Ligand /Complex	Mol. Wt	Color	M.P (^oC)	Elemental Analysis (%) Found (Calculated)			
				C	H	N	M
At-S $C_9H_8N_4O$	188.18	White	170	58.19 (57.90)	4.00 (4.18)	31.90 (28.9)	-
$[Zn((At-S)_2]$ $C_{18}H_{14}N_8O_2Zn$	439.74	Cream	237	49.57 (49.18)	3.12 (3.18)	25.48 (25.50)	14.75 (14.80)
$[Ni(At-S)_2].2H_2O$ $C_{18}H_{18}N_8O_4Ni$	469.08	Bluish Green	280	45.91 (46.07)	3.00 (2.47)	19.10 (19.55)	19.95 (18.60)

Table: 1 Elemental analysis of Schiff base and its derived metal complex

4.1 IR Spectral Studies:

The comperative interpretation of Schiff base and derived metal complexes were shown in table 2. The IR spectra of complexes indicates that the Schiff base (ligand) acts as a tridentate ligand, using phenolic oxygen[16] and azomethine nitrogen and nitrogen of triazole ring as donor atoms. The ligand shows the strong band at 3325 cm^{-1} due to phenolic –OH group. This band is absent in the respective metal complexes indicating the involvement of this group in complex formation.[17-18] The IR spectrum of the Schiff base shows a strong band at 1620 cm^{-1} attributed to $^{\nu}$(HC=N) stretching vibrations of the azomethine group, which gets shifted to higher frequency regions 1638 cm^{-1} and 1645 cm^{-1} in the complexes representing involvement of the nitrogen atom of azomethine group.[19-21] The band at 1469 cm^{-1} is due to the $^{\nu}$(C=N) stretching and this frequency shifted to a lower frequency value of 1545 cm^{-1} and 1522 cm^{-1} in the complexes confirming the involvement of the (C=N) in the coordination with the metal ions[22]. The stretching vibrational band C-O of the ligand lies at 1246 cm^{-1} frequency.[23-24] This band shifts to 1426 cm^{-1} lower frequency side in the complex of Zn(II) and 1373 cm^{-1} a lower frequency side in the complex of Ni(II).

Ligand/ Complex	(HC=N)	C-O	C=N	OH	Chelate ring
AT-S	1620s	1246s	1469s	3325s	1435s
AT-S-Zn	1638s	1426s	1545s	-	1428s
AT-S-Ni	1645s	1373s	1522s	-	1415s

Table: 2 IR Spectra band values

4.2 Electronic Spectra

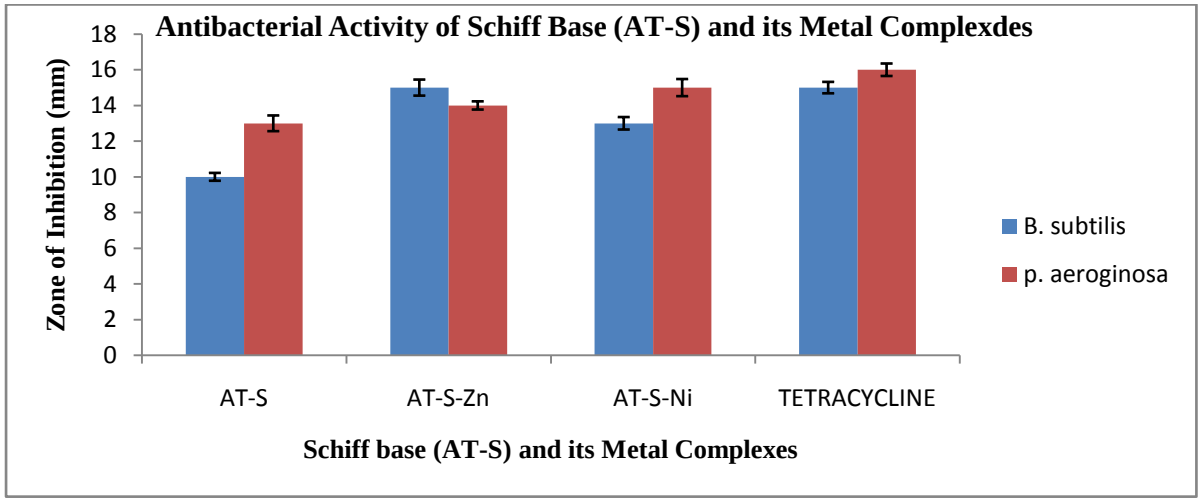
Zn(II) complex are diamagnetic hence shows no transition. The spectrum of Ni (II) complex is consistent with the formation of an octahedral geometry with the appearance of three bands at 22728, 18518 and 10472 cm^1 corresponding to the transitions $^3A_2g \rightarrow ^3T_1g(P)$, $^3A_2g \rightarrow ^3T_1g(F)$ and $^3A_2g \rightarrow ^3T_2g(F)$ [25-26]. The electronic spectrum.

4.3 Biological Activity

The *in vitro* antibacterial investigation results are given in (Table-3 and Fig 1) respectively. It has been observed that all compounds exhibited very significant and better antibacterial activity. The free ligand (Schiff base) shows potent activity against *B. subtilis* bacterial strain with inhibition of 10 mm. Among the metal complexes Zn (II) complex show higher antibacterial activity incase of *B.subtilis* with zone of inhibition of 15 mm. The Ni (II) complex show higher activity incase of *P. aeroginosa* with zone of inhibition of 15 mm. These observations show that both of the metal complexes are more active than the free ligand.

Compound	*B. subtilis*	*p. aeroginosa*
AT-S	10±0.22	13±0.44
AT-S-Zn	15±0.45	14±0.23
AT-S-Ni	13±0.35	15±0.48
TETRACYCLINE	15±0.32	16±0.35

Table: 3- Showing the % Inhibition of Schiff base (AT-S) and its derived metal



5. Conclusion:

On the basis of above results we conclude that the newly synthesized Schiff base acts as a neutral tridentate ligand coordinating through the oxygen of the phenolic group, the nitrogen of the azomethine group and triazole nitrogen. On complexation, complexes show enhanced biological activities than their parents. On complexation, complexes show enhanced biological activities than their parents.

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